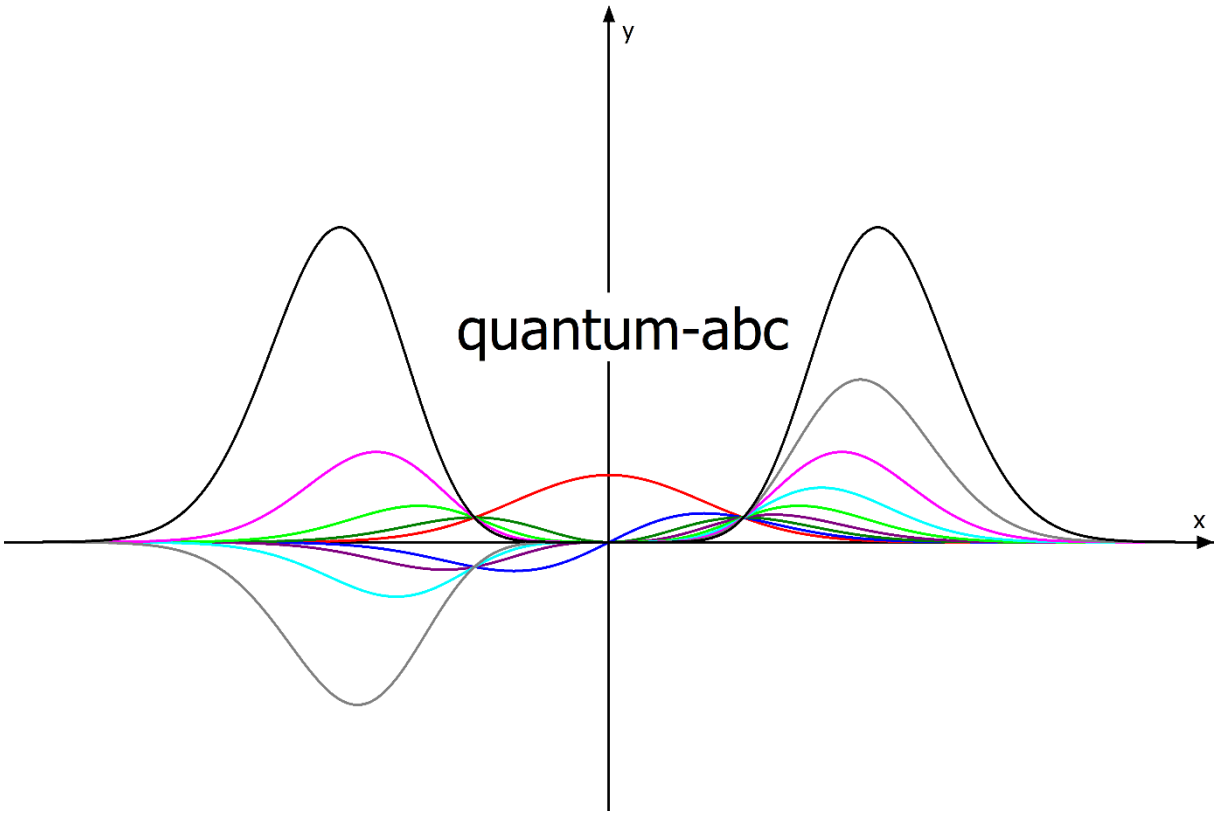
y
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Preface

You are studying physics and have your first lessons in quantum mechanics. You use a lecture script or a textbook in your lessons. Naturally, sometimes some keywords need to be remembered. Here you find a lot of keywords embedded each in a tiny quantum surrounding. Often this delivers a second view to the way your textbook or lecture script presents these topics.

Hope I can help you with learning quantum mechanics.

Sincerely

Dieter Kriesell

Contents

2 x 2 matrices, combining

Let A and B be two 2×2 matrices: $A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{21} \end{pmatrix}$, $B \coloneqq \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{21} \end{pmatrix}$

The matrix version of the tensor product, sometimes called the Kronecker product:

$$A \otimes B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

Note: the matrices need not to be quadratic.

3-vector operators

State-vectors e.g. $|u\rangle$ for “up” and $|d\rangle$ for “down” describe the state of a spin. They are part of a two-dimensional, complex-based vector-space.

The pauli-matrices σ_x, σ_y and σ_z are (complex valued) operators written as matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

They act on state-vectors.

The vector $\vec{\sigma} \coloneqq \sigma_x + \sigma_y + \sigma_z$ is a kind of 3-vector with the components σ_x, σ_y and σ_z and can be written as:

$$\vec{\sigma} \coloneqq \begin{pmatrix} 1 & 1-i \\ 1+i & -1 \end{pmatrix}$$

3-vectors (spatial coordinates):

3-vector means a vector in the ordinary three-dimensional space: $\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ or $\vec{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$.

Orthogonal unit vectors and 3-vectors

The inner or scalar product of orthogonal vectors is zero.

A unit vector has length 1.

Orthogonal unit vectors (cartesian) are e.g. the three basis-vectors $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

To every 3-vector you can calculate the corresponding unit vector by dividing it by its length. The length or the absolute value of a 3-vector is: $\sqrt{x^2 + y^2 + z^2}$.

In bra-ket notation in complex form:

ket $|A\rangle \coloneqq \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, bra $\langle A| \coloneqq (x^* y^* z^*)$,

$$\langle A|A\rangle = (x^* y^* z^*) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = x^* x + y^* y + z^* z$$

Note: this is the square of the absolute value.

4 x 4 matrices, from combined 2 x 2 matrices

Let A and B be two 2×2 matrices: $A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{21} \end{pmatrix}$, $B \coloneqq \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{21} \end{pmatrix}$

The matrix version of the tensor product, sometimes called the Kronecker product.

$$A \otimes B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

Note: the matrices need not to be quadratic.

Addition of complex numbers

Addition of complex numbers is best done in the cartesian representation.

$$z_1 = x + iy, \qquad z_2 = u + iv$$

$$z_1 + z_2 = x + iy + u + iv = (x + u) + i(y + v)$$

Addition of vector, axioms:

Let $|A\rangle$, $|B\rangle$ and $|C\rangle$ be vectors and z, w complex numbers, then:

1. Closure: the sum of two vectors is a vector:
   $|A\rangle + |B\rangle = |C\rangle$
2. Vector addition is commutative:
   $|A\rangle + |B\rangle = |B\rangle + |A\rangle$
3. Vector addition is associative:
   $\{|A\rangle + |B\rangle\} + |C\rangle = |A\rangle + \{|B\rangle + |C\rangle\}$
4. Existence of $|0\rangle$:
   $|A\rangle + |0\rangle = |A\rangle$
5. Existence of the inverse:
   $|A\rangle + (-|A\rangle) = |0\rangle$
6. Multiplication by a scalar produces a new vector:
   $|zA\rangle = z|A\rangle = |B\rangle$
7. Distributive property:
   $z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$
   $\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$

Axioms 6 and 7 taken together are often called *linearity*.

Note: the zero vector $|0\rangle$ is often written simply as 0 because it is a vector containing only zeros.

Amplitude, probability:

Let $|A\rangle$ be a generic state of the up/down-spin, e.g. $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$.

$\langle u^*|A\rangle$ and $\langle d^*|A\rangle$ are called the probability amplitudes.

Note: the probability amplitude is not a probability.

The probability is calculated by $P_u = \langle A|u\rangle\langle u^*|A\rangle$ and $P_d = \langle A|d\rangle\langle d^*|A\rangle$. Remember that we are working with complex numbers.

Multiplying a state by a phase-factor $e^{i\theta}$ changes the probability amplitude but not the probability because in $\langle A|d\rangle\langle d^*|A\rangle$ any phase-factor $e^{i\theta}$ vanishes: $e^{-i\theta}e^{i\theta} = e^{i\theta - i\theta} = e^0 = 1$.

Amplitude, for paths:

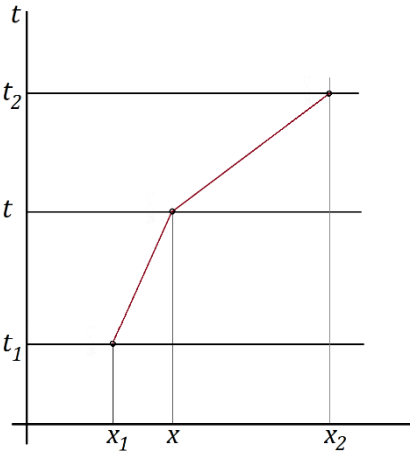
Prerequisite

A classical particle starting at position x_1 at time t_1 and arriving at position x_2 at time t_2 will follow a trajectory according to the principle of the least (stationary) action. Action stands for the Lagrangian between both end points. The standard method of calculus assumes that every function in a tiny interval becomes linear (e.g. Taylor series).

End prerequisite

For quantum mechanical system the probability amplitude $C_{1,2}$ for a particle to go from x_1 to x_2 in the time interval t_1 to t_2:

$$C_{1,2} = \langle x_2 | e^{-iHt} | x_1 \rangle$$



Note: units chosen for which $\hbar = 1$.

Note: H is the Hamilton operator.

Splitting up the path into infinitesimal pieces and replacing e^{-iHt} by $e^{-i\varepsilon H}$ (for each "infinitesimal" $\triangle t$) gives $C_{1,2} = e^{\frac{iA}{\hbar}}$ for each path with A being the action for this individual path.

Finally, we can integrate over all possible paths and get the amplitude for the particle to go from x_1 to x_2:

$$C_{1,2} = \int_{paths} e^{\frac{iA}{\hbar}}$$

And-rule, formal logic:

Prerequisite

A proposition is an expression that can either be $true$ or $false$.

End prerequisite

"and", "or" and "not" are basic rules (operators) to connect propositions. They can be represented by truth tables with "0" for false and "1" for true:

Let A and B be propositions:

A	B	$(A\ or\ B)$	$(A\ and\ B)$
0	0	0	0
0	1	1	0
1	0	1	0
1	1	1	1

There is a special logical operator, the "not", that simply switches the truth value to its opposite:

A	$\neg A$
0	1
1	0

Annihilation operator:

The Hamiltonian can be expressed in terms of momentum operator P and position operator X:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2) = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{i\omega}{2}$$

Note: $\frac{i\omega}{2}$ is needed because P and X do not commute.

$(P + i\omega X)$ is called the raising operator, $(P - i\omega X)$ the lowering (annihilating) operator, written as a^+ and a^-. The raising operator a^+ shifts the energy level of the harmonic oscillator to the next

possible higher level, the lowering operator a^- to the next possible lower level. Applying the lowering operator to the ground level with Energy $E_0 = \frac{\omega\hbar}{2}$ annihilates this ground level. Symbolically this is expressed as:

$$a^-|0\rangle = 0$$

Note: $|0\rangle$ representing the ground level and 0 representing the number zero.

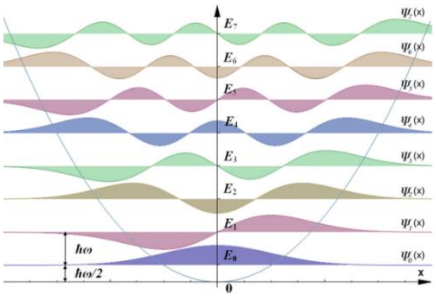
Anti-Hermitian operator:

An operator (a matrix) is called Hermitian if it is identical with its transposed and complex conjugated version: $A = (A^t)^* = (A^*)^t := A^\dagger$.

An operator (a matrix) is called anti-Hermitian if $A^\dagger = -A$.

Antisymmetric eigenfunctions:

A real function is called symmetric if $f(x) = f(-x)$. It is antisymmetric if $f(x) = -f(-x)$. The picture below shows eigenfunctions for the lower states of the harmonic oscillator. Functions for even numbers are symmetric, functions for odd numbers are antisymmetric.

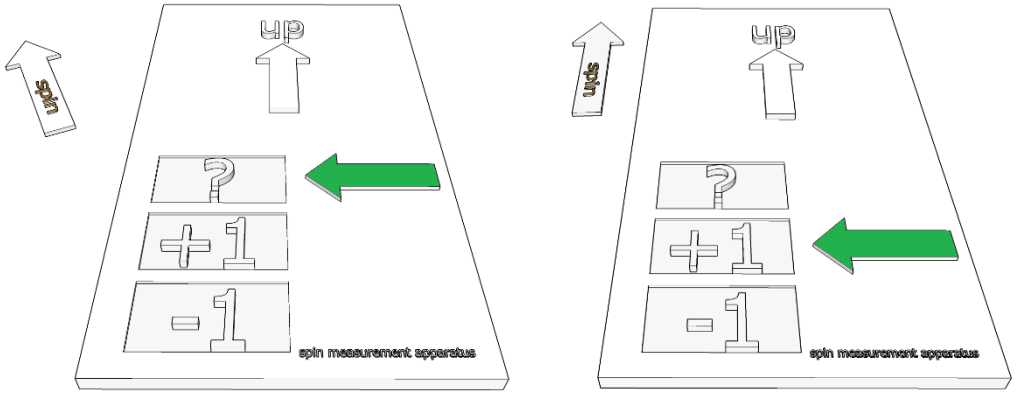


Apparatus, measurement and Apparatus:

An experiment or a measurement can be described by an apparatus or a black box that shows the result. This apparatus is part of the real world.

In case of spin measurement, we orientate the apparatus on any direction in space and measure.

The result will be either -1 or +1 and leave the spin measured in this state.



before measurement after measurement

Note: do not merge “3-vector” in space with “state-vector” of the spin.

Associative property:

This is part 3 of axioms of vector addition:

3. Vector addition is associative: $\{|A\rangle + |B\rangle\} + |C\rangle = |A\rangle + \{|B\rangle + |C\rangle\}$

Atoms:

Atoms made from of neutrons, protons and electrons are the smallest constituent units of ordinary matter (chemical elements). Typical sizes are around 100 picometers ($10^{-10}\ m$) so they are small enough to shatter wave-functions. Quantum principles are needed to (better) explain and predict their behavior.

Atoms in crystal lattice:

Atoms in crystal lattice sometimes behave like oscillators the energy levels of can be explained by the Schrödinger equation.

Atoms, hydrogen-atoms:

(Hydrogen) atoms cannot fully be described by classical physics. Electrons orbiting rapidly get a loss of energy and would fall into the nucleus. This gave rise to the assumption of stable orbits the electron being able only to jump from one to another – the first idea of quantization was born. The Schrödinger equation allows to calculate these stationary states.

Atoms, quantum mechanics and atoms:

Quantum mechanics deals with the behavior of objects so small we humans are not equipped to visualize them at all. Individual atoms are near the upper end of this scale in terms of size.

Atoms, size of atoms:

… about 100 picometers or 10^{-10}m.

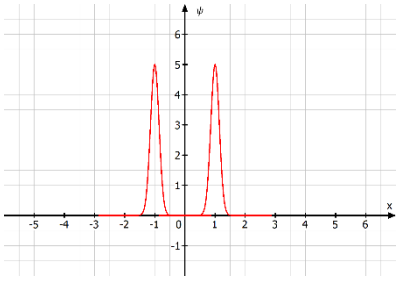
Atoms, spins of atoms:

Some atoms have spins that are described in the same way as electron spins. When two of these atoms are close to each other, the Hamiltonian will depend on the spins and in some situations the Hamiltonian is proportional to the dot-product of both vector-operators. Measuring this energy is a single measurement of the composite operator and does not entail measuring the individual components.

Atoms, wave packets and atoms:

Quantum equation of motion looks classical if the wave packets are unimodal (nice, centered single bump) or coherent and well localized. If wave packets are bimodal (two-humped), it is not always true that the time rate of change of the momentum is the force evaluated at the expectation value of x:

$$\langle F(x)\rangle \neq F(\langle x\rangle)$$



The average of the function of $F(x)$ is not equal the function of the average of x, $F(\langle x\rangle)$.

Average:

a) Statistical, the average for a shifted distribution follows the shifting. If you shift every member of a statistical ensemble, then the average of the shifted ensemble is the same as the shifted average of the original ensemble.
Note: the variance of shifted and unshifted distribution is the same.

b) The probability distribution $P(a,b)$ for two completely uncorrelated variables will factorize: $P(a,b) = P_A(a)P_B(b)$.
Opposite: if two variables are correlated, the probability correlation will not factorize: $\langle\sigma_A\rangle\langle\sigma_B\rangle \neq \langle\sigma_A\sigma_B\rangle$.
c) The average position of a quantum mechanical particle: $\langle\psi|\mathrm{X}|\psi\rangle$. X is the position operator.
d) The velocity of a quantum mechanical particle is the time derivative of the average position: $v = \frac{d}{dt}\langle\psi|\mathrm{X}|\psi\rangle$. With this we get the average momentum: $\langle P\rangle = mv$.
e) Approximating with averages works well if the potential $V(x)$ varies slowly compared to the size of the wave packets.

Average, bra-ket notation for averages:

We have a state A of a quantum system and an observable L and expand L in the orthogonal basis of eigenvectors of L:

$$|A\rangle = \sum_i \alpha_i |\lambda_j\rangle$$

Then $\langle A|L|A\rangle = \sum_i(\alpha_i^*\alpha_i)\lambda_i$ with $\alpha_i^*\alpha_i$ being the probability $P(\lambda_i)$. We express the average as: $\langle L\rangle = \langle A|L|A\rangle$.

Note: $|\lambda_j\rangle$ are the eigenvectors, λ_j the eigenvalues.

Average, defining:

From a mathematical point of view an average is defined:

$$\langle L\rangle = \sum_i \lambda_i P(\lambda_i)$$

Average value:

In statistics the average value is usually denoted by a bar over the quantity: $\bar{x}$. In quantum mechanics the average is noted as $\langle x\rangle$.

Axioms of vector space:

Let $|A\rangle$, $|B\rangle$ and $|C\rangle$ be vectors, then:

1. Closure: the sum of two vectors is a vector:
   $|A\rangle + |B\rangle = |C\rangle$
2. Vector addition is commutative:
   $|A\rangle + |B\rangle = |B\rangle + |A\rangle$
3. Vector addition is associative:
   $\{|A\rangle + |B\rangle\} + |C\rangle = |A\rangle + \{|B\rangle + |C\rangle\}$
4. Existence of the 0:
   $|A\rangle + 0 = |A\rangle$
5. Existence of the inverse:
   $|A\rangle + (-|A\rangle) = 0$
6. Multiplication by a scalar produces a new vector:
   $|zA\rangle = z|A\rangle = |B\rangle$
7. Distributive property:
   $z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$
   $\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$

Axioms 6 and 7 taken together are often called *linearity*.

Basis of simultaneous eigenvectors:

We have a two-spin system and measure with two different operators L and M. If we measure both spins, the system winds up in a state that is simultaneously eigenvector of L and eigenvector of M.

L has eigenvectors $|\lambda_i\rangle$ with eigenvalues λ_i, M has eigenvectors $|\mu_a\rangle$ with eigenvalues μ_a.

We assume that there is a basis of state-vectors $|\lambda_i, \mu_a\rangle$ that are simultaneous eigenvectors of both observables: $L|\lambda_i, \mu_a\rangle = \lambda_i|\lambda_i, \mu_a\rangle$ and $M|\lambda_i, \mu_a\rangle = \mu_a|\lambda_i, \mu_a\rangle$.

Omitting the subscripts for better readability, we write

$$L|\lambda, \mu\rangle = \lambda|\lambda, \mu\rangle$$

$$M|\lambda, \mu\rangle = \mu|\lambda, \mu\rangle$$

Basis vectors:

a) $3 - vectors$: a set of three mutually orthogonal unit vectors, e.g. $\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\0\\1\end{pmatrix}$ for the cartesian space.

b) $|u\rangle$ and $|d\rangle$ as a basis of the state of a spin.
Any state A can be written as $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$

c) If the state vector $|A\rangle$ is normalized, then $\langle A|A\rangle = 1$ or $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$

d) Example: $\alpha_u^* = \alpha_u = \alpha_d^* = \alpha_d = \frac{1}{\sqrt{2}}$ satisfies c)

e) If λ_1 and λ_2 are different eigenvalues of a Hermitian operator, the corresponding eigenvectors are orthogonal, and all of these eigenvectors can form a basis of the state space.

f) If λ_1 and λ_2 are equal eigenvalues of a Hermitian operator, out of the corresponding eigenvectors can be chosen a pair of orthogonal vectors that are necessarily eigenvectors.

g) Orthogonal basis vectors represent two distinguishable states – for all times.

h) Every normalized state $|A\rangle$ of a quantum system can be expanded in the orthonormal basis of eigenvectors of L: $|A\rangle = \sum_i \alpha_i |\lambda_j\rangle$

i) The Hamiltonian applied to the energy eigenvectors of a state delivers the eigenvalues (the energy levels) of the system: $H|E_j\rangle = E_j|E_j\rangle$.
Note: $|E_j\rangle$ are the eigenvectors, E_j the eigenvalues resp. the energies.

j) The elements of a matrix M can be calculated by use of basis vectors:
$m_{jk} = \langle j|M|k\rangle$ with $\langle j|$ and $|k\rangle$ representing the basis vectors.
Note: $\langle j|$ is the complex conjugate to $|j\rangle$.

k) In a single spin system, the basis vector for the $|u\rangle$ state is $\begin{pmatrix}1\\0\end{pmatrix}$, the basis vector for the $|d\rangle$ state is $\begin{pmatrix}0\\1\end{pmatrix}$.

l) In a dual spin system, the basis vectors for the states $|uu\rangle$, $|ud\rangle$, $|du\rangle$ and $|dd\rangle$ are $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$.
Note: these are tensor product states.

m) The sum over the outer product of a set of basis vectors $|i\rangle$ and $\langle i|$ delivers the identity matrix:

$$\sum_j |j\rangle\langle j| = I$$

n) If the measuring apparatus (for spatial spin orientation) comes into play as a quantum system too, in the simplest description it has three states: a blank state and two outcome states with the following basis vectors: $|b\rangle, |(+1)\rangle$ and $|(-1)\rangle$.
The starting state at time 0 is always the blank state.
Note: sometimes these kets are written as $|b\}, |+1\}$ and $|-1\}$ to indicate these are kets of the measuring apparatus.

o) The quantum state of a particle with position x and momentum p: $|x, p\rangle$
Note that the associated operators are the position operator X and momentum operator P.

p) Because momentum and position operators are both Hermitian operators, the sets of $|x\rangle$ and $|p\rangle$ each define basis vectors.

Basis vectors, entangled states:

In case of a two-spin system the maximum entangled states, the singlet state $sing$ and the triplet states T_1, T_2 and T_3 can be written as:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

$$|T_1\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$$

$$|T_2\rangle = \frac{1}{\sqrt{2}}(|uu\rangle + |dd\rangle)$$

$$|T_3\rangle = \frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle)$$

Basis vectors, labelling:

A combined system S_{ab} can be constructed of two systems S_a and S_b by use of the tensor product: $S_{ab} = S_a \otimes S_b$. Basis vectors of the combined system are labeled $|ab\rangle$.

Basis vectors, product states:

Given two states, $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$ and $|B\rangle = \beta_u|u\rangle + \beta_d|d\rangle$.

The product state describing the system is: $|product\ state\rangle = \{\alpha_u|u\rangle + \alpha_d|d\rangle\} \otimes \{\beta_u|u\rangle + \beta_d|d\rangle\}$.

Expanding and switching to composite notation gives

$$|product\ state\rangle = \alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

Bell, John:

John Stewart Bell (1928 – 1990) was a physicist from Northern Ireland and the originator of Bell's theorem.

Bell's theorem:

Bell's theorem proves that quantum physics is incompatible with local hidden variable theories. It was introduced by John Stewart Bell in a 1964 paper titled "On the Einstein Podolsky Rosen Paradox", referring to a 1935 thought experiment that Albert Einstein, Boris Podolsky and Nathan Rosen used to argue that quantum physics is an "incomplete" theory. *(Wikipedia)*

Two computers simulating an entangled spin system can represent a case of Bell's theorem.

Boolean logic:

Boolean logic is a formalized version of the classical logic of propositions.

In classical physics, the order of the measurements (propositions) is not important: (A or B) gives the same results as (B or A). First measuring A and second measuring B gives the same result as first measuring B and second measuring A.

In quantum mechanics measurements are not gentle and can lead to a collapse of the state function. First measuring A can set the system in the state A – and that maybe is not the state it was in before. Analog first measuring B can set the system in the state B. The order of measurements can play a role.

Bracket or Bra-ket notation:

The quantum mechanical notation for the statistical average of a quantity q is Dirac's bracket notation $\langle q \rangle$.

Bra-ket notation for averages:

We have a state A of a quantum system, an observable L and expand L in the orthogonal basis of eigenvectors of L:

$$|A\rangle = \sum_i \alpha_i |\lambda_j\rangle$$

Then $\langle A|L|A\rangle = \sum_i (\alpha_i^* \alpha_i)\lambda_i$ with $\alpha_i^* \alpha_i$ being the probability $P(\lambda_i)$.

We can express the average as follows: $\langle L \rangle = \langle A|L|A\rangle$.

Note: $|\lambda_j\rangle$ are eigenvectors, λ_j eigenvalues.

Bras (bra vectors):

Bra vectors satisfy the same axioms as ket vectors. Please take care of the complex conjugate.

$z|A\rangle$ gives the corresponding $\langle A|z^*$.

If the ket $|A\rangle$ is represented by the column vector $\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}$, then the corresponding bra $\langle A|$ is represented by the row vector $(\alpha_1^* \; \alpha_2^* \; \alpha_3^*)$.

Bras, inner product and bras:

The inner product of bra $\langle B|$ and ket $|A\rangle$ is written as $\langle B|A\rangle$.

The axioms for the inner product:

1. Linearity:
$$\langle C|\{|A\rangle + |B\rangle\} = \langle C|A\rangle + \langle C|B\rangle$$
2. Complex conjugation:
$$\langle B|A\rangle = \langle A|B\rangle^*$$
3. Reality:
$$\langle A|A\rangle \in \mathbb{R}$$

In concrete representation by row and column vectors, the inner product is defined in terms of components (dot product).

$$|A\rangle \coloneqq \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix}$$

$$\langle A| = (\alpha_1^* \; \alpha_2^* \; \alpha_3^* \; \alpha_4^*)$$

$$|B\rangle \coloneqq \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix}$$

$$\langle B| = (\beta_1^* \; \beta_2^* \; \beta_3^* \; \beta_4^*)$$

$$\langle B|A\rangle = (\beta_1^* \; \beta_2^* \; \beta_3^* \; \beta_4^*) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix} = \beta_1^* \alpha_1 + \beta_2^* \alpha_2 + \beta_3^* \alpha_3 + \beta_4^* \alpha_4$$

$$\langle A|B\rangle = (\alpha_1^* \; \alpha_2^* \; \alpha_3^* \; \alpha_4^*) \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} = \alpha_1^* \beta_1 + \alpha_2^* \beta_2 + \alpha_3^* \beta_3 + \alpha_4^* \beta_4$$

For complex values this gives $\langle A|B\rangle \neq \langle B|A\rangle$ and $\langle B|A\rangle = \langle A|B\rangle^*$.

For real values $\langle A|B\rangle = \langle B|A\rangle$.

If the inner product $\langle A|A\rangle = 1$, then the vector is normalized (unit length).

If the inner product $\langle A|B\rangle = 0$, then $|A\rangle$ and $|B\rangle$ are orthogonal.

Bras, linear operators and bras:

We have a linear operator M and a bra $\langle B|$.

The notation for multiplying is: $\langle B|M$.

In detail:

$$(\beta_1^* \; \beta_2^* \; \beta_3^* \; \beta_4^*) \begin{pmatrix} m_{11} & m_{12} & m_{13} & m_{14} \\ m_{21} & m_{22} & m_{23} & m_{24} \\ m_{31} & m_{32} & m_{33} & m_{34} \\ m_{41} & m_{42} & m_{43} & m_{44} \end{pmatrix} =$$

$$\left((\beta_1^* m_{11} + \beta_2^* m_{21} + \beta_3^* m_{31} + \beta_4^* m_{41})(\dots)(\beta_1^* m_{14} + \beta_2^* m_{24} + \beta_3^* m_{34} + \beta_4^* m_{44})\right)$$

Bras, outer products and bras:

The outer product of ket $|A\rangle$ and bra $\langle B|$ is written as $|A\rangle \langle B|$.

In concrete representation by row and column vectors, the outer product is defined in terms of components.

$$|A\rangle \coloneqq \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}, \langle A| = (\alpha_1^* \; \alpha_2^*), |B\rangle \coloneqq \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}, \langle B| = (\beta_1^* \; \beta_2^*), |C\rangle \coloneqq \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix}, \langle C| = (\gamma_1^* \; \gamma_2^*)$$

$$|A\rangle \langle B| = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} (\beta_1^* \; \beta_2^*) = \begin{pmatrix} \alpha_1 \beta_1^* & \alpha_1 \beta_2^* \\ \alpha_2 \beta_1^* & \alpha_2 \beta_2^* \end{pmatrix}$$

The outer product of ket and bra gives an operator.

Operations with bras, kets, and linear operators are left distributive:

$$(|A\rangle\langle B|)|C\rangle = \begin{pmatrix}\alpha_1\beta_1^* & \alpha_1\beta_2^*\\ \alpha_2\beta_1^* & \alpha_2\beta_2^*\end{pmatrix}\begin{pmatrix}\gamma_1\\ \gamma_2\end{pmatrix} = \begin{pmatrix}\alpha_1\beta_1^*\gamma_1 + \alpha_1\beta_2^*\gamma_2\\ \alpha_2\beta_1^*\gamma_1 + \alpha_2\beta_2^*\gamma_2\end{pmatrix} = \begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}(\beta_1^*\gamma_1 + \alpha_1\beta_2^*\gamma_2)$$

$$|A\rangle(\langle B|C\rangle) = \begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}\left((\beta_1^*\ \beta_2^*)\begin{pmatrix}\gamma_1\\ \gamma_2\end{pmatrix}\right) = \begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}(\beta_1^*\gamma_1 + \beta_2^*\gamma_2) = \begin{pmatrix}\alpha_1(\beta_1^*\gamma_1 + \beta_2^*\gamma_2)\\ \alpha_2(\beta_1^*\gamma_1 + \beta_2^*\gamma_2)\end{pmatrix} =$$

$$\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}(\beta_1^*\gamma_1 + \alpha_1\beta_2^*\gamma_2)$$

We get $(|A\rangle\langle B|)|C\rangle = |A\rangle(\langle B|C\rangle)$.

Note: any operation $(|A\rangle\langle B|)|C\rangle$ or $|A\rangle(\langle B|C\rangle)$ corresponds to a multiplication of the first ket $|A\rangle$ by a factor.

Canonical momentum (conjugate to x):

The Lagrangian is kinetic energy minus potential energy:

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2$$

For a one-dimensional system there is only one Lagrange equation, namely:

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

We carry out the operations on the Lagrangian:

right side:

$$\frac{\partial L}{\partial \dot{x}} = \dot{x} \qquad \textit{This is called the canonical momentum p}$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \ddot{x}$$

left side:

$$\frac{\partial L}{\partial x} = -\omega^2 x$$

Result:

$$-\omega^2 x = \ddot{x}$$

The Hamiltonian for the harmonic oscillator:

$$H = p\dot{x} - L \qquad \textit{We have only on degree of freedom}$$

By using the canonical momentum, we calculate:

$$H = p^2 - \frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega^2 x^2 =$$

$$p^2 - \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2 = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

This is the classical Hamiltonian:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

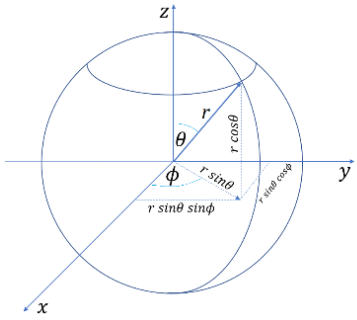
Note: the Hamiltonian represents the total energy of the system and does not change if the system is conservative.

Cartesian coordinates:

Cartesian coordinates are coordinates for the three-dimensional space with the axes x, y and z.

For problems dealing with rotating vectors in space the better choice are spherical coordinates.

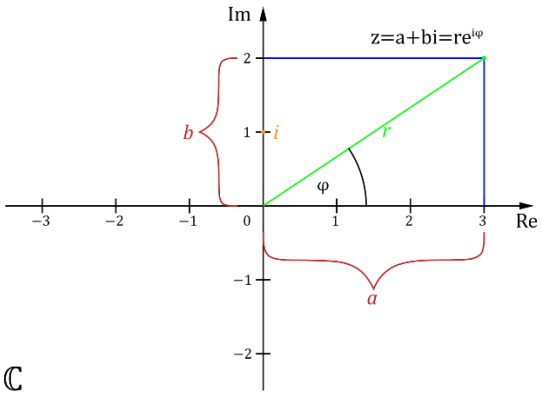
Please do not confuse vectors in space and state-vectors.



Cartesian representation of complex numbers:

A complex number consists of a real part and an imaginary part. We can write it as $z = a + ib$ with $a, b \in \mathbb{R}$. The imaginary unit i has the property $i \cdot i = -1$ or $i^2 = -1$.

We can represent complex numbers by a plane with horizontal real axis and vertical imaginary axis. This is called the cartesian mode.



… graphic courtesy of Wikipedia …

$\mathbb{C}$

A second way of representation describes a complex number by the angle φ it has with the real axis and its length r resp. the absolute value.

This is called the gaussian mode. In this mode we write a complex number as $r \cdot e^{i\varphi}$. Note: r is a real number.

We can switch from one representation to the other:

Given $z = a + ib$: $|z|\ or\ r = \sqrt{a^2 + b^2}$ $\varphi = \arccos\left(\frac{a}{r}\right)$ if $b \geq 0$

resp. $\varphi = -\arccos\left(\frac{a}{r}\right)$ if $b < 0$.

Given $z = re^{i\varphi}$: $a = r \cdot \cos(\varphi)$ $b = r \cdot \sin(\varphi)$

or $z = r \cdot (\cos(\varphi) + i \cdot \sin(\varphi))$

Every complex number z has a complex conjugate number, marked as z^*. The complex conjugate switches the imaginary part to the opposite sign. $z = a + ib$ changes to $z^* = a - ib$ and vice versa.

With that we get new formulas:

$$|z| = \sqrt{zz^*}$$

$$re(z)\ or\ a = \frac{z + z^*}{2}$$

$$im(z)\ or\ b = \frac{z - z^*}{2}$$

Additions and subtraction of complex numbers are best performed with the cartesian representation.

$$(a + ib) + (c + id) = ac + ibd$$

Multiplication and division are best performed with the gaussian representation.

$$r_1 e^{i\varphi} \cdot r_2 e^{i\theta} = r_1 r_2 e^{i(\varphi+\theta)}$$

Cauchy-Schwarz inequality:

For real vector spaces holds:

$$|\vec{X}||\vec{Y}| \geq |\vec{X} \cdot \vec{Y}|$$

This can be derived from the triangle inequality.

Cauchy-Schwarz inequality and triangle inequality:

The triangle inequality for real vectors:

$$|\vec{X}| + |\vec{Y}| \geq |\vec{X} + \vec{Y}|$$

squared:

$$(|\vec{X}| + |\vec{Y}|)^2 \geq |\vec{X} + \vec{Y}|^2$$

left side:

$$(|\vec{X}| + |\vec{Y}|)^2 = |\vec{X}|^2 + |\vec{Y}|^2 + 2|\vec{X}||\vec{Y}|$$

right side:

$$|\vec{X} + \vec{Y}|^2 = (\vec{X} + \vec{Y})(\vec{X} + \vec{Y}) = |\vec{X}|^2 + |\vec{Y}|^2 + 2(\vec{X} \cdot \vec{Y})$$

We get:

$$|\vec{X}||\vec{Y}| \geq |\vec{X} \cdot \vec{Y}|$$

Squared this is called the Cauchy-Schwarz inequality:

$$|\vec{X}|^2|\vec{Y}|^2 \geq |\vec{X} \cdot \vec{Y}|^2$$

Cauchy-Schwarz inequality, triangle inequality for complex valued vectors:

Note: we omit the arrows over the vectors, $\vec{X} \to X$ and write the complex conjugation by an overline, $\bar{X}$.

Note: this will become a little bit tricky …

For complex vector spaces we have to prove:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

We assume vectors X and Y being nonzero.

Let λ be:

$$\lambda = \frac{\langle X|Y\rangle}{\langle Y|Y\rangle} \to \langle X|Y\rangle = \lambda\langle Y|Y\rangle$$

With this we can conclude:

$$\langle Y|X\rangle = \overline{\langle X|Y\rangle} = \overline{\lambda\langle Y|Y\rangle} = \bar{\lambda}\langle Y|Y\rangle$$

We try:

$$0 \leq \langle X - \lambda Y|X - \lambda Y\rangle$$

Right side:

$$\langle X|X\rangle - \bar{\lambda}\langle X|Y\rangle - \lambda\langle Y|X\rangle + \lambda\bar{\lambda}\langle Y|Y\rangle =$$

$$\langle X|X\rangle - \bar{\lambda}\langle X|Y\rangle - \lambda\bar{\lambda}\langle Y|Y\rangle + \lambda\bar{\lambda}\langle Y|Y\rangle =$$

$$\langle X|X\rangle - \bar{\lambda}\langle X|Y\rangle =$$

$$|X|^2 - \frac{\overline{\langle X|Y\rangle}}{|Y|^2}\cdot\langle X|Y\rangle$$

Intermediate result:

$$0 \leq |X|^2 - \frac{\overline{\langle X|Y\rangle}}{|Y|^2}\cdot\langle X|Y\rangle$$

$$\frac{\overline{\langle X|Y\rangle}}{|Y|^2}\cdot\langle X|Y\rangle \leq |X|^2$$

$$\overline{\langle X|Y\rangle}\cdot\langle X|Y\rangle \leq |X|^2|Y|^2$$

$$|\langle X|Y\rangle|^2 \leq |X|^2|Y|^2$$

$$|\langle X|Y\rangle| \leq |X||Y|$$

We multiply the result by 2:

$$2|\langle X|Y\rangle| \leq 2|X||Y|$$

We get the following chain:

$$2|X||Y| \geq 2|\langle X|Y\rangle| = |\langle X|Y\rangle| + |\langle X|Y\rangle| =$$

$$|\langle X|Y\rangle| + |\langle Y|X\rangle| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

We get the form of the Cauchy-Schwarz inequality that is applicable for the uncertainty principle:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

Change in classical physics:

In classical physics, the space of states is a mathematical set, the logic is Boolean and the evolution of states over time is deterministic and reversible. In other words, information is never lost. If two identical systems start out in different states, they stay in different states. Moreover, in the past they were in different states. If two identical systems are in the same state at one point, then their future and past must be identical.

Change, continuity, unitarity and incremental change:

Time-development in quantum mechanics is expressed by use of a unitary time-development operator $U(t)$.

Continuity means that for small periods of time ε the unitary operator $U(\varepsilon)$ is close to the unit operator.

We write

$$U(\varepsilon) = I - i\varepsilon H$$

With $U^{\dagger}(\varepsilon) = I + i\varepsilon H^{\dagger}$ we stick these U's together:

$$U^{\dagger}(\varepsilon)U(\varepsilon) = I = \left(I + i\varepsilon H^{\dagger}\right)(I - i\varepsilon H)$$

We get:

$$I = (I + i\varepsilon H)(I - i\varepsilon H) = I^2 - Ii\varepsilon H + i\varepsilon H^{\dagger}I + \varepsilon^2 H^{\dagger}H =$$

$$I - i\varepsilon H + i\varepsilon H^{\dagger} + \varepsilon^2 H^{\dagger}H$$

Omitting the second order in ε we get:

$$-H + H^{\dagger} = 0 \text{ or } H = H^{\dagger}$$

H is called the quantum Hamiltonian. It is a Hermitian observable (operator) with a complete set of orthonormal eigenvectors and eigenvalues.

Classical equations, quantization and classical equations:

An often-used procedure in quantum mechanics is to quantize a classical system. The procedure is as follows:

1. Start with a classical system, a set of coordinates x_i and momenta p_i and search the classical Hamiltonian.
2. Replace the classical space with a linear vector space and find a wave function $\psi(x_i)$.
3. Replace the $x_i's$ and $p_i's$ with position operators X_i and momentum operators P_i.
   Each X_i multiplies the wave function by x_i.
   Each P_i:
   $$P_i\psi(x_i) \to -i\hbar\frac{\partial\psi(x_i)}{\partial x_i}$$
4. With these replacements the classical Hamiltonian becomes the quantum mechanical Hamiltonian, an operator.

Classical limit:

If a potential V varies slowly compared to the size of a wave packet, then the motion can be described by classical physics. In this situation holds: $\triangle p \triangle x \gg \hbar$.

If a potential V varies rapidly across the wave packet there is a good chance that the wave packet will get broken up. Its behavior must be described by quantum physics.

This situation occurs when $\triangle p \triangle x \approx \hbar$.

Classical physics, change in classical physics:

In classical physics, the space of states is a mathematical set, the logic is Boolean and the evolution of states over time is deterministic and reversible. In other words, information is never lost. If two identical systems start out in different states, they stay in different states. Moreover, in the past they were in different states. If two identical systems are in the same state at one point, then their future and past must be identical.

Classical physics, change in expectation values over time and classical physics:

We use the Poisson bracket formulation of classical mechanics.

Let $L(q,p)$ be an arbitrary function of position in the phase space, varying along the trajectory.

With the Hamilton equations the time derivative of L can be expressed as:

$$\dot{L} = \sum_i \left(\frac{\partial L}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial L}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$$

The right-hand part of this equation is called the Poisson bracket and written as $\{L,H\}$. We get a short form:

$$\dot{L} = \{L,H\}$$

In quantum mechanics the time derivative of an operator L (L being any observable, H being the quantum Hamiltonian) is

$$\frac{dL}{dt} = -\frac{i}{\hbar}[L,H]$$

with $[L,H]$ being the commutator of L and H: $(LH - HL)$.

The formal identification between commutators L, H and Poisson brackets is:

$$[L,H] \leftrightarrow i\hbar\{L,H\}$$

Combining classical physics and quantum mechanics we get:

$$\frac{dL}{dt} = -\frac{i}{\hbar}[L,H] = \{L,H\}$$

Classical physics, commutators and classical physics:

Let X be the observable for position (the position operator) and P the observable for momentum (the momentum operator).

X acts on an arbitrary wave function $\psi(x)$:

$$X\psi(x) = x\psi(x)$$

P acting:

$$P\psi(x) = -i\hbar \frac{d\psi(x)}{dx}$$

Together the product XP acts on $\psi(x)$:

$$X(P\psi(x)) = -i\hbar x \frac{d\psi(x)}{dx}$$

PX acting on $\psi(x)$:

$$P(X\psi(x)) = -i\hbar x \frac{d\big(x\psi(x)\big)}{dx} = -i\hbar \frac{d\psi(x)}{dx} - i\hbar\psi(x)$$

Now we check the commutator relation $[X,P]\psi(x) := (XP - PX)\psi(x)$:

$$(XP - PX)\psi(x) = -i\hbar x \frac{d\psi(x)}{dx} - \left(-i\hbar \frac{d\psi(x)}{dx} - i\hbar\psi(x) \right) = i\hbar\psi(x)$$

From this follows

$$[X, P]\psi(x) = i\hbar\psi(x)$$

$$[X, P] = i\hbar$$

X and P don't commute. We compare this to the corresponding Poisson bracket $\{x, p\}$. With the equivalence $[X, P] \leftrightarrow i\hbar\{x, p\}$ we can conclude that $\{x, p\}$ must be 1 which is the classical relation between coordinates and their conjugate momenta.

Classical physics, momentum in classical physics:

The momentum in classical physics is mass times velocity: $p = mv = m\dot{x}$.

In quantum mechanics we define a differentiation operator D:

$$D\psi(x) \coloneqq \frac{d\psi(x)}{dx}$$

The momentum operator P is defined as:

$$P = -i\hbar D = -i\hbar\frac{d}{dx}$$

Classical physics, particle dynamics and classical physics:

We use a very simple Hamiltonian operator H, a fixed constant times the momentum operator P:

$$H = cP$$

A classical physicist using Hamilton's equations to describe a particle:

$$\frac{\partial H}{\partial p} = \dot{x}$$

and

$$\frac{\partial H}{\partial x} = -\dot{p}$$

Carrying out the partial derivatives with our simple Hamiltonian $H = cP$, these become

$$\frac{\partial H}{\partial p} = \dot{x} = c$$

and

$$\frac{\partial H}{\partial x} = -\dot{p} = 0$$

In the classical description of the particle, the momentum is conserved, and the particle moves with constant speed c.

In quantum mechanical description, the whole probability distribution and the expectation value move with velocity c – quantum description and classical description match.

Note: this resembles the description of a neutrino.

Classical physics, pure/mixed states and classical physics:

Classical physics has its notion of pure and mixed states, although they are not called by those names.

We consider a system of two particles orbiting. According to the rules of classical mechanics, we can calculate the orbits of the particles if we know the values of their positions x_1 and x_2 and momenta p_1 and p_2 at a certain time. The state of the system is completely specified by four numbers x_1, x_2, p_1 and p_2. Knowing these gives a complete description of the two-particle system – there is no more to know. We call this a classical pure state.

Often, we don't know the exact state, but only have in form of a probability density $\rho(x_1, x_2, p_1, p_2)$. The classical pure state is a special case of this with ρ being nonzero at only one point. In general, ρ extends over a range in which case we could call it a classical mixed state.

The difference between classical physics and quantum mechanics: if you are in the pure classical state for the combined two-particle system, you know everything about each single particle.

A pure state for two classical particles implies a pure state for each of the individual particles.

In quantum mechanics this is not true. The state of a composite system can absolutely be pure, but each of its constituents must be described by a mixed state.

Classical physics, quantum mechanics vs. classical physics:

Quantum mechanics differ from classical physics in two ways:

1. Quantum abstractions are fundamentally different from classical ones. The idea of a state in quantum mechanics is conceptually different from its classical counterpart. States are represented by different mathematical objects and have a different logical structure.
2. In classical physics measurements show the state. In quantum mechanics measurements and states are two different things and the relationship between them is nonintuitive.

Collapse of the wave function:

Suppose the state-vector of a system (just before the measurement of L):

$$\sum_j \alpha_j |\lambda_j\rangle$$

with $\sum_j {\alpha_j}^2 = 1$, eigenvectors $|\lambda_j\rangle$ and eigenvalues λ_j.

Any measurement of L will randomly measure an eigenvalue λ_j with probability $|\alpha_j|^2$. After the measurement the system will be in a single eigenstate of L, one of its $|\lambda_j\rangle$.

This we call the collapse of the wave function from a superposition to a single term.

Column vectors:

A column vector:

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix}$$

Column vectors, kets and column vectors:

A column vector:

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix}$$

The corresponding ket might be called $|\alpha\rangle$.

Column vectors, spin states as column vectors:

Spin state vectors usually are labeled as $|u\rangle$ and $|d\rangle$ with the meaning “up” and “down”.

The corresponding column state-vectors are $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ for up and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ for down.

Please do not try to give them a spatial meaning.

Commutation relations:

1)

Commutation relations for operators σ_x, σ_y and σ_z by using the representation as Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The general commutator relation for operators: $[A, B] = AB - BA$

Applied to the operators σ_x and σ_y:

$$[\sigma_x, \sigma_y] = \sigma_x\sigma_y - \sigma_y\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} =$$

$$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = 2i\sigma_z$$

$$[\sigma_x, \sigma_y] = 2i\sigma_z$$

The other pairs:

$$[\sigma_y, \sigma_z] = 2i\sigma_x$$

$$[\sigma_z, \sigma_x] = 2i\sigma_y$$

Note: pairs of the kind $[\sigma_y, \sigma_y]$ always give zero.

2)

Two observables can be measured simultaneously only if the associated operators commute.

No two spin components can be measured simultaneously.

3)

$$[P^2X] = PPX - XPP = PPX - PXP + PXP - XPP =$$

$$P(PX - XP) + (PX - XP)P = P[P, X] + [P, X]P$$

4)

Let X be the observable for position (the position operator) and P the observable for momentum (the momentum operator).

The following commutator relation holds:

$$[X, P] = i\hbar$$

5)

Let X be the observable for position (the position operator) and P the observable for momentum (the momentum operator.

We define:

$a^+ \coloneqq (P + i\omega X)$ the raising operator,

$a^- \coloneqq (P - i\omega X)$ the lowering operator and

$N \coloneqq a^+ a^-$ the number operator.

Note: ω is a real number.

We get a set of operators that closes under commutation:

$$[a^-, a^+] = 1, [a^-, N] = a^- \text{ and } [a^+, N] = -a^+$$

Commutative property:

This is part of axioms of vector addition:

2. Vector addition is commutative: $|A\rangle + |B\rangle = |B\rangle + |A\rangle$

Commutator algebra:

We define:

$a^+ \coloneqq (P + i\omega X)$ the raising operator,

$a^- \coloneqq (P - i\omega X)$ the lowering operator and

$N \coloneqq a^+ a^-$ the number operator.

Note: ω is a real number.

The commutator relations:

$$[a^-, a^+] = 1$$

$$[a^-, N] = a^-$$

$$[a^+, N] = -a^+$$

$$[a^+, N] \coloneqq a^+ N - N a^+ = -a^+ \ (*)$$

With the number operator we write the Hamiltonian:

$$H = \omega\hbar(N + \frac{1}{2})$$

Suppose we have an eigenvector $|n\rangle$ with eigenvalue n of the operator N:

$$N|n\rangle = n|n\rangle$$

Consider a new vector $a^+|n\rangle$, obtained by acting with a^+on $|n\rangle$.

We check (this is a little bit tricky):

$$N(a^+|n\rangle) = \big(a^+N - (a^+N - Na^+)\big)|n\rangle =^{(*)} (a^+N + a^+)|n\rangle =$$

$$a^+(N+1)|n\rangle = a^+(n+1)|n\rangle = (n+1)(a^+|n\rangle)$$

In summa:

$$N(a^+|n\rangle) = (n+1)(a^+|n\rangle)$$

The result of this operation: $a^+|n\rangle$ is eigenvector to the operator N with eigenvalue $n+1$. Analog we can handle the lowering operator and get:

$$N(a^-|n\rangle) = (n-1)(a^-|n\rangle)$$

$a^-|n\rangle$ is eigenvector to the operator N with eigenvalue $n-1$.

Whilst the raising operator raises “endless”, the lowering operator comes to an end. Applying the lowering operator to the lowest energy state, $|0\rangle$ with Energy $E_0 = \frac{\omega\hbar}{2}$, the result will be zero:

$$a^-|0\rangle = 0$$

Note: the vector $|0\rangle$ is a state-vector with a definite energy level. “0” is the zero-vector whose components all are zero. With this commutator algebra we find the entire spectrum of harmonic oscillator energy levels, consisting of energy values:

$$E_n = \omega\hbar\left(n + \frac{1}{2}\right) = \omega\hbar\left(\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\right)$$

Commutators:

1.

Given two operators or matrices, the combination $LM - ML$ is called the commutator of L with M and denoted by $LM - ML = [LM]$.

2.

We can write the change with time of the expectation value of an operator L in a simple form (H is the Hamiltonian):

$$\frac{d}{dt}\langle L\rangle = -\frac{i}{\hbar}\langle [L,H]\rangle$$

3.

Let Q be an observable. The condition for $\langle Q\rangle$ not to change with time is:

$$[Q,H] = 0$$

4.

Any operator commutes with itself:

$$[H, H] = 0$$

H (the total energy of the system) is conserved.

5.

With the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

we get the commutators

$$[\sigma_x, \sigma_y] = 2i\sigma_z, \qquad [\sigma_y, \sigma_z] = 2i\sigma_x, \qquad [\sigma_z, \sigma_x] = 2i\sigma_y$$

Note: pairs of the kind $[\sigma_y, \sigma_y]$ always give zero.

6.

Let $|\psi\rangle$ be any ket and let A and B be any two observables with expectation value zero.

We define $|X\rangle$ and $|Y\rangle$ as follows:

$$|X\rangle = A|\psi\rangle \text{ and } |Y\rangle = iB|\psi\rangle$$

and plug them into the Cauchy-Schwarz inequality:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

We get

$$2\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq |\langle\psi|AB|\psi\rangle - \langle\psi|BA|\psi\rangle| = |\langle\psi|[A, B]|\psi\rangle| = |\langle[A, B]\rangle|$$

A and B have expectation values of zero.

$\langle A^2\rangle$ is the square of the uncertainty in A: $(\triangle A)^2$

$\langle B^2\rangle$ is the square of the uncertainty in B: $(\triangle B)^2$

We rewrite the result as:

$$\triangle A \triangle B \geq \frac{1}{2}|\langle[A, B]\rangle|$$

The product of the uncertainties cannot be smaller than half the magnitude of the expectation value of the commutator.

7.

We replace:

A by X: the observable for position (the position operator)

B by P: the observable for momentum (the momentum operator)

The commutator $[X, P] = i\hbar$

We get the Heisenberg Uncertainty Principle:

$$\triangle X \triangle P \geq \frac{1}{2}|\langle [X,P]\rangle| = \frac{i\hbar}{2}$$

8.

Any potential that is a function of x: $V(x)$ commutes with the observable of position (the position operator) X:

$$[X, V(x)] = 0$$

The classical version of Newton's law:

$$\frac{d}{dt}p = F$$

We transfer it to quantum mechanics via the use of the Hamiltonian: $H = \frac{P^2}{2m} + V(x)$.

$$\frac{d}{dt}\langle P\rangle = \frac{i}{2m\hbar}\langle [P^2, P]\rangle + \frac{i}{\hbar}\langle [V(x), P]\rangle$$

The first term on the right side is zero because an operator commutes with any function of itself.

For the second term holds: $[V(x), P] = i\hbar\frac{d}{dx}V(x)$.

We get:

$$\frac{d}{dt}\langle P\rangle = -\langle \frac{d}{dx}V(x)\rangle$$

Commutators, classical physics and commutators:

Commutators have great similarity to Poisson brackets. If we take the operator symbols L and M, we get:

$$[L, M] \leftrightarrow i\hbar\{L, M\}$$

$[L, M]$ denoting the quantum commutator, $\{L, M\}$ denoting the Poisson brackets.

Let X be the observable for position (position operator) and P the observable for momentum (momentum operator).

X acts on an arbitrary wave function $\psi(x)$:

$$X\psi(x) = x\psi(x)$$

P acts like

$$P\psi(x) = -i\hbar\frac{d\psi(x)}{dx}$$

Together the product XP acts on $\psi(x)$:

$$X(P\psi(x)) = -i\hbar x\frac{d\psi(x)}{dx}$$

PX acting on $\psi(x)$:

$$P(X\psi(x)) = -i\hbar x\frac{d\big(x\psi(x)\big)}{dx} = -i\hbar\frac{d\psi(x)}{dx} - i\hbar\psi(x)$$

Now we check the commutator relation $[X,P]\psi(x)$:= $(XP-PX)\psi(x)$:

$$(XP-PX)\psi(x) = -i\hbar x\frac{d\psi(x)}{dx} - \left(-i\hbar\frac{d\psi(x)}{dx} - i\hbar\psi(x)\right) = i\hbar\psi(x)$$

From this follows

$$[X,P]\psi(x) = i\hbar\psi(x)$$

$$[X,P] = i\hbar$$

X and P don't commute. We compare this to the corresponding Poisson bracket $\{x,p\}$. With the equivalence $[X,P] \leftrightarrow i\hbar\{x,p\}$ we can conclude that $\{x,p\}$ must be 1 which is the classical relation between coordinates and their conjugate momenta.

Commutators, operators and commutators:

The Hamiltonian expressed in terms of position operator X, the observable for position and momentum operator P, the observable for momentum:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2)$$

(*This is a classical as well as a quantum mechanical Hamiltonian, so it would be correct to use the classical lowercase symbols p and x.*)

The idea is to use the properties of X and P, especially the commutation relation $[X,P] = i\hbar$ to construct three new operators, called creation (or raising) operator, annihilation (or lowering) operator and number operator.

The names are program.

The raising operator produces a new eigenvector that has the next higher energy level.

The lowering operator produces a new eigenvector that has the next lower energy level.

The number operator returns the "number" of the energy level.

The construction process.

Using complex numbers, we can split up a sum according to $a^2 + b^2 = (a+ib)(a-ib)$ to

$$H\sim\frac{1}{2}(P + i\omega X)(P - i\omega X)$$

"$\sim$" because of the quantum mechanically behavior of X and P: they don't commute.

We expand the Hamiltonian:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + i\omega XP - i\omega PX - i^2\omega^2 X^2) =$$

$$\frac{1}{2}(P^2 + \omega^2 X^2) + \frac{1}{2}i\omega[X,P]$$

We know the value of the commutator: $[X,P] = i\hbar$ and get:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + \omega^2 X^2) - \frac{1}{2}\hbar\omega$$

Our correct Hamiltonian:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{1}{2}\hbar\omega$$

We define our new raising and lowering operators.

$$a^- \coloneqq (P - i\omega X)$$

$$a^+ \coloneqq (P + i\omega X)$$

$$N \coloneqq a^+ a^-$$

Stated in terms of the number operator, the Hamiltonian becomes:

$$H = \hbar\omega(N + \frac{1}{2})$$

Commutators, Poisson brackets and commutators:

1.

In quantum mechanics we have:

$$\frac{dL}{dt} = -\frac{i}{\hbar}[L, H]$$

We can think of this equation that it tells us how the centers of probability distribution move around. This resembles the Poisson brackets of classical physics. The formal identification between commutators and Poisson brackets is:

$$[L, H] \leftrightarrow i\hbar\{L, H\}$$

We combine and get:

$$\frac{dL}{dt} = -\frac{i}{\hbar}[L, H] = -\frac{i^2\hbar}{\hbar}\{L, H\} = \{L, H\}$$

$$\dot{L} = \{L, H\}$$

2.

Commutators have a great similarity to Poisson brackets. If we take the operator symbols L and M, we get $[L, M] \leftrightarrow i\hbar\{L, M\}$ with $[L, M]$ denoting the quantum commutator, $\{L, M\}$ denoting the Poisson brackets.

Let X be the observable for position (position operator) and P the observable for momentum (momentum operator).

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From this follows

$$[X,P]\psi(x) = i\hbar\psi(x)$$

$$[X,P] = i\hbar$$

X and P do not commute. We compare this with the corresponding Poisson bracket $\{x,p\}$. With the equivalence $[X,P] \leftrightarrow i\hbar\{x,p\}$ we can conclude that $\{x,p\}$ must be 1 which is the classical relation between coordinates and their conjugate momenta.

Commutating variables, complete sets of commutating variables:

Hint: For better readability we omit indices belonging to the respective bases.

In a two-spin system, we measure each spin separately and associate these measurements with two different operators L and M. Every measurement leaves the system in an eigenstate. If we measure both spins in a two-spin system, the system switches to a state that is simultaneously an eigenvector of L and an eigenvector of M.

Every operator has his set of eigenvectors and eigenvalues: L with eigenvalues λ and eigenvectors $|\lambda\rangle$ and M with eigenvalues μ and eigenvectors $|\mu\rangle$.

We assume that there is a basis of state-vectors $|\lambda,\mu\rangle$ that are simultaneous eigenvectors of both observables:

$$L|\lambda,\mu\rangle = \lambda|\lambda,\mu\rangle \text{ and } M|\lambda,\mu\rangle = \mu|\lambda,\mu\rangle$$

$|\lambda,\mu\rangle$ being simultaneous eigenvector of L and M implies:

$$LM|\lambda,\mu\rangle = ML|\lambda,\mu\rangle$$

$$[L,M]|\lambda,\mu\rangle = 0$$

The condition for two observables to be simultaneously measurable is: they must commute.

A set of commuting observables that all commute among themselves is called a complete set of commuting variables.

Commutating variables and wave functions:

Suppose we have a basis of states for some quantum system. The orthonormal basis vectors are called $|a, b, c, \dots\rangle$ with $a, b, c \dots$ the eigenvalues of some complete set of commuting observables $A, B, C, \dots$

Consider an arbitrary state vector $|\psi\rangle$. Since the vectors $|a, b, c, \dots\rangle$ form an orthonormal basis, $|\psi\rangle$ can be expanded in terms of them:

$$|\psi\rangle = \sum_{a,b,c,\dots} \psi(a, b, c, \dots)|a, b, c, \dots\rangle$$

The quantities $\psi(a, b, c, \dots)$ are the coefficients. Each of them is equal to the inner product of the ket $|\psi\rangle$ with one of the basis vectors:

$$\psi(a, b, c, \dots) \coloneqq \langle a, b, c, \dots|\psi\rangle$$

The set of coefficients $\psi(a, b, c, \dots)$ is called the wave function of the system in the basis defined by the observables $A, B, C, \dots$.

The physical meaning of the wave function is important. The squared magnitude of the wave function is the probability for the commuting observables to have values $a, b, c \dots$:

$$P(a, b, c \dots) = \psi^*(a, b, c, \dots)\psi(a, b, c, \dots)$$

The form of the wave function depends on which observable we choose to focus on.

For example, in the case of a single spin the inner products $\psi(u) = \langle u|\psi\rangle$ and $\psi(d) = \langle d|\psi\rangle$ define the wave function in the σ_z basis.

The probabilities of a complete set of commuting observables must sum to 1:

$$\sum_{a,b,c,\dots} P(a, b, c \dots) = \sum_{a,b,c,\dots} \psi^*(a, b, c, \dots)\psi(a, b, c, \dots) = 1$$

This holds in the case of a single observable, a single spin e.g. in the up-down-basis:

$$\sum_{a,b,c,\dots} P(a, b, c \dots) \to \sum_{u,d} P(u, d) = P(u) + P(d) = \psi^*(u)\psi(u) + \psi^*(d)\psi(d)$$

Conclusion: the term wave function refers to the collection of coefficients (components) that are coefficients of the basis vectors in an eigenfunction expansion:

$$|\psi\rangle = \sum_j \alpha_j|\psi_j\rangle$$

with $|\psi_j\rangle$ being orthonormal eigenvectors of a Hermitian operator. The collection of α_j is what we mean by the wave function.

Again, in the example of a single spin in the up-down-basis:

The basis ket vectors: $|u\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |d\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ and their bras $\langle u| = (1\ 0), \langle d| = (0\ 1)$

An arbitrary state-vector: $|\psi\rangle \coloneqq \alpha_1|u\rangle + \alpha_2|d\rangle = \alpha_1\begin{pmatrix}1\\0\end{pmatrix} + \alpha_2\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}\alpha_1\\\alpha_2\end{pmatrix}$

The wave-function $\psi(u,d)$:

$$\psi(u) \coloneqq \langle u|\psi\rangle = (1\ 0)\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} = \alpha_1 \text{ and } \psi^*(u) = {\alpha_1}^*$$

$$\psi(d) \coloneqq \langle d|\psi\rangle = (0\ 1)\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} = \alpha_2 \text{ and } \psi^*(d) = {\alpha_2}^*$$

The set of coefficients $\psi(u,d) = \psi(u), \psi(d)$ is called the wave function of the system in the basis defined by the observable "spin up".

To calculate the probability $\psi^*\psi$ we write this as a vector: $\psi(u,d) = \begin{pmatrix}\psi(u)\\ \psi(d)\end{pmatrix} = \begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}$ and build the dot product with its transposed complex conjugate $((\psi(u,d))^*)^T = \psi(u)^*\psi(d)^* = (\alpha_1^*\alpha_2^*)$:

$$\psi^*\psi = (\alpha_1^*\alpha_2^*)\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} = \alpha_1^*\alpha_1 + \alpha_2^*\alpha_2$$

As this is the total probability it should give 1.

Complex conjugate:

Every complex number z has a complex conjugate number, marked as z^*. The complex conjugate switches the imaginary part to the opposite sign.

In cartesian coordinates: $z = a + ib$ changes to $z^* = a - ib$ and vice versa.

In polar coordinates: $z = re^{i\varphi}$ and $z^* = re^{-i\varphi}$.

Please note that $zz^* = r^2 = |z|^2$

Complex conjugate numbers:

Ket $|A\rangle \coloneqq \begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\\ \alpha_4\end{pmatrix}$, bra $\langle A| = (\alpha_1^*\ \alpha_2^*\ \alpha_3^*\ \alpha_4^*)$.

Inner product: $\langle A|A\rangle = (\alpha_1^*\ \alpha_2^*\ \alpha_3^*\ \alpha_4^*)\begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\\ \alpha_4\end{pmatrix} = \alpha_1^*\alpha_1 + \alpha_2^*\alpha_2 + \alpha_3^*\alpha_3 + \alpha_4^*\alpha_4$

Note: bras are always the complex conjugated and not explicitly written as $\langle A^*|$.

Complex conjugation for operators:

The equation $M|A\rangle = |B\rangle$ needs a counterpart $\langle A|M^\dagger = \langle B|$.

$M^\dagger$ we get out of M by transposing and complex conjugating M:

We transpose a matrix:

$$M = \begin{pmatrix}a & b & c\\ d & e & f\\ g & h & k\end{pmatrix} \rightarrow M^T = \begin{pmatrix}a & d & g\\ b & e & h\\ c & f & k\end{pmatrix}$$

We complex conjugate this matrix:

$$M^T = \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & k \end{pmatrix} \rightarrow M^\dagger = \begin{pmatrix} a^* & d^* & g^* \\ b^* & e^* & h^* \\ c^* & f^* & k^* \end{pmatrix}$$

Please note the symbol: $M^\dagger$ stands for M^{T*}.

Explicit:

Let $|B\rangle := \begin{pmatrix} l \\ m \\ n \end{pmatrix}$ and accordingly $\langle B| := (l^* m^* n^*)$:

$$M|A\rangle = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & k \end{pmatrix} \begin{pmatrix} l \\ m \\ n \end{pmatrix} = \begin{pmatrix} al + bm + cn \\ dl + em + fn \\ gl + hm + kn \end{pmatrix}$$

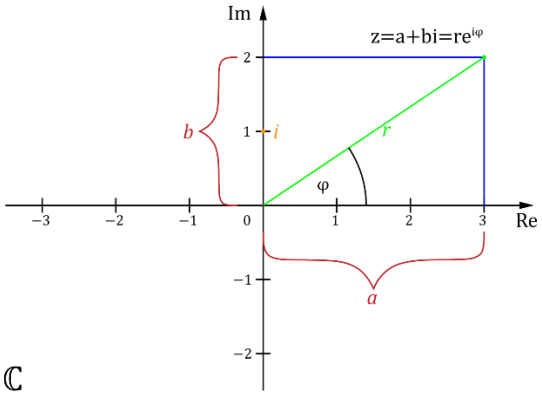
$$\langle A|M^\dagger = (l^* m^* n^*) \begin{pmatrix} a^* & d^* & g^* \\ b^* & e^* & h^* \\ c^* & f^* & k^* \end{pmatrix} = \begin{pmatrix} a^* l^* + b^* m^* + c^* n^* \\ d^* l^* + e^* m^* + f^* n^* \\ g^* l^* + h^* m^* + k^* n^* \end{pmatrix}$$

Obviously $\langle A|M^\dagger = (M|A\rangle)^*$. This fits with the convention that $\langle B|$ is the complex conjugated of $|B\rangle$.

Complex numbers:

A complex number consists of a real part and an imaginary part. We can write it as $z = a + ib$ with $a, b \in \mathbb{R}$. The imaginary unit i has the property $i \cdot i = -1$ or $i^2 = -1$.

We can represent complex numbers by a plane with the horizontal real axis and the vertical imaginary axis. This is called the cartesian mode.



... graphic courtesy of Wikipedia ...

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A second way of representation describes a complex number by the angle it has with the real axis and its length resp. the absolute value. This is called the gaussian mode. In this mode we write a complex number as $r \cdot e^{i\varphi}$.

We can switch from one representation to the other:

Given $z = a + ib$: $\quad |z| \text{ or } r = \sqrt{a^2 + b^2}$ $\quad \varphi = \arccos\left(\frac{a}{r}\right)$ if $b \geq 0$

resp. $\quad \varphi = -\arccos\left(\frac{a}{r}\right)$ if $b < 0$.

Given $z = re^{i\varphi}$: $a = r \cdot \cos(\varphi)$ $b = r \cdot \sin(\varphi)$

or $z = r \cdot (\cos(\varphi) + i \cdot \sin(\varphi))$

Every complex number z has a complex conjugate number, marked as z^*. The complex conjugate switches the imaginary part to the opposite sign. $z = a + ib$ changes to $\bar{z} = a - ib$ and vice versa.

With this we get new formulas:

$$|z| = \sqrt{zz^*}$$

$$re(z)\ or\ a = \frac{z + z^*}{2}$$

$$im(z)\ or\ b = \frac{z - z^*}{2}$$

Additions and subtraction of complex numbers are best performed with the cartesian representation.

$$(a + ib) + (c + id) = ac + ibd$$

Multiplication and division are best performed with the gaussian representation.

$$r_1 e^{i\varphi} \cdot r_2 e^{i\theta} = r_1 r_2 e^{i(\varphi+\theta)}$$

A number of the form $z = e^{i\varphi}$ has the absolute value 1: $\left|e^{i\varphi}\right| = \sqrt{e^{i\varphi} e^{-i\varphi}} = \sqrt{e^0} = \sqrt{1} = 1$. It is called a phase factor. No measurable quantity, no observable is sensitive to an overall phase-factor, so we can ignore it when specifying states.

Note: complex numbers often are used for “a trick” in calculations. With complex numbers you can transform a sum into a product: $(x + iy)(x - iy) = x^2 + y^2$.

Complex numbers, addition of complex numbers:

Additions and subtraction of complex numbers are best performed with the cartesian representation.

$$(a + ib) + (c + id) = ac + ibd$$

Complex numbers, eigenvalues and complex numbers:

An operator M (a Matrix M) can have complex valued eigenvectors:

$$M := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ i \end{pmatrix} = \begin{pmatrix} -i \\ 1 \end{pmatrix} = i \begin{pmatrix} 1 \\ i \end{pmatrix}$$

Complex numbers, multiplication of complex numbers:

Multiplication and division are best performed with the gaussian representation.

$$r_1 e^{i\varphi} \cdot r_2 e^{i\theta} = r_1 r_2 e^{i(\varphi+\theta)}$$

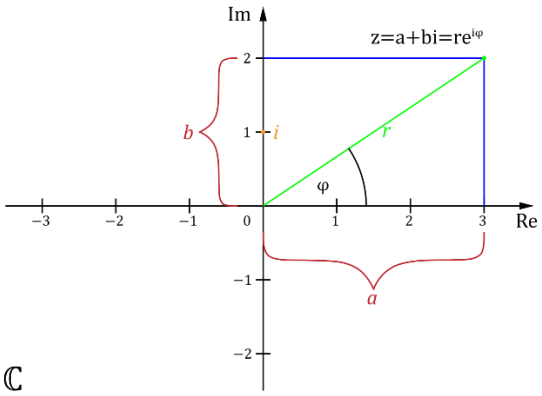
Complex numbers, phase factors of complex numbers:

A number of the form $z = e^{i\varphi}$ has the absolute value 1: $\left|e^{i\varphi}\right| = \sqrt{e^{i\varphi} e^{-i\varphi}} = \sqrt{e^0} = \sqrt{1} = 1$. It is called a phase factor. No measurable quantity, no observable is sensitive to an overall phase-factor, so we can ignore it when specifying states.

An observable is always something like the product of a complex number by its complex conjugated. In this process the phase factors cancel each out.

Complex numbers, representations of complex numbers:

We can represent complex numbers by a plane with the horizontal real axis and the vertical imaginary axis. This is called the cartesian mode.



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resp. $\quad \varphi = -\arccos\left(\frac{a}{r}\right)$ if $b < 0$.

Given $z = re^{i\varphi}$: $\quad a = r \cdot \cos(\varphi)$ $\quad b = r \cdot \sin(\varphi)$

or $\quad z = r \cdot (\cos(\varphi) + i \cdot \sin(\varphi))$

Complex vector spaces, orthonormal basis and complex vector spaces:

The dimension of a space can be defined as the maximum number of mutually orthogonal vectors of length 1, called an orthonormal basis. Any vector $|A\rangle$ in the space can be represented by:

$$|A\rangle = \sum_k \alpha_i |k\rangle$$

$|k\rangle$ representing a set of vectors that form an orthonormal basis.

The same principle is true for complex vector spaces, α_i being complex numbers.

Component matrices and tensor products:

Let A and B be two 2×2 matrices:

$$A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{21} \end{pmatrix}$$

$$B \coloneqq \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{21} \end{pmatrix}$$

The matrix version of the tensor product, sometimes called the Kronecker product:

$$A \otimes B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

We combine state vectors.

The up and $down$ state vectors for each subsystem:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We combine:

$$|uu\rangle = |u\rangle \otimes |u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The same way the other combinations:

$$|ud\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |du\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } |dd\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

We combine operators.

$$\sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tau_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_z \otimes \tau_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & -1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

We apply $\sigma_z \otimes \tau_x$ to $|ud\rangle$:

$$(\sigma_z \otimes \tau_x)|ud\rangle = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |uu\rangle$$

For tensor product holds a kind of distributive rule.

Let A, B be two 2×2 matrices and u, v two 2×1 column vectors:

$$A := \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, B := \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$u := \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, v := \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},$$

$$u \otimes v = \begin{pmatrix} u_1 \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \\ u_2 \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} u_1 v_1 \\ u_1 v_2 \\ u_2 v_1 \\ u_2 v_2 \end{pmatrix}$$

$$A \otimes B := \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix},$$

To prove:

$$(A \otimes B)(u \otimes v) = (Au \otimes Bv)$$

Left side $(A \otimes B)(u \otimes v)$:

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix} \begin{pmatrix} u_1 v_1 \\ u_1 v_2 \\ u_2 v_1 \\ u_2 v_2 \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11}u_1v_1 + a_{11}b_{12}u_1v_2 + a_{12}b_{11}u_2v_1 + a_{12}b_{12}u_2v_2 \\ a_{11}b_{21}u_1v_1 + a_{11}b_{22}u_1v_2 + a_{12}b_{21}u_2v_1 + a_{12}b_{22}u_2v_2 \\ a_{21}b_{11}u_1v_1 + a_{21}b_{12}u_1v_2 + a_{22}b_{11}u_2v_1 + a_{22}b_{12}u_2v_2 \\ a_{21}b_{21}u_1v_1 + a_{21}b_{22}u_1v_2 + a_{22}b_{21}u_2v_1 + a_{22}b_{22}u_2v_2 \end{pmatrix}$$

Right side $(Au \otimes Bv)$:

$$Au = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} a_{11}u_1 + a_{12}u_2 \\ a_{21}u_1 + a_{22}u_2 \end{pmatrix}$$

$$Bv = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix}$$

$$(Au \otimes Bv) = \begin{pmatrix} a_{11}u_1 + a_{12}u_2 \\ a_{21}u_1 + a_{22}u_2 \end{pmatrix} \otimes \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} =$$

$$\begin{pmatrix} (a_{11}u_1 + a_{12}u_2) \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \\ (a_{21}u_1 + a_{22}u_2) \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1(b_{11}v_1 + b_{12}v_2) + a_{12}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{11}u_1(b_{21}v_1 + b_{22}v_2) + a_{12}u_2(b_{21}v_1 + b_{22}v_2) \\ a_{21}u_1(b_{11}v_1 + b_{12}v_2) + a_{22}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{21}u_1(b_{21}v_1 + b_{22}v_2) + a_{22}u_2(b_{21}v_1 + b_{22}v_2) \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1b_{11}v_1 + a_{11}u_1b_{12}v_2 + a_{12}u_2b_{11}v_1 + a_{12}u_2b_{12}v_2 \\ a_{11}u_1b_{21}v_1 + a_{11}u_1b_{22}v_2 + a_{12}u_2b_{21}v_1 + a_{12}u_2b_{22}v_2 \\ a_{21}u_1b_{11}v_1 + a_{21}u_1b_{12}v_2 + a_{22}u_2b_{11}v_1 + a_{22}u_2b_{12}v_2 \\ a_{21}u_1b_{21}v_1 + a_{21}u_1b_{22}v_2 + a_{22}u_2b_{21}v_1 + a_{22}u_2b_{22}v_2 \end{pmatrix}$$

Obviously both sides are equal.

Component:

Component is the collective name for columns, rows, and matrices you use to represent vectors and linear operators.

Component of 3-vector:

1.

A 3-vector $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$ is a vector in "ordinary" space.

$\begin{pmatrix} a \\ b \\ c \end{pmatrix}$ is a short form for using the standard orthonormal basis:

$$\vec{x} = a\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + c\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \coloneqq \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

The coefficients a, b, and c need a basis to be unambiguous.

2.

The operators σ_x, σ_y, and σ_z are the components of the spin operator $\vec{\sigma} \coloneqq (\sigma_x\ \sigma_y\ \sigma_z)$ along the three axes in space.

$\vec{\sigma}$ behaves like a 3-vector because it has three independent components.

To build a spin operator that is oriented along any axis is space we first need the appropriate unit 3-vector $\hat{n} \coloneqq \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$ that goes in this direction. Then we construct the vector-operator:

$$\sigma_n \coloneqq \vec{\sigma} \cdot \hat{n} = \begin{pmatrix} \sigma_x\ \sigma_y\ \sigma_z \end{pmatrix} \cdot \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z$$

This is a new type of vector, a 3-vector operator.

3.

A classical spin (a charged rotor) in a magnetic field $\vec{B} = \begin{pmatrix} B_x\ B_y\ B_z \end{pmatrix}$ has an energy depending on its orientation, the energy proportional to the dot product of spin and magnetic field.

The quantum version of this is:

$$H \sim \vec{\sigma} \cdot \vec{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$$

Note: H is the quantum Hamiltonian, σ_x, σ_y, and σ_z are the spin operators.

Component, addition of components:

The addition of vectors by adding the components:

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} + \begin{pmatrix} d \\ e \\ f \end{pmatrix} = \begin{pmatrix} a+d \\ b+e \\ c+f \end{pmatrix}$$

This holds for matrices analog.

Component of angular momentum:

The classical rotor in a magnetic field (oriented along the z-axis) has an angular momentum that is precessing in the x- and y-components.

In quantum mechanics the expectation values are “precessing” despite of every measurement giving “0” or “1”.

Component of basis vector:

The advantage of representing vectors and linear operators concretely by columns, rows, and matrices (components) is that those components provide a complete, explicit set of arithmetic rules to work with, depending on a specific choice of basis vectors.

The underlying relationships between vectors and operators is independent of any basis, the concrete representation obscures this fact sometimes.

Component of generic state:

The space of states for a single spin has only two dimension, “up” and “$down$”. By choosing $|u\rangle$ and $|d\rangle$ as the two basis vectors we could write any state $|A\rangle$ as a linear superposition of them:

$$|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$$

α_u and α_d are the components of $|A\rangle$ along the basis directions.

Component, inner products and component:

1.

The rule for inner products is essentially the same as for dot products: add the products of corresponding components:

$$\langle B|A\rangle = (\beta_1^* \; \beta_2^* \; \beta_3^*) \cdot \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \beta_1^*\alpha_1 + \beta_2^*\alpha_2 + \beta_3^*\alpha_3$$

Note: row vectors always use the complex conjugated values.

2.

The ket $|A\rangle$ can be written as:

$$|A\rangle = \sum_j \alpha_j \, |j\rangle$$

$|i\rangle$ are basis vectors.

We use $\langle j|A\rangle = \alpha_j$, the components of a vector are its inner products with the basis vectors and write:

$$|A\rangle = \sum_j \langle j|A\rangle \, |j\rangle = \sum_j |j\rangle\langle j|A\rangle$$

Note: $\langle j|A\rangle$ is just a number.

Component, multiplication of component:

A component can be multiplied by a (complex) number:

$$z \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} za \\ zb \\ zc \end{pmatrix}$$

This holds for matrices analog.

Component of phase-factor:

A phase-factor is a complex number z of "length" 1: $|z| = 1$.

For phase-factors holds:

$$zz^* = 1$$

$$z = e^{i\varphi}$$

$$z = cos\varphi + i\ sin\varphi$$

Component of spin:

1. Measuring one component of spin destroys the information about the other components.
2. Proposition A: The z component of the spin is +1.
   Proposition B: the x component of the spin is +1.
   According to classical logic, this could be tested by measuring either
   a) first A and then B,
   b) first B and then A.
   In quantum mechanics this is not possible. First measuring A sets the spin is in state A, subsequent measurements B gives random results +1 and -1.
3. (particle has position x) and (momentum p) is not measurable in quantum mechanics. We can only measure (particle has position x) or (momentum p).
4. The components of spin, $\sigma_x, \sigma_y, \sigma_z$ are observables.
5. Possible values of any of the components of spin are ± 1.
6. A spin operator can only provide information about the spin component in a specific direction.
7. $\sigma_x, \sigma_y, \sigma_z$ are operators (matrices) that correspond to the three measurable components of spin. They behave much like 3-vectors.
8. Any state of a single spin is an eigenvector of some component of the spin.
   Given any state $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$
   there exists some direction $\vec{n}$ such that $(\vec{\sigma} \cdot \vec{n})|A\rangle = |A\rangle$.
   The states of a spin are characterized by a polarization vector, and along that polarization vector the component of the spin is predictably +1.
9. If the expectation value of a component of σ is zero, this means that the experimental outcome is equally likely to +1 or -1.

Component of state-vector:

1.

The state of a system is represented by a unit vector in a vector space of states. The squared magnitudes of the components of the state-vector represent probabilities for various experimental outcomes.

Let $|A\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$, with $|u\rangle$ and $|d\rangle$ as the basis vectors.

$|A\rangle$ is normalized: $\sqrt{\left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2} = 1$, the probabilities for the outcomes are $\left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$ each.

Note: regularly the coefficients are complex so the normalization rule is: $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$ and the probability for outcomes $\alpha_u^*\alpha_u$ resp. $\alpha_d^*\alpha_d$.

2.

You can think of the wave function as a set of components of the state-vector in a particular basis. These components can be stacked up to form a column vector.

$|\psi\rangle$ state-vector

$\psi(\lambda)$ wave function associated with $|\psi\rangle$ in the (one of many possible) L-basis

$|\lambda\rangle$ set of orthonormal eigenvectors of L

λ the according eigenvalues

$\psi(\lambda) = \langle\lambda|\psi\rangle$ the projections of inner products of the state-vector onto the eigenvectors:

$$\begin{pmatrix} \psi(\lambda_1) \\ \vdots \\ \psi(\lambda_1) \end{pmatrix}$$

Component of vector:

The spin-operator σ with its components $\sigma_x, \sigma_y, \sigma_z$ resembles a vector.

Measuring a spin along any axis in space doesn't give fractions but always +1 or -1.

The fraction you get only by the statistics of the +1 and -1 outcomes of several measurements.

Component, wave functions and component:

The term wave function refers to the collection of coefficients (also called components) that multiply the basis vectors in an eigenfunction expansion.

You can think of the wave function as a set of components of the state-vector in a particular basis. These components can be stacked up to form a column vector.

$|\psi\rangle$ state-vector

$\psi(\lambda)$ wave function associated with $|\psi\rangle$ in the (one of many possible) L-basis

$|\lambda\rangle$ set of orthonormal eigenvectors of L

λ the according eigenvalues

$\psi(\lambda) = \langle\lambda|\psi\rangle$ the projections of inner products of the state-vector onto the eigenvectors:

$$\begin{pmatrix} \psi(\lambda_1) \\ \vdots \\ \psi(\lambda_1) \end{pmatrix}$$

A wave function is one of many possible representations of one state-vector.

Component form of addition:

1.

Additions and subtraction of complex numbers are best performed with the cartesian representation.

$$(a + ib) + (c + id) = ac + ibd$$

2.

We construct a vector by stacking up a pair of complex numbers, $\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}$ and identify this with the ket-vector $|A\rangle$. The complex numbers are the components of $|A\rangle$. You can add two column vectors by adding their components:

$$\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}+\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}=\begin{pmatrix}\alpha_1+\beta_1\\ \alpha_2+\beta_2\end{pmatrix}$$

Component form of bra-vectors:

$$\langle B|=(\beta_1^*\ \beta_2^*\ \dots\ \beta_n^*)$$

Note: the values are implicitly complex conjugated.

Component form, equation in component form:

The equation $M|A\rangle=|B\rangle$ in component form:

$$\begin{pmatrix}m_{11}&m_{12}&m_{13}\\ m_{21}&m_{22}&m_{23}\\ m_{31}&m_{32}&m_{33}\end{pmatrix}\begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\end{pmatrix}=\begin{pmatrix}m_{11}\alpha_1+m_{12}\alpha_2+m_{13}\alpha_3\\ m_{21}\alpha_1+m_{22}\alpha_2+m_{23}\alpha_3\\ m_{31}\alpha_1+m_{32}\alpha_2+m_{33}\alpha_3\end{pmatrix}=\begin{pmatrix}\beta_1\\ \beta_2\\ \beta_3\end{pmatrix}$$

The equation $\langle A|M^\dagger=\langle B|$ in component form:

$$(\alpha_1^*\ \alpha_2^*\ \alpha_3^*)\begin{pmatrix}m_{11}^*&m_{21}^*&m_{31}^*\\ m_{12}^*&m_{22}^*&m_{32}^*\\ m_{13}^*&m_{23}^*&m_{33}^*\end{pmatrix}=$$

$$(\alpha_1^*m_{11}^*+\alpha_2^*m_{12}^*+\alpha_3^*m_{13}^*\quad \alpha_1^*m_{21}^*+\alpha_2^*m_{22}^*+\alpha_3^*m_{23}^*\quad \alpha_1^*m_{31}^*+\alpha_2^*m_{32}^*+\alpha_3^*m_{33}^*)=(\beta_1^*\ \beta_2^*\ \beta_3^*)$$

Note: there is an implicit complex conjugation when switching from ket to bra.

The state-vector $|A\rangle=\frac{1}{\sqrt{2}}|u\rangle+\frac{1}{\sqrt{2}}|d\rangle$ written in component form:

$$|A\rangle=\frac{1}{\sqrt{2}}\left|u\right\rangle+\frac{1}{\sqrt{2}}\left|d\right\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix}+\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

Component form of multiplication:

Applying a matrix to a vector normally changes the vector to a new one. Exception from this rule are the eigenvectors of a matrix. Applying a matrix to an eigenvector simply multiplies the eigenvector by a number, its eigenvalue.

$M|A\rangle=\lambda|A\rangle$ in component form:

$$\begin{pmatrix}m_{11}&m_{12}&m_{13}\\ m_{21}&m_{22}&m_{23}\\ m_{31}&m_{32}&m_{33}\end{pmatrix}\begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\end{pmatrix}=\lambda\begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\end{pmatrix}$$

Component form of tensor product operators:

We are working with a two-spin state, σ_z is the operator working with Alice's spin.

We must widen Alice's operator with the tensor product: $\sigma_z\rightarrow\sigma_z\otimes I$.

σ_z is the operator of Alice, $\sigma_z\otimes I$ is the operator of Alice in the two-spin system.

The tensor product: $|ud\rangle=u\otimes d$

We calculate $(\sigma_z)|ud\rangle$. We get:

$$(\sigma_z)|ud\rangle = (\sigma_z \otimes I)(u \otimes d) = \sigma_z|u\rangle \otimes I|d\rangle = |u\rangle \otimes |d\rangle = |ud\rangle$$

Note that $(\sigma_z \otimes I)(u \otimes d)$ can be interpreted in two ways.

In detail

First, there is a kind of distributive rule we used above.

Second, we could work with the matrices.

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, |u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$(\sigma_z \otimes I) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 0\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ 0\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & -1\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$(u \otimes d) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 0\begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$(\sigma_z \otimes I)(u \otimes d) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

If we want to be absolutely correct, we can widen things more.

The coefficients of a Matrix M are the result of: $m_{jk} = \langle j|M|k\rangle$ with $|j\rangle$ and $|k\rangle$ representing basis vectors.

In our two-spin system we have the following four basis vectors:

$$|uu\rangle, |ud\rangle, |du\rangle, |dd\rangle$$

We write $(\sigma_z \otimes I)$:

$$(\sigma_z \otimes I) = \begin{pmatrix} \langle uu|\sigma_z \otimes I|uu\rangle & \langle uu|\sigma_z \otimes I|ud\rangle & \langle uu|\sigma_z \otimes I|du\rangle & \langle uu|\sigma_z \otimes I|dd\rangle \\ \langle ud|\sigma_z \otimes I|uu\rangle & \langle ud|\sigma_z \otimes I|ud\rangle & \langle ud|\sigma_z \otimes I|du\rangle & \langle ud|\sigma_z \otimes I|dd\rangle \\ \langle du|\sigma_z \otimes I|uu\rangle & \langle du|\sigma_z \otimes I|ud\rangle & \langle du|\sigma_z \otimes I|du\rangle & \langle du|\sigma_z \otimes I|dd\rangle \\ \langle dd|\sigma_z \otimes I|uu\rangle & \langle dd|\sigma_z \otimes I|ud\rangle & \langle dd|\sigma_z \otimes I|du\rangle & \langle dd|\sigma_z \otimes I|dd\rangle \end{pmatrix}$$

We are free whether to apply the σ_z to the left and I to the right or vice versa. The outer basis vectors will cancel everything not on the diagonal of the matrix. We will get again:

$$(\sigma_z \otimes I) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Component matrices:

Let A and B be two 2×2 matrices: $A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{21} \end{pmatrix}$, $B \coloneqq \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{21} \end{pmatrix}$

The matrix version of the tensor product, sometimes called the Kronecker product:

$$A \otimes B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

The tensor product of the up and down state vectors:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We combine:

$$|uu\rangle = |u\rangle \otimes |u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The same way the other combinations:

$$|ud\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |du\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } |dd\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

We combine operators. $\sigma_z \coloneqq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\tau_x \coloneqq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$:

$$\sigma_z \otimes \tau_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & -1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

We apply $\sigma_z \otimes \tau_x$ to $|ud\rangle$:

$$(\sigma_z \otimes \tau_x)|ud\rangle \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |uu\rangle$$

For tensor product holds a distributive rule.

Let A, B be two 2×2 matrices and u, v two 2×1 column vectors:

$$A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, B \coloneqq \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$u := \begin{pmatrix} u_1 \\ u_2 \end{pmatrix},\ v := \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},$$

$$u \otimes v = \begin{pmatrix} u_1 \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \\ u_2 \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} u_1 v_1 \\ u_1 v_2 \\ u_2 v_1 \\ u_2 v_2 \end{pmatrix}$$

$$A \otimes B := \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix},$$

To prove:

$$(A \otimes B)(u \otimes v) = (Au \otimes Bv)$$

Left side $(A \otimes B)(u \otimes v)$:

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix} \begin{pmatrix} u_1 v_1 \\ u_1 v_2 \\ u_2 v_1 \\ u_2 v_2 \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11}u_1v_1 + a_{11}b_{12}u_1v_2 + a_{12}b_{11}u_2v_1 + a_{12}b_{12}u_2v_2 \\ a_{11}b_{21}u_1v_1 + a_{11}b_{22}u_1v_2 + a_{12}b_{21}u_2v_1 + a_{12}b_{22}u_2v_2 \\ a_{21}b_{11}u_1v_1 + a_{21}b_{12}u_1v_2 + a_{22}b_{11}u_2v_1 + a_{22}b_{12}u_2v_2 \\ a_{21}b_{21}u_1v_1 + a_{21}b_{22}u_1v_2 + a_{22}b_{21}u_2v_1 + a_{22}b_{22}u_2v_2 \end{pmatrix}$$

Right side $(Au \otimes Bv)$:

$$Au = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} a_{11}u_1 + a_{12}u_2 \\ a_{21}u_1 + a_{22}u_2 \end{pmatrix}$$

$$Bv = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix}$$

$$(Au \otimes Bv) = \begin{pmatrix} a_{11}u_1 + a_{12}u_2 \\ a_{21}u_1 + a_{22}u_2 \end{pmatrix} \otimes \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} =$$

$$\begin{pmatrix} (a_{11}u_1 + a_{12}u_2) \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \\ (a_{21}u_1 + a_{22}u_2) \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1(b_{11}v_1 + b_{12}v_2) + a_{12}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{11}u_1(b_{21}v_1 + b_{22}v_2) + a_{12}u_2(b_{21}v_1 + b_{22}v_2) \\ a_{21}u_1(b_{11}v_1 + b_{12}v_2) + a_{22}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{21}u_1(b_{21}v_1 + b_{22}v_2) + a_{22}u_2(b_{21}v_1 + b_{22}v_2) \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1b_{11}v_1 + a_{11}u_1b_{12}v_2 + a_{12}u_2b_{11}v_1 + a_{12}u_2b_{12}v_2 \\ a_{11}u_1b_{21}v_1 + a_{11}u_1b_{22}v_2 + a_{12}u_2b_{21}v_1 + a_{12}u_2b_{22}v_2 \\ a_{21}u_1b_{11}v_1 + a_{21}u_1b_{12}v_2 + a_{22}u_2b_{11}v_1 + a_{22}u_2b_{12}v_2 \\ a_{21}u_1b_{21}v_1 + a_{21}u_1b_{22}v_2 + a_{22}u_2b_{21}v_1 + a_{22}u_2b_{22}v_2 \end{pmatrix}$$

Obviously both sides are equal.

Composite observables:

We have a two-spin system in an entangled state, the state $|sing\rangle \coloneqq \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$.

Can Alice (σ) and Bob (τ) simultaneously measure their own observable? Only, if the operators commute.

In fact, every component of σ commutes with every component of τ.

Check:

We combine operators. $\sigma_z \coloneqq \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, $\tau_x \coloneqq \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$:

$$\sigma_z \otimes \tau_x = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\\ 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & -1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix} \coloneqq A$$

$$\tau_x \otimes \sigma_z = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} & 1\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\\ 1\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} & 0\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{pmatrix} \coloneqq B$$

The commutation relation: $[A, B] = AB - BA$

$$AB = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix}\begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{pmatrix} = \begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\end{pmatrix}$$

$$BA = \begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{pmatrix}\begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix} = \begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\end{pmatrix}$$

Obviously $AB = BA$, so the operators commute, $[A, B] = 0$.

We try this explicit.

The basis vectors for the states $|uu\rangle, |ud\rangle, |du\rangle$ and $|dd\rangle$ are $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$.

The state$|sing\rangle \coloneqq \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$:

$$|sing\rangle \coloneqq \frac{1}{\sqrt{2}}\left(\begin{pmatrix}0\\1\\0\\0\end{pmatrix} - \begin{pmatrix}0\\0\\1\\0\end{pmatrix}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}$$

We apply operator A to the state $|sing\rangle$:

$$\begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\1\end{pmatrix}$$

Then we apply operator B to the result:

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}$$

We see that $|sing\rangle$ is eigenvector to the observable $\sigma_z\tau_x$ or $\tau_x\sigma_z$ with eigenvalue -1.

Alice and Bob can measure any component of their spin and get opposite results because $|sing\rangle$ is eigenvector to both with eigenvalue -1.

Composite operator, composite vectors and composite operator:

A composite operator $\sigma_z \otimes I$ is operating on a composite vector $|d\rangle \otimes |u\rangle$ to produce a new composite vector $-|d\rangle \otimes |u\rangle$:

$$\sigma_z|du\rangle = (\sigma_z \otimes I\ )(|d\rangle \otimes |u\rangle) = \sigma_z|d\rangle \otimes I|u\rangle = -|d\rangle \otimes |u\rangle = -|du\rangle$$

Alice's composite operator acts only on the left half of the composite vector $|du\rangle$. Analogous Bob's composite operator $I \otimes \tau_z$ acts on the right half.

Composite operator, energy and measurement of composite operator:

Example: Some atoms have spins that are described in the same way as electron spins. When two of these atoms are close to each other – for example, two neighboring atoms in a crystal lattice – the Hamiltonian will depend on the spins. In some situations, the neighboring spins' Hamiltonian is proportional to $\vec{\sigma} \cdot \vec{\tau}$. If that happens to be the case, then measuring $\vec{\sigma} \cdot \vec{\tau}$ is equivalent to measuring the energy of the atomic pair. Measuring this energy is a single measurement of the composite operator and does not entail measuring the individual components of either spin.

Composite state, two spin:

We are working in the z-basis: $|uu\rangle, |ud\rangle, |du\rangle, |dd\rangle$.

The simplest state for the composite system is called a product state, the result of completely independent preparations by Alice and Bob.

Alice prepares her spin in state $\alpha_u|u\rangle + \alpha_d|d\rangle$, Bob prepares his spin in the state $\beta_u|u\rangle + \beta_d|d\rangle$.

Crucial for a composite state is that each state separately is normalized:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1 \text{ and } \beta_u^*\beta_u + \beta_d^*\beta_d = 1.$$

The product state describing the combined system is:

$$|product\ state\rangle = \{\alpha_u|u\rangle + \alpha_d|d\rangle\} \otimes \{\beta_u|u\rangle + \beta_d|d\rangle\} =$$

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

The entangled state superposes the basis vectors in a general way

$$\psi_{uu}|uu\rangle + \psi_{ud}|ud\rangle + \psi_{du}|du\rangle + \psi_{dd}|dd\rangle$$

with only one normalizing condition:

$$\psi_{uu}^*\psi_{uu} + \psi_{ud}^*\psi_{ud} + \psi_{du}^*\psi_{du} + \psi_{dd}^*\psi_{dd} = 1$$

This state has six real parameters and therefore is richer than the combined state, it is entangled.

The four entangled states are the singled state and three triplet states:

$$|singlet\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

$$|t_1\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$$

$$|t_2\rangle = \frac{1}{\sqrt{2}}(|uu\rangle + |dd\rangle)$$

$$|t_3\rangle = \frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle)$$

In the product state there is some direction for which the measurement of spin gives +1. The expectation values satisfy the condition $\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$.

In the entangled state we get $\langle\sigma_x\rangle^2 = \langle\sigma_y\rangle^2 = \langle\sigma_z\rangle^2 = 0$ both for Alice and Bob, we have no access to the single parts of it. This is in contrast to classical physics. If you know the state for two classical particles you also know all about the individual particles.

Composite systems, mixed and pure states and composite systems:

Prerequisite

The trace of an operator Tr (or any square matrix) is the sum of its diagonal elements. The trace of a projection operator is 1.

We have a combined state. Alice prepares her spin with 50% probability either in state $|\varphi\rangle$ or $|\theta\rangle$.

The expectation value of any observable L is:

$$\langle L\rangle = \left(\frac{1}{2}Tr|\varphi\rangle\langle\varphi|L + \frac{1}{2}Tr|\theta\rangle\langle\theta|L\right) = Tr\left(\left(\frac{1}{2}|\varphi\rangle\langle\varphi|L + \frac{1}{2}|\theta\rangle\langle\theta|L\right)\right) =$$

$$Tr\left(\left(\frac{1}{2}|\varphi\rangle\langle\varphi| + \frac{1}{2}|\theta\rangle\langle\theta|\right)L\right)$$

The expression $\frac{1}{2}|\varphi\rangle\langle\varphi| + \frac{1}{2}|\theta\rangle\langle\theta|$ is an operator, called density matrix ρ that encodes Bob's knowledge of Alice's preparation. It can be expanded to a sum of states Alice could prepare with different probabilities P_1, P_2, …:

$$\rho = P_1|\varphi_1\rangle\langle\varphi_1| + P_2|\varphi_2\rangle\langle\varphi_2| + \cdots$$

When the density operator corresponds to a single state, it is a projection operator onto that state, the state called pure. In general, the density operator is a mix of several projection operators and represents a mixed state.

The density matrix ρ comes into life when a basis is chosen for the density operator. Suppose we choose the basis $|a\rangle$, then the matrix representation of the operator ρ is $\rho_{aa'} = \langle a|\rho|a'\rangle$ and the matrix representation of L is $L_{aa'}$. The expectation value $\langle L\rangle$ represents a mixed state and becomes:

$$\langle L\rangle = \sum_{a,a'} L_{a',a}\,\rho_{a,a'} \qquad \bigstar$$

End prerequisite

The state of a composite system can be absolutely pure (~single state), but each of its constituents must be described by a mixed state.

We take a system composed of two part, A and B. We suppose that Alice has complete knowledge of the state of the combined system, she knows the wave function $\psi(ab)$. Alice is interested only in system A and wants to have complete knowledge about system A. She selects an observable L that belongs to A and does nothing to B when it acts. The rule for calculating the expectation value of L:

$$\langle L\rangle = \sum_{ab,a'b'} \psi^*(a'b')L_{a'b',ab}\psi(ab)$$

The observable L was chosen to act on A only and let B unchanged, it acts trivially on the b-index (it leaves b unchanged, so $b' = b$ and the sum over the b separable):

$$\langle L\rangle = \sum_{a,b,a'} \psi^*(a'b)L_{a',a}\psi(ab) = \sum_{a,a'} L_{a',a} \sum_{b} \psi^*(a'b)\psi(ab)$$

The sum

$$\sum_{b} \psi^*(a'b)\psi(ab) = \rho_{a,a'}$$

is the density matrix for all a,a' in the combined system.

We write:

$$\langle L\rangle = \sum_{a,a'} L_{a',a}\,\rho_{a,a'}$$

and get the same expression as ★.

Result:

Despite the fact that the composite system is described by a pure state, the subsystem A must be described by a mixed state.

Composite systems, observables in composite systems:

We are in a two-spin system of Alice and Bob. The operators of Alice: $\sigma_x, \sigma_y, \sigma_z$ act on her state vectors $|u\rangle$ and $|d\rangle$. The same holds for Bob with his operators τ_x, τ_y, τ_z and state vectors $|u\rangle$ and $|d\rangle$.

In a composite system we use the tensor product to combine both operators and state vectors and get a four-dimensional system, a product state.

We write $\sigma_x|uu\rangle, \sigma_x|ud\rangle, \sigma_x|du\rangle, \sigma_x|dd\rangle$ with σ_x acting only on Alice's half, the left half of $|uu\rangle$ $etc.$ and analog $\tau_x|uu\rangle, \tau_x|ud\rangle, \tau_x|du\rangle, \tau_x|dd\rangle$ for Bob with Bob's operator acting only on the right half of $|uu\rangle$ $etc.$

We extend:

σ_x was $\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ is now $\sigma_x \otimes I = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix} 0\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} & 1\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \\ 1\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} & 0\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\end{pmatrix}$

τ_x was $\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ is now $I\otimes\tau_x = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\otimes\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\\ 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & 1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}$

The combination of state-vectors:

$$|uu\rangle = |u\rangle\otimes|u\rangle = \begin{pmatrix}1\\ 0\end{pmatrix}\otimes\begin{pmatrix}1\\ 0\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}1\\ 0\end{pmatrix}\\ 0\begin{pmatrix}1\\ 0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix}$$

$$|ud\rangle = |u\rangle\otimes|d\rangle = \begin{pmatrix}1\\ 0\end{pmatrix}\otimes\begin{pmatrix}0\\ 1\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}0\\ 1\end{pmatrix}\\ 0\begin{pmatrix}0\\ 1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0\\ 1\\ 0\\ 0\end{pmatrix}$$

We check whether an operator of Bob is acting on Bob's observable. $\tau_x|uu\rangle$ should give $|ud\rangle$ because $\tau_x|u\rangle$ in the one spin system gives $|d\rangle$.

$$\tau_x|uu\rangle = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}\begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix} = \begin{pmatrix}0\\ 1\\ 0\\ 0\end{pmatrix} = |ud\rangle$$

In a composite system the expectation values of the components satisfy:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$$

We check this with σ_z and $|uu\rangle$: $\langle\sigma_z\rangle = \langle uu|\sigma_z|uu\rangle$ with $\langle uu| = (1\ 0\ 0\ 0)$.

σ_z is now $\sigma_z\otimes I = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\otimes\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} & 0\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\\ 0\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} & -1\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}$

$$|uu\rangle = \begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix}$$

$$\langle\sigma_z\rangle = \langle uu|\sigma_z|uu\rangle = \langle uu|\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}\begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix} =$$

$$\langle uu|\begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix} = (1\ 0\ 0\ 0)\begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix} = 1$$

The other expectation values with $|uu\rangle$ will give 0. The equation $\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$ is valid.

This is not true for entangled system. We show this in the symbolic representation only …

In the up-down-basis the entangled state $|sing\rangle \coloneqq \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$ and $\langle sing| \coloneqq \frac{1}{\sqrt{2}}(\langle ud| - \langle du|)$. Remember that basis vectors are orthogonal.

We calculate the expectation value of $\langle\sigma_z\rangle$.

$$\langle\sigma_z\rangle = \langle sing|\sigma_z|sing\rangle = \left\langle sing\left|\sigma_z\right|\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)\right\rangle = \left\langle sing\left|\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)\right\rangle =$$

$$\left\langle\frac{1}{\sqrt{2}}(\langle ud| - \langle du|)\left|\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)\right\rangle = \frac{1}{2}(\langle ud|ud\rangle + \langle ud|du\rangle - \langle du|ud\rangle - \langle du|du\rangle) =\right.$$

$$\frac{1}{2}(1 + 0 - 0 - 1) = 0$$

The same holds for the other variants. We get $\langle\sigma_x\rangle = \langle\sigma_y\rangle = \langle\sigma_z\rangle = 0$

Composite systems, product states:

The simplest state for the composite system is called a product state, the result of completely independent preparations by Alice and Bob. Alice prepares her spin in state $\alpha_u|u\rangle + \alpha_d|d\rangle$, Bob prepares his in the state $\beta_u|u\rangle + \beta_d|d\rangle$.

In a composite state each state is normalized separately:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1 \text{ and } \beta_u^*\beta_u + \beta_d^*\beta_d = 1.$$

The product state describing the combined system is:

$$|product\ state\rangle = \{\alpha_u|u\rangle + \alpha_d|d\rangle\}\otimes\{\beta_u|u\rangle + \beta_d|d\rangle\} =$$

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

Composite systems, tensor products and composite systems:

Imagine two systems. Alice throws a coin, Bob a die.

The system of Alice has two states and two basis vectors $\binom{H}{0}$ and $\binom{0}{T}$, represented as $\binom{H}{T}$.

In classical physics they are exclusive, a coin can giver either H or T when thrown, so the above representation in $\binom{H}{T}$ makes sense with exclusive $H = 1$ or $T = 1$.

In quantum mechanics there is allowed also every superposition:

$$\alpha_H\binom{H}{0} + \alpha_T\binom{0}{T}$$

$$\binom{\alpha_H H}{\alpha_T T}$$

$$\alpha_H|H\rangle + \alpha_T|T\rangle$$

The system of Bob has six states and accordingly six basis vectors $|1\rangle$ through $|6\rangle$, represented as:

$$\begin{pmatrix}1\\2\\3\\4\\5\\6\end{pmatrix} \text{ or, more detailed } \begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix} + \begin{pmatrix}0\\2\\0\\0\\0\\0\end{pmatrix} + \cdots + \begin{pmatrix}0\\0\\0\\0\\0\\6\end{pmatrix}$$

Again, in classical physics a die could show only one number, one of these basis vectors, but in quantum mechanics any superposition:

$$\alpha_1|1\rangle + \alpha_2|2\rangle + \alpha_3|3\rangle + \alpha_4|4\rangle + \alpha_5|5\rangle + \alpha_6|6\rangle \text{ or } \begin{pmatrix}\alpha_1 1\\ \alpha_2 2\\ \alpha_3 3\\ \alpha_4 4\\ \alpha_5 5\\ \alpha_6 6\end{pmatrix}$$

The combination of both basis vector systems is performed by the tensor product:

$$\binom{H}{T} \otimes \begin{pmatrix}1\\2\\3\\4\\5\\6\end{pmatrix} = \begin{pmatrix} H\begin{pmatrix}1\\2\\3\\4\\5\\6\end{pmatrix} \\ T\begin{pmatrix}1\\2\\3\\4\\5\\6\end{pmatrix} \end{pmatrix} = \begin{pmatrix}H1\\H2\\H3\\H4\\H5\\H6\\T1\\T2\\T3\\T4\\T5\\T6\end{pmatrix} = \begin{pmatrix}H1\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\end{pmatrix} + \begin{pmatrix}0\\H2\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\end{pmatrix} + \cdots + \begin{pmatrix}0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\T6\end{pmatrix}$$

For example, the state-label H4 denotes a state in which Alice's coin shows H and Bob's die shows 4.

We could represent the $H4$ state explicit by writing $|H\rangle\otimes|4\rangle$ or $|H\rangle|4\rangle$. Usually it is more convenient to take the composite notation $|H4\rangle$. This emphasizes that we are talking about a single state with a two-part label. The left half labels Alice's subsystem, the right half labels Bob's subsystem.

Once the basis vectors are listed – in this case, twelve of them, the basis vectors for the S_{AB} system – we can combine them linearly to form arbitrary superpositions. A superposition of two basis vectors might look like:

$$\alpha_{h3}|H3\rangle + \alpha_{t4}|T4\rangle$$

In each case, the first half of the state-label describes the state of Alice's coin, and the second half describes the state of Bob's die. The coefficient α_{h3} results out of the multiplication of α_h from Alice's system and α_3 from Bob's system – it is a (complex) number.

Sometimes, we will need to refer to an arbitrary basis vector in S_{AB}. To do that, we will use ket-vectors that look like $|ab\rangle$ or $|a'b'\rangle$.

There is one aspect of this notion that is tricky. Even though our S_{AB} state-labels have a double index, ket-vectors like $|ab\rangle$ or $|H3\rangle$ represent a single state of the combined system. We are using a double index to label a single state – this will take some getting used to. Alice's part of the state-label is always on the left, Bob's part is always on the right.

Composite vectors, composite operators and composite vectors:

A composite operator $\sigma_z\otimes I$ acts on a composite vector $|d\rangle\otimes|u\rangle$ and produces a new composite vector $-|d\rangle\otimes|u\rangle$, in this case only on Alice's half of the system.

The composite operator $I\otimes\tau_x$ acts on a composite vector $|d\rangle\otimes|u\rangle$ and produces a new composite vector $|d\rangle\otimes|d\rangle$, in this case only on Bob's half of the system.

Both composite operators act only on their half of the composite vector. We check this explicitly. $\tau_x|uu\rangle$ should give $|ud\rangle$ because $\tau_x|u\rangle$ in the one spin system gives $|d\rangle$.

$$\tau_x|uu\rangle = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = |ud\rangle$$

Conservation:

Conservation of distinctions:

Let us consider a closed system (no external forces etc.) and two distinguishable states that changes with time t: $|\varphi(t)\rangle$ and $|\theta(t)\rangle$.

The states at time t are given by some operation that we call $U(t)$, an operator acting on the states at time zero:

$$|\varphi(t)\rangle = U(t)|\varphi(0)\rangle$$

$$\langle\varphi(t)| = \langle\varphi(0)|U^\dagger$$

$$|\theta(t)\rangle = U(t)|\theta(0)\rangle$$

U is called the time-development operator for the system.

If $|\varphi(0)\rangle$ and $|\theta(0)\rangle$ are two distinguishable states in a closed system, this must be valid for all times. Distinguishable states are orthogonal, so $\langle\varphi(0)|\theta(0)\rangle = \langle\varphi(t)|\theta(t)\rangle = 0$.

We take a look at $\langle\varphi(t)|\theta(t)\rangle$:

$$\langle\varphi(t)|\theta(t)\rangle = 0 = \langle\varphi(0)|U^\dagger(t)U(t)|\theta(0)\rangle$$

From this follows that $U^\dagger(t)U(t)$ must be the identity operator I:

$$U^\dagger(t)U(t) = I$$

An operator that satisfies $U^\dagger(t)U(t) = I$ is called unitary, therefore time evolution is unitary in quantum mechanics.

Conservation of energy:

The condition for an observable Q to call it conserved is that its expectation value $\langle Q\rangle$ does not change with time (or the expectation value of any power of Q, e.g. $\langle Q^n\rangle$).

The change over time for an observable Q in quantum mechanics:

$$\frac{d\langle Q\rangle}{dt} = -\frac{i}{\hbar}\langle[Q,H]\rangle$$

or shorthand

$$\frac{dQ}{dt} = -\frac{i}{\hbar}[Q,H]$$

The right side of this equation becomes zero if Q and H commute: $[Q,H] = 0$. H is the Hamiltonian, the energy of a system both in classical physics and in quantum mechanics. Every operator commutes with itself, so:

$$\frac{dH}{dt} = -\frac{i}{\hbar}[H,H] = 0$$

Energy is conserved in quantum mechanics under very general conditions. From

$$\frac{dQ}{dt} = -\frac{i}{\hbar}[Q, H]$$

we can derive:

$$\frac{dQ^2}{dt} = 2Q\frac{dQ}{dt} = -\frac{2iQ}{\hbar}[Q, H]$$

and again, this is zero if Q and H commute. This holds for every power of Q.

Conservation of overlaps:

If A and B are any two state vectors, the inner product of $|A\rangle$ and $|B\rangle$ is the same as the inner product of $U|A\rangle$ and $U|B\rangle$ provided U is unitary.

We check:

$$U|A\rangle \rightarrow \langle A|U^\dagger$$

$$\langle A|U^\dagger U|B\rangle = \langle A|B\rangle \rightarrow U^\dagger U = I$$

This is called the conservation of overlaps and expresses the fact that logical relations between states are preserved with time.

Continuity:

Continuity is a principle when working with incremental changes. It means that state-vectors changes smoothly. The time-development operator $U(t)$ for ε-amounts of time becomes $U(\varepsilon) = I - i\varepsilon H$. With this $U^\dagger(\varepsilon) = I + i\varepsilon H^\dagger$.

$U^\dagger(t)U(t) = I$, so $U^\dagger(\varepsilon)U(\varepsilon)$ must be I too.

$$I = U^\dagger(\varepsilon)U(\varepsilon) = \left(I + i\varepsilon H^\dagger\right)(I - i\varepsilon H) =$$

$$I \cdot I - Ii\varepsilon H + i\varepsilon H^\dagger I + \varepsilon^2 H^\dagger H =$$

$$I - i\varepsilon H + i\varepsilon H^\dagger + \varepsilon^2 H^\dagger H$$

We omit the second order in ε and get:

$$I = I - i\varepsilon H + i\varepsilon H^\dagger$$

$$0 = -i\varepsilon H + i\varepsilon H^\dagger$$

$$0 = -H + H^\dagger$$

$$H = H^\dagger$$

H must be a Hermitian operator too and it follows that H is an observable with a complete set of orthonormal eigenvectors and eigenvalues – it is the quantum Hamiltonian.

Continuous functions:

We begin by picking an observable L with eigenvalues λ and eigenvectors $|\lambda\rangle$.

Let $|\psi\rangle$ be a state-vector. Since the eigenvectors of a Hermitian operator form a complete orthonormal basis, the vector $|\psi\rangle$ can be expanded as $\sum_{i=1}^{n} \psi(\lambda_i)|\lambda_i\rangle$.

The quantities $\psi(\lambda_i)$ are called the wave function in the L-basis of the system, so their actual form depends on the observable chosen.

Note: other observable – other wave functions, even if we talk about the same state.

The eigenvectors are orthogonal to each other: $\langle\lambda_i|\lambda_j\rangle = \delta_{ij}$.

We can identify the wave functions with the inner product, the projections of the state-vector $|\psi\rangle$ onto the eigenvectors $|\lambda\rangle$: $\psi(\lambda) = \langle\lambda|\psi\rangle$.

You can think of the wave function in two ways. First of all, it is a set of components of the state-vector in a particular basis, the components forming a column vector:

$$\begin{pmatrix} \psi(\lambda_1) \\ \vdots \\ \psi(\lambda_n) \end{pmatrix}$$

You also can think of the wave function as a complex valued function of the discrete variable λ: $\psi(\lambda)$.

A single spin system has a two-dimensional space of state.

In contrast the coordinates of a particle, moving on the x-axis can be found on any real value of x, the observable has an infinite number of possible values: $x \in \mathbb{R}$.

The former discrete wave function $\psi(x_i)$ becomes a function of a continuous variable $\psi(x)$.

Continuous functions as vectors:

Let us consider the set of complex functions $\varphi(x)$ of a single variable x: $x \to \varphi(x)$ with $\varphi(x) \in \mathbb{C}$. With appropriate restrictions, functions like $\varphi(x)$ satisfy the mathematical axioms that define a vector space (algebraic structure):

1. Closure: $\varphi(x) + \theta(x) = \vartheta(x)$
2. Commutative property: $\varphi(x) + \theta(x) = \theta(x) + \varphi(x)$
3. Associative property: $\big(\varphi(x) + \theta(x)\big) + \vartheta(x) = \varphi(x) + (\theta(x) + \vartheta(x))$
4. Zero: $\varphi(x) + 0 = \varphi(x)$
5. Inverse: $\varphi(x) + (-\varphi(x)) = 0$
6. Multiplying property: $z\varphi(x) = \tau(x)$
7. Distributive properties:
    a. $z[\varphi(x) + \theta(x)] = z\varphi(x) + z\theta(x)$
    b. $[z + w]\,\varphi(x) = z\varphi(x) + w\varphi(x)$

We can identify the functions $\varphi(x)$ with the ket-vectors $|\varphi\rangle$ in an abstract vector space. The corresponding bra vectors are $\varphi^*(x)$.

Continuous functions require:

a) Integral replaces sum
b) Probability density replaces probability
c) Dirac delta function replaces Kronecker delta

a) Integral replaces sum:

The inner product $\langle\varphi|\theta\rangle$:

was:

$$\sum_{i,j}\varphi_i^*\theta_j\delta_{ij}$$

is:

$$\int_{-\infty}^{\infty}\varphi^*(x)\theta(x)dx$$

b) Probability density replaces probability:

was:

$|A\rangle$ state-vector, observable L, the probability to observe value λ_i:

$$P(\lambda_i)=\langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$

is:

probability density: $P(a,b)$:

$$\int_a^b P(x)dx=\int_a^b\varphi^*(x)\varphi(x)dx$$

Analog to the discrete case we define a normalization condition:

$$\int_{-\infty}^{\infty}\varphi^*(x)\varphi(x)dx=1$$

c) Dirac delta function replaces Kronecker delta:

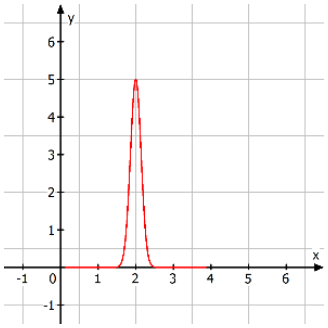
Consider a vector F_i in a discrete, finite dimensional space.

$\sum_{i,j}\left(\delta_{ij}F_j\right)$ gives F_j because δ_{ij} is nonzero only for $i=j$.

The Dirac delta function performs this: $\delta(x-x')$ is something that returns zero for all $x\neq x'$ and "∞" for $x=x'$. With this:

$$\int_{-\infty}^{\infty}\delta(x-x')\,f(x')dx'=f(x)$$

Note: the Dirac delta function can be thought of as $\lim_{n\to\infty} ne^{-(nx)^2}$.



Continuous functions, integration by parts:

The rule for integration by parts:

$$\int_a^b FdG = FG|_a^b - \int_a^b GdF$$

We work with normalized functions that span the entire x-axis and go to zero at infinity, so the expression $FG|_a^b$ becomes zero. With this we get an expression that is often used in physics:

$$\int FdG = -\int GdF$$

Continuous functions, linear operators:

An operator L acting on wave functions is linear:

Additivity: $L\big(\varphi(x) + \theta(x)\big) = L\varphi(x) + L\theta(x)$

Homogeneity: $L\big(z\varphi(x)\big) = zL\varphi(x)$

Note: z is a (complex) number.

Two examples:

a) The "multiply by x" operator with the symbol X: $X\varphi(x) = x\varphi(x)$ with $x \in \mathbb{R}$
b) The "differentiate" operator with the symbol D: $D\varphi(x) = \frac{d\varphi(x)}{dx}$

Both are linear operators.

X is called the position operator, D transforms to the momentum operator P.

Continuous functions, Hermitian linear operators:

By definition, a Hermitian operator: $L^\dagger = L$. Note: $(L^*)^t \coloneqq L^\dagger$

For a Hermitian operator L holds: $\langle\varphi(x)|L|\theta(x)\rangle = \langle\theta(x)|L|\varphi(x)\rangle$

The position operator X is Hermitian: $X\varphi(x) = x\varphi(x)$:

Discrete:

$$\langle\varphi(x)|X|\theta(x)\rangle = \langle\varphi(x)|x\theta(x)\rangle = x\langle\varphi(x)|\theta(x)\rangle = x\varphi^*(x)\theta(x)$$

$$\langle\theta(x)|X|\varphi(x)\rangle = \langle\theta(x)|x\varphi(x)\rangle = x\langle\theta(x)|\varphi(x)\rangle = x\theta^*(x)\varphi(x)$$

$$\big(\varphi^*(x)\theta(x)\big)^* = \varphi(x)\theta^*(x) = \theta^*(x)\varphi(x)$$

We get $\langle\varphi(x)|X|\theta(x)\rangle = \langle\theta(x)|X|\varphi(x)\rangle$, the operator X is Hermitian. Remember $x \in \mathbb{R}$.

Continuous:

In the continuous version the inner product of two wave functions is defined as

$$\langle\varphi|\theta\rangle = \int_{-\infty}^{\infty} \varphi^*(x)\theta(x)dx$$

For the X operator we get:

$$\langle\varphi|X|\theta\rangle = \langle\varphi|x\theta\rangle = \int_{-\infty}^{\infty} x\varphi^*(x)\theta(x)dx$$

$$\langle\theta|X|\varphi\rangle = \langle\theta|x\varphi\rangle = \int_{-\infty}^{\infty} x\theta^*(x)\varphi(x)dx$$

Again, we use $\big(\varphi^*(x)\theta(x)\big)^* = \varphi(x)\theta^*(x) = \theta^*(x)\varphi(x)$ and the two integrals are the same.

Is the "differentiate" operator D, $D\varphi(x) = \frac{d\varphi(x)}{dx}$, Hermitian?

We have no discrete case, so we check the continuous case. The inner product of two wave functions is defined as

$$\langle\varphi|\theta\rangle = \int_{-\infty}^{\infty} \varphi^*(x)\theta(x)dx$$

For the D operator we get:

$$\langle\varphi|D|\theta\rangle = \left\langle\varphi\middle|\frac{d\theta(x)}{dx}\right\rangle = \int_{-\infty}^{\infty} \varphi^*(x)\frac{d\theta(x)}{dx}dx = \int_{-\infty}^{\infty} \varphi^*(x)d\theta(x)$$

For better "workability" we write this as $\int \varphi^* d\theta$.

$$\langle\theta|D|\varphi\rangle = \left\langle\theta\middle|\frac{d\varphi(x)}{dx}\right\rangle = \int_{-\infty}^{\infty} \theta^*(x)\frac{d\varphi(x)}{dx}dx = \int_{-\infty}^{\infty} \theta^*(x)d\varphi(x)$$

We write this as $\int \theta^* d\varphi$.

We use integration by parts $\int FdG = -\int GdF$ and rewrite $\int \theta^* d\varphi = -\int \varphi d\theta^*$.

We get:

$$\langle\varphi|D|\theta\rangle = -\langle\theta|D|\varphi\rangle^*$$

The D operator is not Hermitian, instead, it satisfies $D = -D^\dagger$. This is called anti-Hermitian.

We can construct a new Hermitian operator out of D by multiplying D with $-i\hbar$ (the $\hbar$ for convenience purposes in later applications, the $-i$ would be sufficient in this place).

The new operator $-i\hbar D$ is Hermitian:

$$-i\hbar D\varphi(x) = -i\hbar\frac{d\varphi(x)}{dx}$$

Continuous functions, wave functions and continuous functions:

We begin by picking an observable L with eigenvalues λ and eigenvectors $|\lambda\rangle$.

Let $|\psi\rangle$ be a state-vector.

Since the eigenvectors of a Hermitian operator form a complete orthonormal basis, the vector $|\psi\rangle$ can be expanded as $\sum_{i=1}^{n}\psi(\lambda_i)|\lambda_i\rangle$.

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The former discrete wave function $\psi(x_i)$ becomes a function of a continuous variable $\psi(x)$.

Note: in the appendix you find a complete transformation from a discrete wave function to a continuous one.

Correlation:

Correlation of near singlet state:

For near singlet states (partially entangled states) correlation is between -1 and +1, but neither $-1/+1$ nor exactly 0. They are partially correlated.

Correlation of product state:

For product states the correlation is zero because they are independent.

Correlation of singlet state:

For singlet states (maximum entanglement) the correlation is -1. Whenever you measure the first spin the other one takes the opposite direction, they are maximal correlated.

Correlation test for entanglement:

Correlation between observables is defined in terms of average (expectation) values. The correlation $C(A, B)$ between two observables A and B is defined:

$$C(A, B) = \langle AB\rangle - \langle A\rangle\langle B\rangle$$

$C(A, B)$ is in the range $[-1, +1]$.

If $C(A, B) = 0$, then A and B are not correlated.

The more the magnitude of $|C(A, B)|$ approaches the value 1, the more entangled the state is. If $|C(A, B)| = 1$, then A and B are maximum correlated.

Note: in a product state the correlation is zero, there is no correlation.

Creation operators:

The Hamiltonian expressed in terms of operators X, the observable for position and P, the observable for momentum:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2)$$

(*This is a classical as well as a quantum mechanical Hamiltonian, so it would be correct to use the classical lowercase symbols p and x.*)

The idea is to use the properties of X and P, especially the commutation relation $[X, P] = i\hbar$ to construct three new operators, called creation (or raising) operator, annihilation (or lowering) operator and number operator. The names are program. The raising operator shall produce a new eigenvector that has the next higher energy level, the lowering operator shall produce a new eigenvector that has the next lower energy level. The number operator returns the "number" of the energy level.

The construction process.

Using complex numbers, we can split up the sum according to $a^2 + b^2 = (a + ib)(a - ib)$ to

$$H \sim \frac{1}{2}(P + i\omega X)(P - i\omega X)$$

"$\sim$" because of the quantum mechanically behavior of X and P: they do not commute. The problem are the products PX and XP.

We expand the Hamiltonian:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + i\omega XP - i\omega PX - i^2\omega^2 X^2) =$$

$$\frac{1}{2}(P^2 + \omega^2 X^2) + \frac{1}{2}i\omega[X, P]$$

We know the value of the commutator: $[X, P] = i\hbar$ and get:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + \omega^2 X^2) - \frac{1}{2}\hbar\omega$$

Our correct Hamiltonian:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{1}{2}\hbar\omega$$

We define the creation operator a^+ and the annihilating operator a^-:

$$a^- \coloneqq (P - i\omega X)$$

$$a^+ \coloneqq (P + i\omega X)$$

Note: the number operator is defined as $N \coloneqq a^+ a^-$ and "returns" the number of the energy level.

Crystal lattice:

If an atom in a crystal lattice is displaced slightly from its equilibrium position, it gets pushed back with an approximately linear restoring force – so we have the case of a harmonic oscillator in three dimensions and three independent oscillations.

Degeneracy

Observable quantities in quantum mechanics are represented by Hermitian operators – this is a fundamental theorem.

- The eigenvectors of a Hermitian operator are a complete set, any vector the operator can generate can be expressed by a sum of its eigenvectors.
- If λ_1 and λ_2 are two eigenvalues of a Hermitian operator with $\lambda_1 \neq \lambda_2$ then the corresponding eigenvectors are orthogonal.
- If two eigenvalues are equal, the corresponding eigenvectors span a subspace. For the corresponding subspace can be found an orthonormal basis via the *Gram-Schmidt* procedure.
  Two eigenvalues being equal is called degeneracy.

Density matrices

The scenario: suppose Alice has prepared a spin using an apparatus oriented along some axis. Bob only has the information that the spin might be oriented along the x-axis or the y-axis.

What does Bob do? How can he use this information to make predictions?

If Alice prepared a spin in the state $|\psi\rangle$, then the expectation value of any observable L is

$$\langle\psi|L|\psi\rangle = Tr|\psi\rangle\langle\psi|L$$

with Tr being the trace of an operator or a square matrix. The trace of an operator is the sum of its diagonal elements. The trace of a projection operator is 1.

Check $\langle\psi|L|\psi\rangle$:

We try this explicitly.

Let $|\psi\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}$ and the observable L be "spin up" or σ_z: $\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$.

Then $\langle\psi| = \frac{1}{\sqrt{2}}\langle u| + \frac{1}{\sqrt{2}}\langle d| = \left(\frac{1}{\sqrt{2}}\ \frac{1}{\sqrt{2}}\right)$ (real coefficients only).

The expectation value $\langle L\rangle = \langle\psi|L|\psi\rangle = \left\langle \frac{1}{\sqrt{2}}\langle u| + \frac{1}{\sqrt{2}}\langle d|\middle|L\middle|\frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle\right\rangle =$

$$\left(\frac{1}{\sqrt{2}}\ \frac{1}{\sqrt{2}}\right)\left(\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\cdot\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\right) = \left(\frac{1}{\sqrt{2}}\ \frac{1}{\sqrt{2}}\right)\cdot\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix} = 0$$

This is according to the laws of quantum mechanics, "spin up" and "spin down" appears with equal possibilities, so the average is zero.

Check $Tr|\psi\rangle\langle\psi|L$:

$$|\psi\rangle\langle\psi|L = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\left(\left(\frac{1}{\sqrt{2}}\ \frac{1}{\sqrt{2}}\right)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right) = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\left(\frac{1}{\sqrt{2}}\ -\frac{1}{\sqrt{2}}\right) = \begin{pmatrix}\frac{1}{2} & -\frac{1}{2}\\ \frac{1}{2} & -\frac{1}{2}\end{pmatrix}$$

$$Tr|\psi\rangle\langle\psi|L = Tr\begin{pmatrix}\frac{1}{2} & -\frac{1}{2}\\ \frac{1}{2} & -\frac{1}{2}\end{pmatrix} = \frac{1}{2} - \frac{1}{2} = 0$$

giving the same result.

If Alice prepared the spin in the state $|\theta\rangle$, then the expectation value of any observable L is

$$\langle\theta|L|\theta\rangle = Tr|\theta\rangle\langle\theta|L$$

Bob assumes a 50:50 probability giving an expectation value of $\langle L\rangle$:

$$\langle L\rangle = \left(\frac{1}{2}Tr|\psi\rangle\langle\psi|L + \frac{1}{2}Tr|\theta\rangle\langle\theta|L\right) = Tr\left(\left(\frac{1}{2}|\psi\rangle\langle\psi|L + \frac{1}{2}|\theta\rangle\langle\theta|L\right)\right) =$$

$$Tr\left(\left(\frac{1}{2}|\psi\rangle\langle\psi| + \frac{1}{2}|\theta\rangle\langle\theta|\right)L\right)$$

$\left(\frac{1}{2}|\psi\rangle\langle\psi| + \frac{1}{2}|\theta\rangle\langle\theta|\right)$ is the density matrix ρ, half the projection operator onto $|\psi\rangle$ plus half the projection operator onto $|\theta\rangle$.

$|\psi\rangle\langle\psi|$ and $|\theta\rangle\langle\theta|$ are square matrices of the same rank.

With this density matrix computing the expectation values becomes:

$$\langle L\rangle = Tr(\rho L)$$

Note: ρ is an operator and becomes a matrix if a basis is chosen. Suppose we have the basis $|a\rangle$, then the density matrix with respect to this basis is $\rho_{aa'} = \langle a|\rho|a'\rangle$. If the matrix representation of L with respect to this basis is: $L_{a'a} = \langle a'|L|a\rangle$, we can write the expectation value of L:

$$\langle L\rangle = \sum_{a,a'} L_{a',a}\rho_{a,a'}$$

Density matrices, calculating density matrices:

Suppose we know the wave function of a composite system, $\psi(a,b)$, but we are only interested in the subsystem of Alice. Let L be an observable of Alice's system. L can be represented as a matrix:

$$L_{a'b',ab} = \langle a'b'|L|ab\rangle$$

$L_{a'b',ab}$ is a matrix index L_{ij} you get by sandwiching the Matrix with the appropriate basis vectors $\langle i|$ and $|j\rangle$.

Explicitly:

$$L = \begin{pmatrix} l_{uu,uu} & l_{uu,ud} & l_{uu,du} & l_{uu,dd}\\ l_{ud,uu} & l_{ud,ud} & l_{ud,du} & l_{ud,dd}\\ l_{du,uu} & l_{du,ud} & l_{du,du} & l_{du,dd}\\ l_{dd,uu} & l_{dd,ud} & l_{dd,du} & l_{dd,dd}\end{pmatrix}$$

By multiplication with the basis vectors e.g. $(0\ 1\ 0\ 0)$ and $\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ we get

$$(0\ 1\ 0\ 0)\begin{pmatrix} l_{uu,uu} & l_{uu,ud} & l_{uu,du} & l_{uu,dd} \\ l_{ud,uu} & l_{ud,ud} & l_{ud,du} & l_{ud,dd} \\ l_{du,uu} & l_{du,ud} & l_{du,du} & l_{du,dd} \\ l_{dd,uu} & l_{dd,ud} & l_{dd,du} & l_{dd,dd} \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = (0\ 1\ 0\ 0)\begin{pmatrix} l_{uu,du} \\ l_{ud,du} \\ l_{du,du} \\ l_{dd,du} \end{pmatrix}$$

$$(0\ 1\ 0\ 0)\begin{pmatrix} l_{uu,du} \\ l_{ud,du} \\ l_{du,du} \\ l_{dd,du} \end{pmatrix} = l_{ud,du}$$

The index of row 3, column 2, so we can say: $L_{ud,du} = \langle ud|L|du\rangle$

L shall be an Alice-observable meaning it does nothing to Bob's subsystem, so any elements of L that could have an effect to Bob's system must be filtered out by setting it to zero.

This L gets the special form:

$$L_{a'b',ab} = L_{a'a} \otimes \delta_{b'b}$$

The expectation value of $\langle L\rangle = \langle\psi|L|\psi\rangle = \sum_{a,b,a',b'} \psi^*(a',b')L_{a'b',ab}\psi(a,b)$

Because of $b' = b$:

$$\langle L\rangle = \langle\psi|L|\psi\rangle = \sum_{a',b,a} \psi^*(a',b)L_{a',a}\psi(a,b) = \sum_{a',b,a} \psi^*(a,b)\psi(a',b)L_{a,a'} =$$

$$\sum_{a',a}\sum_{b} \psi^*(a,b)\psi(a',b)\, L_{a,a'}$$

The quantity

$$\sum_{b} \psi^*(a,b)\psi(a',b) \coloneqq \rho_{a'a}$$

is the density matrix of Alice.

We get the expectation value of L (the 2×2 version):

$$\langle L\rangle = \sum_{a'a} \rho_{a',a}L_{a,a'}$$

Consider the state-vector $|\psi\rangle = 0|uu\rangle + \frac{1}{\sqrt{2}}|ud\rangle + \frac{1}{\sqrt{2}}|du\rangle + 0|dd\rangle$.

The values of $\psi(a,b)$ are:

$$\psi(u,u) = 0, \psi(u,d) = \frac{1}{\sqrt{2}}, \psi(d,u) = \frac{1}{\sqrt{2}}, \psi(d,d) = 0$$

Next, we expand the factors in the density matrix $\rho_{a',a} = \sum_b \psi^*(a,b)\psi(a',b)$.

Remember that we are summing over the second index b, the first index a being unchanged:

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = 0 \cdot 0 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} = \frac{1}{2}$$

$$\rho_{ud} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = 0$$

$$\rho_{du} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = 0$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = \frac{1}{2}$$

These values are elements of a 2×2 matrix:

$$\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

The trace of this density matrix is 1 as it should be for density matrices.

Density matrices, entanglement and density matrices:

The state of a composite system can be absolutely pure (~single state), but each of its constituents must be described by a mixed state.

We take a system composed of two subsystems, A and B. We suppose that Alice has complete knowledge of the state of the combined system, she knows the wave function $\psi(a,b)$. Alice is interested only in system A and want to have complete knowledge about system A. She selects an observable L that belongs to A and does nothing to B when it acts.

The rule for calculating the expectation value of L is:

$$\langle L \rangle = \sum_{ab,a'b'} \psi^*(a'b')L_{a'b',ab}\psi(ab)$$

The observable L was chosen to act on A only and let B unchanged, so it acts trivially on the b-index (it leaves b unchanged, so $b' = b$ and the sum over the b separable):

$$\langle L \rangle = \sum_{a,b,a'} \psi^*(a'b)L_{a',a}\psi(ab) = \sum_{a,a'} L_{a',a} \sum_b \psi^*(a'b)\psi(ab)$$

The sum

$$\sum_b \psi^*(a'b)\psi(ab) = \rho_{a,a'}$$

gives the density matrix in the combined system.

With this we can write:

$$\langle L \rangle = \sum_{a,a'} L_{a',a}\, \rho_{a,a'}$$

the expectation value of a mixed state.

Note: in $\sum_b \psi^*(a'b)\psi(ab) = \rho_{a,a'}$ the right-hand index of $\rho_{a,a'}$ (the index a') belongs to the complex conjugate vector $\psi^*(a'b)$. This is a consequence of our convention $L_{aa'} = \langle a|L|a' \rangle$ for labeling the matrix elements of an operator L.

Applying this convention to

$$\rho = |\psi\rangle\langle\psi|$$

results in

$$\rho_{a,a'} = \langle a|\psi\rangle\langle\psi|a'\rangle = \psi(a)\psi^*(a')$$

Density matrices of near singlet state:

The near-singlet state is a state of partial entanglement and has the state-vector $\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$.

The state-vector leads to the following wave-function:

$\psi_{uu} = 0|uu\rangle$ $\psi_{ud} = \sqrt{0.6}|ud\rangle$ $\psi_{du} = -\sqrt{0.4}|du\rangle$ $\psi = 0|dd\rangle$

As the values are all real, the complex conjugated are identical: $\psi_{uu} = \psi^*{}_{uu}$ etc.

The wave function is normalized: $0^2 + \sqrt{0.6}^2 + (-\sqrt{0.4})^2 + 0^2 = 1$

$\psi(a,b)$ takes the form $\psi(a,b) = \psi_{ud} + \psi_{du} = \sqrt{0.6}|ud\rangle - \sqrt{0.4}|du\rangle$

and results in: $\psi_{uu} = 0,\ \psi_{ud} = \sqrt{0.6},\ \psi_{du} = -\sqrt{0.4},\ \psi_{dd} = 0$

The density matrix of Alice: $\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$

expanded a, a' (with $\psi^* = \psi$ due to all coefficients being real):

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = 0.6$$

$$\rho_{ud} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = 0$$

$$\rho_{du} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = 0$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = 0.4$$

Alice's density matrix:

$$\rho := \begin{pmatrix} 0.6 & 0 \\ 0 & 0.4 \end{pmatrix}$$

Density matrices, notation for density matrices:

$$\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b) = \psi^*(a)\psi(a')$$

Please note the reverse order of indices in $\rho_{a'a}$ and the product of the wave functions $\psi^*(a)\psi(a')$.

Density matrices of product state:

The product state is a state of independent subsystems and has a generalized state-vector:

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

The normalization conditions are $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$ and $\beta_u^*\beta_u + \beta_d^*\beta_d = 1$.

The state-vector leads to the following wave-function:

$\psi_{uu} = \alpha_u\beta_u|uu\rangle$ $\psi_{ud} = \alpha_u\beta_d|ud\rangle$ $\psi_{du} = \alpha_d\beta_u|du\rangle$ $\psi_{dd} = \alpha_d\beta_d|dd\rangle$

$$\psi_{uu} = \alpha_u\beta_u,\ \psi_{ud} = \alpha_u\beta_d,\ \psi_{du} = \alpha_d\beta_u,\ \psi_{dd} = \alpha_d\beta_d$$

The density matrix of Alice: $\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$

expanded a, a':

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) =$$

$$\alpha_u^*\beta_u^*\alpha_u\beta_u + \alpha_u^*\beta_d^*\alpha_u\beta_d = \alpha_u^*\alpha_u(\beta_u^*\beta_u + \beta_d^*\beta_d) = \alpha_u^*\alpha_u$$

$$\rho_{ud} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) =$$

$$\alpha_u^*\beta_u^*\alpha_d\beta_u + \alpha_u^*\beta_d^*\alpha_d\beta_d = \alpha_u^*\alpha_d(\beta_u^*\beta_u + \beta_d^*\beta_d) = \alpha_u^*\alpha_d$$

$$\rho_{du} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) =$$

$$\alpha_d^*\beta_u^*\alpha_u\beta_u + \alpha_d^*\beta_d^*\alpha_u\beta_d = \alpha_d^*\alpha_u(\beta_u^*\beta_u + \beta_d^*\beta_d) = \alpha_d^*\alpha_u$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) =$$

$$\alpha_d^*\beta_u^*\alpha_d\beta_u + \alpha_d^*\beta_d^*\alpha_d\beta_d = \alpha_d^*\alpha_d(\beta_u^*\beta_u + \beta_d^*\beta_d) = \alpha_d^*\alpha_d$$

Alice's density matrix:

$$\rho := \begin{pmatrix} \alpha_u^*\alpha_u & \alpha_u^*\alpha_d \\ \alpha_d^*\alpha_u & \alpha_d^*\alpha_d \end{pmatrix}$$

We check a) a density matrix must be Hermitian and b) the trace of a density matrix must be 1.

Our density matrix fulfills these conditions: it is Hermitian, $\alpha_u^*\alpha_d = (\alpha_d^*\alpha_u)^*$ and the trace is 1: $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$, this is the normalization condition.

Note: the density matrix in case of a product state is independent of Bob's variables β.

Density matrices, properties of density matrices:

- Density matrices are Hermitian: $\rho_{aa'} = \rho_{a'a}^*$ (please note the reverse order of indices)
- The trace of a density matrix is 1: $Tr(\rho) = 1$
- The eigenvalues of a density matrix are all positive between $[0,1]$
- For pure states hold:
  $\rho^2 = \rho$ meaning the matrix has a single entry "1" on the diagonal
  $Tr(\rho^2) = 1$
- For mixed states hold:
  $\rho^2 \neq \rho$
  $Tr(\rho^2) \neq 1$

Note: every Hermitian matrix can be diagonalized.

Note: let A, B be two matrices, then $Tr(AB) = Tr(BA)$ even if $AB \neq BA$.

Density matrices for a single spin:

For a single spin we have the state-vector $|\psi\rangle = \alpha|u\rangle + \beta|d\rangle$ giving the wave-functions $\psi(u) = \alpha$, $\psi(d) = \beta$ and accordingly $\psi^*(u) = \alpha^*$, $\psi^*(d) = \beta^*$.

The density matrix:

$$\rho_{a'a} := \begin{pmatrix} \alpha^*\alpha & \alpha^*\beta \\ \alpha\beta^* & \beta^*\beta \end{pmatrix}$$

Density matrices of singlet state:

The singlet state is a state of maximum entanglement and has the state-vector $\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$.

The state-vector leads to the following wave-function:

$\psi_{uu} = 0|uu\rangle \qquad \psi_{ud} = \frac{1}{\sqrt{2}}|ud\rangle \qquad \psi_{du} = -\frac{1}{\sqrt{2}}|du\rangle \qquad \psi = 0|dd\rangle$

The values are all real, the complex conjugated are identical: $\psi_{uu} = \psi^*{}_{uu}$ etc.

The wave function is normalized: $0^2 + \frac{1}{\sqrt{2}}^2 + (-\frac{1}{\sqrt{2}})^2 + 0^2 = 1$

$\psi(a,b)$ takes the form $\psi(a,b) = \psi_{ud} + \psi_{du} = \frac{1}{\sqrt{2}}|ud\rangle - \frac{1}{\sqrt{2}}|du\rangle$

and results in: $\psi_{uu} = 0,\ \psi_{ud} = \frac{1}{\sqrt{2}},\ \psi_{du} = -\frac{1}{\sqrt{2}},\ \psi_{dd} = 0$

The density matrix of Alice: $\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$

expanded a, a' (with $\psi^* = \psi$ due to all coefficients being real):

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = \frac{1}{2}$$

$$\rho_{ud} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = 0$$

$$\rho_{du} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = 0$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = \frac{1}{2}$$

Alice's density matrix:

$$\rho := \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

Alice knows nothing about her system, all outcomes are equally likely.

Density matrices, two-spin system and density matrices:

For a single spin (Alice only) we have the state-vector $|\psi\rangle = \alpha|u\rangle + \beta|d\rangle$ giving the wave-functions $\psi(u) = \alpha, \psi(d) = \beta$ and accordingly $\psi^*(u) = \alpha^*, \psi^*(d) = \beta^*$.

The density matrix:

$$\rho_{a'a} := \begin{pmatrix} \alpha^*\alpha & \alpha^*\beta \\ \alpha\beta^* & \beta^*\beta \end{pmatrix}$$

For a two-spin system the composite state has a generalized state-vector:

$$\alpha_1|uu\rangle + \alpha_2|ud\rangle + \alpha_3|du\rangle + \alpha_4|dd\rangle$$

The normalization conditions is $\alpha_1^*\alpha_1 + \alpha_2^*\alpha_2 + \alpha_3^*\alpha_3 + \alpha_4^*\alpha_4 = 1$

The state-vector leads to the following wave-function:

$$\psi_{uu} = \alpha_1|uu\rangle \qquad \psi_{ud} = \alpha_2|ud\rangle \qquad \psi_{du} = \alpha_3|du\rangle \qquad \psi_{dd} = \alpha_4|dd\rangle$$

$$\psi_{uu} = \alpha_1,\ \psi_{ud} = \alpha_2,\ \psi_{du} = \alpha_3,\ \psi_{dd} = \alpha_4$$

and

$$\psi^*_{uu} = \alpha^*_1, \psi^*_{ud} = \alpha^*_2, \psi^*_{du} = \alpha^*_3, \psi^*_{dd} = \alpha^*_4$$

The density matrix of Alice: $\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$

expanded a, a' – note that we are summing over the second index b:

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = \alpha^*_1\alpha_1 + \alpha^*_2\alpha_2$$

$$\rho_{ud} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = \alpha^*_1\alpha_3 + \alpha^*_2\alpha_4$$

$$\rho_{du} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = \alpha^*_3\alpha_1 + \alpha^*_4\alpha_2$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = \alpha^*_3\alpha_3 + \alpha^*_4\alpha_4$$

Alice's density matrix:

$$\rho \coloneqq \begin{pmatrix} \alpha^*_1\alpha_1 + \alpha^*_2\alpha_2 & \alpha^*_1\alpha_3 + \alpha^*_2\alpha_4 \\ \alpha^*_3\alpha_1 + \alpha^*_4\alpha_2 & \alpha^*_3\alpha_3 + \alpha^*_4\alpha_4 \end{pmatrix}$$

This matrix fulfills the properties of a density matrix. The trace of the matrix is $\alpha^*_1\alpha_1 + \alpha^*_2\alpha_2 + \alpha^*_3\alpha_3 + \alpha^*_4\alpha_4 = 1$, this is exactly the normalizing condition. The matrix is Hermitian because $(\alpha^*_1\alpha_3 + \alpha^*_2\alpha_4)^* = \alpha_1\alpha^*_3 + \alpha_2\alpha^*_4$.

Note: in the composite case the density matrix of Alice depends on all four parameters of the state-vector.

In case of a product state we have two independent subsystems. The state vector is generalized:

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

The normalization conditions:

$$\alpha^*_u\alpha_u + \alpha^*_d\alpha_d = 1 \text{ and } \beta^*_u\beta_u + \beta^*_d\beta_d = 1$$

The state-vector leads to the following wave-function:

$$\psi_{uu} = \alpha_u\beta_u|uu\rangle \qquad \psi_{ud} = \alpha_u\beta_d|ud\rangle \qquad \psi_{du} = \alpha_d\beta_u|du\rangle \qquad \psi_{dd} = \alpha_d\beta_d|dd\rangle$$

$$\psi_{uu} = \alpha_u\beta_u,\ \psi_{ud} = \alpha_u\beta_d,\ \psi_{du} = \alpha_d\beta_u,\ \psi_{dd} = \alpha_d\beta_d$$

The density matrix of Alice:

$$\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$$

expanded a, a'– note that we are summing over the second index b:

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) =$$

$$\alpha^*_u\beta^*_u\alpha_u\beta_u + \alpha^*_u\beta^*_d\alpha_u\beta_d = \alpha^*_u\alpha_u(\beta^*_u\beta_u + \beta^*_d\beta_d) = \alpha^*_u\alpha_u$$

$$\rho_{ud} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) =$$

$$\alpha^*_u\beta^*_u\alpha_d\beta_u + \alpha^*_u\beta^*_d\alpha_d\beta_d = \alpha^*_u\alpha_d(\beta^*_u\beta_u + \beta^*_d\beta_d) = \alpha^*_u\alpha_d$$

$$\rho_{du} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) =$$

$$\alpha_d^*\beta_u^*\alpha_u\beta_u + \alpha_d^*\beta_d^*\alpha_u\beta_d = \alpha_d^*\alpha_u(\beta_u^*\beta_u + \beta_d^*\beta_d) = \alpha_d^*\alpha_u$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) =$$

$$\alpha_d^*\beta_u^*\alpha_d\beta_u + \alpha_d^*\beta_d^*\alpha_d\beta_d = \alpha_d^*\alpha_d(\beta_u^*\beta_u + \beta_d^*\beta_d) = \alpha_d^*\alpha_d$$

This gives Alice's density matrix:

$$\rho := \begin{pmatrix} \alpha_u^*\alpha_u & \alpha_u^*\alpha_d \\ \alpha_d^*\alpha_u & \alpha_d^*\alpha_d \end{pmatrix}$$

We check a) a density matrix must be Hermitian and b) the trace of a density matrix must be 1.

Our density matrix fulfills these conditions: it is Hermitian, $\alpha_u^*\alpha_d = (\alpha_d^*\alpha_u)^*$ and the trace is 1: $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$, this is the normalization condition.

Note: the density matrix in the case of a product state is independent of Bob's variables β.

Density matrices test for entanglement:

To calculate correlations, you have to know about both Bob's part and Alice's part of the system, along with the system wave function. But there is another test for entanglement that only requires to know Alice's or Bob's matrix. Suppose the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$. Then the composite wave function also is product of Bob's factor and Alice's factor:

$$\psi(a,b) = \vartheta(a)\theta(b)$$

Alice's density matrix:

$$\rho_{a'a} = \vartheta^*(a)\vartheta(a')\sum_b \theta^*(b)\theta(b)$$

As the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$, both Alice's and Bob's state separately are normalized, so:

$$\sum_b \theta^*(b)\theta(b) = 1$$

Alice's density matrix becomes $\rho_{a'a} = \vartheta^*(a)\vartheta(a')$.

We prove a theorem: for product states the density matrix of Alice or Bob has exactly one eigenvalue of value one.

The eigenvalue equation for Alice's matrix $\rho_{a'a}$:

$$\sum_a \rho_{a'a}\alpha_a = \lambda\alpha_a =$$

$$\sum_a \vartheta^*(a)\vartheta(a')\alpha_a = \vartheta(a')\sum_a \vartheta^*(a)\alpha_a$$

$\sum_a \vartheta^*(a)\alpha_a$ has the form of an inner product. If the column vector α is orthogonal to ϑ, then $\sum_a \vartheta^*(a)\alpha_a$ is zero giving an eigenvector with eigenvalue zero.

In a space state of dimension N we have $N-1$ vectors orthogonal to ϑ, so we have only one possible direction for an eigenvector with nonzero eigenvalue $\vartheta(a)$:

$$\vartheta^*(a)\alpha_a = 0 \text{ for all } \alpha_a \neq \vartheta(a) \text{ and } 1 \text{ for } \alpha_a = \vartheta(a).$$

Alice's system is in a pure state, all of her observations are described as if Bob never existed.

In a maximally entangled system on the other hand Alice's density matrix is proportional to the unit matrix with all equal eigenvalues $\frac{1}{N}$:

$$\rho_{a'a} = \frac{1}{N}\delta_{a'a}$$

As the density matrix gives the probability for an outcome this means that every outcome has equal possibility.

For partial entanglement the weights of $\rho_{a'a}$ move from the equal distribution towards a concentration on a single value 1 on the diagonal of the density matrix.

Although in a maximum entangled state Alice can't predict the outcome of her experiments, she knows (after the experiment has been done) exactly about the relation between her and Bob's outcomes.

Determinism

Determinism in classical physics:

In classical physics, the space of states is a mathematical set, the logic is Boolean, and the evolution of states over time is deterministic and reversible.

An alternative formulation: information is never lost. If two identical isolated systems start out in different states, they stay in different states and formerly were in different states. If two identical isolated systems start out in identical states, they stay in identical states and formerly were in identical states.

A third formulation: classical physics allows to predict the results of experiments.

A fourth formulation: in classical physics there is no difference between states and measurements.

Determinism in quantum mechanics:

Quantum evolution of states allows to predict the probabilities of later measurements.

In quantum mechanics we get statistical expectation values.

Differentiation operator:

The differentiation operator D applied to a wave function $\psi(x)$:

$$D\psi(x) = \frac{d\psi(x)}{dx}$$

The differentiation operator D is a linear operator but not a Hermitian operator (it is anti-Hermitian).

Dimensions:

We throw a dice – the result will be a number between one and six.

We are interested only in the result.

The dice shows any number, e.g. the two. We throw the dice – it shows e.g. the $five$.

The mathematical model to describe this immediate transition is the model of a vector space. We can do the transit from two to $five$ in one step without the need to go the route $2-1-2-3-4-5$ or something like this. It is a kind of random access as used in the memory of a computer.

The vector space for this model has 6 dimensions.

The same holds for a pair of dice. All possible results from $1{,}1$ to $6{,}6$ can be accessed randomly, so we describe it best by a vector space of 36 dimensions.

This model gives us the advantage to use all properties of a vector space, especially that of orthogonality and the use of matrices.

Note: in the beginning, especially with the model of spins, this can be confusing. The space of states of the spin is two-dimensional, it can be up or $down$ or anything in between. The conditions up and $down$ are mutually exclusive – orthogonal, the spatial directions itself are not.

Dirac, Paul:

1.

Dirac invented the bra-ket notation for the expectation value of an observable L:

$$\langle L\rangle = \sum_i \lambda_i P(\lambda_i)$$

The expectation value is a sum weighted with the Probability function P.

2.

Dirac formulated the structural connection between classical mechanics and quantum mechanics in respect to commutators $[F,G]$ and Poisson brackets $\{F,G\}$:

$$[F,G] \leftrightarrow i\hbar\{F,G\}$$

Especially if we replace G by the Hamiltonian H:

$$[F,H] \leftrightarrow i\hbar\{F,H\}$$

which leads to

$$\frac{dF}{dt} = \{F,H\}$$

3.

Dirac established the theoretical basis for antiparticles.

Dirac delta functions:

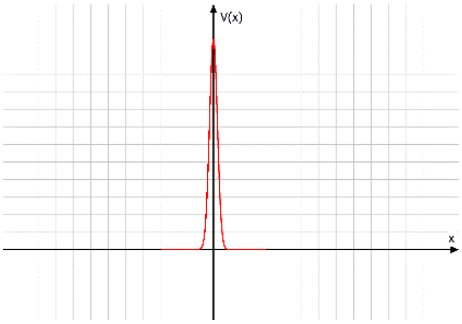
The transition from discrete functions to continuous functions requires the Kronecker delta function to be replaced by an appropriate function that works with integrals.

Remember the Kronecker delta. Let F_i be a vector in a discrete, finite dimensional space:

$$\sum\nolimits_{i,j}\left(\delta_{ij}F_j\right)$$

gives F_j because δ_{ij} is nonzero only for $i=j$.

In the integration concept the Dirac delta function performs the same: $\delta(x - x')$ is something that returns zero for all $x \neq x'$ and "∞" for $x = x'$.



With this:

$$\int_{-\infty}^{\infty} \delta(x - x_0)\, f(x) dx = f(x_0)$$

Note: the Dirac delta function can be thought of as $\lim_{n\to\infty} ne^{-(n(x-x_0))^2}$.

Example: let X be the position operator in a one-dimensional vector space, e.g. the x-axis. The position operator should give back the position of a particle:

$$X|\psi\rangle = x_0|\psi\rangle$$

In terms of wave function this becomes:

$$x\psi(x) = x_0\psi(x)$$

We rewrite this:

$$(x - x_0)\psi(x) = 0$$

The property of the Dirac delta function is to be zero on every $x \neq x_0$ and to be nonzero at $x = x_0$.

The wave function $\psi(x) = \delta(x - x_0)$ represent the state in which the particle is located exactly at the point x_0 on the x-axis.

Dirac, bracket notation:

Dirac invented the bra-ket notation for the expectation value of an observable L:

$$\langle L \rangle = \sum_i \lambda_i P(\lambda_i)$$

The expectation value follows statistics, it is a sum weighted with the Probability function P.
Example:

We begin with a spin A oriented along $\vec{m}$ and confirm that measuring of σ gives +1 (fixing that spin A is oriented in this direction).

Then subsequent measurements in direction $\vec{n}$ with unchanged spin A gives the statistical result $\langle A \rangle = \vec{m} \cdot \vec{n}$. To a certain degree, averages of quantum measurements follow the laws of classical physics.

Distributive property:

This is part of axioms of vector addition:

7. Distributive property:

$$z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$$
$$\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$$

Dot product:

1.

Analogous to the dot product for spatial 3-vectors is the inner product of bra $\langle B|$ and ket $|A\rangle$, written as $\langle B|A\rangle$. The axioms for the inner product:

1. Linearity:
$$\langle C|\{|A\rangle + |B\rangle\} = \langle C|A\rangle + \langle C|B\rangle$$
2. Complex conjugation:
$$\langle B|A\rangle = \langle A|B\rangle^*$$
3. Reality:
$$\langle A|A\rangle \in \mathbb{R}$$

In concrete representation by row and column vectors, the inner product is defined in terms of components.

$$|A\rangle \coloneqq \begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\\ \alpha_4\end{pmatrix}, \langle A| = (\alpha_1^* \ \alpha_2^* \ \alpha_3^* \ \alpha_4^*), |B\rangle \coloneqq \begin{pmatrix}\beta_1\\ \beta_2\\ \beta_3\\ \beta_4\end{pmatrix}, \langle B| = (\beta_1^* \ \beta_2^* \ \beta_3^* \ \beta_4^*)$$

$$\langle B|A\rangle = (\beta_1^* \ \beta_2^* \ \beta_3^* \ \beta_4^*)\begin{pmatrix}\alpha_1\\ \alpha_2\\ \alpha_3\\ \alpha_4\end{pmatrix} = \beta_1^*\alpha_1 + \beta_2^*\alpha_2 + \beta_3^*\alpha_3 + \beta_4^*\alpha_4$$

$$\langle A|B\rangle = (\alpha_1^* \ \alpha_2^* \ \alpha_3^* \ \alpha_4^*)\begin{pmatrix}\beta_1\\ \beta_2\\ \beta_3\\ \beta_4\end{pmatrix} = \alpha_1^*\beta_1 + \alpha_2^*\beta_2 + \alpha_3^*\beta_3 + \alpha_4^*\beta_4$$

For complex values this gives $\langle A|B\rangle \neq \langle B|A\rangle$ and $\langle B|A\rangle = \langle A|B\rangle^*$. For real values $\langle A|B\rangle = \langle B|A\rangle$.

If the inner product $\langle A|A\rangle = 1$, then the vector is normalized.

If the inner product $\langle A|B\rangle = 0$, then $|A\rangle$ and $|B\rangle$ are orthogonal.

2.

The Cauchy-Schwarz inequality states that, given any two vectors $\vec{X}$ and $\vec{Y}$, the product of their lengths is greater than or equal to their dot product:

$$\left|\vec{X}\right|\left|\vec{Y}\right| \geq \left|\vec{X}\cdot\vec{Y}\right|$$

Squared this is called the Cauchy-Schwarz inequality:

$$\left|\vec{X}\right|^2\left|\vec{Y}\right|^2 \geq \left|\vec{X}\cdot\vec{Y}\right|^2$$

3.

In a two-spin system of Alice and Bob both can measure their spin with individual apparatuses, Alice measuring $\vec{\sigma}$, Bob measuring $\vec{\tau}$. Quantum mechanics insists that some kind of apparatus can be build that measures the observable $\vec{\sigma}\cdot\vec{\tau} = \sigma_x\tau_x + \sigma_y\tau_y + \sigma_z\tau_z$. As Alice and Bob cannot simultaneously measure the individual components of their spin, because they do not commute, the observable $\vec{\sigma}\cdot\vec{\tau}$ is not accessible for them.

Example: some atoms have spins that are described in the same way as electron spins. When two of these atoms are close to each other – for example, two neighboring atoms in a crystal lattice – the Hamiltonian will depend on the spins. In some situations, the neighboring spins' Hamiltonian is proportional to $\vec{\sigma} \cdot \vec{\tau}$. If that happens to be the case, then measuring $\vec{\sigma} \cdot \vec{\tau}$ is equivalent to measuring the energy of the atomic pair, a single measurement of the composite operator without measuring its components.

Down state:

The basis vector for the up-state $|u\rangle$ is $\binom{1}{0}$, the basis vector for the down-state $|d\rangle$ is $\binom{0}{1}$.

Dual number systems:

Every complex number z has a complex conjugate z^*:

$$z \coloneqq x + iy \;\rightarrow\; z^* = x - iy$$

$$z \coloneqq r \cdot e^{i\theta} \;\rightarrow\; z^* = r \cdot e^{-i\theta}$$

Every complex conjugate is itself a complex number, but it is often helpful to think of z and z^* as belonging to separate "dual" number system. Dual here means that for every z there is a unique z^* and vice versa.

Eigen-equation for momentum:

Let P be the momentum operator, defined in terms of the derivation operator: $P = -i\hbar\frac{d}{dx}$. The "$minus\ i$" is necessary to make the operator P Hermitian.

The eigen-equation in abstract vector notation is:

$$P|\psi\rangle = p|\psi\rangle$$

with p as an eigenvalue of P. We can write the eigen-equation as:

$$P|\psi\rangle = -i\hbar\frac{d\psi(x)}{dx} = p\psi(x)$$

or

$$\frac{d\psi(x)}{dx} = \frac{ip}{\hbar}\psi(x)$$

This is a differential equation with a solution of the form:

$$\psi_p(x) = Ae^{\frac{ipx}{\hbar}}$$

The subscript p is a reminder that $\psi_p(x)$ is eigenvector of P with the specific eigenvalue p. It is a function of x, but labeled by an eigenvalue of P.

Eigenfunctions of position operator:

Let X be the position operator. We can write the eigen-equation as:

$$X|\psi\rangle = x_0|\psi\rangle$$

In terms of wave functions:

$$x\psi(x) = x_0\psi(x)$$

We rewrite the equation:

$$(x - x_0)\psi(x) = 0$$

The properties of $\psi(x)$: $\psi(x)$ must be zero for all $x \neq x_0$ and can be anything for $x = x_0$. This is the property of the Dirac delta function:

$$\psi(x) := \delta(x - x_0)$$

$\psi(x)$ is eigenfunction of the position operator X with eigenvalue x_0:

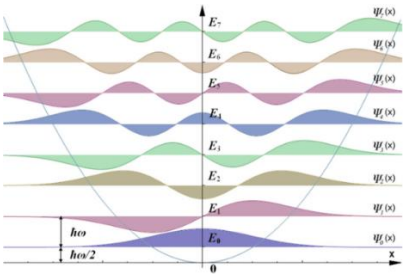
$$x\psi(x) = x\delta(x - x_0) = x_0\delta(x - x_0) = x_0\psi(x)$$

Note: for discrete vector spaces it would be sufficient for $\delta(x - x_0)$ to be 1 at $x = x_0$, the Dirac delta function thus becoming the Kronecker δ.

For continuous functions “one wouldn’t be enough”. The Dirac delta function can be approximated by $\lim_{n\to\infty} ne^{-(n(x-x_0))^2}$.

Eigenfunctions, symmetric and antisymmetric:

A real function is called symmetric, if $f(x) = f(-x)$. It is antisymmetric, if $f(x) = -f(-x)$. The picture below shows eigenfunctions for the lower states of the harmonic oscillator. Functions for even numbers are symmetric, functions for odd numbers are antisymmetric.



Picture courtesy AllenMcC. CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=11623546

Eigenfunctions for energy levels of harmonic oscillator:

If we apply the raising operator $a^+ \coloneqq (P + i\omega X)$ to the ground-state wave function, $e^{-\frac{\omega}{2\hbar}x^2}$, we get the first energy level:

$$\psi_1(x) = (P + i\omega X)\psi_0(x) =$$

$$\left(-i\hbar\frac{\partial}{\partial x} + i\omega x\right)e^{-\frac{\omega}{2\hbar}x^2} = i\hbar\frac{2x\omega}{2\hbar}e^{-\frac{\omega}{2\hbar}x^2} + i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\psi_0(x)(i\omega x + i\omega x) = 2i\omega x\psi_0(x)$$

$$\psi_1(x) = 2i\omega x\psi_0(x)$$

Applying the raising operator to $\psi_1(x)$, omitting the factor $2i\omega$ we get:

$$\psi_2(x) = (P + i\omega X)\psi_1(x) = \left(-i\hbar\frac{\partial}{\partial x} + i\omega x\right)x\psi_0(x) =$$

$$\left(-i\hbar\frac{\partial}{\partial x} + i\omega x\right)xe^{-\frac{\omega}{2\hbar}x^2} =$$

$$-i\hbar\frac{\partial}{\partial x}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right) + i\omega x^2e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-i\hbar\left(e^{-\frac{\omega}{2\hbar}x^2} + x\left(\frac{-x\omega}{\hbar}\right)e^{-\frac{\omega}{2\hbar}x^2}\right) + i\omega x^2e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-i\hbar\left(\psi_0(x) + x\left(\frac{-x\omega}{\hbar}\right)\psi_0(x)\right) + i\omega x^2\psi_0(x) =$$

$$\psi_0(x)(-i\hbar - ix(-x\omega)) + i\omega x^2\psi_0(x) =$$

$$\psi_0(x)(-i\hbar + i\omega x^2 + i\omega x^2) =$$

$$\psi_0(x)(-i\hbar + 2i\omega x^2) =$$

$$i\psi_0(x)(-\hbar + 2\omega x^2)$$

$$\psi_2(x) \sim \psi_0(x)(-\hbar + 2\omega x^2)$$

The important pattern we see here is, that each eigenfunction is a polynomial in x of increasing degree. This explains why successive eigenfunctions alternate between being symmetric and antisymmetric.

Note: the polynomials in this sequence are the Hermite polynomials.

Eigenstate, collapse of wave function and eigenstate:

Experimental physics is measuring observables. Even if we know the state-vector exactly, we don't know the result of any given measurement although the state-vector evolves in a perfectly definite way, according to the Schrödinger equation.

Explicit: suppose the state vector just before the measurement of L is:

$$\sum_j \alpha_j |\lambda_j\rangle$$

Randomly, with probability $|\alpha_j|^2$, the apparatus measures value λ_j and leaves the system in a single eigenstate of L, namely $|\lambda_j\rangle$. The entire superposition of states collapses to a single term.

Eigenvalues:

1.

In general, if a linear operator acts on a vector, it will change the direction of the vector. But for particular linear operators M there will be certain vectors $|\lambda\rangle$ whose directions are the same after the action. These special vectors are called eigenvectors, and they will be multiplied by a factor λ, the eigenvalue:

$$M|\lambda\rangle = \lambda|\lambda\rangle$$

Note: λ is a real or complex value, $|\lambda\rangle$ is a vector.

Example: $M := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $|\lambda\rangle = \begin{pmatrix} 1 \\ i \end{pmatrix}$:

$$M|\lambda\rangle = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ i \end{pmatrix} = \begin{pmatrix} -i \\ 1 \end{pmatrix} = i\begin{pmatrix} 1 \\ i \end{pmatrix}$$

The eigenvalue λ in this case is the imaginary unit i.

2.

The possible results of a measurement are the eigenvalues of the operator that represents the observable, usually called λ_j with the according eigenvector $|\lambda_j\rangle$.

Eigenvalues of density matrix:

1.

The eigenvalues of a density matrix are all positive and lie between 0 and 1 (a probability density). If there is an eigenvalue with value 1, all other eigenvalues are 0, the corresponding state being a pure state. If not – mixed state. This can be used to distinguish between entangled and unentangled states.

2.

In a product state of Alice and Bob the density matrix of Alice (and analog Bob) depends on the variables of Alice. Both systems are unentangled (product state), so the density matrix of Alice has exactly one eigenvalue 1, the rest being zero.

Explicit:

The density matrix of Alice:

$$\rho_{a'a} = \psi^*(a)\,\psi(a')$$

The eigenvalue equation for the density matrix ρ of Alice:

$$\sum_a \rho_{a'a}\alpha_a = \sum_a \psi^*(a)\psi(a')\alpha_a =$$

$$\psi(a')\sum_a \psi^*(a)\alpha_a = \lambda\alpha_{a'}$$

The quantity $\sum_a \psi^*(a)\alpha_a$ has the form of an inner product. If the column vector α is orthogonal to ψ, the sum becomes zero and so the left side of the equation – we have an eigenvector with eigenvalue zero.

There is only one possible direction for an eigenvector with nonzero eigenvalue, namely the vector $\psi(a)$. Together with the normalizing convention we get, that $\alpha_a := \psi(a)$ is eigenvector of ρ with eigenvalue 1.

Note: the decomposition of the phase-state in eigenvectors of an operator is complete, so all eigenvectors are orthogonal to each other.

Eigenvalues, energy:

Let H be the Hamilton operator, E_j eigenvalues and $|E_j\rangle$ eigenvectors. The equation:

$$H|E_j\rangle = E_j|E_j\rangle$$

is the time-independent Schrödinger equation. Because H represents energy, E_j are the energy eigenvalues with $|E_j\rangle$ the energy eigenvectors.

Note: you can read this equation in two ways.

a) you put in a particular value of Energy E_j and look for the ket-vector $|E_j\rangle$ that solves the equation.

b) you put in an arbitrary value of E_j. In general, there will exist no solution, so you can search for possible energy eigenvalues of the system.

Explicit:

$$H|\psi_E\rangle = E|\psi_E\rangle$$

If we compose the Hamiltonian out of the position operator X and the momentum operator P, we get:

$$-\frac{\hbar^2}{2}\frac{\partial^2\psi_E(x)}{\partial x^2} + \frac{1}{2}\omega^2 x^2\psi_E(x) = E\psi_E(x)$$

To solve this equation, we must:

a) Find allowable values of E (the energies) that permit a mathematical solution,
b) Find eigenvectors and possible eigenvalues of the energy.

The problem is that for every value for E including all complex numbers, there is a solution for this equation, but most of them makes physical no sense. Physically solutions of the Schrödinger equation must be normalizable. $\psi_E(x)$ must become zero for x approaching $\pm\infty$.

Eigenvalues of Hermitian operators:

Eigenvalues of Hermitian operators must be real.

Hermitian operators satisfy:

$$M = M^{\dagger}$$

In terms of matrix elements, this can be stated as:

$$m_{ij} = m_{ij}^{*}$$

Flipping a Hermitian matrix about the main diagonal and taking the complex conjugates delivers the original matrix.

Suppose λ and $|\lambda\rangle$ represent an eigenvalue and its corresponding eigenvector of the Hermitian operator L.

In symbolic style:

$$L|\lambda\rangle = \lambda|\lambda\rangle \rightarrow \langle\lambda|L|\lambda\rangle = \langle\lambda|\lambda|\lambda\rangle$$

Working with the corresponding bra:

$$\langle\lambda|L^{\dagger} = \langle\lambda|\lambda^{*}$$

As L is Hermitian:

$$\langle\lambda|L = \langle\lambda|\lambda^{*}$$

We have:

$$\langle\lambda|L = \langle\lambda|\lambda^{*} \rightarrow \langle\lambda|L|\lambda\rangle = \langle\lambda|\lambda^{*}|\lambda\rangle$$

It follows:

$$\langle\lambda|\lambda|\lambda\rangle = \langle\lambda|\lambda^{*}|\lambda\rangle \rightarrow \lambda = \lambda^{*}$$

$\lambda = \lambda^{*}$ requests λ being real.

Eigenvalues of operators:

1. Operators are used to calculate eigenvalues and eigenvectors.
2. Operators act on state-vectors, not on actual physical system.
3. If an operator acts on a state-vector, it produces a new state vector.

Note: measuring an observable is **not always** the same as operating with the corresponding operator on the state.

Example: we have a spin is prepared in the right-state $|r\rangle$. This is not an eigenvector of σ_z.

In the $up - down$-system we describe $|r\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

We act with the operator σ_z on this state vector, the result is the state-vector $\frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$.

But, a measurement of the spin in the z-axis would either set the spin in this direction or would not change the spin at all.

Eigenvalues of position:

Prerequisite

The inner product in terms of wave functions:

$$\langle\psi|\theta\rangle = \int_{-\infty}^{+\infty} \psi^*(x)\theta(x)dx$$

End prerequisite

If the position of a particle is an observable, there must be a Hermitian operator associated with it. The "multiply by x" operator X is a suitable candidate.

$$X\psi(x) \coloneqq x\psi(x)$$

The eigen-equation for X is:

$$X|\psi\rangle = x_0|\psi\rangle$$

In terms of wave functions this becomes:

$$x\psi(x) = x_0\psi(x)$$

We rewrite this:

$$(x - x_0)\psi(x) = 0$$

This is the property of the Dirac delta function $\delta(x - x_0)$. The wave function

$$\psi(x) = \delta(x - x_0)$$

represents the state in which the particle is located exactly at the x_0 on the x-axis. Every real number x_0 is eigenvalue of the operator X. The corresponding eigenvectors (eigenfunctions) are concentrated at $x = x_0$.

Consider the inner product of a state $|\psi\rangle$ and a position eigenstate $|x_0\rangle$:

$$\langle x_0|\psi\rangle$$

We can write this:

$$\langle x_0|\psi\rangle = \int_{-\infty}^{+\infty} x_0\psi(x)dx = \int_{-\infty}^{+\infty} x_0\delta(x - x_0)dx =$$

$$x_0\int_{-\infty}^{+\infty} \delta(x - x_0)dx = x_0$$

We use:

$$x_0 = \psi(x_0)$$

Because this is true for every x_0, we can drop the subscript and write:

$$\langle x|\psi\rangle = \psi(x)$$

$\psi(x)$ is referred to as the *wave function in the position representation*.

Eigenvalues of spin operator:

The spin operators are σ_x, σ_y and σ_z:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Eigenvectors of σ_x are:

$$|r\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|l\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Both vectors are orthogonal to each other:

$$\langle r|l\rangle = \frac{1}{\sqrt{2}}(1\ 1) \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{2}(1\ 1) \cdot \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{2}(1 \cdot 1 + 1 \cdot (-1)) = 0$$

Note: the bra $\langle r|$ to the ket $|r\rangle$ is the complex conjugated, but as $|r\rangle$ is real $\langle r^*|$ = $\langle r|$.

We check the eigenvector property:

$$\langle \sigma_x|r\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \cdot 1 + 1 \cdot 1 \\ 1 \cdot 1 + 0 \cdot 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$|r\rangle$ is eigenvector to the operator σ_x with eigenvalue 1.

$$\langle \sigma_x|l\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \cdot 1 + 1 \cdot (-1) \\ 1 \cdot 1 + 0 \cdot (-1) \end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$|l\rangle$ is eigenvector to the operator σ_x with eigenvalue -1.

Eigenvectors of σ_y are:

$$|i\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{i}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$|o\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{i}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Both vectors are orthogonal to each other:

$$\langle i|o\rangle = \frac{1}{\sqrt{2}}(1\ (-i)) \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{2}(1\ (-i)) \cdot \begin{pmatrix} 1 \\ -i \end{pmatrix} =$$

$$\frac{1}{2}(1 \cdot 1 + (-i) \cdot (-i)) = \frac{1}{2}(1 + i^2) = 0$$

Note: $\langle i|$ is the vector "in".

Note: the bra $\langle i|$ to the ket $|i\rangle$ is the complex conjugated.

We check the eigenvector property:

$$\langle\sigma_y|i\rangle = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 - i^2\\ i\cdot 1 + 0\cdot i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}$$

$|i\rangle$ is eigenvector to the operator σ_y with eigenvalue 1.

$$\langle\sigma_y|o\rangle = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 + i^2\\ i\cdot 1 + 0\cdot(-i)\end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}$$

$|o\rangle$ is eigenvector to the operator σ_y with eigenvalue -1.

Eigenvectors of σ_z are:

$$|u\rangle \coloneqq \begin{pmatrix}1\\ 0\end{pmatrix}$$

$$|d\rangle \coloneqq \begin{pmatrix}0\\ 1\end{pmatrix}$$

Both vectors are orthogonal to each other:

$$\langle u|d\rangle = (1\ 0)\cdot\begin{pmatrix}0\\ 1\end{pmatrix} = (1\cdot 0 + 0\cdot 1) = 0$$

Note: the bra $\langle u|$ to the ket $|u\rangle$ is the complex conjugated, but as $|u\rangle$ is real $\langle u^*|$ = $\langle u|$.

We check the eigenvector property:

$$\langle\sigma_z|u\rangle = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\cdot\begin{pmatrix}1\\ 0\end{pmatrix} = \begin{pmatrix}1\cdot 1 + 0\cdot 0\\ 0\cdot 1 - 1\cdot 0\end{pmatrix} = \begin{pmatrix}1\\ 0\end{pmatrix}$$

$|u\rangle$ is eigenvector to the operator σ_z with eigenvalue 1.

$$\langle\sigma_z|d\rangle = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\cdot\begin{pmatrix}0\\ 1\end{pmatrix} = \begin{pmatrix}1\cdot 0 + 0\cdot 0\\ 0\cdot 0 - 1\cdot 1\end{pmatrix} = -\begin{pmatrix}0\\ 1\end{pmatrix}$$

$|d\rangle$ is eigenvector to the operator σ_z with eigenvalue -1.

Eigenvectors:

1.

For particular operators M there will be certain vectors $|\lambda\rangle$ the directions are the same after the operator acted on them. These vectors are called eigenvectors, normally multiplied by a factor, the eigenvalue:

$$M|\lambda\rangle = \lambda|\lambda\rangle$$

Note: λ denotes a number, the eigenvalue, $|\lambda\rangle$ the eigenvector.

Example:

$$M|\lambda\rangle \coloneqq \begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}\begin{pmatrix}1\\ 1\end{pmatrix} = \begin{pmatrix}1\cdot 1 + 2\cdot 1\\ 2\cdot 1 + 1\cdot 1\end{pmatrix} = \begin{pmatrix}3\\ 3\end{pmatrix} = 3\begin{pmatrix}1\\ 1\end{pmatrix}$$

$\begin{pmatrix}1\\ 1\end{pmatrix}$ is eigenvector to the operator $\begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}$ with eigenvalue 3.

$$M|\lambda\rangle \coloneqq \begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}\begin{pmatrix}1\\ -1\end{pmatrix} = \begin{pmatrix}1\cdot 1 - 2\cdot 1\\ 2\cdot 1 - 1\cdot 1\end{pmatrix} = \begin{pmatrix}-1\\ 1\end{pmatrix} = -1\begin{pmatrix}1\\ -1\end{pmatrix}$$

$\begin{pmatrix}1\\ -1\end{pmatrix}$ is eigenvector to the operator $\begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}$ with eigenvalue -1.

Eigenvectors form an orthogonal base of the vector space:

$$\begin{pmatrix}1\\ 1\end{pmatrix}\cdot\begin{pmatrix}1\\ -1\end{pmatrix} = 1 - 1 = 0$$

For all other vectors this is not valid.

Example:

$$M|\lambda\rangle \coloneqq \begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \begin{pmatrix}1\cdot 1 + 2\cdot 0\\ 2\cdot 1 + 1\cdot 0\end{pmatrix} = \begin{pmatrix}1\\ 2\end{pmatrix} \neq \begin{pmatrix}1\\ 0\end{pmatrix}$$

$\begin{pmatrix}1\\ 0\end{pmatrix}$ is not an eigenvector to the operator $\begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}$.

Note: eigenvectors and eigenvalues can have complex values.

Example:

$$M|\lambda\rangle \coloneqq \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\ i\end{pmatrix} = \begin{pmatrix}0\cdot 1 - 1\cdot i\\ 1\cdot 1 - 0\cdot i\end{pmatrix} = \begin{pmatrix}-i\\ 1\end{pmatrix} = -i\begin{pmatrix}1\\ i\end{pmatrix}$$

$\begin{pmatrix}1\\ i\end{pmatrix}$ is eigenvector to the operator $\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$ with eigenvalue $-i$.

This holds for bra-vectors too:

$$\langle\lambda|M = \langle\lambda|\lambda$$

Example:

$$\langle\lambda|M \coloneqq (1\ 1)\begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix} = \big((1\cdot 1 + 1\cdot 2) + (1\cdot 2 + 1\cdot 1)\big) = (3\ 3) = 3(1\ 1)$$

$(1\ 1)$ is eigenvector to the operator $\begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}$ with eigenvalue 3.

Note: switching from ket to bra implies complex conjugation.

Example:

$$\langle\lambda|M \coloneqq (1(-i))\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} = \big((1\cdot 0 - i\cdot 1) + (1\cdot(-1) - i\cdot 0)\big) = \big((-i)(-1)\big) = -i(1(-i))$$

$(1(-i))$ is eigenvector to the operator $\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$ with eigenvalue $-i$.

2.

If $|A\rangle$ is the state-vector of a system, and the observable L is measured, the probability to observe values λ_i is:

$$P(\lambda_i) = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$

Note: in $P(\lambda_i)$, λ_i are the eigenvalues of L. In $\langle A|\lambda_i\rangle$ and $\langle\lambda_i|A\rangle$ we have the eigenvectors in bra and ket form.

Eigenvectors of annihilation operator:

Note: annihilation operator and lowering operator are used synonym.

Note: What meant here is the annihilation operator acting on the eigenfunctions of the harmonic oscillator.

Applying the lowering operator to the ground state of a harmonic oscillator “destroys” it to zero.

Applying the lowering operator to excited energy wave-functions (eigenfunctions) brings up the wave-function (eigenfunction) of the previous lower energy level.

We begin with the Hamiltonian expressed in terms of the position operator X and the momentum operator P:

$$H = \frac{P^2 + \omega^2 X^2}{2}$$

Out of this we can extract the annihilation operator:

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X) = \frac{i}{\sqrt{2\omega\hbar}}\left(-i\hbar\frac{d}{dx} - i\omega x\right) =$$

$$\frac{1}{\sqrt{2\omega\hbar}}\left(\hbar\frac{d}{dx} + \omega x\right)$$

The annihilation operator applied to the ground state wave-function annihilates it:

$$a^-\big(\psi_0(x)\big) = 0$$

This leads to a differential equation:

$$\left(\hbar\frac{d}{dx} + \omega x\right)\psi_0(x) = 0$$

Solution:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

The energy eigenfunctions of a harmonic oscillator (by subsequent applying the raising operator a^+) in ascending order are:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

$$\psi_1(x) = \sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} = \sqrt{\frac{2\omega}{\hbar}}x\psi_0(x)$$

$$\psi_2(x) = \left(-1 + \frac{2\omega}{\hbar}x^2\right)e^{-\frac{\omega}{2\hbar}x^2} = \left(-1 + \frac{2\omega}{\hbar}x^2\right)\psi_0(x)$$

…

Applying the annihilation operator to the first excited energy state $\psi_1(x)$:

$$a^-\left(\sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$\frac{1}{\sqrt{2\omega\hbar}}\left(\hbar\frac{d}{dx}+\omega x\right)\left(\sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2}\right)=$$

$$\frac{d}{dx}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right)+\frac{\omega x^2}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}=;$$

First part: $\frac{d}{dx}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right)$

$$\frac{d}{dx}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right)=$$

$$\left(e^{-\frac{\omega}{2\hbar}x^2}+xe^{-\frac{\omega}{2\hbar}x^2}\left(-\frac{\omega x}{\hbar}\right)\right)=$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(1-\frac{\omega x^2}{\hbar}\right)$$

Second part: $\frac{\omega x^2}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}$

Merging:

$$e^{-\frac{\omega}{2\hbar}x^2}\left(1-\frac{\omega x^2}{\hbar}\right)+\frac{\omega x^2}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}=$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(1-\frac{\omega x^2}{\hbar}+\frac{\omega x^2}{\hbar}\right)=$$

$$e^{-\frac{\omega}{2\hbar}x^2}$$

The annihilation operator grades the first excited state down to the ground state.

Eigenvectors of creation operator:

Note: creation operator and raising operator are used synonym.

Note: What meant here is the raising operator acting on the eigenfunctions of the harmonic oscillator.

Applying the raising operator to the ground state of a harmonic oscillator “raises” it up to the next level … and so on …

We begin with the Hamiltonian expressed in terms of the position operator X and the momentum operator P:

$$a^+=\frac{-i}{\sqrt{2\omega\hbar}}(P+i\omega X)=\frac{-i}{\sqrt{2\omega\hbar}}\left(-i\hbar\frac{d}{dx}+i\omega x\right)=$$

$$\frac{-i}{\sqrt{2\omega\hbar}}(-i)\left(\hbar\frac{d}{dx}-\omega x\right)=\frac{-1}{\sqrt{2\omega\hbar}}\left(\hbar\frac{d}{dx}-\omega x\right)=$$

$$\frac{1}{\sqrt{2\omega\hbar}}\left(-\hbar\frac{d}{dx}+\omega x\right)$$

The raising operator applied to the ground state wave-function:

$$a^+\left(\psi_0(x)\right)=\psi_1(x)$$

The energy eigenfunctions of a harmonic oscillator (by subsequent applying the raising operator a^+) in ascending order are:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

$$\psi_1(x) = \sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} = \sqrt{\frac{2\omega}{\hbar}}x\psi_0(x)$$

$$\psi_2(x) = \left(-1+\frac{2\omega}{\hbar}x^2\right)e^{-\frac{\omega}{2\hbar}x^2} = \left(-1+\frac{2\omega}{\hbar}x^2\right)\psi_0(x)$$

…

Applying the raising operator to the ground level energy state $\psi_0(x)$:

$$a^+\left(e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$\frac{1}{\sqrt{2\omega\hbar}}\left(-\hbar\frac{d}{dx}+\omega x\right)\left(e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$-\sqrt{\frac{\hbar}{2\omega}}\frac{d}{dx}e^{-\frac{\omega}{2\hbar}x^2} + \frac{1}{\sqrt{2\omega\hbar}}\omega x e^{-\frac{\omega}{2\hbar}x^2}$$

First part: $-\sqrt{\frac{\hbar}{2\omega}}\frac{d}{dx}e^{-\frac{\omega}{2\hbar}x^2}$

$$-\sqrt{\frac{\hbar}{2\omega}}\frac{d}{dx}e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\sqrt{\frac{\hbar}{2\omega}}\frac{\omega x}{\hbar}e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\sqrt{\frac{\omega}{2\hbar}}xe^{-\frac{\omega}{2\hbar}x^2}$$

Second part: $\frac{1}{\sqrt{2\omega\hbar}}\omega x e^{-\frac{\omega}{2\hbar}x^2}$

$$\frac{1}{\sqrt{2\omega\hbar}}\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\sqrt{\frac{\omega}{2\hbar}}xe^{-\frac{\omega}{2\hbar}x^2}$$

Merging:

$$\sqrt{\frac{\omega}{2\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} + \sqrt{\frac{\omega}{2\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} =$$

$$\sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} =$$

$$\sqrt{\frac{2\omega}{\hbar}}x\psi_0(x)$$

The raising operator raises the ground state to the first excited state.

Eigenvectors of energy:

1.

Matrix representation

The Hamiltonian H represents energy:

$$H|E_j\rangle = E_j|E_j\rangle$$

This is called the time independent Schrödinger equation and works in a specific matrix basis.

Note: E_j is a number, the energy eigenvalue. $|E_j\rangle$ is the corresponding energy eigenvector.

2.

Wave function

$$H|\varphi_E\rangle = E|\psi_E\rangle$$

Again, this is the time independent Schrödinger equation.

The classical Hamiltonian:

$$H = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega^2 x^2$$

In quantum mechanics we do not have a velocity operator. With the Lagrangian $\mathcal{L}$ we can translate velocity in momentum:

$$p = \frac{\partial \mathcal{L}}{\partial \dot{x}} = \dot{x}$$

We rewrite the Hamiltonian:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

Again, this is a classical Hamiltonian. We turn it into a quantum mechanical equation by reinterpreting x and p as operators acting on $\psi(x)$.

The position operator X multiplies the wave function by x:

$$X|\psi_E(x)\rangle \to x\psi_E(x)$$

The momentum operator is the derivative:

$$P|\psi_E(x)\rangle \to -i\hbar\frac{\partial}{\partial x}\psi_E(x)$$

Both operators operate twice. The position operator is ok, for the momentum operator we get:

$$(P|\psi_E(x))^2 \to -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\psi_E(x)\right) = -\hbar^2\frac{\partial^2}{\partial x^2}\psi_E(x)$$

Our quantum Hamiltonian:

$$H|\psi_E\rangle = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi_E(x) + \frac{1}{2}\omega^2 x^2 \psi_E(x) = E\psi_E(x)$$

A solution to this are the energy eigenfunctions:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

$$\psi_1(x) = \sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} = \sqrt{\frac{2\omega}{\hbar}}x\psi_0(x)$$

$$\psi_2(x) = \left(-1 + \frac{2\omega}{\hbar}x^2\right)e^{-\frac{\omega}{2\hbar}x^2} = \left(-1 + \frac{2\omega}{\hbar}x^2\right)\psi_0(x)$$

with the according eigenvalues 1, $\sqrt{\frac{2\omega}{\hbar}}x$, $\left(-1 + \frac{2\omega}{\hbar}x^2\right)$, …

Eigenvectors of Hermitian operator:

The fundamental theorem:

a) The eigenvectors of a Hermitian operator form a complete set. Any vector the operator can generate can be expanded as a sum of its eigenvectors.
b) If λ_1 and λ_2 are two unequal eigenvalues of a Hermitian operator, then the corresponding eigenvectors are orthogonal.
c) Even if two eigenvalues are equal, the corresponding eigenvectors can be chosen to be orthogonal. This situation is called degeneracy.

Note: the eigenvectors of a Hermitian operator form an orthonormal basis.

Check a)

For the example of the R^3 we change the basis vectors.

Let $\begin{pmatrix}1\\0\\1\end{pmatrix}, \begin{pmatrix}1\\1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\\1\end{pmatrix}$ be a set of vectors B_1, B_2 and B_3 that form a basis B of $\mathbb{R}^3$.

They are linear independent:

$$a\begin{pmatrix}1\\0\\1\end{pmatrix} + b\begin{pmatrix}1\\1\\0\end{pmatrix} + c\begin{pmatrix}0\\1\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$$

$$\begin{array}{cccc} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{array}$$

We transform this:

$$\begin{array}{cccc} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{array} \rightarrow \begin{array}{cccc} 1 & 0 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{array} \rightarrow \begin{array}{cccc} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{array} \rightarrow \begin{array}{cccc} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{array} \rightarrow \begin{array}{cccc} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array}$$

The only solution to this is a = b = c = 0.

The linear independent vectors define a matrix P, a linear map:

$$P \coloneqq \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$$

Let $\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ be a vector with respect to this basis B: $\overline{x} = x_1 B_1 + x_2 B_2 + x_3 B_3$.

Then $P \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ give the coordinates of $\overline{x}$ in the canonical basis E_1, E_2 and E_3: $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

$$P \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_1 + x_2 \\ x_2 + x_3 \\ x_1 + x_3 \end{pmatrix}$$

Check:

$$P \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$$P \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$P \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

To get this the other way around we must find the inverse matrix P^{-1}:

$$\left(\begin{array}{ccc|ccc} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \end{array}\right)$$

$$\left(\begin{array}{ccc|ccc} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & -1 & 1 & -1 & 0 & 1 \end{array}\right)$$

$$\left(\begin{array}{ccc|ccc} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 2 & -1 & 1 & 1 \end{array}\right)$$

$$\left(\begin{array}{ccc|ccc} 1 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 2 & -1 & 1 & 1 \end{array}\right)$$ line 3 divided by 2

$$\left(\begin{array}{ccc|ccc} 1 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{array}\right)$$

The inverse matrix P^{-1}:

$$\frac{1}{2}\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{pmatrix}$$

Applied to the linear independent vectors B_1, B_2 and B_3 this gives the canonical basis E_1, E_2 and E_3.

Check:

$$P^{-1}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$P^{-1}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$P^{-1}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Check b)

According to the definition of eigenvectors and eigenvalues, we can write:

$$L|\lambda_1\rangle = \lambda_1|\lambda_1\rangle$$

$$L|\lambda_2\rangle = \lambda_2|\lambda_2\rangle$$

Note: λ_i is an eigenvalue, a number. $|\lambda_i\rangle$ is an eigenvector. L is a Hermitian operator, we can switch from ket to bra in the first equation without modification:

$$\langle\lambda_1|L = \lambda_1\langle\lambda_1|$$

We have:

$$\langle\lambda_1|L = \lambda_1\langle\lambda_1|$$

$$L|\lambda_2\rangle = \lambda_2|\lambda_2\rangle = |\lambda_2\rangle\lambda_2$$

We form the inner product of the first equation with $|\lambda_2\rangle$ and the inner product of the second equation with $\langle\lambda_1|$:

$$\langle\lambda_1|L|\lambda_2\rangle = \lambda_1\langle\lambda_1|\lambda_2\rangle$$

$$\langle\lambda_1|L|\lambda_2\rangle = \langle\lambda_1|\lambda_2\rangle\lambda_2 = \lambda_2\langle\lambda_1|\lambda_2\rangle$$

The left side of both equations is identic, so we get:

$$\lambda_1\langle\lambda_1|\lambda_2\rangle = \lambda_2\langle\lambda_1|\lambda_2\rangle$$

It follows:

$$\lambda_1\langle\lambda_1|\lambda_2\rangle - \lambda_2\langle\lambda_1|\lambda_2\rangle = 0$$

$$(\lambda_1 - \lambda_2)\langle\lambda_1|\lambda_2\rangle = 0$$

If the eigenvalues λ_1 and λ_2 are different, the inner product $\langle\lambda_1|\lambda_2\rangle$ must be zero.

Check c)

Even if two eigenvalues are equal, the corresponding eigenvectors can be chosen to be orthogonal. This situation is called degeneracy. Again, we write

$$L|\lambda_1\rangle = \lambda_1|\lambda_1\rangle$$

$$L|\lambda_2\rangle = \lambda_2|\lambda_2\rangle$$

with $\lambda_1 = \lambda_2 \coloneqq \lambda$ but $|\lambda_1\rangle \neq |\lambda_2\rangle$. We choose a linear combination of both eigenvectors:

$$|A\rangle = \alpha|\lambda_1\rangle + \beta|\lambda_2\rangle$$

We apply the operator L on both sides:

$$L|A\rangle = L\alpha|\lambda_1\rangle + L\beta|\lambda_2\rangle = \alpha L|\lambda_1\rangle + \beta L|\lambda_2\rangle =$$

$$\alpha\lambda|\lambda_1\rangle + \beta\lambda|\lambda_2\rangle = \lambda(\alpha|\lambda_1\rangle + \beta|\lambda_2\rangle)$$

Result: any linear combination of both eigenvectors is eigenvector again.

Out of two non-parallel vectors we can construct a pair of orthonormal vectors by the Gram-Schmidt procedure (not shown here).

Eigenvectors of momentum:

The momentum operator in quantum mechanics is called P, it is defined in terms of the operator $-i\hbar D$:

$$P \coloneqq -i\hbar D = -i\hbar\frac{d}{dx}$$

Note: the factor $-i$ is necessary to make the operator Hermitian, the factor $\hbar$ is needed to be dimensional correct.

In terms of wave functions:

$$P\big(\psi(x)\big) = -i\hbar\frac{d\psi(x)}{dx}$$

In terms of vector notation:

$$P|\psi\rangle = p|\psi\rangle$$

Note: P is the momentum operator, p an eigenvalue of P.

We combine both equations:

$$-i\hbar\frac{d\psi(x)}{dx} = p\psi(x)$$

We get:

$$\frac{d\psi(x)}{dx} = \frac{p}{-i\hbar}\psi(x) = \frac{ip}{\hbar}\psi(x)$$

This is a differential equation with the solution:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}}e^{\frac{ipx}{\hbar}}$$

It represents the momentum eigenvector (eigenfunction) in the position basis. It is a function of x.

The factor $\frac{1}{\sqrt{2\pi}}$ is result of normalization.

Eigenvectors of operators:

a) Operators are the objects we use to calculate eigenvalues and eigenvectors.
b) Operators act on state-vectors, not on real physical systems.
c) Operators acting on state-vectors produce new state-vectors.
d) If the new state-vectors are the old ones, multiplied by a constant, they are called eigenvectors, the constant called eigenvalue.

Eigenvectors of position:

Prerequisite

$|x\rangle$ is an eigenvector of position.

The inner product in terms of wave functions:

$$\langle\psi|\theta\rangle = \int_{-\infty}^{+\infty} \psi^*(x)\theta(x)dx$$

End prerequisite

If the position of a particle is an observable, there must be a Hermitian operator associated with it. The "multiply by x" operator X is a suitable candidate.

$$X\psi(x) \coloneqq x\psi(x)$$

The eigen-equation for X is:

$$X|\psi\rangle = x_0|\psi\rangle$$

In terms of wave functions this becomes:

$$x\psi(x) = x_0\psi(x)$$

We rewrite this:

$$(x - x_0)\psi(x) = 0$$

This is the property of the Dirac delta function $\delta(x - x_0)$.

The wave function

$$\psi(x) = \delta(x - x_0)$$

represents the state in which the particle is located x_0 on the x-axis.

Every real number x_0 is eigenvalue of the operator X because it is a potential candidate for a position on the x-axis.

The corresponding eigenvectors (eigenfunctions) are infinitely concentrated at $x = x_0$.

Consider the inner product of a state $|\psi\rangle$ and a position eigenstate (eigenvector) $|x_0\rangle$:

$$\langle x_0|\psi\rangle$$

We can write:

$$\langle x_0|\psi\rangle = \int_{-\infty}^{+\infty} x_0\psi(x)dx = \int_{-\infty}^{+\infty} x_0\delta(x-x_0)dx =$$

$$x_0\int_{-\infty}^{+\infty}\delta(x-x_0)dx = x_0$$

and

$$x_0 = \psi(x_0)$$

Because this is true for every x_0, we can drop the subscript and write:

$$\langle x|\psi\rangle = \psi(x)$$

The wave function $\psi(x)$ of a particle moving in the x-direction is the projection of a state-vector $|\psi\rangle$ onto the eigenvectors of position $|x\rangle$. $\psi(x)$ is referred to as the *wave function in the position representation*.

Eigenvectors of projection operator:

The outer product of a normalized ket with its corresponding bra is called a projection operator:

$$|\psi\rangle\langle\psi|$$

A projection operator acting on another vector $|A\rangle$:

$$(|\psi\rangle\langle\psi|)\ |A\rangle = |\psi\rangle\ (\langle\psi|A\rangle)$$

As $\langle\psi|A\rangle$ is a number, the result is a vector proportional to $|\psi\rangle$.

A projection operator projects a vector $|A\rangle$ onto the direction defined by $|\psi\rangle$.

Properties of projection operators:

- Projection operators are Hermitian
- The vector $|\psi\rangle$ is eigenvector to its projection operator with eigenvalue 1:
$$(|\psi\rangle\langle\psi|)\ |A\psi\rangle = |\psi\rangle\ (\langle\psi|\psi\rangle) = |\psi\rangle$$
- Any vector orthogonal to $|\psi\rangle$ is eigenvector to $(|\psi\rangle\langle\psi|)$ with eigenvalue 0.
- The square of a projection vector is the same as the projection operator itself:
$$(|\psi\rangle\langle\psi|)^2 = (|\psi\rangle\langle\psi|)$$
- If we add all the projection operators for a basis system, we obtain the identity operator:
$$\sum_i |\psi\rangle\langle\psi| = I$$
- The trace of a projection operator is 1:
$$Tr\ |\psi\rangle\langle\psi| = 1$$
- The expectation value of any observable L in state $|\psi\rangle$ is given by:
$$\langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|\ L$$

We check the last property:

$$Tr\ |\psi\rangle\langle\psi|\ L = \sum_i \langle\psi|L|i\rangle\langle i|\psi\rangle$$

Using

$$\sum_i |\psi\rangle\langle\psi| = I$$

we get:

$$\sum_i \langle\psi|L|i\rangle\langle i|\psi\rangle = \langle\psi|L|\psi\rangle$$

Eigenvectors, simultaneous eigenvectors:

In complex systems, we may have multiple observables that are compatible, their values can be known (exactly) simultaneously. Example: a composite system of two independent spins. We can measure each spin separately and associate these measurements with two different operators, called L and M.

If we measure both spins in a two spin (composite) system, the system changes into a state that is simultaneously eigenvector of L and eigenvector of M, a simultaneous eigenvector of the operators L and M.

Example:

We have an operator L and an operator M. There is a basis of state-vectors $|\lambda_i, \mu_j\rangle$ that are simultaneous eigenvectors of both observables. The eigenvalues λ_i belong to operator L, the eigenvalues μ_j belong to operator M with the subscripts running over all possible outcomes of measurements of L and M:

$$L|\lambda_i, \mu_j\rangle = \lambda_i|\lambda_i, \mu_j\rangle$$

$$M|\lambda_i, \mu_j\rangle = \mu_j|\lambda_i, \mu_j\rangle$$

For better readability we omit the subscripts and write:

$$L|\lambda, \mu\rangle = \lambda|\lambda, \mu\rangle$$

$$M|\lambda, \mu\rangle = \mu|\lambda, \mu\rangle$$

In order to have a basis of simultaneous eigenvectors, the operators L and M must commute:

$$LM|\lambda, \mu\rangle = L\mu|\lambda, \mu\rangle = \lambda\mu|\lambda, \mu\rangle = \mu\lambda|\lambda, \mu\rangle = M\lambda|\lambda, \mu\rangle = ML|\lambda, \mu\rangle$$

$$LM|\lambda, \mu\rangle = ML|\lambda, \mu\rangle$$

$$LM|\lambda, \mu\rangle - ML|\lambda, \mu\rangle = 0$$

With the commutator:

$$[L, M] = LM - ML$$

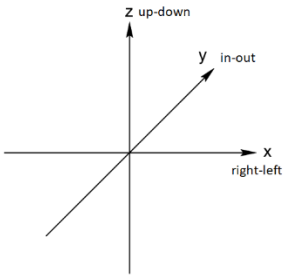
we can write

$$[L, M]|\lambda, \mu\rangle = 0$$

Note: “0” means the zero-vector $|0\rangle$.

Eigenvectors of spin operator:

Note: the names up-down, left-right, in-out refer to the spatial arrangement:



Note: the ordering z, y and x is due to the fact that we chose up-down as starting point, so the other pairs are derived from this.

The three spin operators (Pauli-matrices) are $\sigma_x, \sigma_y, \sigma_z$:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The up and down state-vectors are $|u\rangle$ and $|d\rangle$, written as state-vectors:

$$|u\rangle \coloneqq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |d\rangle \coloneqq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The in and out state-vectors are $|i\rangle$ and $|o\rangle$. They are linear superpositions of $|u\rangle$ and $|d\rangle$:

$$|i\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle$$

Note: $|i\rangle$ is a vector, i the imaginary unit.

Written as state-vectors:

$$|i\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{i}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

The right and left state-vectors are $|r\rangle$ and $|l\rangle$. They are linear superpositions of $|u\rangle$ and $|d\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

$$|l\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

Written as state-vectors:

$$|r\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$$|l\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

We check the eigenvector/eigenvalue properties.

For $|u\rangle$ and $|d\rangle$:

$$\sigma_z|u\rangle = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\cdot 1 + 0\cdot 0\\0\cdot 1 - 1\cdot 0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}$$

$|u\rangle$ is eigenvector to σ_z with eigenvalue 1.

$$\sigma_z|d\rangle = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\cdot 0 + 0\cdot 1\\0\cdot 0 - 1\cdot 1\end{pmatrix} = \begin{pmatrix}0\\-1\end{pmatrix} = -\begin{pmatrix}0\\1\end{pmatrix}$$

$|d\rangle$ is eigenvector to σ_z with eigenvalue -1.

For $|i\rangle$ and $|o\rangle$:

$$\sigma_y|i\rangle = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 - i\cdot i\\i\cdot(-1) + 0\cdot i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}$$

$|i\rangle$ is eigenvector to σ_y with eigenvalue 1.

$$\sigma_y|o\rangle = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 - i\cdot(-i)\\i\cdot 1 - 0\cdot i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\i\end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$$

$|o\rangle$ is eigenvector to σ_y with eigenvalue -1.

For $|r\rangle$ and $|l\rangle$:

$$\sigma_x|r\rangle = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 + 1\cdot 1\\1\cdot 1 + 0\cdot 1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$|r\rangle$ is eigenvector to σ_x with eigenvalue 1.

$$\sigma_x|l\rangle = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 + 1\cdot(-1)\\1\cdot 1 - 0\cdot 1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

$|l\rangle$ is eigenvector to σ_x with eigenvalue -1.

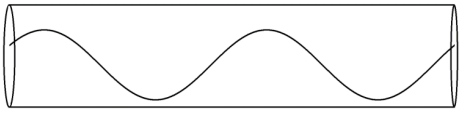
Einstein, Albert:

Einstein realized, in accepting quantum mechanics we are radically leaving the classical view. It seems that in quantum mechanics, we can know everything about some composite systems – everything there is to know – and still know nothing about their constituent parts. This weirdness of entanglement disturbed him, together with the “spooky action at a distance” that he claimed was implied by quantum mechanics.

Electric current:

In the context of harmonic oscillator, the electric current in a circuit of low resistance often oscillates with a characteristic frequency. The mathematics of these circuits is identical to the mathematics of masses attached to springs.

Electromagnetic radiation in cavity:



Consider the example of electromagnetic radiation in a cavity, a region of space bracketed by a pair of perfectly reflecting mirrors that keep the radiation bouncing endlessly back and forth.

There is only one important number associated with a harmonic oscillator, its frequency and the corresponding wavelength:

$$\omega = \frac{2\pi c}{\lambda}$$

In classical physics, the frequency is just the frequency.

In quantum mechanics, the frequency determines the quantum energy of the oscillator. The energy contained in waves of length λ has to be:

$$\left(n + \frac{1}{2}\right)\hbar\omega$$

The term $\frac{1}{2}\hbar\omega$ is the zero-point energy which we ignore here. Then the energy of waves of length λ becomes:

$$\frac{2\pi\hbar c}{\lambda} \cdot n$$

The energy of an electromagnetic wave is quantized in indivisible units of $\frac{2\pi\hbar c}{\lambda}$. These units are called photons, the quantized unit of energy in a quantum harmonic oscillator.

Electromagnetic waves:

Just like any other wave, a light wave or a radio wave oscillates when it passes you. The same mathematics that describes the oscillation particle also applies to electromagnetic waves.

Electrons:

1.

Electrons are frequently used as objects of study. Our sensory organs are simply not built to perceive the motion of an electron. The best we can do is to try to understand electrons and their motion as mathematical abstractions.

2.

Atoms are collections of nucleons and electrons, each of which could be considered a quantum system in its own right.

3.

Large masses and smooth potentials characterize the classical limit. A particle with low mass, moving through an abrupt potential, behaves like a quantum mechanical system. This holds for electrons too. They behave classically e.g. if you place it between two capacitor plates separated by a centimeter. In the smooth electric field between them, the electron crosses the gap like a coherent, almost classical particle. On the other hand, the potential associated with the nucleus of an atom always has a sharp feature in it. If an electron wave packet hits this potential, it will scatter.

Electrons, spin of electrons:

1.

Electrons have an extra degree of freedom called its spin.

2.

When a classical spin (a charged rotor) is put into a magnetic field, it has an energy that depends on its orientation. The energy is proportional to the dot product of the spin and the magnetic field.

3.

Some atoms have spins that are described in the same way as electron spins. When two of these atoms are close to each other, the Hamiltonian will depend on the spins.

Electrons, wave packets and electrons:

Electrons behave classically e.g. if you place it between two capacitor plates separated by a centimeter. In the smooth electric field between them, the electron crosses the gap like a classical particle. On the other hand, the potential associated with the nucleus of an atom always has a sharp feature in it. If an electron wave packet hits this potential, it will scatter.

Energy:

Composite operator and energy:

Let there be an observable that can be thought of as the dot product of the vector operators of Alice and Bob, $\vec{\sigma}$ and $\vec{\tau}$:

$$\vec{\sigma} \cdot \vec{\tau} = \sigma_x \tau_x + \sigma_y \tau_y + \sigma_z \tau_z$$

The observable $\vec{\sigma} \cdot \vec{\tau}$ could not be measured because Alice and Bob only can measure one component at a time. To measure $\vec{\sigma} \cdot \vec{\tau}$ a new apparatus must be built that measures $\vec{\sigma} \cdot \vec{\tau}$ without measuring the components.

Some atoms have spins that are described in the same way as electron spins. When two of these atoms are close to each other – for example, two neighboring atoms in a crystal lattice – the Hamiltonian will depend on the spins. In some situations, the neighboring spins' Hamiltonian is proportional to $\vec{\sigma} \cdot \vec{\tau}$. If that happens to be the case, then measuring $\vec{\sigma} \cdot \vec{\tau}$ is equivalent to measuring the energy of the atomic pair. Measuring this energy is a single measurement of the composite operator and does not entail measuring the individual components of either spin.

Conservation of energy:

The commutator of two operators A, B is defined as:

$$[A, B] = AB - BA$$

Two operators commute if the commutator is 0:

$$[A, B] = AB - BA = 0$$

Every operator commutes with itself:

$$[A, A] = AA - AA = 0$$

If an operator Q commutes with the Hamiltonian H, the expectation values of all functions of Q are conserved:

$$[Q,H] = QH - HQ = 0$$

As the Hamiltonian is the energy of the system, we see that the energy is conserved:

$$[H,H] = HH - HH = 0$$

Creation and annihilation operators and energy:

Note: annihilation operator and lowering operator are used synonym as well as raising operator and creating operator.

We begin with the Hamiltonian expressed in terms of the position operator X and the momentum operator P:

$$H = \frac{P^2 + \omega^2 X^2}{2}$$

With complex numbers we can rewrite the sum of squares:

$$a^2 + b^2 = (a - ib)(a + ib)$$

Applied to the right side of the Hamiltonian equation:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(PP - i\omega PX + i\omega XP + \omega^2 XX) =$$

$$\frac{1}{2}\big(P^2 + \omega^2 X^2 + i\omega(XP - PX)\big) =$$

$$\frac{P^2 + \omega^2 X^2}{2} + \frac{1}{2}\big(i\omega(XP - PX)\big)$$

We know the value of the commutator $[X,P] = XP - PX$, it has the value $i\hbar$.

We write:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{P^2 + \omega^2 X^2}{2} + \frac{1}{2}(i\omega i\hbar) =$$

$$\frac{P^2 + \omega^2 X^2}{2} - \frac{\omega\hbar}{2}$$

The term $\frac{1}{2}(P + i\omega X)(P - i\omega X)$ is smaller than the term $\frac{P^2+\omega^2X^2}{2}$ by $-\frac{\omega\hbar}{2}$.

If we want to substitute $\frac{P^2+\omega^2X^2}{2}$ by $\frac{1}{2}(P + i\omega X)(P - i\omega X)$ we must add the correction factor $\frac{\omega\hbar}{2}$ and get the new Hamiltonian:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{\omega\hbar}{2}$$

The two factors $(P + i\omega X)$ and $(P - i\omega X)$ are called raising and lowering operator.

The official definitions are:

$$a^{+} = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

$$a^{-} = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

The annihilation operator applied to the ground state wave-function annihilates it:

$$a^{-}\big(\psi_0(x)\big) = 0$$

This leads to a differential equation:

$$\left(\hbar\frac{d}{dx} + \omega x\right)\psi_0(x) = 0$$

Solution is the ground state:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

The lowering operator acting on a valid energy level of the spectrum of harmonic oscillator energy is stepping down to the next lower level. Analog the raising operator is stepping upwards.

Frequency and energy:

Prerequisite

If we know the Hamiltonian, the time-dependent Schrödinger equation tells us how the state-vector of an undisturbed system changes with time:

$$\hbar\frac{\partial|\psi\rangle}{\partial t} = -iH|\psi\rangle \text{ or } i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

The time-independent Schrödinger equation, written with the Hamiltonian in ket-style:

$$H|E_j\rangle = E_j|E_j\rangle$$

The Hamiltonian operator H acting on an energy eigenvector $|E_j\rangle$ delivers the eigenvalue of this eigenvector E_j.

End prerequisite

Suppose we found all energy eigenvalues E_j and the corresponding eigenvectors $|E_j\rangle$. We use that information to solve the time-dependent Schrödinger equation by the fact that eigenvectors form an orthonormal basis. We expand the state-vector $|\psi\rangle$ in that basis:

$$|\psi(t)\rangle = \sum_j \alpha_j|E_j\rangle$$

Since the state-vector $|\psi\rangle$ changes with time and the basis vectors $|E_j\rangle$ do not, it follows that the coefficients α_j must depend on time:

$$\frac{\partial}{\partial t}|\psi(t)\rangle = \sum_j \dot{\alpha_j}(t)|E_j\rangle$$

We feed this back into the time-dependent Schrödinger equation $\hbar \frac{\partial|\psi\rangle}{\partial t} = -iH|\psi\rangle$ and get:

$$\hbar \sum_j \dot{\alpha}_j(t)|E_j\rangle = -iH|\psi\rangle$$

$$\sum_j \dot{\alpha}_j(t)|E_j\rangle = -\frac{i}{\hbar}H|\psi\rangle$$

$$\sum_j \dot{\alpha}_j(t)|E_j\rangle = -\frac{i}{\hbar}H\sum_j \alpha_j(t)|E_j\rangle$$

With $H|E_j\rangle = E_j|E_j\rangle$ we build the final result:

$$\sum_j \dot{\alpha}_j(t)|E_j\rangle = -\frac{i}{\hbar}\sum_j E_j\alpha_j(t)|E_j\rangle$$

We rearrange this:

$$\sum_j \dot{\alpha}_j(t)|E_j\rangle + \frac{i}{\hbar}\sum_j E_j\alpha_j(t)|E_j\rangle = 0$$

$$\sum_j \left(\dot{\alpha}_j(t) + \frac{i}{\hbar}E_j\alpha_j(t)\right)|E_j\rangle = 0$$

As the $|E_j\rangle$ are basis vectors, every coefficient must be zero. For each eigenvalue E_j we have the differential equation:

$$\dot{\alpha}_j(t) = -\frac{i}{\hbar}E_j\alpha_j(t)$$

The solution is:

$$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$$

The real part (the result of any measurement must be real) is oscillating with $\cos(-\frac{E_j}{\hbar}t)$. Frequency and energy are connected throughout quantum mechanics.

Harmonic oscillator and energy:

Prerequisite

The classical oscillator with kinetic energy $\frac{1}{2}m\dot{x}^2$ and potential energy $\frac{1}{2}kx^2$.

The Lagrangian:

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2$$

The equations of motion for a one-dimensional system:

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

Note: $\frac{\partial L}{\partial \dot{x}}$ is the canonical momentum conjugate p to x.

Right side:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{d}{dt}\dot{x} = \ddot{x}$$

Left side:

$$\frac{\partial L}{\partial x} = -\omega^2 x$$

We get:

$$\ddot{x} = -\omega^2 x$$

End prerequisite

We need the Hamiltonian to find the possible energies of the one-dimensional harmonic oscillator.

The state of a particle moving on a line is represented by a wave function $\psi(x)$.

$\psi^*(x)\psi(x)$ is the probability density $P(x)$ to find a particle at position x:

$$\psi^*(x)\psi(x) = P(x)$$

The canonical momentum conjugate to x (classical):

$$p = \frac{\partial L}{\partial \dot{x}} = \dot{x}$$

The Hamiltonian for the harmonic oscillator is

$$H = p\dot{x} - \mathcal{L}$$

The Lagrangian is kinetic energy minus potential energy.

The Hamiltonian is kinetic energy plus potential energy – the total energy:

$$H = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega^2 x^2$$

There is no velocity operator in quantum mechanics, only position x and momentum p. We take the classical momentum:

$$p = \frac{\partial L}{\partial \dot{x}} = \dot{x}$$

and rewrite the Hamiltonian:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

We interpret x and p as operators, defined by their action on $\psi(x)$. The operator X multiplies the wave function by the position variable:

$$X|\psi(x)\rangle \to x\psi(x)$$

The operator P derives:

$$P|\psi(x)\rangle \to -i\hbar\frac{d}{dx}\psi(x)$$

We replace p and x in the classical Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$ and get the quantum Hamiltonian:

Both operators act twice. For the momentum operator we get:

$$(P|\psi(x)\rangle)^2 \to -i\hbar\frac{d}{dx}\left(-i\hbar\frac{d}{dx}\psi(x)\right) = -\hbar^2\frac{d^2}{dx^2}\psi(x)$$

Our quantum Hamiltonian:

$$H|\psi(x)\rangle = -\frac{\hbar^2}{2}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}\omega^2 x^2\psi(x)$$

The Hamiltonian is the energy of the system, the energy of the quantum mechanics harmonic oscillator:

$$-\frac{\hbar^2}{2}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}\omega^2 x^2\psi(x) = E\psi(x)$$

Note: instead of $\frac{d}{dx}$ we should better write $\frac{\partial}{\partial x}$ because ψ depends on time. The partial derivative would indicate that we are describing the system at a fixed time.

Energy of particle with negative momentum:

In general, the energy of a particle with negative momentum is negative, and the energy of a particle with positive momentum is positive. The problem of negative energy for particles with positive momentum was solved by Dirac, who used it to establish the theoretical basis for antiparticles.

Energy of photon:

$$E(\lambda) = \frac{2\pi\hbar c}{\lambda}$$

The shorter the wavelength of a photon, the higher its energy.

Energy eigenvalues and Energy eigenvectors:

1.

Matrix representation

The Hamiltonian H represents energy:

$$H|E_j\rangle = E_j|E_j\rangle$$

This is called the time independent Schrödinger equation and works in a specific matrix basis.

Note: E_j is a number, the energy eigenvalue. $|E_j\rangle$ is the corresponding energy eigenvector.

2.

Wave function

$$H|\psi_E\rangle = E|\psi_E\rangle$$

Again, this is the time independent Schrödinger equation.

The classical Hamiltonian:

$$H = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega^2 x^2$$

In quantum mechanics we do not have a velocity operator. With the Lagrangian $\mathcal{L}$ we can translate velocity in momentum:

$$p = \frac{\partial \mathcal{L}}{\partial \dot{x}} = \dot{x}$$

We rewrite the Hamiltonian:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

Again, this is a classical Hamiltonian. We turn it into a quantum mechanical equation by reinterpreting x and p as operators acting on $\psi(x)$.

The position operator X multiplies the wave function by x:

$$X|\psi_E(x)\rangle \to x\psi_E(x)$$

The momentum operator is the derivative:

$$P|\psi_E(x)\rangle \to -i\hbar\frac{\partial}{\partial x}\psi_E(x)$$

Both operators operate twice. For the momentum operator we get:

$$(P|\psi_E(x))^2 \to -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\psi_E(x)\right) = -\hbar^2\frac{\partial^2}{\partial x^2}\psi_E(x)$$

Our quantum Hamiltonian:

$$H|\psi_E\rangle = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi_E(x) + \frac{1}{2}\omega^2 x^2\psi_E(x) = E\psi_E(x)$$

A solution to this are the energy eigenfunctions:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

$$\psi_1(x) = \sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} = \sqrt{\frac{2\omega}{\hbar}}x\psi_0(x)$$

$$\psi_2(x) = \left(-1 + \frac{2\omega}{\hbar}x^2\right)e^{-\frac{\omega}{2\hbar}x^2} = \left(-1 + \frac{2\omega}{\hbar}x^2\right)\psi_0(x)$$

…

with the according eigenvalues 1, $\sqrt{\frac{2\omega}{\hbar}}x$, $\left(-1 + \frac{2\omega}{\hbar}x^2\right)$, …

Energy levels, eigenfunctions for energy levels:

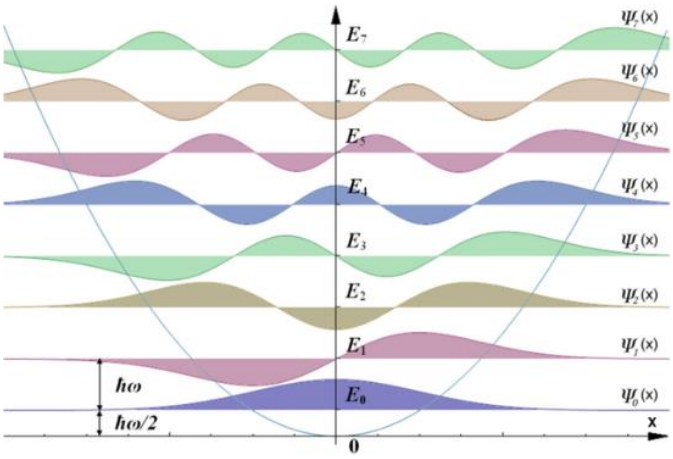
The energy eigenfunctions of a harmonic oscillator in ascending order:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

$$\psi_1(x) = \sqrt{\frac{2\omega}{\hbar}}xe^{-\frac{\omega}{2\hbar}x^2} = \sqrt{\frac{2\omega}{\hbar}}x\psi_0(x)$$

$$\psi_2(x) = \left(-1+\frac{2\omega}{\hbar}x^2\right)e^{-\frac{\omega}{2\hbar}x^2} = \left(-1+\frac{2\omega}{\hbar}x^2\right)\psi_0(x)$$

...



Picture courtesy AllenMcC. CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=11623546

Energy levels, harmonic oscillators and energy levels:

The quantum Hamiltonian for the harmonic oscillator (time-independent Schrödinger equation):

$$H|\psi_E\rangle = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi_E(x) + \frac{1}{2}\omega^2x^2\psi_E(x) = E\psi_E(x)$$

To solve this equation, we must find the allowable values of E that permit a mathematical solution, filter out the solutions that make physically sense and find the eigenvectors and eigenvalues for the energy.

Physical solutions of the Schrödinger equation must be normalizable.

The solution for the ground state energy eigenfunction is:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

Applying the Hamiltonian to this eigenfunction delivers the eigenvalue:

$$H|\psi_0(x)\rangle = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi_0(x) + \frac{1}{2}\omega^2x^2\psi_0(x) =$$

$$-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}e^{-\frac{\omega}{2\hbar}x^2} + \frac{1}{2}\omega^2x^2e^{-\frac{\omega}{2\hbar}x^2} =;$$

Left part of the sum (without the multiplying factor $-\frac{\hbar^2}{2}$):

$$\frac{\partial}{\partial x} e^{-\frac{\omega}{2\hbar}x^2} = -\frac{\omega}{\hbar} x e^{-\frac{\omega}{2\hbar}x^2}$$

$$\frac{\partial}{\partial x}\left(-\frac{\omega}{\hbar} x e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$-\frac{\omega}{\hbar} e^{-\frac{\omega}{2\hbar}x^2} + \left(-\frac{\omega}{\hbar} x\right)\left(-\frac{\omega}{\hbar} x\right) e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-\frac{\omega}{\hbar} e^{-\frac{\omega}{2\hbar}x^2} + \left(-\frac{\omega}{\hbar} x\right)^2 e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\left(\frac{\omega^2}{\hbar^2} x^2 - \frac{\omega}{\hbar}\right) e^{-\frac{\omega}{2\hbar}x^2}$$

multiplying the factor $-\frac{\hbar^2}{2}$:

$$-\frac{\hbar^2}{2}\left(\frac{\omega^2}{\hbar^2} x^2 - \frac{\omega}{\hbar}\right) e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\left(-\frac{\omega^2}{2} x^2 + \frac{\omega\hbar}{2}\right) e^{-\frac{\omega}{2\hbar}x^2}$$

Right part:

$$\frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2}$$

Merging:

$$\left(-\frac{\omega^2}{2} x^2 + \frac{\omega\hbar}{2}\right) e^{-\frac{\omega}{2\hbar}x^2} + \frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\left(-\frac{\omega^2}{2} x^2 + \frac{\omega\hbar}{2} + \frac{1}{2}\omega^2 x^2\right) e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\frac{\omega\hbar}{2} e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\frac{\omega\hbar}{2}\psi_0(x)$$

$\psi_0(x)$ is eigenfunction to the Hamiltonian operator with eigenvalue $\frac{\omega\hbar}{2}$.

We can rewrite the Hamiltonian in terms of the position operator X and the momentum operator P:

$$H = \frac{P^2 + \omega^2 X^2}{2}$$

We write the sum as complex product:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{\omega\hbar}{2}$$

Note: $\frac{\omega\hbar}{2}$ is needed because the product $\frac{1}{2}(P + i\omega X)(P - i\omega X)$ does not exactly give $\frac{P^2+\omega^2X^2}{2}$

The two factors $(P + i\omega X)$ and $(P - i\omega X)$ are the raising operator a^+ and lowering operator a^-. The official definitions are:

$$a^+ = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

The lowering operator applied to the ground state wave-function annihilates it:

$$a^-\big(\psi_0(x)\big) = 0$$

The lowering operator applied to any other state produces an eigenvector whose eigenvalue is one unit lower. Analog the raising operator applied to any state produces an eigenvector whose eigenvalue is on unit higher.

Entangled states:

Prerequisite

Suppose Alice prepares her spin in state:

$$\alpha_u|u\rangle + \alpha_d|d\rangle$$

Bob prepares his spin in state:

$$\beta_u|u\rangle + \beta_d|d\rangle$$

As they are separate, each state is normalized:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

$$\beta_u^*\beta_u + \beta_d^*\beta_d = 1$$

The product state is combined with the tensor product:

$$\{\alpha_u|u\rangle + \alpha_d|d\rangle\}\otimes\{\beta_u|u\rangle + \beta_d|d\rangle\}$$

In composite notation:

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

As there are two normalizing conditions and two overall phase factors, out of the eight factors α_u etc. remaining 4 independent parameters – two for every spin system.

End prerequisite

The most general vector in the composite space of states:

$$\psi_{uu}|uu\rangle + \psi_{ud}|ud\rangle + \psi_{du}|du\rangle + \psi_{dd}|dd\rangle$$

In contrast to the product state we have only one normalizing condition:

$$\psi_{uu}^*\psi_{uu} + \psi_{ud}^*\psi_{ud} + \psi_{du}^*\psi_{du} + \psi_{dd}^*\psi_{dd} = 1$$

and there is only one overall or global phase to ignore.

Note: global phase means that a state $|A\rangle$ is equivalent to the state $e^{i\theta}|A\rangle$.

With this we can conclude that out of the eight factors ψ_{uu} etc. there remain six independent parameter.

Obviously, the composite state is richer than the product state – it is an entangled state.

Entanglement:

In classical physics knowing all about a combined state means knowing all about its components.

In quantum mechanics knowing all about an entangled systems not necessarily means knowing all about its components.

Entanglement, Bells Theorem and entanglement:

The non-locality in quantum mechanics only relates to the specific spin-information of two entangled spins. A measurement of Alice's spin cannot be used to instantly transmit any other information to Bob at great distances, and even Bob will not be able to tell independently whether or not Alice has measured her spin. So, there is no information travelling faster than the speed of light.

Entanglement, classical entanglement:

If we perform a number of separate measurements σ_a and σ_b in classical physics (always the same measurement σ_a and σ_b) we can calculate the average of the respective results, $\langle\sigma_a\rangle$ and $\langle\sigma_b\rangle$.

If the measurements are independent, then $\langle\sigma_a\rangle\langle\sigma_b\rangle = \langle\sigma_a\sigma_b\rangle$, the product of the averages of single measurements will be equal to the average of the product of both measurements.

If this is not the case: $\langle\sigma_a\rangle\langle\sigma_b\rangle \neq \langle\sigma_a\sigma_b\rangle$, then there is a correlation between the two measurements, they are not independent – a kind of classical entanglement. In classical physics this leads to an investigation to find the cause of the correlation, to search for the missing information.

Entanglement, combining quantum systems:

We use two single spin system of Alice and Bob. The basis vectors in the system of Alice are $|u\rangle$ and $|d\rangle$, the basic vectors in the system of Bob are $|u\}$ and $|d\}$.

If we combine the two systems to one, we write $|ab\rangle$ to label a single basis vector of the combined system, in our case: $|uu\rangle$, $|ud\rangle$, $|du\rangle$ and $|dd\rangle$. The corresponding bra to $|ab\rangle$ is $\langle a'b'|$.

Example: consider a linear operator M acting on the space of states of the composite system of Alice and Bob. It can be represented as a matrix. The elements of the matrix can be extracted by sandwiching the operator between the basis vectors:

$$\langle a'b'|M|ab\rangle = M_{a'b',ab}$$

Basis vectors usually are orthonormal, this means that the inner product $\langle a'b'|ab\rangle$ gives the Kronecker delta:

$$\langle a'b'|ab\rangle = \delta_{aa'}\delta_{bb'}$$

With the basis vectors we can write any state vector in the composite system as:

$$|\psi\rangle = \sum_{a,b} \psi(a,b)|ab\rangle$$

For a product state of Alice and Bob this gives:

$$|\psi\rangle = \psi(u,u)|uu\rangle + \psi(u,d)|ud\rangle + \psi(d,u)|du\rangle + \psi(d,d)|dd\rangle$$

In summa:

The basis vectors in the two-dimensional system of Alice are $|u\rangle$ and $|d\rangle$, the basic vectors in the two-dimensional system of Bob are $|u\}$ and $|d\}$. If we combine the two systems to one, we get a four-dimensional combined system with basis vectors $|uu\rangle$, $|ud\rangle$, $|du\rangle$ and $|dd\rangle$.

$|uu\rangle$ is one four-dimensional basis vector. The labelling $|uu\rangle$ etc. is chosen to indicate the origin: $|uu\rangle$ is composed out of $|u\rangle$ Alice and $|u\}$ Bob.

Entanglement, composite observables:

We have a two-spin system in an entangled state, the state $|sing\rangle \coloneqq \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$. Alice (σ) and Bob (τ) simultaneously can measure their own observable if the operators commute. In fact, every component of σ commutes with every component of τ.

Check:

We combine operators. $\sigma_z \coloneqq \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, $\tau_x \coloneqq \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$:

$$\sigma_z \otimes \tau_x = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\\ 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & -1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix} \coloneqq A$$

$$\tau_x \otimes \sigma_z = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} & 1\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\\ 1\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} & 0\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{pmatrix} \coloneqq B$$

The commutation relation: $[A, B] = AB - BA$

$$AB = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix}\begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{pmatrix} = \begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\end{pmatrix}$$

$$BA = \begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{pmatrix}\begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix} = \begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\end{pmatrix}$$

$AB = BA$, the operators commute, $[A, B] = 0$.

We try this explicit.

The basis vectors for the states $|uu\rangle$, $|ud\rangle$, $|du\rangle$ and $|dd\rangle$ are $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}$, $\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$, $\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$.

The state$|sing\rangle \coloneqq \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$:

$$|sing\rangle \coloneqq \frac{1}{\sqrt{2}}\left(\begin{pmatrix}0\\1\\0\\0\end{pmatrix} - \begin{pmatrix}0\\0\\1\\0\end{pmatrix}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}$$

We apply operator A to the state $|sing\rangle$:

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Then we apply operator B to the result:

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}$$

We see that $|sing\rangle$ is eigenvector to the observable $\sigma_z\tau_x$ or $\tau_x\sigma_z$ with eigenvalue -1.

Alice and Bob can measure any component of their spin and get opposite results because $|sing\rangle$ is eigenvector to both with eigenvalue -1.

This has no classical analog.

What Alice and Bob are not able to do is: measure the dot-product $\vec{\sigma} \cdot \vec{\tau} \coloneqq \sigma_x\tau_x + \sigma_y\tau_y + \sigma_z\tau_z$. They are not able to measure simultaneously even two components of the sum, because they (the operators for this) do not commute.

Entanglement, correlation test for entanglement:

The correlation between two observables A and B is defined in terms of average values:

$$C(A,B) = \langle AB\rangle - \langle A\rangle\langle B\rangle$$

The expectation value of the product minus the product of the expectation values. If $C(A,B) \neq 0$ then A and B are correlated and the state is entangled.

Correlation lie in the range $-1, +1$. The greater the magnitude of $C(A,B)$, the more entangled. If $C(A,B) = 0$, there is no correlation and no entanglement.

Entanglement, density matrices and entanglement:

The state of a composite system can be absolutely pure (~single state), but each of its constituents must be described by a mixed state.

We take a system composed of two part, A and B. We suppose that Alice has complete knowledge of the state of the combined system, she knows the wave function $\psi(a,b)$. Alice is interested only in system A and wants to have complete knowledge about system A. She selects an observable L that belongs to A and does nothing to B when it acts. The rule for calculating the expectation value of L:

$$\langle L\rangle = \sum_{ab,a'b'} \psi^*(a'b')L_{a'b',ab}\psi(ab)$$

The observable L was chosen to act on A only and let B unchanged, so it acts trivially on the b-index (it leaves b unchanged, so $b' = b$ and the sum over the b separable):

$$\langle L\rangle = \sum_{a,b,a'} \psi^*(a'b)L_{a',a}\psi(ab) = \sum_{a,a'} L_{a',a} \sum_{b} \psi^*(a'b)\psi(ab)$$

The sum

$$\sum_b \psi^*(a'b)\psi(ab) = \rho_{a,a'}$$

gives the density matrix in the combined system.

With this we can write:

$$\langle L \rangle = \sum_{a,a'} L_{a',a}\, \rho_{a,a'}$$

the expectation value of a mixed state.

Note: in $\sum_b \psi^*(a'b)\psi(ab) = \rho_{a,a'}$ in the right-hand index of $\rho_{a,a'}$ the index a' belongs to the complex conjugate vector $\psi^*(a'b)$. This is a consequence of our convention $L_{aa'} = \langle a|L|a' \rangle$ for labeling the matrix elements of an operator L.

Applying this convention to

$$\rho = |\psi\rangle\langle\psi|$$

results in:

$$\rho_{a,a'} = \langle a|\psi\rangle\langle\psi|a'\rangle = \psi(a)\psi^*(a')$$

A concrete example for this.

Let L be an observable of Alice's system. L can be represented as a matrix:

$$L_{a'b',ab} = \langle a'b'|L|ab\rangle$$

L shall be an Alice-observable meaning it does nothing to Bob's subsystem, so any elements of L that could have an effect to Bob's system must be filtered out by setting it to zero. This L gets the special form:

$$L_{a'b',ab} = L_{a'a} \otimes \delta_{b'b}$$

The expectation value of $\langle L \rangle = \langle\psi|L|\psi\rangle = \sum_{a,b,a',b'} \psi^*(a',b')L_{a'b',ab}\psi(a,b)$

Because of $b' = b$:

$$\langle L \rangle = \langle\psi|L|\psi\rangle = \sum_{a',b,a} \psi^*(a',b)L_{a',a}\psi(a,b) = \sum_{a',b,a} \psi^*(a,b)\psi(a',b)L_{a,a'} =$$

$$\sum_{a',a}\sum_b \psi^*(a,b)\psi(a',b)\, L_{a,a'}$$

The quantity

$$\sum_b \psi^*(a,b)\psi(a',b) \coloneqq \rho_{a'a}$$

is the density matrix of Alice.

We get the expectation value of L (the 2×2 version):

$$\langle L \rangle = \sum_{a'a} \rho_{a',a} L_{a,a'}$$

Consider the state-vector $|\psi\rangle = 0|uu\rangle + \frac{1}{\sqrt{2}}|ud\rangle + \frac{1}{\sqrt{2}}|du\rangle + 0|dd\rangle$.

The values of $\psi(a,b)$ are:

$$\psi(u,u) = 0, \psi(u,d) = \frac{1}{\sqrt{2}}, \psi(d,u) = \frac{1}{\sqrt{2}}, \psi(d,d) = 0$$

Next, we expand the factors in the density matrix $\rho_{a',a} = \sum_b \psi^*(a,b)\psi(a',b)$. Remember that we are summing over the second index b, the first index a being unchanged:

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = 0 \cdot 0 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} = \frac{1}{2}$$

$$\rho_{ud} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = 0$$

$$\rho_{du} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = 0$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = \frac{1}{2}$$

These values are elements of a 2×2 matrix:

$$\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

The trace of this density matrix is 1 as it should be for density matrices.

Entanglement, density matrix test for entanglement:

Prerequisite

Suppose the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$. Then the composite wave function also is product of Bob's factor and Alice's factor:

$$\psi(a,b) = \vartheta(a)\theta(b)$$

Alice's density matrix:

$$\rho_{a',a} = \vartheta^*(a)\vartheta(a') \sum_b \theta^*(b)\theta(,b)$$

As the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$, both Alice's and Bob's state separately are normalized, so:

$$\sum_b \theta^*(b)\theta(,b) = 1$$

And Alice's density matrix becomes $\rho_{a',a} = \vartheta^*(a)\vartheta(a')$.

End prerequisite

We prove a theorem about the eigenvalues of Alice's density matrix that is only true for product states but not for entangled states and thus can serve to identify them: for product states the density matrix of Alice or Bob has exactly one eigenvalue of value one.

The eigenvalue equation for Alice's matrix $\rho_{a'a}$:

$$\sum_a \rho_{a'a}\alpha_a = \lambda\alpha_a =$$

$$\sum_a \vartheta^*(a)\vartheta(a')\alpha_a = \vartheta(a')\sum_a \vartheta^*(a)\alpha_a$$

$\sum_a \vartheta^*(a)\alpha_a$ has the form of an inner product. If the column vector α is orthogonal to ϑ, then $\sum_a \vartheta^*(a)\alpha_a$ is zero giving an eigenvector with eigenvalue zero.

In a space state of dimension N we have $N-1$ vectors orthogonal to ϑ, so we have only one possible direction for an eigenvector with nonzero eigenvalue $\vartheta(a)$:

$$\vartheta^*(a)\alpha_a = 0 \text{ for all } \alpha_a \neq \vartheta(a) \text{ and } 1 \text{ for } \alpha_a = \vartheta(a).$$

Alice's system is in a pure state, all of her observations are described as if Bob never existed.

In a maximally entangled system on the other hand Alice's density matrix is proportional to the unit matrix with all equal eigenvalues $\frac{1}{N}$:

$$\rho_{a'a} = \frac{1}{N}\delta_{a'a}$$

As the density matrix gives the probability for an outcome this means that every outcome has equal possibility.

For partial entanglement the weights of $\rho_{a'a}$ move from the equal distribution towards a concentration on a single value 1 on the diagonal of the density matrix.

Although in a maximum entangled state Alice can't predict the outcome of her experiments, she knows (after the experiment has been done) exactly about the relation between her and Bob's outcomes.

Entanglement, locality and entanglement:

The quantum field theorist's point of view: locality means that it is impossible to send a signal (information) faster than the speed of light. Quantum mechanics enforces this rule.

We begin with the definition of Alice's system and Bob's system in an expanded meaning. The system of Alice consists of herself, the apparatus she is using, the experimental surrounding etc. The same holds for Bob and his system.

To easy distinguish between both systems we write the basis kets of Alice $|a\rangle$, the basis kets of Bob $|b\rangle$. $|a\rangle$ and $|b\rangle$ describe everything that Alice and Bob can interact with.

The tensor product states $|ab\rangle$ describe the combination of Alice's and Bob's world.

The Alice-Bob wave function is:

$$\psi(ab)$$

Alice's complete description of her system (apparatus, herself, …) is contained in her density matrix ρ:

$$\rho_{aa'} = \sum_b \psi^*(a'b)\psi(ab)$$

Note: the index is b, because in the product states both states are independent, in summing up over b we get all transitions aa'.

Consider this question: Can Bob do anything to instantly change Alice's density matrix?

All Bob can do are things that follow the laws of quantum mechanics. In particular, Bob's evolution must be unitary, it must be described by a unitary matrix:

$$U_{bb'}$$

The matrix U represents whatever happens to Bob's system. It acts on the wave function to produce a new wave function which we will call the "final" wave function:

$$\psi_{final}(ab) = \sum_{b'} U_{bb'}\psi(ab')$$

and the complex conjugate of it:

$$\psi^*{}_{final}(a'b) = \sum_{b'} \psi^*(a'b){U^\dagger}_{b'b}$$

With this we calculate Alice's new density matrix, using the "final" wave function:

$$\rho_{aa'} = \sum_{b} \psi^*(a'b)\psi(ab) \rightarrow$$

$$\sum_{b,b'} \psi^*(a'b){U^\dagger}_{b'b}U_{bb'}\psi(ab')$$

The product of the two unitary matrices ${U^\dagger}_{b'b}U_{bb'}$ is the unit matrix $\delta_{b'b}$, meaning all indices collapsing to b:

$$\rho_{aa'} = \sum_{b} \psi^*(a'b)\psi(ab)$$

This is exactly the same density matrix. In other words, it is exactly the same it was before U (Bob) acted. Nothing that happens at Bob's end has any immediate effect on Alice's density matrix, even if Bob's and Alice's system are maximally entangled. There is no information transfer.

Note: we can write the complex conjugate with other indexing as

$$\psi^*{}_{final}(a'b) = \sum_{b''} \psi^*(a'b''){U^\dagger}_{b''b}$$

to indicate another sequence in the "b's".

This would lead to:

$$\rho_{aa'} = \sum_{b,b',b''} \psi^*(a'b''){U^\dagger}_{b''b}U_{bb'}\psi(ab')$$

In this case the product ${U^\dagger}_{b''b}U_{bb'}$ would become the unit matrix $\delta_{b''b'}$ and this amounts to a sum where $b'' = b'$. All b, b' and b'' build the same set of basis vectors, this collapses to the simple sum over b.

Entanglement of near singlet state:

The near-singlet state stands for partial entanglement with the state-vector:

$$\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$$

It has some information about the composite system and some about each subsystem – incomplete in each case.

Entanglement, observables and entanglement:

For a product space holds, that for any state of a single spin, there is some direction for which the spin is $+1$. This meets our expectations in a way that the spin must have exactly one direction, even if we do not know it.

This means that the expectation values of the components must sum up to 1:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$$

This classical expectation does not hold for entangled states, especially not for the entangled state $|sing\rangle$.

The entangled state $|sing\rangle$ is defined:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

The expectation value $\langle\sigma_z\rangle \coloneqq \langle sing|\sigma_z|sing\rangle$

$$\langle\sigma_z\rangle \coloneqq \langle sing|\sigma_z|sing\rangle =$$

$$\left\langle sing\middle|\sigma_z\middle|\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)\right\rangle =$$

$$\left\langle sing\middle|\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)\right\rangle =$$

$$\left(\frac{1}{\sqrt{2}}(\langle ud| - \langle du|)\right)\left(\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)\right) =$$

$$\frac{1}{2}(\langle ud|ud\rangle + \langle ud|du\rangle - \langle du|ud\rangle - \langle du|du\rangle) =$$

$$\frac{1}{2}(1 + 0 - 0 - 1) = 0$$

The same result we get for $\langle\sigma_y\rangle$ and $\langle\sigma_x\rangle$. Our sum of expectation values:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2$$

is shrinking to zero. In plain words – we can measure whatever direction we want we don't find the spin orientation.

If the expectation value of a component of σ is zero, this means that the experimental outcome is equally likely to be $+1$ or -1, the outcome is completely uncertain. Even though we know the exact state-vector $|sing\rangle$, we know nothing about the outcome of any measurement of any component of either spin.

Entanglement, process of measurement and entanglement:

In the process of measurement, the apparatus (for measuring etc.) combine with the objects to measure to a bigger system. For simplicity we chose a single spin system and an apparatus that has three states: $|b\}$ for the initial state, $|-1\}$ and $|+1\}$ as possible results of measurement. Our spin system has the states $|u\rangle$ up and $|d\rangle$ down.

By use of the tensor product we build a space of states that has six basis vectors $|u,b\rangle$, $|u,+1\rangle$, $|u,-1\rangle$, $|d,b\rangle$, $|d,+1\rangle$, $|d,-1\rangle$.

We assume the following sequences.

Apparatus starts in the blank state (as always) and the spin in the up-state. The final spin state shall be the up-state:

$$|u,b\rangle \rightarrow |u,+1\rangle.$$

Apparatus starts in the blank state (as always) and the spin in the $down$-state. The final spin state shall be the $down$-state:

$$|d,b\rangle \rightarrow |d,-1\rangle.$$

Looking at the apparatus after the measurements allows telling how the spin was oriented initially.

Let the initial spin more general $\alpha_u|u\rangle + \alpha_d|d\rangle$.

The initial state becomes:

$$\alpha_u|u,b\rangle + \alpha_d|d,b\rangle$$

a product state completely unentangled.

With this the system evolves to the final state:

$$\alpha_u|u,b\rangle + \alpha_d|d,b\rangle \rightarrow \alpha_u|u,+1\rangle + \alpha_d|d,-1\rangle$$

This final state is an entangled state and, if $\alpha_u = -\alpha_d$ a maximally entangled state. The entanglement evolves by unitary evolution of the state-vector.

By looking at the apparatus we can read the spin state – up or down.

We can even calculate the probability of the outcomes: $\alpha_u^*\alpha_u$ for up and $\alpha_d^*\alpha_d$ for $down$.

Entanglement of product state (classical state):

Given two states, $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$ and $|B\rangle = \beta_u|u\rangle + \beta_d|d\rangle$.

Each state is normalized: $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$ and $\beta_u^*\beta_u + \beta_d^*\beta_d = 1$

The product state describing the system is: $|product\ state\rangle = \{\alpha_u|u\rangle + \alpha_d|d\rangle\}\otimes\{\beta_u|u\rangle + \beta_d|d\rangle\}$.

Expanding and switching to composite notation gives:

$$|product\ state\rangle = \alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

This state vector of the combined system is automatically normalized too:

$$\alpha_u\beta_u + \alpha_u\beta_d + \alpha_d\beta_u + \alpha_d\beta_d = 1$$

The density matrix A as well as the density matrix B have exactly one nonzero eigenvalue 1, the eigenvector with this eigenvalue is the wave function of system A resp. B.

The wave function is factorized: $\psi(a)\psi(b)$.

The expectation values are: $\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$ and $\langle\tau_x\rangle^2 + \langle\tau_y\rangle^2 + \langle\tau_z\rangle^2 = 1$

The correlation between the two systems is zero: $\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = 0$

The main feature of a product state is that each subsystem behaves independently of the other.

Entanglement of singlet state (maximum entangled):

In case of a two-spin system the maximum entangled state, the singlet state can be written as:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

or in the extended form:

$$|sing\rangle = 0|uu\rangle + \frac{1}{\sqrt{2}}|ud\rangle - \frac{1}{\sqrt{2}}|du\rangle + 0|dd\rangle$$

We have only one normalization condition:

$$\psi^*_{uu}\psi_{uu} + \psi^*_{ud}\psi_{ud} + \psi^*_{du}\psi_{du} + \psi^*_{dd}\psi_{dd} = 1$$

in this case reducing to:

$$\psi^*_{ud}\psi_{ud} + \psi^*_{du}\psi_{du} = 1$$

The density matrix A as well as the density matrix B is a diagonal matrix with equal values that sum up to one, hence each outcome is equally likely.

The wave function is not factorized: $\psi(a,b)$.

The expectation values for each single system are zero:

$\langle\sigma_x\rangle^2 = \langle\sigma_y\rangle^2 = \langle\sigma_z\rangle^2 = 0$ and $\langle\tau_x\rangle^2 = \langle\tau_y\rangle^2 = \langle\tau_z\rangle^2 = 0$.

The expectation values for the combined system are 1:

$\langle\sigma_x\tau_x\rangle^2 = \langle\sigma_y\tau_y\rangle^2 = \langle\sigma_z\tau_z\rangle^2 = 1$ and $\langle\sigma_x\tau_x\rangle = \langle\sigma_y\tau_y\rangle = \langle\sigma_z\tau_z\rangle = -1$

The correlation between the two systems is -1:

$$\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = -1$$

The main feature of an entangled state is that the composite system as a whole is fully characterized but there is no information about the subsystems.

Entanglement, tests for entanglement:

Note:

> Entanglement is the quantum mechanical generalization of correlation. The mathematical indication:
>
> Suppose we have a probability distribution $P(a,b)$. If the variables are independent (in quantum mechanics: the two systems are completely uncorrelated), then:
>
> $$P(a,b) = P(a)P(b)$$
>
> The probability function $P(a,b)$ factorizes.

If the variables are not independent (in quantum mechanics: the two systems are partially or totally entangled), then:

$$P(a,b) \neq P(a)P(b)$$

The probability function $P(a,b)$ does not factorize.

End note

Suppose the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$. Then the composite wave function also is product of Bob's factor and Alice's factor:

$$\psi(a,b) = \vartheta(a)\theta(b)$$

Alice's density matrix:

$$\rho_{a'a} = \vartheta^*(a)\vartheta(a')\sum_b \theta^*(b)\theta(,b)$$

As the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$, both Alice's and Bob's state separately are normalized, so

$$\sum_b \theta^*(b)\theta(,b) = 1$$

and Alice's density matrix becomes $\rho_{a'a} = \vartheta^*(a)\vartheta(a')$.

We prove a theorem about the eigenvalues of Alice's density matrix that is only true for product states but not for entangled states and thus can serve to identify them: for product states the density matrix of Alice or Bob has exactly one eigenvalue of value one.

The eigenvalue equation for Alice's matrix $\rho_{a'a}$:

$$\sum_a \rho_{a'a}\alpha_a = \lambda\alpha_a =$$

$$\sum_a \vartheta^*(a)\vartheta(a')\alpha_a = \vartheta(a')\sum_a \vartheta^*(a)\alpha_a$$

$\sum_a \vartheta^*(a)\alpha_a$ has the form of an inner product. If the column vector α is orthogonal to ϑ, then $\sum_a \vartheta^*(a)\alpha_a$ is zero giving an eigenvector with eigenvalue zero.

In a space state of dimension N we have $N-1$ vectors orthogonal to ϑ, so we have only one possible direction for an eigenvector with nonzero eigenvalue $\vartheta(a)$:

$\vartheta^*(a)\alpha_a = 0$ for all $\alpha_a \neq \vartheta(a)$ and 1 for $\alpha_a = \vartheta(a)$.

Alice's system is in a pure state, all of her observations are described as if Bob never existed.

In a maximally entangled system on the other hand Alice's density matrix is proportional to the unit matrix with all equal eigenvalues $\frac{1}{N}$:

$$\rho_{a'a} = \frac{1}{N}\delta_{a'a}$$

As the density matrix gives the probability for an outcome this means that every outcome has equal possibility.

For partial entanglement the weights of $\rho_{a'a}$ move from the equal distribution towards a concentration on a single value 1 on the diagonal of the density matrix.

Entanglement for two spins:

Imagine two spins of Alice and Bob attached two to fixed particles in space. Alice and Bob each have their own apparatuses A and B they can use independently to prepare and measure spin components. We name the spins σ for Alice and τ for Bob:

$$\sigma_x, \sigma_y, \sigma_z \text{ and } \tau_x, \tau_y, \tau_z$$

In a basis in which the z components of both spins are specified, the basis vectors are:

$$|uu\rangle, |ud\rangle, |du\rangle, |dd\rangle$$

The first part of each label represents the state of σ, the second part the state of τ. $|uu\rangle$ represents the state in which both spins are up, $|ud\rangle$ the state with Alice's spin up, Bob's spin down etc.

Alice has only a single spin, her density matrix is:

$$\rho_{aa\prime} = \psi^*(a')\psi(a)$$

For the special form of $|\psi\rangle = \alpha|u\rangle + \beta|d\rangle$ we have:

$$\psi(u) = \alpha, \psi^*(u) = \alpha^*, \psi(d) = \beta, \psi^*(d) = \beta^*$$

The density matrix:

$$\rho_{aa\prime} = \begin{pmatrix} \alpha^*\alpha & \alpha^*\beta \\ \beta^*\alpha & \beta^*\beta \end{pmatrix}$$

Suppose we know the wave function of the composite system $\psi(a, b)$, but we are only interested in a (complete) knowledge of Alice's subsystem.

Let L be an observable of Alice's system. L can be represented as a matrix:

$$L_{a'b',ab} = \langle a'b'|L|ab\rangle$$

Note: for the composite system, ab is a single index labelling one basis vector.

L shall do nothing to Bob's system, L must have the form:

$$L_{a'b',ab} = L_{a\prime a}\delta_{b\prime b}$$

No transitions in Bob's system.

The left side is an element of a 4×4 matrix because ab and $a'b'$ represent each 4 distinct values uu, ud, du, dd.

The right side also must be an element of a 4×4 matrix, it is an element of the tensor product of two 2×2 matrices. One matrix is $L_{a\prime a}$, the other matrix is $\delta_{b\prime b}$, the 2×2 identity matrix.

The expectation value of L in the composite system:

$$\langle\psi|L|\psi\rangle = \sum_{a,b,a',b\prime} \psi^*(a', b')L_{a'b',ab}\psi(a, b)$$

With the restriction (L should do nothing on Bob's system) we can use the L above and get:

$$\langle\psi|L|\psi\rangle = \sum_{a,b,a',b\prime} \psi^*(a', b')L_{a'a}\delta_{b'b}\psi(a, b) =$$

$$\sum_{a,b,a'} \psi^*(a',b) L_{a'a} \psi(a,b)$$

We concentrate on the index b. If we are summing over b, the term $L_{a'a}$ plays no role and we get:

$$\sum_{b} \psi^*(a,b)\psi(a',b) = \rho_{aa'}$$

This is a 2×2 matrix, the density matrix of Alice. It does not depend on any b-index, it is purely a function of Alice's variables a and a'.

We plug the density matrix of Alice into the sum above and get:

$$\langle \psi|L|\psi\rangle = \langle L\rangle = \sum_{a,a'} L_{a'a}\rho_{aa'}$$

This is the sum over diagonal elements of a matrix, it is the trace Tr of the matrix $L\rho$, so we can write:

$$\langle L\rangle = Tr\ L\rho$$

Result: to calculate Alice's density matrix ρ, we may need the full wave function of the composite system, including the dependencies on Bob's variables. Once we know ρ, we can forget where it came from, and use it to calculate anything about Alice's observations.

Example

We can use ρ to calculate the probability $P(a)$ that Alice's system will be left in the state a if a measurement is made.

$P(a,b)$ is the probability that the combined system is in state $|ab\rangle$:

$$P(a,b) = \psi^*(a,b)\psi(a,b)$$

Summing over b we get the (total) probability for a:

$$P(a) = \sum_{b} \psi^*(a,b)\psi(a,b)$$

This is just one diagonal entry in the density matrix:

$$P(a) = \rho_{aa}$$

Euler-Lagrange equations:

In Lagrangian mechanics, according to Hamilton's principle of stationary action, the evolution of a physical system is described by the solutions to the Euler equation for the action of the system. In this context Euler equations are usually called Lagrange equations. In classical mechanics, it is equivalent to Newton's laws of motion, but it has the advantage that it takes the same form in any system of generalized coordinates, and it is better suited to generalizations.
(https://en.wikipedia.org/wiki/Euler%E2%80%93Lagrange_equation)

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0$$

Example:

The length S of a path, defined by $f(x)$:

$$S = \int_a^b \sqrt{dx^2 + dy^2} = \int_a^b \sqrt{1 + (f(x)')^2}dx$$

The integrand function is $L(x, y, y')$. For better readability we use $y = f(x)$ and the general integral:

$$S = \int \sqrt{1 + (y')^2}dx$$

$$L = \sqrt{1 + (y')^2}$$

$$\frac{\partial L}{\partial y} = 0$$

$$\frac{\partial L}{\partial y'} = \frac{y'}{\sqrt{1 + (y')^2}}$$

The Lagrangian equation:

$$\frac{d}{dx}\frac{y'}{\sqrt{1 + (y')^2}} = 0$$

Solution:

$$\frac{y'}{\sqrt{1 + (y')^2}} = c$$

$$y' = c\sqrt{1 + (y')^2}$$

$$(y')^2 = c^2(1 + (y')^2) = c^2 + c^2(y')^2$$

$$\frac{(y')^2}{c^2(y')^2} = \frac{c^2}{c^2(y')^2}$$

$$\frac{1}{c^2} = \frac{1}{(y')^2}$$

$$c^2 = (y')^2$$

$$y' = |c| \rightarrow y = c \cdot x + d$$

Result: a straight line. The straight line is the shortest connection between two points.

Expectation values:

From a mathematical point of view, we have the expectation value of an operator L:

$$\langle L \rangle = \sum_i \lambda_i P(\lambda_i)$$

This is the standard formula for an average value, a weighted sum, weighted with the probability function P.

Alternatively, we can define the average experimental. We do an experiment several times and use the Laplace formula to determine the probabilities. If the number of experiments is large enough the experimental results converge to the mathematical results.

Suppose that the normalized state of a quantum system is $|A\rangle$. We expand $|A\rangle$ in the orthonormal basis of eigenvectors of L:

$$|A\rangle = \sum_i \alpha_i |\lambda_i\rangle$$

and

$$\langle A| = \sum_i \langle\lambda_i|\alpha_i^*$$

We compute the quantity $\langle A|L|A\rangle$:

$$\langle A|L|A\rangle = \langle A|L|\sum_i \alpha_i|\lambda_i\rangle\rangle = \langle A|\sum_i \alpha_i L|\lambda_i\rangle =$$

$$\langle A|\sum_i \alpha_i\lambda_i|\lambda_i\rangle = \langle A|\sum_i \alpha_i\lambda_i|\lambda_i\rangle =$$

$$\sum_i \langle\lambda_i|\alpha_i^*\alpha_i\lambda_i|\lambda_i\rangle = \sum_i \alpha_i^*\alpha_i\lambda_i\langle\lambda_i|\lambda_i\rangle =$$

$$\sum_i \alpha_i^*\alpha_i\lambda_i$$

In summa:

$$\langle A|L|A\rangle = \sum_i \alpha_i^*\alpha_i\lambda_i$$

This has the same form as:

$$\langle L\rangle = \sum_i P(\lambda_i)\lambda_i$$

We can identify:

$$\langle L\rangle = \langle A|L|A\rangle$$

with

$$P(\lambda_i) = \alpha_i^*\alpha_i$$

This gives a rule to compute averages. Just sandwich the observable between the bra and ket representations of the state vector.

Change over time in expectation values:

Prerequisite: The Schrödinger equation:

$$\frac{d\psi(t)}{dt} = -\frac{iH}{\hbar}\psi(t)$$

end prerequisite:

Expectation values change with time according to the system change with time. Suppose the state at time t is represented by ket $|\psi(t)\rangle$ and bra $\langle\psi(t)|$.

The expectation value of the observable L at time t is:

$$\langle\psi(t)|L|\psi(t)\rangle$$

We differentiate:

$$\frac{d}{dt}\langle\psi(t)|L|\psi(t)\rangle = \langle\dot{\psi}(t)|L|\psi(t)\rangle + \langle\psi(t)|L|\dot{\psi}(t)\rangle$$

Plugging in the bra and ket versions of Schrödinger's equation:

$$\langle\dot{\psi}(t)|L|\psi(t)\rangle + \langle\psi(t)|L|\dot{\psi}(t)\rangle = \left\langle\frac{iH}{\hbar}\psi(t)\middle|L\middle|\psi(t)\right\rangle + \left\langle\psi(t)\middle|L\middle|-\frac{iH}{\hbar}\psi(t)\right\rangle =$$

$$\left\langle\frac{iH}{\hbar}\psi(t)\middle|L\middle|\psi(t)\right\rangle + \left\langle\psi(t)\middle|L\middle|-\frac{iH}{\hbar}\psi(t)\right\rangle =$$

$$\left\langle\frac{i}{\hbar}\psi(t)\middle|HL\middle|\psi(t)\right\rangle + \left\langle\psi(t)\middle|LH\middle|-\frac{i}{\hbar}\psi(t)\right\rangle =$$

$$\frac{i}{\hbar}\langle\psi(t)|[HL-LH]|\psi(t)\rangle$$

Note: there is no change in time if the operators H and L commute.

Conservation of expectation values:

An observable Q is conserved if it does not change with time (unless the system itself is disturbed).

With the Hamiltonian

$$\frac{dQ}{dt} = -\frac{i}{\hbar}[Q,H]$$

we get that $\frac{dQ}{dt} = 0$ if Q and H commutes, $[Q,H] = QH - HQ = 0$.

From $[Q,H] = 0$ we can see that $[Q^2,H] = 0$:

$$[Q^2,H] = Q^2H - HQ^2 = Q^2H + QH - HQ - HQ^2 =$$

$$[Q^2,H] = Q^2H - HQ^2 = Q^2H + QH - (HQ + HQ^2) =$$

$$QH(Q+1) - HQ(Q+1) =$$

$$(QH - HQ)(Q+1) = 0$$

This holds for all powers of Q, so we can conclude: if Q commutes with the Hamiltonian, the expectation values of all functions of Q are conserved.

Note: the Hamiltonian itself is a conserved quantity, because $[H,H] = 0$.

Correlation test for entanglement and expectation values:

Assume Alice with observable A and Bob with observable B. The expectation values (average values) are $\langle A\rangle$ and $\langle B\rangle$.

The correlation $C(A,B)$ between them is defined:

$$C(A,B) = \langle AB\rangle - \langle A\rangle\langle B\rangle$$

Correlations lie in the range $-1;+1$. If the correlation $C(A,B) \neq 0$, then the states are entangled. The greater the magnitude of $C(A,B)$, the more entangled are the states. If $C(A,B) = 0$ then there is no entanglement, both states are independent (e.g. in the product state).

Expectation values for density matrix:

Suppose Alice has prepared a spin using an apparatus oriented along some axis. She gives the spin to Bob but doesn't tell him along which axis the apparatus was oriented. Perhaps she gives him some partial information, such as that the axis was either the z axis or the x-axis. What does Bob do? How can he use this information to make predictions?

If Alice prepared the spin in the state $|\psi\rangle$, then the expectation value of any observable L is

$$\langle\psi|L|\psi\rangle = Tr|\psi\rangle\langle\psi|L$$

with Tr being the trace of an operator or a square matrix. The trace of an operator is the sum of its diagonal elements. The trace of a projection operator is 1.

If Alice prepared the spin in the state $|\theta\rangle$, then the expectation value of any observable L is

$$\langle\theta|L|\theta\rangle = Tr|\theta\rangle\langle\theta|L$$

If Bob knows nothing, he assumes a 50:50 probability giving an expectation value of $\langle L\rangle$:

$$\langle L\rangle = \left(\frac{1}{2}Tr|\psi\rangle\langle\psi|L + \frac{1}{2}Tr|\theta\rangle\langle\theta|L\right) = Tr\left(\left(\frac{1}{2}|\psi\rangle\langle\psi|L + \frac{1}{2}|\theta\rangle\langle\theta|L\right)\right) =$$

$$Tr\left(\left(\frac{1}{2}|\psi\rangle\langle\psi| + \frac{1}{2}|\theta\rangle\langle\theta|\right)L\right)$$

$\left(\frac{1}{2}|\psi\rangle\langle\psi| + \frac{1}{2}|\theta\rangle\langle\theta|\right)$ is the density matrix ρ, half the projection operator onto $|\psi\rangle$ plus half the projection operator onto $|\theta\rangle$.

$|\psi\rangle\langle\psi|$ and $|\theta\rangle\langle\theta|$ are square matrices of the same rank.

With this density matrix computing the expectation values becomes:

$$\langle L\rangle = Tr(\rho L)$$

Note: ρ is an operator and becomes a matrix when a basis is chosen. Suppose we have the basis $|a\rangle$, then the density matrix with respect to this basis is $\rho_{aa'} = \langle a|\rho|a'\rangle$. If the matrix representation of L with respect to this basis is: $L_{a'a} = \langle a'|L|a\rangle$, we can write the expectation value of L:

$$\langle L\rangle = \sum_{a,a'} L_{a',a}\rho_{a,a'}$$

Expectation values of entangled state:

For a product space holds that for any state of a single spin there is some direction for which the spin is $+1$. This meets our expectations in a way that the spin must have exactly one direction, even if we do not know it.

This means that the expectation values of the components must sum up to 1:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$$

This classical expectation does not hold for entangled states, especially not for the entangled state $|sing\rangle$.

The entangled state $|sing\rangle$ is defined:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

The expectation value $\langle\sigma_z\rangle \coloneqq \langle sing|\sigma_z|sing\rangle$

$$\langle\sigma_z\rangle \coloneqq \langle sing|\sigma_z|sing\rangle =$$

$$\left\langle sing\left|\sigma_z\right|\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)\right\rangle =$$

$$\left\langle sing\left|\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)\right\rangle =\right.$$

$$\left(\frac{1}{\sqrt{2}}(\langle ud| - \langle du|)\right)\left(\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)\right) =$$

$$\frac{1}{2}(\langle ud|ud\rangle + \langle ud|du\rangle - \langle du|ud\rangle - \langle du|du\rangle) =$$

$$\frac{1}{2}(1 + 0 - 0 - 1) = 0$$

The same result we get for $\langle\sigma_y\rangle$ and $\langle\sigma_x\rangle$. Our sum of expectation values:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 0$$

is shrinking to zero. In plain words – we can measure whatever direction we want we don't find the spin orientation.

If the expectation value of a component of σ is zero, this means that the experimental outcome is equally likely to be $+1$ or -1, the outcome is completely uncertain. Even though we know the exact state-vector $|sing\rangle$, we know nothing at all about the outcome of any measurement of any component of either spin.

Expectation values of near singlet state:

The near singlet state is a partially entangled state.

The state-vector:

$$\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$$

or in the extended form:

$$|nearsing\rangle = 0|uu\rangle + \sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle + 0|dd\rangle$$

We have only one normalization condition:

$$\psi^*_{uu}\psi_{uu} + \psi^*_{ud}\psi_{ud} + \psi^*_{du}\psi_{du} + \psi^*_{dd}\psi_{dd} = 1$$

in this case reducing to:

$$\psi^*_{ud}\psi_{ud} + \psi^*_{du}\psi_{du} = 1$$

The density matrix for the full composite system: $\rho^2 = \rho, Tr(\rho^2) = 1.$

The density matrix for Alice's subsystem A: $\rho^2 \neq \rho, Tr(\rho^2) < 1$

The wave function is not factorized: $\psi(a, b).$

The expectation values:

$\langle\sigma_z\rangle = 0{,}2\ \langle\sigma_x\rangle = \langle\sigma_y\rangle = 0$

$\langle\tau_z\rangle = -0{,}2\ \langle\tau_x\rangle = \langle\tau_y\rangle = 0$

$\langle\tau_z\sigma_z\rangle = -1$

$\langle\tau_x\sigma_x\rangle = -2\sqrt{0{,}24}$

The correlation between the two systems: $\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = -0{,}96$

The main feature of a partially entangled state is that the composite system as a whole is fully characterized but there is no complete information about the subsystems.

Particle dynamics and expectation values:

Classic: a particle is moving on the x-axis. The momentum is conserved, the particle moving with fixed velocity.

Quantum mechanical: an expectation value (of a probability distribution) is "moving" on the x-axis. The expectation value of position behaves according to the classical equations of motion.

Expectation values of product state:

The product state is a not entangled state, its two constituting states are independent, we have classical behavior.

The state-vector:

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

Note: the parameter α standing for Alice's subsystem, the parameter β for Bob's subsystem.

We have two normalization conditions:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

$$\beta_u^*\beta_u + \beta_d^*\beta_d = 1$$

The density matrix for Alice's subsystem A has exactly one nonzero eigenvalue 1. The eigenvector with this eigenvalue is the wave function of Alice's subsystem – same for Bob.

The wave function is factorized: $\psi(a)\theta(b)$.

Note: $\psi(a)$ is the wave function of Alice, $\theta(b)$ for Bob.

The expectation values for Alice's subsystem:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$$

The expectation values for Bob's subsystem:

$$\langle\tau_x\rangle^2 + \langle\tau_y\rangle^2 + \langle\tau_z\rangle^2 = 1$$

The correlation between the two systems: $\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = 0$

Expectation values and projection operator:

Let $|\psi\rangle$ be normalized, $||\psi\rangle| = 1$. The outer product is called a projection operator:

$$|\psi\rangle\langle\psi|$$

We apply the projection operator to an operator L:

$$(|\psi\rangle\langle\psi|)\ |L\rangle = |\psi\rangle\ (\langle\psi|L\rangle)$$

$\langle\psi|L\rangle$ is a (complex) number, the result of the operation is proportional to $|\psi\rangle$.

Note: The trace Tr of an operator or any square matrix is the sum of its diagonal elements:
$Tr\ L = \sum_i \langle i|L|i\rangle$

Properties of projection operators:

- Projection operators are Hermitian
- The vector $|\psi\rangle$ is eigenvector of its projection operator $|\psi\rangle\langle\psi|$ with eigenvalue 1:
$$(|\psi\rangle\langle\psi|)\ |\psi\rangle = |\psi\rangle\ (\langle\psi|\psi\rangle) = |\psi\rangle$$
- Any vector orthogonal to $|\psi\rangle$ is eigenvector with eigenvalue zero. The eigenvalues of $|\psi\rangle\langle\psi|$ are all either 0 or 1. There is only one eigenvector with eigenvalue 1, $|\psi\rangle$ itself.
- The square of a projection operator is the same as the projection operator itself:
$$(|\psi\rangle\langle\psi|)^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|$$
- The trace of a projection operator is 1.
- If we add all the projection operators for a basis system, we obtain the identity operator:
$$\sum_i |i\rangle\langle i| = I$$
- The expectation value for any operator (observable) $|L\rangle$ in state $|\psi\rangle$ is given by:

$$\langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|\ L$$

We check the last property:

$$Tr\ |\psi\rangle\langle\psi|\ L = \sum_i \langle i|\psi\rangle\langle\psi|L|i\rangle =$$

$$\sum_i \langle\psi|L|i\rangle\ \langle i|\psi\rangle = \langle\psi|L|\psi\rangle = \langle L\rangle$$

Expectation values of singlet state:

In case of a two-spin system the maximum entangled state, the singlet state can be written as:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

or in the extended form:

$$|sing\rangle = 0|uu\rangle + \frac{1}{\sqrt{2}}|ud\rangle - \frac{1}{\sqrt{2}}|du\rangle + 0|dd\rangle$$

We have only one normalization condition:

$$\psi^*_{uu}\psi_{uu} + \psi^*_{ud}\psi_{ud} + \psi^*_{du}\psi_{du} + \psi^*_{dd}\psi_{dd} = 1$$

This is reducing to:

$$\psi_{ud}^{*}\psi_{ud} + \psi_{du}^{*}\psi_{du} = 1$$

For the full composite system, the density matrix:

$$\rho^2 = \rho$$

The trace Tr of the density matrix:

$$Tr(\rho^2) = 1$$

The density matrix A of Alice as well as the density matrix B of Bob is a diagonal matrix with equal values that sum up to one, hence each outcome for the single-spin systems is equally likely.

For both systems:

$$\rho^2 \neq \rho$$

$$Tr(\rho^2) < 1$$

The wave function is not factorized: $\psi(a, b)$.

The expectation values for each single system are zero:

$\langle\sigma_x\rangle^2 = \langle\sigma_y\rangle^2 = \langle\sigma_z\rangle^2 = 0$ and $\langle\tau_x\rangle^2 = \langle\tau_y\rangle^2 = \langle\tau_z\rangle^2 = 0$.

The expectation values for the combined system are 1:

$\langle\sigma_x\tau_x\rangle^2 = \langle\sigma_y\tau_y\rangle^2 = \langle\sigma_z\tau_z\rangle^2 = 1$ and $\langle\sigma_x\tau_x\rangle = \langle\sigma_y\tau_y\rangle = \langle\sigma_z\tau_z\rangle = -1$

The correlation between the two systems is -1:

$\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = -1$

The main feature of an entangled state is that the composite system as a whole is fully characterized but there is no information about the subsystems.

Expectation values in spin over time:

A spin in a magnetic field will not stay constant but change with time. The classical analog would be the precession of a charged rotor, the energy being proportional to the dot product of the spin and the magnetic field. The quantum version:

$$H \sim \vec{\sigma} \cdot \vec{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$$

Note: $\sigma_x, \sigma_y, \sigma_z$ represent the components of the spin operator.

The magnetic field lies along the z-axis, so the Hamiltonian is proportional to σ_z.

For convenience, all numerical constants without $\hbar$ go into the constant ω:

$$H = \frac{\hbar\omega}{2}\sigma_z$$

We want to know how the expectation value of the spin changes with time:

$$\langle\sigma_x(t)\rangle, \langle\sigma_y(t)\rangle, \langle\sigma_z(t)\rangle$$

The change of an operator with time:

$$\frac{dL}{dt} = -\frac{i}{\hbar}[L, H]$$

Note: this is a shorthand form of:

$$\frac{d}{dt}\langle\psi(t)|L|\psi(t)\rangle = \frac{i}{\hbar}\langle\psi(t)|[HL - LH]|\psi(t)\rangle$$

We get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i}{\hbar}\langle[\sigma_x, H]\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i}{\hbar}\langle\left[\sigma_y, H\right]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i}{\hbar}\langle[\sigma_z, H]\rangle$$

We replace H by $\frac{\hbar\omega}{2}\sigma_z$:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i\omega}{2}\langle\left[\sigma_y, \sigma_z\right]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i\omega}{2}\langle[\sigma_z, \sigma_z]\rangle$$

We check this for the first case $\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$:

$$\langle\dot{\sigma_x}\rangle = -\frac{i}{\hbar}\langle[\sigma_x, H]\rangle = -\frac{i}{\hbar}\langle\left[\sigma_x, \frac{\hbar\omega}{2}\sigma_z\right]\rangle =$$

$$-\frac{i}{\hbar}\langle\frac{\hbar\omega}{2}\sigma_x\sigma_z - \frac{\hbar\omega}{2}\sigma_z\sigma_x\rangle =$$

$$-\frac{i\hbar\omega}{2\hbar}\langle\sigma_x\sigma_z - \sigma_z\sigma_x\rangle =$$

$$-\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$$

The operators $\sigma_x, \sigma_y, \sigma_z$ represent the Pauli matrices:

$$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

We calculate the results of $[\sigma_x, \sigma_z]$, $[\sigma_y, \sigma_z]$ and $[\sigma_z, \sigma_z]$:

$$[\sigma_x, \sigma_z] = \sigma_x\sigma_z - \sigma_z\sigma_x =$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} =$$

$$\begin{pmatrix} 0\cdot 1 + 1\cdot 0 & 0\cdot 0 + 1\cdot(-1) \\ 1\cdot 1 + 0\cdot 0 & 1\cdot 0 + 0\cdot(-1) \end{pmatrix} - \begin{pmatrix} 1\cdot 0 + 0\cdot 1 & 1\cdot 1 + 0\cdot 0 \\ 0\cdot 0 + (-1)\cdot 1 & 0\cdot 1 + (-1)\cdot 0 \end{pmatrix} =$$

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} =$$

$$= 2\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = 2\begin{pmatrix} 0 & i\cdot i \\ -i\cdot i & 0 \end{pmatrix} = -2i\sigma_y$$

$$[\sigma_y, \sigma_z] = \sigma_y\sigma_z - \sigma_z\sigma_y =$$

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} =$$

$$\begin{pmatrix} 0\cdot 1 + (-i)\cdot 0 & 0\cdot 0 + (-i)\cdot(-1) \\ i\cdot 1 + 0\cdot 0 & i\cdot 0 + 0\cdot(-1) \end{pmatrix} - \begin{pmatrix} 1\cdot 0 + 0\cdot i & 1\cdot(-i) + 0\cdot 0 \\ 0\cdot 0 + (-1)\cdot i & 0\cdot(-i) + (-1)\cdot 0 \end{pmatrix} =$$

$$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} =$$

$$= 2i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = 2i\sigma_x$$

$$[\sigma_z, \sigma_z] = \sigma_z\sigma_z - \sigma_z\sigma_z = 0$$

We take the results and get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle -2i\sigma_y\rangle = -\omega\langle\sigma_y\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i\omega}{2}\langle 2i\sigma_x\rangle = \omega\langle\sigma_x\rangle$$

$$\langle\dot{\sigma_z}\rangle = 0$$

The 3-vector-operator $\vec{\sigma}$ is precessing like a gyroscope around the direction of the magnetic field with constant angular velocity ω.

Note: the difference between classical precession and "quantum precession" is, that in quantum mechanics the expectation value is precessing. The expectation value for measuring σ_z does not change with time, but the other expectation values σ_y and σ_x do.

Experiments, apparatus and two-state system:

Simple

We have a spin that either can be up or $down$. This is a two-state system (a bit) with two states.

Formally we have a degree of freedom called σ that can take two values, $+1$ and -1. With this we can replace the state up by $\sigma = +1$ and the state $down$ by $\sigma = -1$.

An experiment involves an apparatus A to record the state of the spin, the result being shown in a window. The apparatus starts with a blank window and after a measurement shall show an arrow up if the spin is up so we know $\sigma = +1$. Analog for spin $down$.

Subsequent experiments will confirm this state.

In classical physics we would say, the first measurement detects the position of the spin.

In quantum mechanics we would say, the first measurement determines the position of the spin.

Extended

The first measurement with the spin oriented up – the apparatus shows an arrow up or $\sigma = +1$.

After that we turn the apparatus upside down and measure again. Now the apparatus records $\sigma = -1$.

We do this sequence again, but this time turning the apparatus by 90° for the second measurement. This time the apparatus will give for every measurement $+1$ or -1 with an average of 0.

Feynman, Richard:

Richard Phillips Feynman (1918 – 1988) was an American theoretical physicist, known for his work in the path integral formulation of quantum mechanics, the theory of quantum electrodynamics, the physics of the superfluidity of supercooled liquid helium, as well as his work in particle physics for which he proposed the parton model. For contributions to the development of quantum electrodynamics, Feynman received the Nobel Prize in Physics in 1965 jointly with Julian Schwinger and Shin'ichirō Tomonaga. *(Courtesy Wikipedia)*

Forces:

Prerequisite

The connection between the classical notion of momentum $v = \frac{p}{m}$ and the momentum operator P:

$$\langle P \rangle = mv$$

The average momentum equals mass times velocity.

The time derivative of the expectation value of any observable L:

$$\frac{d}{dt}\langle L \rangle = \frac{i}{\hbar}\langle [H, L] \rangle$$

Note: $[H, L]$ is the commutator $HL - LH$.

End prerequisite

We usually work with a potential energy function for the particle we are studying in classical physics as well as in quantum mechanics.

The potential energy is denoted by $V(x)$. In classical mechanics it is related to the force on a particle:

$$F(x) = -\frac{\partial V}{\partial x}$$

We combine this with Newton's second law, $F = ma$:

$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

In quantum mechanics we write the Hamiltonian and solve the Schrödinger equation. The potential energy $V(x)$ becomes an operator V.

When the operator V acts on any wave function $\psi(x)$, it multiplies the wave function by the function $V(x)$:

$$V|\psi\rangle \rightarrow V(x)\psi(x)$$

Once forces are included, the momentum of a particle is not conserved:

$$\frac{dp}{dt} = F = -\frac{\partial V}{\partial x}$$

We add $V(x)$ to the Hamiltonian:

$$H = \frac{P^2}{2m} + V(x)$$

We modify the Schrödinger equations:

$$H\psi(x) = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)$$

We check whether $\langle P\rangle = mv$ still is valid. Because a new term has been added to H, there will be the new term $V(x)$ in the commutator of X and H, it involves the commutator of X with $V(x)$.
Multiplying by x and multiplying by a function of x are operations that commute, so:

$$[X, V] = [X, V(x)] = 0$$

The connection between velocity and momentum is unaffected by forces, in classical physics as well as in quantum mechanics.

We calculate the time derivative of the expectation value of P, $\frac{d}{dt}\langle P\rangle$ by commuting P with the Hamiltonian $H = \frac{P^2}{2m} + V$:

$$\frac{d}{dt}\langle P\rangle = \frac{i}{\hbar}\langle[H, P]\rangle = \frac{i}{\hbar}\left\langle\left[\left(\frac{P^2}{2m} + V\right), P\right]\right\rangle =$$

$$\frac{i}{2m\hbar}\langle[P^2, P]\rangle + \frac{i}{\hbar}\langle[V, P]\rangle$$

Left part of the sum: $\frac{i}{2m\hbar}\langle[P^2, P]\rangle$ is zero because an operator commutes with any function of itself.

Right part of the sum with $V(x)$ instead of V because we apply it to $\psi(x)$:

$$[V(x), P]\psi(x) =$$

$$V(x)\left(-i\hbar\frac{d}{dx}\right)\psi(x) - \left(-i\hbar\frac{d}{dx}\right)\left(V(x)\psi(x)\right) =$$

$$V(x)\left(-i\hbar\frac{d\psi(x)}{dx}\right) - \left(-i\hbar\frac{dV(x)}{dx}\psi(x) - i\hbar\frac{d\psi(x)}{dx}V(x)\right) =$$

$$V(x)\left(-i\hbar\frac{d\psi(x)}{dx}\right) + i\hbar\frac{dV(x)}{dx}\psi(x) + i\hbar\frac{d\psi(x)}{dx}V(x) =$$

$$-i\hbar\frac{d\psi(x)}{dx}V(x) + i\hbar\frac{dV(x)}{dx}\psi(x) + i\hbar\frac{d\psi(x)}{dx}V(x) =$$

$$i\hbar\frac{dV(x)}{dx}\psi(x)$$

Omitting the $\psi(x)$ we get:

$$[V(x), P] = i\hbar\frac{dV(x)}{dx}$$

For $\frac{i}{\hbar}\langle[V, P]\rangle$ this gives:

$$\frac{i}{\hbar}\langle[V(x), P]\rangle = -\frac{d}{dx}V(x)$$

We add the results:

$$\frac{d}{dt}\langle P\rangle = -\frac{d}{dx}V(x)$$

This is the quantum analog of Newton's equation for the time rate change of the expectation value of momentum.

Fourier transforms:

Prerequisite

The inner product of a position eigenvector $|x\rangle$ and a momentum eigenvector $|p\rangle$:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}e^{\frac{ipx}{\hbar}}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}}e^{-\frac{ipx}{\hbar}}$$

Please note the minus sign.

End prerequisite

The wave function gives the probability for finding a particle at position x:

$$P(x) = \psi^*(x)\psi(x)$$

As we will see, no experiment can determine both the position and the momentum of a particle simultaneously, analog to the impossibility to measure both the x and z component of a spin.

The probability that a momentum measurement will give p is:

$$P(p) = |\langle P|\psi\rangle|^2$$

$\langle P|\psi\rangle$ is called the wave function of $|\psi\rangle$ in the momentum representation. It is denoted by:

$$\tilde{\psi}(p) = \langle P|\psi\rangle$$

The state vector can be represented in two ways, the position basis or the momentum basis. Both wave functions, the position wave function $\psi(x)$ and the momentum wave function $\tilde{\psi}(p)$ represent exactly the same state-vector $|\psi\rangle$. The transformation between them is the Fourier transformation.

Given a basis of a phase state in basis vectors $|i\rangle$. We can rewrite the identity operator I in terms of the outer product:

$$I = \sum_i |i\rangle\langle i|$$

Because momentum and position are both Hermitian, the sets of vectors $|x\rangle$ and $|p\rangle$ each define basis vectors.

We replace the sum by an integral:

$$I = \int |x\rangle\langle x|\, dx \text{ or } I = \int |p\rangle\langle p|\, dp$$

Suppose we know the wave function of the vector $|\psi\rangle$ in the position representation: By definition, it is equal to:

$$\psi(x) = \langle x|\psi\rangle$$

We build the wave function $\tilde{\psi}(p)$ in the momentum representation.

1. We use the definition of the momentum-representation wave function:
$$\tilde{\psi}(p) = \langle p|\psi\rangle$$
2. We insert the unit operator:
$$\tilde{\psi}(p) = \int \langle p|x\rangle\langle x|\psi\rangle \, dx$$
3. $\langle x|\psi\rangle$ is just the wave function $\psi(x)$.
$\langle p|x\rangle$ is given by:
$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$
4. Result:
$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{ipx}{\hbar}} \psi(x) dx$$

If we know $\psi(x)$ in the position representation we can calculate the corresponding wave function in the momentum representation.

This works also the other way around. We know the wave function in the momentum representation and calculate the position representation:

1. We use the definition of the position-representation wave function:
$$\psi(x) = \langle x|\psi\rangle$$
2. We insert the unit operator:
$$\psi(x) = \int \langle x|p\rangle\langle p|\psi\rangle \, dp$$
3. $\langle p|\psi\rangle$ is just the wave function $\tilde{\psi}(p)$.
$\langle x|p\rangle$ is given by:
$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$
4. Result:
$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{\frac{ipx}{\hbar}} \tilde{\psi}(p) dp$$

Position and momentum representation are reciprocal Fourier transforms of each other.

Frequency, energy and frequency:

Prerequisite:

The time-dependent Schrödinger equation:

$$\hbar \frac{\partial}{\partial t} |\psi\rangle = -iH|\psi\rangle$$

The time-independent Schrödinger equation:

$$H|E_j\rangle = E_j|E_j\rangle$$

Note: E_j are the eigenvalues, $|E_j\rangle$ the eigenvectors. Eigenvalues of Hermitian operators always are real.

End prerequisite

Let us suppose we have found all energy eigenvalues E_j and corresponding eigenvectors $|E_j\rangle$.

We solve the time-dependent Schrödinger equation.

The state-vector:

$$|\psi\rangle = \sum_j \alpha_j |E_j\rangle$$

The state-vector changes with time, the basis vectors $|E_j\rangle$ do not, so the α_j have to:

$$|\psi(t)\rangle = \sum_j \alpha_j(t) |E_j\rangle$$

We feed this result back into the time-dependent Schrödinger equation:

$$\hbar \frac{\partial}{\partial t} \sum_j \alpha_j(t) |E_j\rangle = -iH \sum_j \alpha_j(t) |E_j\rangle$$

$$\hbar \sum_j \dot{\alpha}_j(t) |E_j\rangle = -iH \sum_j \alpha_j(t) |E_j\rangle$$

$$\sum_j \dot{\alpha}_j(t) |E_j\rangle = -\frac{i}{\hbar} H \sum_j \alpha_j(t) |E_j\rangle$$

We use $H|E_j\rangle = E_j|E_j\rangle$ and regroup the result:

$$\sum_j \dot{\alpha}_j(t) |E_j\rangle + \frac{i}{\hbar} \sum_j \alpha_j(t) E_j |E_j\rangle = 0$$

$$\sum_j \left(\dot{\alpha}_j(t) |E_j\rangle + \frac{i}{\hbar} \alpha_j(t) E_j |E_j\rangle \right) = 0$$

The $|E_j\rangle$ build a basis, every coefficient must be zero. We get:

$$\dot{\alpha}_j(t) |E_j\rangle + \frac{i}{\hbar} \alpha_j(t) E_j |E_j\rangle = 0$$

$$\dot{\alpha}_j(t) |E_j\rangle = -\frac{i}{\hbar} \alpha_j(t) E_j |E_j\rangle$$

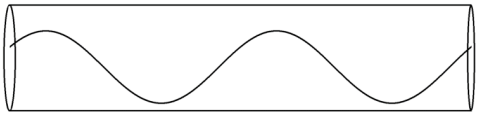
This is a differential equation with the solution:

$$a_j(t) = a_j(0) e^{-\frac{i}{\hbar} E_j \cdot t}$$

Observables always are real. The “observable part” of $a_j(t)$ is something of the kind:

$$a_j(t) = a_j(0) \cos\left(-\frac{E_j}{\hbar} \cdot t \right) \sim r \, cos(\omega t)$$

Frequency of harmonic oscillator:



Consider the example of electromagnetic radiation in a cavity, a region of space bracketed by a pair of perfectly reflecting mirrors that keep the radiation bouncing endlessly back and forth.

There is only one important number associated with a harmonic oscillator, its frequency and the corresponding wavelength:

$$\omega = \frac{2\pi c}{\lambda}$$

In classical physics, the frequency is just the frequency.

In quantum mechanics, the frequency determines the quantum energy of the oscillator. The energy contained in waves of length λ has to be:

$$\left(n + \frac{1}{2}\right)\hbar\omega$$

The term $\frac{1}{2}\hbar\omega$ is the zero-point energy which we ignore here. The energy of waves of length λ becomes:

$$\frac{2\pi\hbar c}{\lambda} \cdot n$$

The energy of an electromagnetic wave is quantized in indivisible units of $\frac{2\pi\hbar c}{\lambda}$. These units are called photons, the quantized unit of energy in a quantum harmonic oscillator.

Functions:

Functions, the Dirac delta function:

Replacing discrete functions by continuous functions require the Kronecker delta function to be replaced by an appropriate function that works with integrals. Remember the Kronecker delta δ_{ij}.

Let F_i be a vector in a discrete, finite dimensional space.

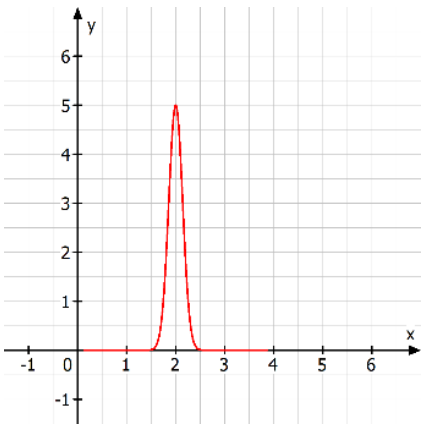
$$\sum\nolimits_{i,j}(\delta_{ij}F_j)$$

gives F_j because δ_{ij} is $zero$ for $i \neq j$ and 1 for $i = j$.

In the integration concept the Dirac delta function performs the same: $\delta(x - x')$ is something that returns zero for all $x \neq x'$ and "∞" for $x = x'$. With this:

$$\int_{-\infty}^{\infty} \delta(x - x_0)\, f(x)dx = f(x_0)$$

Note: the Dirac delta function can be thought of as $\lim_{n\to\infty} ne^{-(n(x-x_0))^2}$.



Example: let X be the position operator in a one-dimensional vector space, e.g. the x-axis. The position operator should give back the position of a particle:

$$X|\psi\rangle = x_0|\psi\rangle$$

In terms of wave function this becomes:

$$x\psi(x) = x_0\psi(x)$$

We rewrite this:

$$(x - x_0)\psi(x) = 0$$

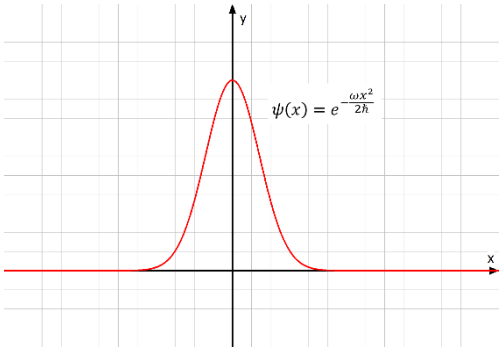
It is the property of the Dirac delta function $\delta(x - x_0)$ to be zero on every $x \neq x_0$ and to be nonzero at a single point.

The wave function $\psi(x) = \delta(x - x_0)$ represents the state in which the particle is located exactly at the point x_0 on the x-axis.

Functions, the Gaussian function:

The ground state wave function is the Gaussian function:

$$\psi(x) = e^{-\frac{\omega x^2}{2\hbar}}$$



The ground state energy $E_0 = \frac{\hbar\omega}{2}$.

Note: the maximum height of the ground state function is 1.

Note: the Gaussian function cannot be integrated elementary.

Note: the Gaussian function is also used in statistics as normal distribution.

Functions, normalizable functions:

The probability density to find a particle at position x:

$$\psi^*(x)\psi(x) = P(x)$$

The total probability to find a particle at any position must be 1:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1$$

Obviously, this requires the function go to zero "fast enough" on both sides. Functions that meet this condition are called normalizable. The Gaussian function is a good candidate for this.

Functions, potential functions:

The potential energy function is denoted by $V(x)$. In classical mechanics it is related to the force on a particle:

$$F(x) = -\frac{\partial V}{\partial x}$$

We combine this with Newton's second law:

$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

In quantum mechanics we use the operator V instead. If the operator V acts on any wave function $\psi(x)$, it multiplies the wave function $\psi(x)$ by the function $V(x)$:

$$V|\psi\rangle \rightarrow V(x)\psi(x)$$

If $V(x)$ is a smooth function in respect to the "size" of the wave packets, then the wave packets have a good chance to cross this region as wave packets. If $V(x)$ has sharp spikes, the wave packets tend to break up.

Electrons e.g. act like solid objects in the electric field of a capacitor. The potential associated with the nucleus of an atom has sharp features in it. Electrons hitting this potential spikes tend to scatter.

Functions, probability functions:

1.

Suppose we have an experiment that measures an observable L. The outcome must be one of the eigenvalues of L with the probability $P(\lambda_i)$. $P(\lambda_i)$ is the probability function.

The average of an observable L:

$$\langle L\rangle = \sum_i \lambda_i P(\lambda_i)$$

This is a weighted sum, weighted with the probability function P.

Note: $0 \leq P(\lambda_i) \leq 1, \sum_i P(\lambda_i) = 1$.

2.

Suppose you have a probability distribution $P(a,b)$ for two variables a and b. If the variables are completely uncorrelated, the probability will factorize:

$$P(a,b) = P_A(a)P_B(b)$$

Note: the subscripts A and B are a reminder that P_A and P_B could be different functions of their arguments.

Functions, as vectors:

The single spin system is described by a two-dimensional space of states, the observables having only a finite number of possible observable values. The coordinates of a particle have an infinite number of possible values, x is a continuously variable. The idea of vectors have to be expanded to include functions – a Hilbert space.

Consider a set of complex functions $\psi(x)$ of a single real variable x: x is real, $\psi(x)$ has complex values. With appropriate restrictions $\psi(x)$ satisfies the mathematical axioms that define a vector space:

1. The sum of any two functions is a function.
2. The addition of functions is commutative.
3. The addition of functions is associative.
4. There exists a zero function for addition.
5. There exists an inverse function for addition.
6. Multiplying a function by a complex number gives a new function and is linear.
7. The distributive property holds:
    a. $z[\varphi(x) + \theta(x)] = z\varphi(x) + z\theta(x)$
    b. $[z + w]\psi(x) = z\,\psi(x) + w\psi(x)$

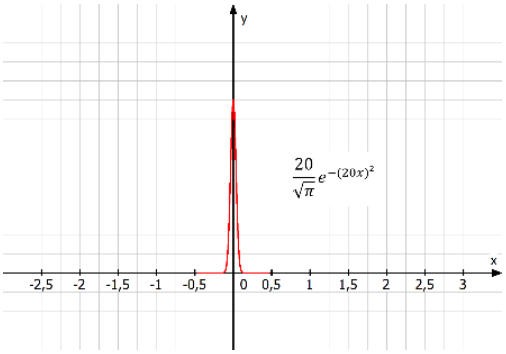
With this we can identify functions $\psi(x)$ with ket-vectors $|\psi\rangle$. The bra-vector $\langle\psi|$ corresponds to the complex conjugate function $\psi^*(x)$.

We have to replace:

a) Integrals replace sums,
$$\langle\psi|\theta\rangle = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx$$
our new inner product.

b) Probability densities replace probabilities. The probability of a continuous variable at exactly one point is zero, so we can only determine the probability the variable lies in between boundaries a and b:
$P(a,b) = \int_a^b P(x)dx = \int_a^b \psi^*(x)\psi(x)dx.$
$P(x)$ becomes a probability density.
For probability densities holds:
$$\int_{-\infty}^{\infty} P(x)dx = 1$$

c) Dirac delta functions replace Kronecker deltas.
The Kronecker delta satisfies:
$$\sum_j \delta_{ij}F_j = F_i$$
The Dirac delta functions $\delta(x - x')$ does the same job for integrals:
$$\int_{-\infty}^{\infty} \delta(x - x')F(x')dx' = F(x)$$



Note: the Dirac delta function can be approximated by e.g.:
$$\frac{n}{\sqrt{\pi}}e^{-(nx)^2}$$

Functions, vector space of functions:

Functions

Consider a set of continuous functions $A(x)$. You can add any two such functions $A_1(x) + A_2(x)$ and multiply them by complex numbers $z \cdot A$. You will get a new continuous function.

Vectors

Two-dimensional column vectors provide another example. We construct them by stacking up a pair of complex numbers, α_1 and α_2:
$$\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}$$
This is the ket-vector $|A\rangle$. You can add any two such vectors $\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} + \begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}$ and multiply them by complex numbers $z \cdot \begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}$. You will get a new vector.

Note: the corresponding bra $\langle A|$ is $(\alpha_1^* \ \alpha_2^*)$.

Functions, zero functions:

This means part 4 of the mathematical axioms defining a vector space:

1. The sum of any two functions is a function.
2. The addition of functions is commutative.
3. The addition of functions is associative.
4. **There exists a zero function for addition.**
5. There exists an inverse function for addition.
6. Multiplying a function by a complex number gives a new function and is linear.

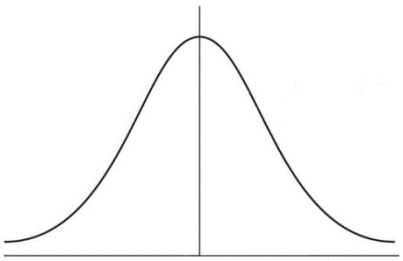
Fundamental theorem of quantum mechanics:

- The eigenvectors of a Hermitian operator are a complete set. Any vector the operator can generate can be expressed by a sum of its eigenvectors.
- If λ_1 and λ_2 are two eigenvalues of a Hermitian operator with $\lambda_1 \neq \lambda_2$, then the corresponding eigenvectors are orthogonal.
- If two eigenvalues are equal, the corresponding eigenvectors span a subspace. For the corresponding subspace can be found an orthonormal basis via the *Gram-Schmidt* procedure.
  Two eigenvalues being equal is called degeneracy.

Gaussian curve and Gaussian wave packets:

For wave packets holds that $\triangle x \triangle p \geq \frac{\hbar}{2}$.

There are minimum uncertainty wave packets where $\triangle x \triangle p = \frac{\hbar}{2}$.

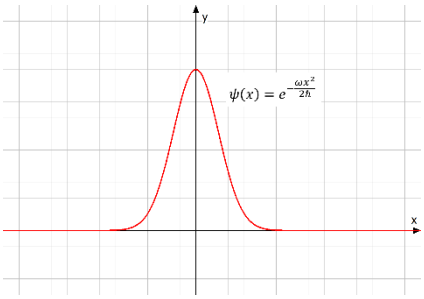


These wave packets have the form of a Gaussian curve, and they are often called Gaussian wave packets.

Note: the Gaussian function is also the probability density function of the normal distribution.

Gaussian function:

The ground state wave function is the Gaussian function:



$$\psi(x) = e^{-\frac{\omega x^2}{2\hbar}}$$

The ground state energy $E_0 = \frac{\hbar\omega}{2}$.

Note: the maximum height of the ground state function is 1.

Note: the Gaussian function cannot be integrated elementary.

Note: the Gaussian function is also used in statistics as normal distribution.

General Schrödinger equation:

The generalized or time-dependent Schrödinger equation:

$$\frac{\partial|\psi\rangle}{\partial t} = -iH|\psi\rangle$$

The time dependent Schrödinger equation describes the time-development of the state-vector. The essential ingredient is the Hamiltonian H, which in both classical and quantum mechanics represents the total energy of a system.

General uncertainty principle:

Prerequisite

Let X and Y be vectors. The Cauchy-Schwarz inequality:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

End prerequisite

Let $|\psi\rangle$ be any normalized ket and let A and B be any two observables. Observables are always real. We define $|X\rangle$ and $|Y\rangle$:

$$|X\rangle = A|\psi\rangle \text{ and } \langle X| = \langle\psi|A$$

$$|Y\rangle = iB|\psi\rangle \text{ and } \langle Y| = \langle\psi| - iB$$

With these the Cauchy-Schwarz inequality becomes:

$$\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq \frac{1}{2}|\langle\psi|AB|\psi\rangle - \langle\psi|BA|\psi\rangle|$$

Written with the commutator:

$$\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq \frac{1}{2}|\langle\psi|[AB]|\psi\rangle|$$

In detail:

$$\langle A\rangle = \langle\psi|A|\psi\rangle \text{ and } \langle B\rangle = \langle\psi|B|\psi\rangle$$

$$|X| = \sqrt{\langle X|X\rangle} = \sqrt{\langle\psi|AA|\psi\rangle} = \sqrt{\langle A^2\rangle}$$

$$|Y| = \sqrt{\langle Y|Y\rangle} = \sqrt{\langle\psi|{-iBiB}|\psi\rangle} = \sqrt{\langle B^2\rangle}$$

$$\langle X|Y\rangle = \langle\psi|AiB|\psi\rangle = i\langle\psi|AB|\psi\rangle$$

$$\langle Y|X\rangle = \langle\psi|{-iBA}|\psi\rangle = -i\langle\psi|BA|\psi\rangle$$

$$\langle X|Y\rangle + \langle Y|X\rangle = i(\langle\psi|AB|\psi\rangle - \langle\psi|BA|\psi\rangle)$$

$$|\langle X|Y\rangle + \langle Y|X\rangle| = |\langle\psi|AB|\psi\rangle - \langle\psi|BA|\psi\rangle|$$

Note: bras are implicitly defined as complex conjugated. If the ket $|\psi\rangle$ is written as a column vector:

$$|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

then the corresponding bra is:

$$\langle\psi| = (a^* b^*)$$

End detail

For simplicity reasons let A and B have expectation values of zero. In that case, $\langle A^2\rangle$ is the square of the uncertainty in $A \coloneqq (\triangle A)^2$ and similar $B \coloneqq (\triangle B)^2$. We get:

$$\sqrt{\langle A^2\rangle\langle B^2\rangle} \rightarrow \triangle A \triangle B$$

$$\triangle A \triangle B \geq \frac{1}{2}|\langle\psi|[AB]|\psi\rangle|$$

In plain words: the product of the uncertainties cannot be smaller than half the magnitude of the expectation value of the commutator. If the commutator of A and B is not zero, both observables cannot simultaneous be certain.

Note: if A and B do not have expectation values of zero, we can shift them and build two new variables:

$$\bar{A} \coloneqq A - \langle A\rangle$$

$$\bar{B} \coloneqq B - \langle B\rangle$$

For these new variables hold:

$$\triangle A^2 = \langle \bar{A}^2 \rangle$$

$$\triangle B^2 = \langle \bar{B}^2 \rangle$$

$$[\bar{A}, \bar{B}] = [AB]$$

For the case of position operator X and momentum operator P we know that applying the commutator onto any wave function $\psi(x)$:

$$[X, P]\psi(x) = i\hbar\psi(x)$$

We express this by writing:

$$[X, P] = i\hbar$$

The fact that X and P do not commute is the key to understanding that they are not simultaneously measurable. We insert them into

$$\triangle X \triangle P \geq \frac{1}{2}|\langle\psi|[XP]|\psi\rangle|$$

and get:

$$\triangle X \triangle P \geq \frac{1}{2}|\langle\psi|i\hbar|\psi\rangle| =$$

$$\frac{1}{2}|i\hbar\langle\psi|\psi\rangle| = \frac{1}{2}|i\hbar| = \frac{1}{2}\hbar$$

$$\triangle X \triangle P \geq \frac{1}{2}|i\hbar| = \frac{1}{2}\hbar$$

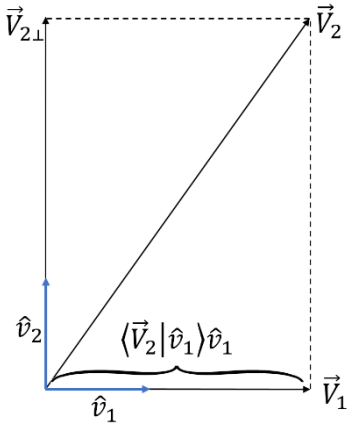
Remember $|\psi\rangle$ is normalized.

This is the Heisenberg Uncertainty Principle.

Gluons:

A gluon is an elementary particle that acts as the exchange particle (or gauge boson) for the strong force between quarks. It is analogous to the exchange of photons in the electromagnetic force between two charged particles. In layman's terms, they "glue" quarks together, forming hadrons such as protons and neutrons. *Courtesy Wikipedia*

Gram-Schmidt procedure:



Given two vectors $\vec{V}_1$ and $\vec{V}_2$ in $\mathbb{R}^2$ that are not orthogonal.

We construct two orthonormal vectors, $\hat{v}_1$ and $\hat{v}_2$.

From $\vec{V}_1$ we get the unit vector $\hat{v}_1$:

$$\hat{v}_1 = \frac{\vec{V}_1}{|\vec{V}_1|}$$

We need the projection of $\vec{V}_2$ onto $\vec{V}_1$:

$$\langle\vec{V}_2|\hat{v}_1\rangle\hat{v}_1$$

We construct $\vec{v}_{2\perp}$:

$$\vec{V}_{2\perp} = \vec{V}_2 - \langle \vec{V}_2 | \hat{v}_1 \rangle \hat{v}_1$$

We build $\hat{v}_2$:

$$\hat{v}_2 = \frac{\vec{V}_{2\perp}}{|\vec{V}_{2\perp}|}$$

Vectors $\hat{v}_1$ and $\hat{v}_2$ are orthonormal.

Gravitons:

Massless particles can move at the velocity of light c, and they can only move at that velocity. All particles other than photons and gravitons are massive and can move at any velocity less than c.

In theories of quantum gravity, the graviton is the hypothetical quantum of gravity, an elementary particle that mediates the force of gravity. There is no complete quantum field theory of gravitons due to an outstanding mathematical problem with renormalization in general relativity. In string theory, believed to be a consistent theory of quantum gravity, the graviton is a massless state of a fundamental string. *Courtesy Wikipedia*

Ground state:

Prerequisite

The Hamiltonian:

$$H|\psi(x)\rangle = -\frac{\hbar^2}{2}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}\omega^2 x^2 \psi(x)$$

The Hamiltonian gives the energy of the state:

$$H|\psi(x)\rangle \coloneqq E|\psi(x)\rangle$$

End prerequisite

In classical physics the lowest possible energy level for a harmonic oscillator is zero.

In quantum mechanics the uncertainty principle says that it is not possible to set both x and p to zero. Best that can be done is to find a state in which x and p are not too spread out.

The lowest energy level the ground state $\psi_0(x)$ is not zero.

The ground state wave function:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

To calculate the energy of the ground state we apply the Hamiltonian:

$$H|\psi_0(x)\rangle = -\frac{\hbar^2}{2}\frac{\partial^2 e^{-\frac{\omega}{2\hbar}x^2}}{\partial x^2} + \frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2}$$

Omitting $-\frac{\hbar^2}{2}$ in the left term we get:

$$\frac{\partial^2}{\partial x^2} e^{-\frac{\omega}{2\hbar}x^2} = \frac{\partial}{\partial x}\left(-\frac{x\omega}{\hbar}\right) e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-\frac{\omega}{\hbar}\frac{\partial}{\partial x} x e^{-\frac{\omega}{2\hbar}x^2} = -\frac{\omega}{\hbar}\left(e^{-\frac{\omega}{2\hbar}x^2} + x\left(-\frac{x\omega}{\hbar}\right) e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$-\frac{\omega}{\hbar} e^{-\frac{\omega}{2\hbar}x^2}\left(1 - \frac{x^2\omega}{\hbar}\right)$$

Reinserting $-\frac{\hbar^2}{2}$:

$$\frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2}\left(1 - \frac{x^2\omega}{\hbar}\right)$$

The right term remains:

$$\frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2}$$

Combining both terms:

$$H|\psi_0(x)\rangle = \frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2}\left(1 - \frac{x^2\omega}{\hbar}\right) + \frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2} =$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(\frac{\hbar\omega}{2} - \frac{x^2\omega^2}{2}\right) + \frac{x^2\omega^2}{2} e^{-\frac{\omega}{2\hbar}x^2} =$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(\frac{\hbar\omega}{2} - \frac{x^2\omega^2}{2} + \frac{x^2\omega^2}{2}\right) =$$

$$\frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2}$$

As $H|\psi_0(x)\rangle = E_0|\psi_0(x)\rangle$ we have the energy E of the ground state:

$$E_0 = \frac{\hbar\omega}{2}$$

Ground state, annihilation of ground state:

Prerequisite

The Hamiltonian can be expressed in terms of the momentum operator P and position operator X:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2) = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{i\omega}{2}$$

because P and X do not commute.

End prerequisite

$(P + i\omega X)$ is called the raising operator, $(P - i\omega X)$ the lowering operator, written as a^+ and a^-.

The raising operator a^+ shifts the energy level of the harmonic oscillator to the next possible higher level, the lowering operator a^- to the next possible lower level.

Applying the lowering operator to the ground level with Energy $E_0 = \frac{\omega\hbar}{2}$ annihilates this ground level. Symbolically this is expressed as

$$a^-|0\rangle = 0$$

with $|0\rangle$ representing the ground level.

Ground state, wave function for the ground state:

Assume we have no explicit ground state wave function $\psi_0(x)$. We know the ground state is "annihilated" by the lowering operator:

$$a^-|0\rangle = 0$$

We rewrite that in terms of the position and momentum operator and the ground state wave function:

$$\frac{i}{\sqrt{2\hbar\omega}}(P - i\omega X)\psi_0(x) = 0$$

We divide the equation by the constant factor $\frac{i}{\sqrt{2\hbar\omega}}$:

$$(P - i\omega X)\psi_0(x) = 0$$

We replace the momentum operator P and the position operator X by their effect on $\psi_0(x)$:

$$\left(-i\hbar\frac{d}{dx} - i\omega x\right)\psi_0(x) = 0$$

$$-i\hbar\frac{d\psi_0(x)}{dx} - i\omega x\psi_0(x) = 0$$

$$\frac{d\psi_0(x)}{dx} = -\frac{\omega x}{\hbar}\psi_0(x)$$

We get a first order differential equation with the solution:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

This is our ground state function.

Hamiltonian:

Prerequisite

The change of the state-vector with time:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

U is called the time-development operator for the system, U must be unitary.

End prerequisite

The basic idea is that of an incremental change in time, valid both for classical physics and quantum mechanics. We need two principles.

Principle one is unitarity:

$$U^\dagger(\epsilon)U(\epsilon) = I$$

Principle two is continuity:

$$U(\epsilon) = I - i\epsilon H$$

"Small changes are represented by the identity matrix minus a small change."

The Hermitian conjugate of $U(\epsilon)$:

$$U^\dagger(\epsilon) = I + i\epsilon H^\dagger$$

We plug this into $U^\dagger(\epsilon)U(\epsilon) = I$ and get:

$$\left(I + i\epsilon H^\dagger\right)(I - i\epsilon H) = I$$

$$II - Ii\epsilon H + i\epsilon H^\dagger I + \epsilon^2 H^\dagger H = I$$

$$I - Ii\epsilon H + i\epsilon H^\dagger I + \epsilon^2 H^\dagger H = I$$

We omit the second order in ϵ:

$$I - Ii\epsilon H + i\epsilon H^\dagger I = I$$

$$-H + H^\dagger = 0$$

$$H = H^\dagger$$

Out of our two principles we get, that H must be a Hermitian operator. Hermitian operators are observables having a complete set of orthonormal eigenvectors and eigenvalues.

H is the quantum Hamiltonian. Its eigenvalues are the energy of a quantum system.

We take the change of a state-vector with time

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

and apply it to the incremental change $t = \epsilon$:

$$|\psi(\epsilon)\rangle = U(\epsilon)|\psi(0)\rangle$$

$$|\psi(\epsilon)\rangle = (I - i\epsilon H)|\psi(0)\rangle$$

$$|\psi(\epsilon)\rangle = |\psi(0)\rangle - i\epsilon H|\psi(0)\rangle$$

This we can turn into a differential equation:

$$|\psi(\epsilon)\rangle = |\psi(0)\rangle - i\epsilon H|\psi(0)\rangle$$

$$|\psi(\epsilon)\rangle - |\psi(0)\rangle = -i\epsilon H|\psi(0)\rangle$$

$$\frac{|\psi(\epsilon)\rangle - |\psi(0)\rangle}{\epsilon} = -iH|\psi(0)\rangle$$

Taking the limit $\epsilon \to 0$ and being valid for all other times t too, it becomes the time derivative of the state-vector:

$$\frac{\partial\psi(t)}{\partial x} = -iH|\psi(t)\rangle$$

This is the generalized Schrödinger equation or the time-dependent Schrödinger equation.

Hamiltonian, canonical momentum and Hamiltonian:

Prerequisite

The harmonic oscillator has the kinetic energy $\frac{1}{2}m\dot{x}^2$ and the potential energy $\frac{1}{2}k\dot{x}^2$.

By replacing x with $x\sqrt{m}$ and defining $\omega = \sqrt{\frac{k}{m}}$ we get the Lagrangian L:

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2$$

The canonical momentum conjugate p to x is defined as:

$$p = \frac{\partial L}{\partial \dot{x}} = \dot{x}$$

End prerequisite

The Hamiltonian for the harmonic oscillator, written with the Lagrangian L and the canonical momentum conjugate p:

$$H = p\dot{x} - L$$

The Hamiltonian written as the sum of kinetic energy plus potential energy:

$$H = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega^2 x^2$$

We rewrite this with the canonical momentum:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

For changing H into a quantum mechanical operator, we must reinterpret x and p as operators, the position operator X and the momentum operator P.

X multiplies the wave function by the position variable x:

$$X|\psi(x)\rangle = x\psi(x)$$

P derivates:

$$P|\psi(x)\rangle \to -i\hbar\frac{\partial}{\partial x}\psi(x)$$

We replace these in the Hamiltonian:

$$H = \frac{1}{2}\left(-i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial\psi(x)}{\partial x}\right)\right) + \frac{1}{2}\omega^2 x^2\psi(x)$$

$$H = -\frac{\hbar^2}{2}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}\omega^2 x^2\psi(x)$$

This is the quantum mechanical Hamiltonian.

Hamiltonian, conservation of Hamiltonian:

Prerequisite

The change of the expectation value of an operator L with time:

$$\frac{d}{dt}\langle L\rangle = -\frac{i}{\hbar}\langle[L,H]\rangle$$

This is often written as:

$$\frac{dL}{dt} = -\frac{i}{\hbar}[L,H]$$

Note: H is the quantum mechanical Hamiltonian, $[L,H]$ denotes the commutator $LH - HL$.

End prerequisite

The condition for the expectation value of an operator L not to change is:

$$[L,H] = 0$$

Every operator commutes with itself:

$$[H,H] = 0$$

H is conserved, the total energy of a (closed) system does not change with time.

Hamiltonian, entanglement and Hamiltonian:

Prerequisite

The spin operator $\vec{\sigma}\cdot\vec{\tau} = \sigma_x\tau_x + \sigma_y\tau_y + \sigma_z\tau_z$

The state $|sing\rangle$:

$$\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

The triple states $|T_1\rangle$, $|T_2\rangle$ und $|T_3\rangle$:

$$|T_1\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$$

$$|T_2\rangle = \frac{1}{\sqrt{2}}(|uu\rangle + |dd\rangle)$$

$$|T_3\rangle = \frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle)$$

The Hamilton-operator for the 2-spin-system:

$$H = \frac{\omega\hbar}{2}\vec{\sigma}\cdot\vec{\tau}$$

The entangled state $|sing\rangle$ is eigenvector of the spin operator $\vec{\sigma}\cdot\vec{\tau}$ with eigenvalue 3.

The entangled states $|T_1\rangle$, $|T_2\rangle$ und $|T_3\rangle$ are eigenvectors of the spin operator $\vec{\sigma}\cdot\vec{\tau}$ with each eigenvalue 1.

End prerequisite

We apply the Hamiltonian to the state $|sing\rangle$:

$$H|sing\rangle = \frac{\omega\hbar}{2}\vec{\sigma}\cdot\vec{\tau}|sing\rangle = \frac{3\omega\hbar}{2}|sing\rangle$$

Applying the Hamiltonian to a state vector gives the energy of this state. The energy of $|sing\rangle$ = $\frac{3\omega\hbar}{2}$.

Analog the energy of each entangled state $|T_1\rangle$, $|T_2\rangle$ und $|T_3\rangle$ is $\frac{\omega\hbar}{2}$.

Hamiltonian for harmonic oscillator:

The classical Hamiltonian:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

The quantum mechanical Hamiltonian:

$$H = -\frac{\hbar^2}{2}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}\omega^2 x^2\psi(x)$$

We care about the energy levels. The time-independent Schrödinger equation:

$$H|\psi_E\rangle = E|\psi_E\rangle$$

Note: the index E indicates that $|\psi_E\rangle$ is eigenvector for a particular eigenvalue E.

We insert the Hamiltonian:

$$-\frac{\hbar^2}{2}\frac{\partial^2\psi_E(x)}{\partial x^2} + \frac{1}{2}\omega^2 x^2\psi_E(x) = E\psi_E(x)$$

To solve this equation, we must:

- Find the values of E that permit a mathematical solution,
- Find eigenvectors and eigenvalues of energy.

This is no simple task, but most solutions can be sorted out because they make physically no sense. We need a solution $\psi_E(x)$ that can be normalized:

$$\int_{-\infty}^{\infty}\psi_E(x)\,dx = 1$$

A function that works is:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

This is the harmonic oscillator ground state function.

We check this by applying the Hamiltonian to this function:

$$H|\psi_0(x)\rangle = \frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2}\left(1 - \frac{x^2\omega}{\hbar}\right) + \frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2} =$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(\frac{\hbar\omega}{2} - \frac{x^2\omega^2}{2}\right) + \frac{x^2\omega^2}{2} e^{-\frac{\omega}{2\hbar}x^2} =$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(\frac{\hbar\omega}{2} - \frac{x^2\omega^2}{2} + \frac{x^2\omega^2}{2}\right) =$$

$$\frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2} \coloneqq E_0\psi_0(x)$$

We get the energy E of the ground state:

$$E_0 = \frac{\hbar\omega}{2}$$

To find the other energy levels of the harmonic oscillator, we rewrite the Hamiltonian in terms of position operator X and momentum operator P:

$$H = \frac{P^2 + \omega^2 X^2}{2}$$

We use the property of the commutation relation $[X, P] = (XP - PX) = i\hbar$ and get:

$$H \sim \frac{1}{2}(P + i\omega X)(P - i\omega X)$$

As X and P does not commute, we get the correction term $i\hbar$ and can complete:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{\hbar\omega}{2}$$

Note: $\frac{\hbar\omega}{2}$ is the zero-energy level of the harmonic oscillator.

$(P + i\omega X)$ called the raising operator:

$$a^+ \coloneqq \frac{i}{\sqrt{2\hbar\omega}}(P + i\omega X)$$

$(P - i\omega X)$ the lowering operator or annihilation operator:

$$a^- \coloneqq \frac{i}{\sqrt{2\hbar\omega}}(P - i\omega X)$$

Note: the factor $\frac{i}{\sqrt{2\hbar\omega}}$ comes out of historical reasons.

The product of raising operator and annihilation operator is called the number operator:

$$N \coloneqq a^+ a^-$$

The three operators have important properties.

For reasons of simplicity we rewrite the eigenvalues by numbering them n and rewrite the eigenvectors:

$$e.g. |\psi_1\rangle \rightarrow |1\rangle$$

With this convention the raising operator a^+ applied to the ground state function gives the next energy level:

$$a^+|n\rangle = |n+1\rangle$$

The lowering operator a^- applied to any state except the ground state gives:

$$a^-|n\rangle = |n-1\rangle$$

The lowering operator a^- applied to the ground state gives:

$$a^-|0\rangle = 0$$

Note: $|0\rangle$ is the ground state wave function $e^{-\frac{\omega}{2\hbar}x^2}$ with energy $\frac{\hbar\omega}{2}$. The annihilation operator destroys this to zero.

The numbering operator N applied to any state gives the energy or the "number" of the respective state:

$$N|n\rangle = n|n\rangle$$

With the operators a^-, a^- and N we find the entire spectrum of harmonic oscillator energy levels:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

Hamiltonian, motion of particles and Hamiltonian:

We take the momentum operator $P := -i\hbar\frac{\partial}{\partial x}$ and build a simple Hamiltonian with c being a constant:

$$H = cP$$

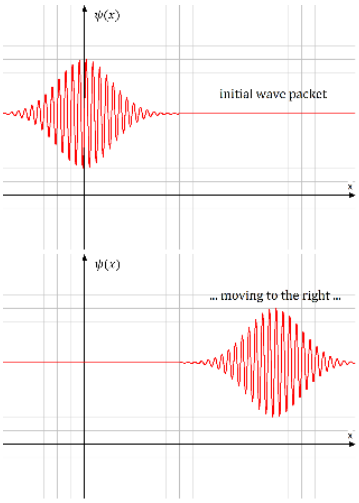
The time-dependent Schrödinger equation:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

We insert the Hamiltonian:

$$i\hbar\frac{\partial|\psi(x,t)\rangle}{\partial t} = -ci\hbar\frac{\partial|\psi(x,t)\rangle}{\partial x}$$

$$\frac{\partial|\psi(x,t)\rangle}{\partial t} = -c\frac{\partial|\psi(x,t)\rangle}{\partial x}$$



Note: $\psi(x,t)$ is function of two variables x and t.

Any function of the argument $(x-ct)$ is a solution to this time-dependent Schrödinger equation.

We need a function that is concentrated at a finite area in space:

$$\int_{-\infty}^{\infty}\psi^*(x)\psi(x)dx = 1$$

Let $\psi(x)$ be a wave packet like in the schematic on the right.

If we replace the argument (x) by $(x-ct)$ we get with increasing time t a left shift of the argument, so the function moves to the right with "speed" c.

Hamiltonian, nonrelativistic free particles and Hamiltonian:

A nonrelativistic free particle has kinetic energy:

$$T = \frac{1}{2}mv^2$$

In terms of momentum $p = mv$:

$$T = \frac{p^2}{2m}$$

The Hamiltonian is the energy:

$$H = \frac{p^2}{2m}$$

We replace the classical momentum by the momentum operator P:

$$P = -i\hbar\frac{\partial}{\partial x}$$

We get the quantum Hamiltonian:

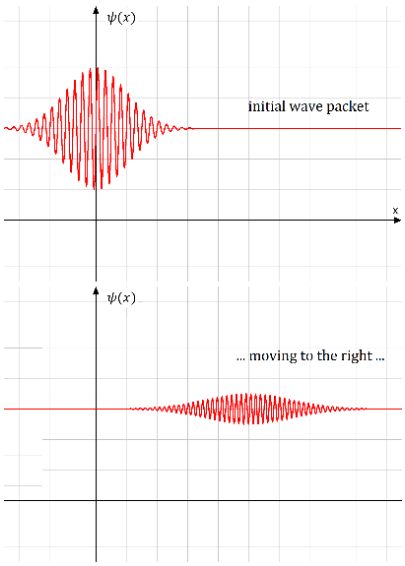
$$H = \frac{P^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

We use the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle \rightarrow i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

We insert the quantum Hamiltonian:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$



This is the traditional Schrödinger equation for a nonrelativistic free particle. The solution gives a wave packet with different wavelengths, moving with different velocities.

The effect: dispersion of the wave packet, it tends to spread out and fall apart.

Hamiltonian, quantum Hamiltonian:

Prerequisite

The change of the state-vector with time:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

U is called the time-development operator for the system and U must be unitary.

End prerequisite

The basic idea is that of an incremental change in time, valid both for classical physics and quantum mechanics.

We need two principles.

Principle one is unitarity:

$$U^\dagger(\epsilon)U(\epsilon) = I$$

Principle two is continuity:

$$U(\epsilon) = I - i\epsilon H$$

“Small changes are represented by the identity matrix minus a small change.”

The Hermitian conjugate of U:

$$U^\dagger(\epsilon) = I + i\epsilon H^\dagger$$

We plug this into $U^\dagger(\epsilon)U(\epsilon) = I$ and get:

$$\left(I + i\epsilon H^\dagger\right)(I - i\epsilon H) = I$$

$$II - Ii\epsilon H + i\epsilon H^\dagger I + \epsilon^2 H^\dagger H = I$$

$$I - Ii\epsilon H + i\epsilon H^\dagger I + \epsilon^2 H^\dagger H = I$$

We omit the second order in ϵ:

$$I - Ii\epsilon H + i\epsilon H^\dagger I = I$$

$$-H + H^\dagger = 0$$

$$H = H^\dagger$$

H must be a Hermitian operator. Hermitian operators are observables having a complete set of orthonormal eigenvectors and eigenvalues.

H is the quantum Hamiltonian. Its eigenvalues are the energy of a quantum system.

We take the change of a state-vector with time

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

and apply it to the incremental change $t = \epsilon$:

$$|\psi(\epsilon)\rangle = U(\epsilon)|\psi(0)\rangle$$

$$|\psi(\epsilon)\rangle = (I - i\epsilon H)|\psi(0)\rangle$$

$$|\psi(\epsilon)\rangle = |\psi(0)\rangle - i\epsilon H|\psi(0)\rangle$$

This we can turn into a differential equation:

$$|\psi(\epsilon)\rangle = |\psi(0)\rangle - i\epsilon H|\psi(0)\rangle$$

$$|\psi(\epsilon)\rangle - |\psi(0)\rangle = -i\epsilon H|\psi(0)\rangle$$

$$\frac{|\psi(\epsilon)\rangle - |\psi(0)\rangle}{\epsilon} = -iH|\psi(0)\rangle$$

Taking the limit $\epsilon \to 0$ it becomes the time derivative of the state-vector:

$$\frac{\partial\psi(t)}{\partial x} = -iH|\psi(t)\rangle$$

This is the generalized Schrödinger equation or the time-dependent Schrödinger equation.

If we do a dimensional check, we see that there is a mismatch. The left side is of dimension $\frac{1}{t}$, the Hamiltonian (energy) is of dimension joules or $\frac{kg \cdot m^2}{s^2}$. We need a factor of dimension $\frac{kg \cdot m^2}{s}$ on the left side:

$$[\hbar] = \frac{kg \cdot m^2}{s}$$

Note: $\hbar = \frac{h}{2\pi} = 1{,}054571726 \ldots \times 10^{-34}\ \frac{kg \cdot m^2}{s}$

With this we complete the time-dependent Schrödinger equation to make it dimensionally correct:

$$\hbar\frac{\partial\psi(t)}{\partial x} = -iH|\psi(t)\rangle$$

Hamiltonian of spin in magnetic field:

Prerequisite

The Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Let $|\psi(t)\rangle$ be a state vector and L an operator. The change of the expectation value of an operator L with time:

$$\frac{d}{dt}\langle\psi(t)|L|\psi(t)\rangle = -\frac{i}{\hbar}\langle[L, H]\rangle$$

Written in shorthand form:

$$\dot{L} = -\frac{i}{\hbar}\langle[L, H]\rangle$$

End prerequisite

When a classical spin (a charged rotor) is put into a magnetic field, it has an energy depending on its orientation. It is proportional to the dot product of the spin and the magnetic field.

The quantum version:

$$H \sim \vec{\sigma} \cdot \vec{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$$

Note: σ_x, σ_y and σ_z represents the components of the spin operator.

The magnetic field lies along the z axis. We absorb all numerical constants without $\hbar$ into a single constant ω and get the quantum Hamiltonian:

$$H = \frac{\hbar\omega}{2}\sigma_z$$

We search how the expectation value of the spin changes with time, $\langle\sigma_x(t)\rangle$, $\langle\sigma_y(t)\rangle$ and $\langle\sigma_z(t)\rangle$. We use:

$$\langle\dot{\sigma_x}\rangle = -\frac{i}{\hbar}\langle\sigma_x, H\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i}{\hbar}\langle[\sigma_y, H]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i}{\hbar}\langle[\sigma_z, H]\rangle$$

We plug in the quantum Hamiltonian $H = \frac{\hbar\omega}{2}\sigma_z$ and get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i\omega}{2}\langle[\sigma_y, \sigma_z]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i\omega}{2}\langle[\sigma_z, \sigma_z]\rangle$$

We check this explicitly for $\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$ by using the Pauli-matrices:

$$[\sigma_x, \sigma_z] = \sigma_x\sigma_z - \sigma_x\sigma_z =$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} =$$

$$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} - \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = \begin{pmatrix}0 & -2\\ 2 & 0\end{pmatrix} =$$

$$-2i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = -2i\sigma_y$$

We get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle -2i\sigma_y\rangle = -\omega\langle\sigma_y\rangle$$

The results:

$$\langle\dot{\sigma_x}\rangle = -\omega\langle\sigma_y\rangle$$

$$\langle\dot{\sigma_y}\rangle = \omega\langle\sigma_x\rangle$$

$$\langle\dot{\sigma_z}\rangle = 0$$

In classical mechanics, the x and y components of angular momentum are precessing around the z axis.

In quantum mechanics the expectation values for $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ will be precessing, but each single measurement will always give +1 or -1. The expectation value for $\langle\sigma_z\rangle$ remains unchanged.

Hamiltonian, time evolution of a system and Hamiltonian:

In quantum mechanics the Hamiltonian controls the time evolution of a system by the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\psi(t)}{\partial x} = H|\psi(t)\rangle$$

Hamiltonian operator, Schrödinger ket and Hamiltonian operator:

Prerequisite

We have a Hamiltonian and we know the initial state $|\psi(0)\rangle$ of a system.

End prerequisite

We find the eigenvalues and eigenvectors of H by solving the time-independent Schrödinger equation:

$$H|E_j\rangle = E_j|E_j\rangle$$

Note: $|E_j\rangle$ is eigenvector to H with eigenvalue E_j.

We want to rewrite $|\psi(0)\rangle$ in terms of eigenvectors $|E_j\rangle$:

$$|\psi(0)\rangle = \sum_j \alpha_j(0)|E_j\rangle$$

For this we need the initial coefficients $\alpha_j(0)$:

$$\alpha_j(0) = \langle E_j|\psi(0)\rangle$$

As the eigenvectors $|E_j\rangle$ build a basis of the state and this basis does not change with time, the coefficients α_j must change with time:

$$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$$

We get the "Schrödinger ket":

$$|\psi(t)\rangle = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}|E_j\rangle$$

Hamilton's equations:

In both classical and quantum mechanics states change in a way that information and distinctions are never erased.

In classical mechanics, this principle led to Hamilton's equations and Liouville's theorem.

In quantum mechanics, this principle led to unitarity and in the end to the general Schrödinger equation:

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial x} = H|\psi(t)\rangle$$

Note: $|\psi(t)\rangle$ is a state vector, H is the Hamiltonian.

Harmonic oscillator:

Harmonic oscillator, annihilation (lowering) operators:

The Hamiltonian can be expressed in terms of the momentum operator P and position operator X:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2) = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{i\omega}{2}$$

Note: $\frac{i\omega}{2}$ is necessary because P and X do not commute.

$(P + i\omega X)$ is called the raising operator, $(P - i\omega X)$ the lowering operator, written as a^+ and a^-. The raising operator a^+ shifts the energy level of the harmonic oscillator to the next possible higher level, the lowering operator a^- to the next possible lower level. Applying the lowering operator to the ground level with Energy $E_0 = \frac{\omega\hbar}{2}$ annihilates this ground level. Symbolically this is expressed as

$$a^-|0\rangle = 0$$

with $|0\rangle$ representing the ground level.

Harmonic oscillator, classical description:

Graphic courtesy Wikipedia by Svjo

For convenience we switch the coordinates from y to x. Then kinetic and potential energy are $\frac{1}{2}m\dot{x}^2$ and $\frac{1}{2}kx^2$.

For more convenience we aggregate the variable x to

$$x \coloneqq \sqrt{m}x$$

and use a new variable, the frequency of the oscillator:

$$\omega = \sqrt{\frac{k}{m}}$$

The Lagrangian is kinetic energy minus potential energy:

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2$$

In this form, oscillators are distinguished from each other only by their frequency ω.

From the Lagrangian we can work out the equations of motion. We have a one-dimensional system with one Lagrangian:

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

Left side:

$$\frac{\partial L}{\partial x} = -\omega^2 x$$

Right side:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} =$$

$$\frac{d}{dt}\frac{\partial}{\partial \dot{x}}\left(\frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2\right) =$$

$$\frac{d}{dt}(\dot{x}) = \ddot{x}$$

We combine both results:

$$\ddot{x} = -\omega^2 x$$

This is a differential equation with the general solution:

$$x = A\,cos(\omega t) + B\,sin(\omega t)$$

Harmonic oscillator, creation operators:

The Hamiltonian expressed in terms of operators X, the observable for position and P, the observable for momentum:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2)$$

(*This is a classical as well as a quantum mechanical Hamiltonian, so it would be correct to use the classical lowercase symbols p and x.*)

The idea is to use the properties of X and P, especially the commutation relation $[X, P] = i\hbar$ to construct two (three) new operators, called creation (or raising) operator, annihilation (or lowering) operator and number operator. The names are program. The raising operator shall produce a new eigenvector that has the next higher energy level, the lowering operator shall produce a new eigenvector that has the next lower energy level. The number operator returns the "number" of the energy level.

The construction process.

Using complex numbers, we can split up the sum according to $a^2 + b^2 = (a + ib)(a - ib)$ to

$$H \sim \frac{1}{2}(P + i\omega X)(P - i\omega X)$$

and that is almost correct, because of the quantum mechanically behavior of X and P: they don't commute. The problem are the products PX and XP.

We expand the Hamiltonian:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + i\omega XP - i\omega PX - i^2\omega^2 X^2) =$$

$$\frac{1}{2}(P^2 + \omega^2 X^2) + \frac{1}{2}i\omega[X, P]$$

We know the value of the commutator: $[X, P] = i\hbar$ and get:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + \omega^2 X^2) - \frac{1}{2}\hbar\omega$$

Our correct Hamiltonian:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{1}{2}\hbar\omega$$

We now can define the creation operator a^+ and the annihilating operator a^-:

$$a^- \coloneqq (P - i\omega X)$$

$$a^+ \coloneqq (P + i\omega X)$$

Note: the number operator is defined as $N \coloneqq a^+ a^-$ and "returns" the number of the energy level.

Harmonic oscillator, energy levels:

The quantum Hamiltonian for the harmonic oscillator (time-independent Schrödinger equation):

$$H|\psi_E\rangle = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi_E(x) + \frac{1}{2}\omega^2 x^2 \psi_E(x) = E\psi_E(x)$$

To solve this equation, we must find the allowable values of E that permit a mathematical solution, filter out the solutions that make physically sense and find the eigenvectors and eigenvalues for the energy.

Physical solutions of the Schrödinger equation must be normalizable.

The solution for the ground state energy eigenfunction is:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

Applying the Hamiltonian to this eigenfunction delivers the eigenvalue:

$$H|\psi_0(x)\rangle = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi_0(x) + \frac{1}{2}\omega^2 x^2 \psi_0(x) =$$

$$-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}e^{-\frac{\omega}{2\hbar}x^2} + \frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2} =;$$

Left part (without the multiplying factor $-\frac{\hbar^2}{2}$):

$$\frac{\partial}{\partial x}e^{-\frac{\omega}{2\hbar}x^2} = -\frac{\omega}{\hbar}xe^{-\frac{\omega}{2\hbar}x^2}$$

$$\frac{\partial}{\partial x}\left(-\frac{\omega}{\hbar}xe^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$-\frac{\omega}{\hbar}e^{-\frac{\omega}{2\hbar}x^2} + \left(-\frac{\omega}{\hbar}x\right)\left(-\frac{\omega}{\hbar}x\right)e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-\frac{\omega}{\hbar}e^{-\frac{\omega}{2\hbar}x^2} + \left(-\frac{\omega}{\hbar}x\right)^2 e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\left(\frac{\omega^2}{\hbar^2}x^2 - \frac{\omega}{\hbar}\right)e^{-\frac{\omega}{2\hbar}x^2}$$

multiplying the factor $-\frac{\hbar^2}{2}$:

$$-\frac{\hbar^2}{2}\left(\frac{\omega^2}{\hbar^2}x^2 - \frac{\omega}{\hbar}\right)e^{-\frac{\omega}{2\hbar}x^2} =$$

$$\left(-\frac{\omega^2}{2}x^2 + \frac{\omega\hbar}{2}\right)e^{-\frac{\omega}{2\hbar}x^2}$$

Right part:

$$\frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2}$$

Merging:

$$\left(-\frac{\omega^2}{2}x^2+\frac{\omega\hbar}{2}\right)e^{-\frac{\omega}{2\hbar}x^2}+\frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2}=$$

$$\left(-\frac{\omega^2}{2}x^2+\frac{\omega\hbar}{2}+\frac{1}{2}\omega^2 x^2\right)e^{-\frac{\omega}{2\hbar}x^2}=$$

$$\frac{\omega\hbar}{2}e^{-\frac{\omega}{2\hbar}x^2}=$$

$$\frac{\omega\hbar}{2}\psi_0(x)$$

$\psi_0(x)$ is eigenfunction to the Hamiltonian operator with eigenvalue $\frac{\omega\hbar}{2}$.

We can rewrite the Hamiltonian in terms of the position operator X and the momentum operator P:

$$H=\frac{P^2+\omega^2X^2}{2}$$

We write the sum as complex product:

$$H=\frac{1}{2}(P+i\omega X)(P-i\omega X)+\frac{\omega\hbar}{2}$$

Note: $\frac{\omega\hbar}{2}$ is needed because the product $\frac{1}{2}(P+i\omega X)(P-i\omega X)$ does not exactly give $\frac{P^2+\omega^2X^2}{2}$

The two factors $(P+i\omega X)$ and $(P-i\omega X)$ are the raising operator a^+ and lowering operator a^-.
The official definitions are:

$$a^+=\frac{-i}{\sqrt{2\omega\hbar}}(P+i\omega X)$$

$$a^-=\frac{i}{\sqrt{2\omega\hbar}}(P-i\omega X)$$

The lowering operator applied to the ground state wave-function annihilates it:

$$a^-\big(\psi_0(x)\big)=0$$

The lowering operator applied to any other state produces an eigenvector whose eigenvalue is one unit lower. Analog the raising operator applied to any state produces an eigenvector whose eigenvalue is on unit higher. With this we get all energy levels of the Harmonic oscillator.

Harmonic oscillator, ground state:

Prerequisite

The Hamiltonian:

$$H|\psi(x)\rangle=-\frac{\hbar^2}{2}\frac{\partial^2\psi(x)}{\partial x^2}+\frac{1}{2}\omega^2x^2\psi(x)$$

The Hamiltonian gives the energy of the state:

$$H|\psi(x)\rangle \coloneqq E|\psi(x)\rangle$$

End prerequisite

In classical physics the lowest possible energy level for a harmonic oscillator is zero because the Hamiltonian has a x^2 term and a p^2 term.

In quantum mechanics the uncertainty principle says that it is not possible to set both x and p to zero. Best that can be done is to find a state in which x and p are not too spread out.

The lowest energy level the ground state $\psi_0(x)$ is not zero.

The ground state wave function:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

To calculate the energy of the ground state we apply the Hamiltonian:

$$H|\psi_0(x)\rangle = -\frac{\hbar^2}{2}\frac{\partial^2 e^{-\frac{\omega}{2\hbar}x^2}}{\partial x^2} + \frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2}$$

Omitting $-\frac{\hbar^2}{2}$ in the left term we get:

$$\frac{\partial^2}{\partial x^2} e^{-\frac{\omega}{2\hbar}x^2} = \frac{\partial}{\partial x}\left(-\frac{x\omega}{\hbar}\right) e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-\frac{\omega}{\hbar}\frac{\partial}{\partial x} x e^{-\frac{\omega}{2\hbar}x^2} = -\frac{\omega}{\hbar}\left(e^{-\frac{\omega}{2\hbar}x^2} + x\left(-\frac{x\omega}{\hbar}\right) e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$-\frac{\omega}{\hbar} e^{-\frac{\omega}{2\hbar}x^2}\left(1 - \frac{x^2\omega}{\hbar}\right)$$

Reinserting $-\frac{\hbar^2}{2}$:

$$\frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2}\left(1 - \frac{x^2\omega}{\hbar}\right)$$

The right term remains:

$$\frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2}$$

Combining both terms:

$$H|\psi_0(x)\rangle = \frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2}\left(1 - \frac{x^2\omega}{\hbar}\right) + \frac{1}{2}\omega^2 x^2 e^{-\frac{\omega}{2\hbar}x^2} =$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(\frac{\hbar\omega}{2} - \frac{x^2\omega^2}{2}\right) + \frac{x^2\omega^2}{2} e^{-\frac{\omega}{2\hbar}x^2} =$$

$$e^{-\frac{\omega}{2\hbar}x^2}\left(\frac{\hbar\omega}{2} - \frac{x^2\omega^2}{2} + \frac{x^2\omega^2}{2}\right) =$$

$$\frac{\hbar\omega}{2} e^{-\frac{\omega}{2\hbar}x^2}$$

As $H|\psi_0(x)\rangle = E_0|\psi_0(x)\rangle$ we have the energy E of the ground state:

$$E_0 = \frac{\hbar\omega}{2}$$

Harmonic oscillator, prevalence in physics:

In contrast to objects like a hydrogen atom the harmonic oscillator is a mathematical framework for understanding a huge number of phenomena. What is characterizing these systems is that the potential energy function looks like a parabola:

$$V(x) = \frac{k}{2}x^2$$

The force on an object is minus the gradient of V:

$$F = -kx$$

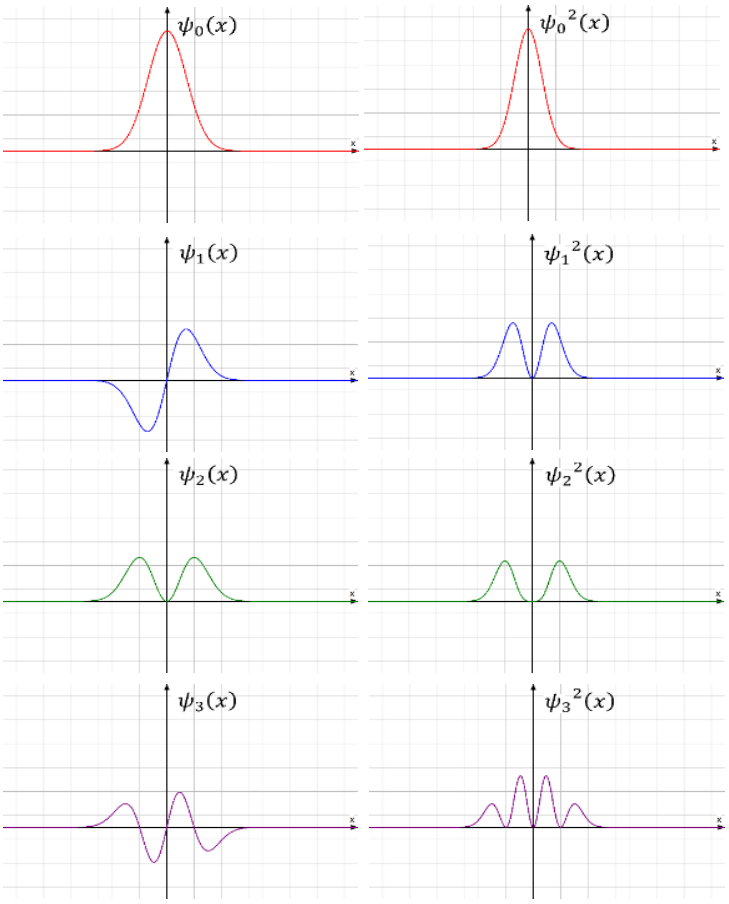
Harmonic oscillators are prevalent in physics because almost any smooth function looks like a parabola close to local extrema, a minimum or maximum of the function.

Many kinds of systems are characterized by an energy function that can be approximated by a quadratic function of some variable representing a displacement from equilibrium. When disturbed, these systems will oscillate about the equilibrium point.

Examples:

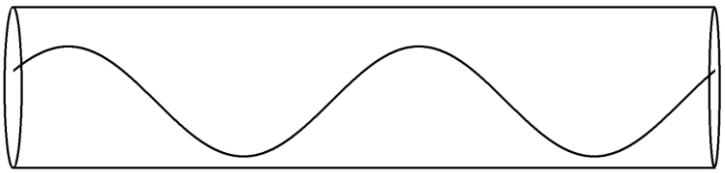
- If an atom situated in a crystal lattice is displaced slightly from its equilibrium position, it gets pushed back with an approximately linear restoring force.
- The electric current in a circuit often oscillates with a characteristic frequency. The mathematics for describing this is identical to the mathematics of masses attached to springs.
- If the surface of a pond is disturbed, waves appear on the surface. The oscillation of the water particles can be described as harmonic oscillation.
- The mathematics to describe electromagnetic waves is the same mathematics that describes oscillation particles.

Harmonic oscillator, quantization and harmonic oscillator:



Harmonic oscillator Eigenfunctions. Amplitudes are shown on the left, probabilities on the right. The higher-energy wave functions oscillate faster and are more spread out.

Consider the example of electromagnetic radiation in a cavity, a region of space bracketed by a pair of perfectly reflecting mirrors that keep the radiation bouncing endlessly back and forth.



There is only one important number associated with a harmonic oscillator, its frequency and the corresponding wavelength:

$$\omega = \frac{2\pi c}{\lambda}$$

In classical physics, the frequency is just the frequency.

In quantum mechanics, the frequency determines the quantum energy of the oscillator. The energy contained in waves of length λ has to be:

$$\left(n + \frac{1}{2}\right)\hbar\omega$$

The term $\frac{1}{2}\hbar\omega$ is the zero-point energy which we ignore here. Then the energy of waves of length λ becomes:

$$\frac{2\pi\hbar c}{\lambda} \cdot n$$

The energy of an electromagnetic wave is quantized in indivisible units of $\frac{2\pi\hbar c}{\lambda}$. These units are called photons, the quantized unit of energy in a quantum harmonic oscillator.

We can describe this another way. Photons can be thought of as particles, a wave excited to its nth quantum state can be thought of as a collection of n photons. In this picture, the energy of a single photon is what is needed to add one more unit:

$$E(\lambda) = \frac{2\pi\hbar c}{\lambda}$$

Harmonic oscillator, quantum mechanical description:

We try to translate the classical harmonic oscillator into a quantum mechanical one. For this we need a space of states. A particle moving on a line is represented by a wave function $\psi(x)$. $\psi(x)$ is defined in such a way that $\psi^*(x)\psi(x)$ is the probability density to find a particle at position x:

$$\psi^*(x)\psi(x) = P(x)$$

Note: $\psi^*(x)$ is the complex conjugated to $\psi(x)$.

A probability density has the restriction:

$$\int_{-\infty}^{\infty} P(x)dx = 1$$

Our function $\psi^*(x)\psi(x)$ must fulfill this condition:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx = 1$$

Note: this condition is called normalizable.

The (classical) Hamiltonian is kinetic energy plus potential energy, the total energy:

$$H = \frac{1}{2}\dot{p}^2 + \frac{1}{2}\omega^2 x^2$$

In quantum mechanics, we need to represent observables as operators. We do not have a velocity operator, so we have to recast in terms of position operator and momentum operator.

The position operator X multiplies the wave function by the position variable:

$$X|\psi(x)\rangle \coloneqq x\psi(x)$$

Accordingly:

$$X^2|\psi(x)\rangle \coloneqq x^2\psi(x)$$

The momentum operator differentiates:

$$P|\psi(x)\rangle \coloneqq -i\hbar\frac{\partial}{\partial x}\psi(x)$$

Accordingly:

$$P^2|\psi(x)\rangle \coloneqq -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x) = -\hbar^2\frac{\partial^2}{\partial x^2}\psi(x)$$

We insert this in the Hamiltonian:

$$H = \frac{1}{2}\dot{p}^2 + \frac{1}{2}\omega^2x^2 \rightarrow -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}\omega^2x^2\psi(x)$$

We get the quantum mechanical Hamiltonian:

$$H = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}\omega^2x^2\psi(x)$$

Harmonic oscillator, Schrödinger equation and harmonic oscillator:

The time-dependent Schrödinger equation:

$$i\frac{\partial\psi}{\partial t} = \frac{1}{\hbar}H\psi$$

We insert the quantum mechanical Hamiltonian:

$$i\frac{\partial\psi}{\partial t} = -\frac{\hbar}{2}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2\hbar}\omega^2x^2\psi$$

Note: the equation is complex valued.

If we know ψ, both real and imaginary parts at some point in time, we can predict what it will be next in future. Under certain circumstances, ψ will form a wave packet that moves around like a harmonic oscillator.

Harmonic oscillator, wave functions and harmonic oscillator:

Prerequisite

The annihilation or lowering operator:

$$a^- \coloneqq \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

The raising operator:

$$a^+ \coloneqq \frac{i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

The position operator X multiplies the wave function by the position variable:

$$X|\psi(x)\rangle \coloneqq x\psi(x)$$

The momentum operator P differentiates:

$$P|\psi(x)\rangle \coloneqq -i\hbar\frac{\partial}{\partial x}\psi(x)$$

End prerequisite

We begin with the ground state of the harmonic oscillator:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

The raising operator acting on the ground state:

$$(P + i\omega X)e^{-\frac{\omega}{2\hbar}x^2}$$

Note: for better readability we omit the constant factor $\frac{i}{\sqrt{2\omega\hbar}}$.

We replace the operators:

$$i\left(-\hbar\frac{\partial}{\partial x} + \omega x\right)e^{-\frac{\omega}{2\hbar}x^2} =$$

$$i\hbar\frac{\omega x}{\hbar}e^{-\frac{\omega}{2\hbar}x^2} + i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$i\omega x e^{-\frac{\omega}{2\hbar}x^2} + i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$2i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$2i\omega x\psi_0(x) = \psi_1(x)$$

Applying the raising operator to the ground state we get the next excited state.

The presence of the factor x in the first excited state causes the wave function of the first excited state to have a zero (a node) at $x = 0$.

We repeat this process. Applying the raising operator to the first excited state will give the second excited state. Again, we omit the constant factor $\frac{i}{\sqrt{2\omega\hbar}}$ and get:

$$i\left(-\hbar\frac{\partial}{\partial x} + \omega x\right)\psi_1(x) =$$

$$i\left(-\hbar\frac{\partial}{\partial x} + \omega x\right)x\psi_0(x) =$$

$$-i\hbar\frac{\partial}{\partial x}(x\psi_0(x)) + i\omega x^2\psi_0(x) =$$

$$-i\hbar\left(\psi_0(x) + x\frac{\partial}{\partial x}\psi_0(x)\right) + i\omega x^2\psi_0(x) =$$

$$-i\hbar\left(\psi_0(x) - \frac{\omega x^2}{\hbar}\psi_0(x)\right) + i\omega x^2\psi_0(x) =$$

$$\left(-i\hbar + \frac{i\hbar\omega x^2}{\hbar} + i\omega x^2\right)\psi_0(x) =$$

$$(-i\hbar + i\omega x^2 + i\omega x^2)\psi_0(x) =$$

$$(-i\hbar + 2i\omega x^2)\psi_0(x)$$

Again, omitting the constant factor i we get the result

$$(P + i\omega X)\psi_1(x) = \psi_2(x)$$

with:

$$\psi_2(x) = (-\hbar + 2\omega x^2)\psi_0(x)$$

In summa we have the first 3 energy states of the harmonic oscillator:

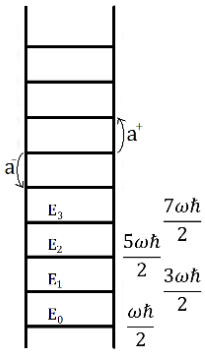
$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

$$\psi_1(x) = 2i\omega x\psi_0(x)$$

$$\psi_2(x) = (-\hbar + 2\omega x^2)\psi_0(x)$$

Note: there may be some constants missing.

Harmonic oscillator, energy level ladder/tower:



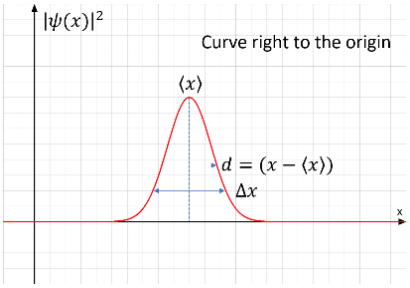
We can view at the rising sequence of energy levels as a ladder, beginning with the lowest energy level as eigenvalue of eigenfunction $\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$ and then stepping higher. The difference between two steps is always $\hbar\omega$.

Heisenberg, Werner:

Heisenberg liked algebra, matrices and, had he known what to call then, linear operators. Erwin Schrödinger, in contrast, thought in terms of wave functions and wave equations, the Schrödinger equation being one famous example.

The two ways of thinking are not contradictory because functions form a vector space and derivatives are operators. This connection is not intuitive and hard to bridge.

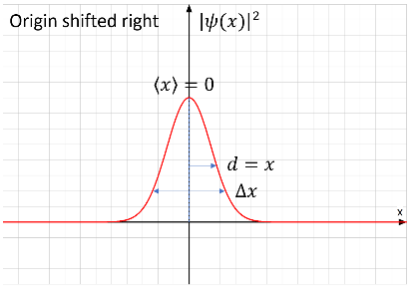
Heisenberg Uncertainty Principle:



Prerequisite:

A general statistical theorem allows that we always can modify an operator A in a way that its expectation value is zero. In this case $\triangle A$ is the uncertainty in A. This simplifies calculation.

End prerequisite



The Heisenberg Uncertainty Principle in its original form deals with position and momentum of a particle and can be expanded into a general principle that applies to any two observables not commuting: the product of the uncertainty of two operators cannot be less than $\frac{\hbar}{2}$.

Let A and B be two observables, then:

$$\triangle A \triangle B \geq \frac{1}{2}|\langle\psi|[AB]|\psi\rangle|$$

The product of the uncertainties cannot be smaller than half the magnitude of the expectation value of the commutator.

If the commutator of A and B is not zero, both observables cannot simultaneous be certain.

For the case of position operator X and momentum operator P we know that applying the commutator onto any wave function $\psi(x)$ results in:

$$[X, P]\psi(x) = i\hbar\psi(x)$$

We express this by writing:

$$[X, P] = i\hbar$$

The fact that X and P do not commute is the key to understanding that they are not simultaneously measurable. We insert them into:

$$\triangle X \triangle P \geq \frac{1}{2}|\langle\psi|[XP]|\psi\rangle|$$

We get:

$$\triangle X \triangle P \geq \frac{1}{2}|\langle\psi|i\hbar|\psi\rangle| =$$

$$\frac{1}{2}|i\hbar\langle\psi|\psi\rangle| = \frac{1}{2}|i\hbar| = \frac{1}{2}\hbar$$

$$\triangle X \triangle P \geq \frac{1}{2}\hbar$$

Remember $|\psi\rangle$ is normalized.

This is the Heisenberg Uncertainty Principle.

Hermite, Charles:

Charles Hermite (1822 – 1901) was a French mathematician who did research concerning number theory, quadratic forms, invariant theory, orthogonal polynomials, elliptic functions, and algebra. Hermite polynomials, Hermite interpolation, Hermite normal form, Hermitian operators, and cubic Hermite splines are named in his honor. *(Courtesy Wikipedia)*

Hermite polynomials:

Prerequisite:

The energy states of the harmonic oscillator, beginning with the ground state:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

$$\psi_1(x) = 2i\omega x\psi_0(x)$$

$$\psi_2(x) = (-\hbar + 2\omega x^2)\psi_0(x)$$

...

End prerequisite

Each eigenfunction of the energy states is a polynomial in x multiplied by $e^{-\frac{\omega}{2\hbar}x^2}$ or $\psi_0(x)$. These polynomials are called the Hermite polynomials.

Note: the exponential functions ensures that the functions converge fast enough to zero to fulfill normalization condition.

Note: this leads to a small but finite chance of finding a particle outside any borders the potential energy function defines.

Hermitian

density matrices as Hermitian matrices:

Density matrices are Hermitian:

$$\rho_{aa'} = \rho^*_{a'a}$$

Note: Hermitian matrices can be diagonalized by use of a special basis.

Momentum and position as Hermitian matrices:

The momentum operator P and position operator X are Hermitian matrices.

Projection operators as Hermitian matrices:

Let $|\psi\rangle$ be a normalized ket with its corresponding bra $\langle\psi|$.

The outer product:

$$|\psi\rangle\langle\psi|$$

is called a projection operator.

Projection operators are Hermitian (a Hermitian matrix).

Hermitian conjugation:

You take a matrix M, transpose it $M \to M^T$ and complex conjugate the result $M^T \to (M^T)^*$.

$(M^T)^*$ is called the Hermitian conjugate to M, written as $M^\dagger$.

Note: a matrix M that satisfies $M^\dagger M = I$ is called unitary.

Hermitian matrix:

An example of a 2×2 Hermitian matrix with r_1 and r_2 real numbers and z a complex number:

$$\begin{pmatrix} r_1 & z \\ z^* & r_2 \end{pmatrix}$$

Any 2×2 Hermitian matrix can be written as the sum of four matrices:

$$a\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + b\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + c\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + d\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Note: a, b, c, d are real numbers.

Note: the matrices are called the Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

Note: Hermitian matrices can be diagonalized by use of a special basis.

Note: The diagonal of a Hermitian matrix only has real values.

Hermitian observable:

A Hermitian observable is an observable represented by a Hermitian matrix. Momentum P and Position X are Hermitian observables and can be represented by Hermitian matrices.

Note: by help of the "trick of resolving the identity" we can transform a wave function $\psi(x)$ in position representation into the corresponding wave function in momentum representation $\tilde{\psi}(p)$.

Hermitian operators:

1.

Operators corresponding to physical observables must be Hermitian as well as linear.

2.

Hermitian operators have a complete set of orthonormal eigenvectors and eigenvalues building a basis of the vector space.

3.

The commutator of Hermitian operators must not be Hermitian.

4.

Any 2×2 Hermitian matrix can be written as the sum of the three Pauli-matrices and the identity matrix.

5.

The differentiation operator $D \coloneqq \frac{d}{dx}$ by itself is not Hermitian. By multiplying with the imaginary unit $-i$ it becomes Hermitian:

$$-iD = -i\frac{d}{dx}$$

Hermitian operator, action on state-vector:

By sandwiching a Hermitian operator A with a state-vector $|r\rangle$:

$$\langle r|A|r\rangle$$

we get the expectation value of the state-vector – the probabilities for the outcome of each measurement A.

Hermitian operators in composite space of states:

Prerequisite

In a single-spin system of Alice we have e.g. the state vectors $|u\rangle$ and $|d\rangle$ and a Hermitian operator σ_z. The action of σ_z onto a state vector is written as e.g. $\sigma_z|d\rangle = -|d\rangle$. The same holds for Bob's system.

We combine the two systems by the tensor product. The composite state-vectors are written e.g.:

$$|du\rangle = |d\rangle \otimes |u\rangle$$

End prerequisite

Assume we have a two-spin system of each Alice and Bob with the Hermitian operator σ_z for the system of Alice and τ_z for Bob. We get the composite system by the tensor product. To properly apply the operator σ_z of Alice in the composite system we have to build the tensor product too.

For Alice: $\sigma_z \to \sigma_z \otimes I$

For Bob: $\tau_z \to I \otimes \tau_z$

Note: I is the 2×2 identity matrix.

With this we write the action of Alice's operator onto the combined system as:

$$(\sigma_z \otimes I)(|d\rangle \otimes |u\rangle) = (\sigma_z|d\rangle \otimes I|u\rangle) = (-|d\rangle \otimes |u\rangle)$$

We abbreviate this and write:

$$\sigma_z|du\rangle = -|du\rangle$$

Hermitian operators, eigenvector of Hermitian operator:

1.

If a state is eigenvector of a Hermitian operator A, then it will not be eigenvector of other operators that do not commute with A.

2.

Eigenvectors of a Hermitian operator form a complete orthonormal basis of the state, so every vector can be expressed in this basis.

3.

Let A be any Hermitian operator with basis vectors $|i\rangle$. We can rewrite the identity operator I:

$$I = \sum_i |i\rangle\langle i|$$

Note: this is called "resolving the identity".

Hermitian operator, linear operator as Hermitian operator:

Prerequisite

An operator A is called linear:

a) $A(f(x)) = h(x)$
b) $A\big(f(x) + g(x)\big) = A\big(f(x)\big) + A(g(x))$
c) $A\big(z \cdot f(x)\big) = z \cdot A(f(x))$

Note: z may be a complex number.

The formula for the inner product:

$$\langle\psi|\theta\rangle = \int \psi^*(x)\theta(x)$$

For normalized functions f holds: $f(-\infty) = f(+\infty) = 0$

Integration by parts for the special case of normalized functions:

$$\int_{-\infty}^{\infty} u\,dv = [uv]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} v\,du = -\int_{-\infty}^{\infty} v\,du$$

Note: this is caused by the fact that the functions are normalized – they are zero in infinity.

End prerequisite

Principle 1 of quantum mechanics: the observable or measurable quantities of quantum mechanics are represented by linear, Hermitian operators.

For a linear, Hermitian operator A holds:

$$\langle\psi|A|\theta\rangle = \langle\theta|A|\psi\rangle^*$$

We take a look at two examples, the position operator X that multiplies any function by x, and the differentiation operator D that differentiates any function:

$$X\psi(x) = x\psi(x)$$

$$D\psi(x) = \frac{d\psi(x)}{dx}$$

Both operators are linear.

We check whether X is Hermitian:

$$\langle\psi|X|\theta\rangle = \int \psi^*(x)x\theta(x)$$

$$\langle\theta|X|\psi\rangle^* = \left(\int \theta^*(x)x\psi(x)\right)^* = \int \theta(x)x\psi^*(x) =$$

$$\int \theta(x)x\psi^*(x) = \int \psi^*(x)x\theta(x) = \langle\psi|X|\theta\rangle$$

X is Hermitian.

We check whether D is Hermitian:

$$\langle\psi|D|\theta\rangle = \int \psi^*(x)\frac{d\theta(x)}{dx}dx = \int \psi^*(x)d\theta(x)$$

$$\langle\theta|D|\psi\rangle^* = \left(\int \theta^*(x)\frac{d\psi(x)}{dx}dx\right)^* = \int \theta(x)d\psi^*(x)$$

Integration by parts of $\int \theta(x)d\psi^*(x)$:

$$\int \theta(x)d\psi^*(x) = -\int \psi^*(x)d\theta(x)$$

We calculate:

$$\langle\psi|D|\theta\rangle - \langle\theta|D|\psi\rangle^* =$$

$$\int \psi^*(x)d\theta(x) + \int \psi^*(x)d\theta(x) = 2\int \psi^*(x)d\theta(x) \neq 0$$

Result: D is not Hermitian, instead D satisfies:

$$D^\dagger = -D$$

An operator with this property is called anti-Hermitian. Multiplying an anti-Hermitian operator by $-i$ gives a Hermitian operator, so $-iD$ is Hermitian:

$$-iD\psi(x) = -i\frac{d\psi(x)}{dx}$$

This is called the momentum operator.

Hermitian operator, orthonormal bases and Hermitian operator:

Fundamental Theorem:

- Eigenvectors of a Hermitian operator are a complete set. Any vector the operator can generate can be expanded as a sum of its eigenvectors.
- Eigenvectors with unequal eigenvalues are orthogonal.
- Out of eigenvectors with equal eigenvalues can be chosen two orthogonal eigenvectors via the Gram-Schmidt procedure.

We prove the second item, two eigenvectors $|\lambda_1\rangle$ and $|\lambda_2\rangle$ with unequal eigenvalues λ_1 and λ_2.

According to the definition of eigenvectors and eigenvalues:

$$L|\lambda_1\rangle = \lambda_1|\lambda_1\rangle$$

The operator L is Hermitian:

$$\langle\lambda_1|L = \lambda_1\langle\lambda_1|$$

The second eigenvector:

$$L|\lambda_2\rangle = \lambda_2|\lambda_2\rangle$$

We multiply with the eigenvectors $|\lambda_2\rangle$ and $\langle\lambda_1|$:

$$\langle\lambda_1|L|\lambda_2\rangle = \lambda_1\langle\lambda_1|\lambda_2\rangle$$

$$\langle\lambda_1|L|\lambda_2\rangle = \lambda_1\langle\lambda_1|\lambda_2\rangle$$

We get:

$$\lambda_1\langle\lambda_1|\lambda_2\rangle - \lambda_1\langle\lambda_1|\lambda_2\rangle = 0$$

$$(\lambda_1 - \lambda_1)\langle\lambda_1|\lambda_2\rangle = 0$$

$(\lambda_1 - \lambda_1) \neq 0$ implies that $\langle\lambda_1|\lambda_2\rangle$ must be 0. Both vectors must be orthogonal.

We prove the third item, two eigenvectors $|\lambda_1\rangle$ and $|\lambda_2\rangle$ with equal eigenvalues $\lambda \coloneqq \lambda_1 = \lambda_2$.

According to the definition of eigenvectors and eigenvalues:

$$L|\lambda_1\rangle = \lambda|\lambda_1\rangle$$

$$L|\lambda_2\rangle = \lambda|\lambda_2\rangle$$

We chose a linear combination of both:

$$|A\rangle = \alpha|\lambda_1\rangle + \beta|\lambda_1\rangle$$

We apply the operator L on both sides:

$$L|A\rangle = \alpha L|\lambda_1\rangle + \beta L|\lambda_1\rangle = \alpha\lambda|\lambda_1\rangle + \beta\lambda|\lambda_1\rangle =$$

$$\lambda(\alpha|\lambda_1\rangle + \beta|\lambda_1\rangle) = \lambda|A\rangle$$

Any linear combination of both eigenvectors is eigenvector to eigenvalue λ again.

Out of two linear independent vectors we can always form an orthogonal pair by the Gram-Schmidt procedure.

Hermitian operator, overview:

1.

Hermitian operators L are their own complex conjugated and transposed:

$$L = L^{\dagger}$$

In terms of matrix elements:

$$l_{ji} = l_{ij}^{*}$$

2.

Eigenvectors of Hermitian operators have real eigenvalues.

Suppose $|\lambda\rangle$ is eigenvector to the Hermitian operator L with eigenvalue λ:

$$L|\lambda\rangle = \lambda|\lambda\rangle$$

The bra version:

$$\langle\lambda|L^{\dagger} = \langle\lambda|L = \langle\lambda|\lambda^{*}$$

We sandwich with corresponding bra $\langle\lambda|$ and ket $|\lambda\rangle$:

$$\langle\lambda|L|\lambda\rangle = \langle\lambda|\lambda|\lambda\rangle$$

$$\langle\lambda|L^{\dagger}|\lambda\rangle = \langle\lambda|L|\lambda\rangle = \langle\lambda|\lambda^{*}|\lambda\rangle$$

We get:

$$\lambda^{*} = \lambda$$

The eigenvalue must be a real number.

Hermitian operator, particles and Hermitian operator:

The important information about a particle on the x axis is position and momentum. We need a Hermitian position operator X and a Hermitian momentum operator P. Both operators do not commute, so we cannot measure both without uncertainty.

Hermitian operator, trace of a Hermitian operator:

Prerequisite

Let $|\psi\rangle$ be a normalized state vector. The outer product $|\psi\rangle\langle\psi|$ is called a projection operator.

The sum of all projection operators for a basis system $|i\rangle$ is the identity operator I:

$$\sum_{i}|i\rangle\langle i| = I$$

The trace Tr of a matrix (an operator) L is the sum of its diagonal elements and can be written as:

$$Tr\ L = \sum_{i}\langle i|L|i\rangle$$

Note: $|i\rangle$ and $\langle i|$ preferably the canonical basis but can be any basis.

End prerequisite

The expectation value of a Hermitian operator (an observable) L in state $|\psi\rangle$:

$$\langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|L$$

Proof: let $|i\rangle$ be basis of the Hermitian operator L.

$$Tr\ |\psi\rangle\langle\psi|L = \sum_i \langle i|\psi\rangle\langle\psi|L|i\rangle =$$

$$\sum_i \langle\psi|L|i\rangle\,\langle i|\psi\rangle = \langle\psi|LI|\psi\rangle = \langle\psi|L|\psi\rangle$$

Hilbert, David:

In a broader view vectors can be seen as a set of mathematical objects satisfying certain postulates. In this view functions form a vector space, often called a Hilbert space.

David Hilbert; 1862 – 1943) was a German mathematician and one of the most influential and universal mathematicians of the 19th and early 20th centuries. Hilbert discovered and developed a broad range of fundamental ideas in many areas, including invariant theory, the calculus of variations, commutative algebra, algebraic number theory, the foundations of geometry, spectral theory of operators and its application to integral equations, mathematical physics, and foundations of mathematics (particularly proof theory). *(courtesy Wikipedia)*

Hilbert spaces:

In quantum mechanics the term Hilbert space refers to the space of states with finite or infinite number of dimensions.

Note: spaces with infinite number of dimensions are hard to compute with finite computers.

Hooke's law:

An idealized spring satisfies Hooke's law. The force on the displaced mass is proportional to the distance it has been displaced:

$$F = -kx$$

The characteristic potential energy function:

$$V(x) = \frac{k}{2}x^2$$

The characteristic potential energy function looks like a parabola. As almost any smooth function looks like a parabola close to a local minimum Hooke's law and with it the harmonic oscillator are applicable to a lot of physical problems.

Graphic courtesy Wikipedia by Svjo

Identity, resolving the identity:

Given a basis of a phase state in orthonormal basis vectors $|i\rangle$. We can rewrite the identity operator I in terms of the outer product:

$$I = \sum_i |i\rangle\langle i|$$

Because momentum and position are both Hermitian, the sets of vectors $|x\rangle$ and $|p\rangle$ each define a set of orthonormal basis vectors.

We replace the sum by an integral in position x:

$$I = \int |x\rangle\langle x| \, dx$$

Or in momentum p:

$$I = \int |p\rangle\langle p| \, dp$$

Resolving the identity in "position mode" and "momentum mode" allows us to choose the appropriate representation.

We can switch between $\psi(x) = \langle x|\psi\rangle$ in position mode and $\tilde{\psi}(p) = \langle p|\psi\rangle$ in momentum mode by help of reciprocal Fourier transformations.

Identity operator, from projection operators:

The outer product of a normalized ket $|\psi\rangle$ with its corresponding bra $\langle\psi|$ is a projection operator:

$$|\psi\rangle\langle\psi|$$

The trace Tr of a projection operator is 1.

The sum of all projection operators of a set of orthonormal basis vectors $|i\rangle\langle i|$ gives the identity operator I:

$$\sum_i |i\rangle\langle i| = I$$

Note: there are n basis vectors in a n-dimensional space, so we get the n entries in the diagonal matrix each with value 1.

Inner products:

The inner product for bras and kets $\langle B|A\rangle$ is defined analogous to the dot product for spatial vectors.

The result of the inner product is a (complex) number.

The inner product is linear:

$$\langle C| \{ |A\rangle + |B\rangle \} = \langle C|A\rangle + \langle C|B\rangle$$

Interchanging bra and ket corresponds to complex conjugation:

$$\langle B|A\rangle = \langle A|B\rangle^*$$

Note: Switching from ket $|A\rangle$ to bra $\langle A|$ implies complex conjugation:

$$|A\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_n \end{pmatrix} \rightarrow \langle A| = (\alpha_1^* \, \alpha_2^* \dots \alpha_n^*)$$

This is a kind of implicit complex conjugation. If you have kets $|A\rangle$ and $|B\rangle$

$$|A\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_n \end{pmatrix} \text{ and } |B\rangle = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \dots \\ \beta_n \end{pmatrix}$$

then $\langle B|A\rangle$:

$$(\beta_1^* \, \beta_2^* \dots \beta_n^*) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_n \end{pmatrix}$$

Integrals, replacing sums, schematically:

In general:

$$\sum_i \quad \rightarrow \int dx$$

We redefine the inner product from the discrete case

$$\langle A|B\rangle = \sum_{i=1}^{n} \alpha_i^* \beta_i$$

to the continuous case:

$$\int_{-\infty}^{\infty} \alpha^*(x)\beta(x)dx$$

Note: $\alpha^*(x)$ and $\beta(x)$ are wave functions and must be normalized for the integral to have a finite value.

Integration by parts:

The formula for integration by parts:

$$\int_a^b FdG = \int_a^b d(FG) - \int_a^b GdF$$

In the special case of quantum mechanics, we use normalized function and integrate from $-\infty$ to ∞:

$$\int_{-\infty}^{\infty} FdG = \int_{-\infty}^{\infty} d(FG) - \int_{-\infty a}^{\infty} GdF$$

$$\int_{-\infty}^{\infty} FdG = [FG]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} GdF$$

A normalized function must go to zero, so $[FG]_{-\infty}^{\infty} = 0$.

We get:

$$\int FdG = -\int GdF$$

Switching the derivative from one factor of the integrand to the other require a minus sign.

Ket vectors:

A complex vector has a dual version that is essentially the complex conjugate vector space.

For every ket vector $|A\rangle$, there is a bra vector $\langle A|$:

$$|A\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_n \end{pmatrix} \rightarrow \langle A| = (\alpha_1^* \; \alpha_2^* \dots \alpha_n^*)$$

This leads to a little complication when multiplying a ket $|A\rangle$ with a complex number z.

To the ket

$$z|A\rangle$$

the corresponding bra is

$$\langle A|z^*$$

Ket vectors, axioms of ket vectors:

Let $|A\rangle$, $|B\rangle$ and $|C\rangle$ be ket vectors, z a complex number, then:

1. Closure: the sum of two vectors is a vector:
   $|A\rangle + |B\rangle = |C\rangle$
2. Vector addition is commutative:
   $|A\rangle + |B\rangle = |B\rangle + |A\rangle$
3. Vector addition is associative:
   $\{\, |A\rangle + |B\rangle \,\} + |C\rangle = |A\rangle + \{\, |B\rangle + |C\rangle \,\}$
4. Existence of the 0:
   $|A\rangle + 0 = |A\rangle$
5. Existence of the inverse:
   $|A\rangle + (-|A\rangle) = 0$
6. Multiplication by a scalar produces a new vector:
   $|zA\rangle = z|A\rangle = |B\rangle$
7. Distributive property:
   $z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$
   $\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$

Axioms 6 and 7 taken together are often called *linearity*.

Ket vectors, composite systems and ket vectors:

We take the composite system of Alice (coin) and Bob (die). Obviously, the combined system has 12 dimensions because we have 12 basis vectors $T1, H1, \dots$

		state labels of Bob					
		1	2	3	4	5	6
State labels of Alice	Head	H1	H2	H3	H4	H5	H6
	Tail	T1	T2	T3	T4	T5	T6

We could represent e.g. the H4 state in explicit notation:

$$|H\rangle \otimes |4\rangle$$

Usually we use the composite notation:

$$|H4\rangle$$

Note: despite the two identifiers "H" and "4" the ket $|H4\rangle$ represents a single state of the combined system. The identifiers show something like the origin and help with understanding what happens to the single subsystems in a combined system.

A superposition of two state vectors could be:

$$\alpha_{H3}|H3\rangle + \beta_{T4}|T4\rangle$$

Ket vectors, inner product of ket vectors:

The inner product for bras and kets $\langle B|A\rangle$ is defined analogous to the dot product for spatial vectors.

The result of the inner product is a (complex) number.

The inner product is linear:

$$\langle C|\{|A\rangle + |B\rangle\} = \langle C|A\rangle + \langle C|B\rangle$$

Interchanging bra and ket corresponds to complex conjugation:

$$\langle B|A\rangle = \langle A|B\rangle^*$$

Note: Switching from ket $|A\rangle$ to bra $\langle A|$ implies complex conjugation:

$$|A\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_n \end{pmatrix} \rightarrow \langle A| = (\alpha_1^* \; \alpha_2^* \dots \alpha_n^*)$$

This is a kind of implicit complex conjugation. If you have kets $|A\rangle$ and $|B\rangle$

$$|A\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_n \end{pmatrix} \text{ and } |B\rangle = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \dots \\ \beta_n \end{pmatrix}$$

This gives $\langle B|A\rangle$:

$$(\beta_1^* \; \beta_2^* \dots \beta_n^*) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_n \end{pmatrix}$$

For a normalized (vector) ket $|A\rangle$:

$$\langle A|A\rangle = 1$$

For orthogonal (vectors) kets $|A\rangle, |B\rangle$:

$$\langle B|A\rangle = 0$$

Ket, recipe for a Schrödinger ket:

1. Derive, look up, guess, borrow or steal the Hamiltonian operator H for the system.
2. Prepare an initial state $|\psi(0)\rangle$.
3. Find the eigenvalues and eigenvectors of H by solving the time-independent Schrödinger equation:

   $$H|E_j\rangle = E_j|E_j\rangle$$

   You will get:

   $$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$$

Note 1: "E_j" is eigenvalue to the eigenvector $|E_j\rangle$.

Note 2: $H|E_j\rangle = E_j|E_j\rangle$ leads to a differential equation that determines $\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$.

4. Calculate the initial coefficients $\alpha_j(0) = \langle E_j|\psi(0)\rangle$.
5. Rewrite $|\psi(0)\rangle$ in terms of eigenvectors $|E_j\rangle$ and initial coefficients $\alpha_j(0)$:

$$|\psi(0)\rangle = \sum_j \alpha_j(0)\,|E_j\rangle$$

6. Replace each $\alpha_j(0)$ with $\alpha_j(t)$ to capture its time-dependence. As the basis vectors $|E_j\rangle$ do not change, this leads to:

$$|\psi(t)\rangle = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}\,|E_j\rangle$$

Kronecker delta:

In mathematics, the Kronecker delta is a function of two variables for (non-negative) integers:

$$\delta_{ij} = \begin{cases} 0 \; if \; i \neq j \\ 1 \; if \; i = j \end{cases}$$

It is used in summing up:

$$\sum_{i,j} a_i b_j \delta_{ij} = \sum_i a_i b_i$$

This is important e.g. for orthonormal basis vectors:

$$\langle \lambda_i|\lambda_j\rangle = \delta_{ij}$$

Kronecker delta, replaced by Dirac delta function:

Replacing discrete functions by continuous functions require the Kronecker delta function to be replaced by an appropriate function that works with integrals. Remember the Kronecker delta:

Let F_i be a vector in a discrete, finite dimensional space.

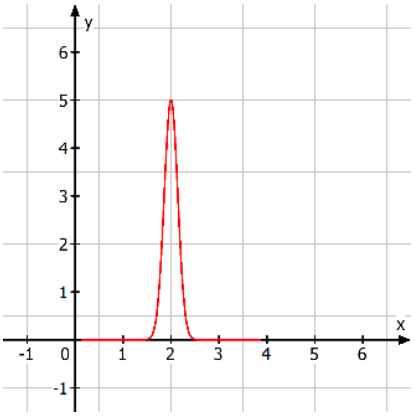
$$\sum\nolimits_{i,j} (\delta_{ij} F_j)$$

gives F_j because δ_{ij} is nonzero only for $i = j$.

In the integration concept the Dirac delta function performs the same: $\delta(x - x')$ is something that returns zero for all $x \neq x'$ and "∞" for $x = x'$. With this:

$$\int_{-\infty}^{\infty} \delta(x - x_0)\, f(x) dx = f(x_0)$$

Note: the Dirac delta function can be thought of as $\lim_{n\to\infty} ne^{-(n(x-x_0))^2}$.



Example: let X be the position operator in a one-dimensional vector space, e.g. the x-axis. The position operator should give back the position of a particle:

$$X|\psi\rangle = x_0|\psi\rangle$$

In terms of wave function this becomes:

$$x\psi(x) = x_0\psi(x)$$

We rewrite this:

$$(x - x_0)\psi(x) = 0$$

This is exactly the property of the Dirac delta function $\delta(x - x_0)$ to be zero on every $x \neq x_0$ and to be nonzero at a single point.

The wave function $\psi(x) = \delta(x - x_0)$ represents the state in which the particle is located exactly at the point x_0 on the x-axis.

Kronecker delta, tensor product:

The Kronecker product is the matrix version of the tensor product.

Let A and B be two 2×2 matrices: $A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{21} \end{pmatrix}$, $B \coloneqq \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{21} \end{pmatrix}$

The Kronecker product (tensor product):

$$A \otimes B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

We apply this to state vectors. The tensor product of the up and down state vectors:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We combine:

$$|uu\rangle = |u\rangle \otimes |u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The same way the other combinations:

$$|ud\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |du\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } |dd\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

We combine operators $\sigma_z \coloneqq \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, $\tau_x \coloneqq \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$:

$$\sigma_z \otimes \tau_x = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\\ 0\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} & -1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix}$$

We apply $\sigma_z \otimes \tau_x$ to $|ud\rangle$:

$$(\sigma_z \otimes \tau_x)|ud\rangle \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix}\begin{pmatrix}0\\ 1\\ 0\\ 0\end{pmatrix} = \begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix} = |uu\rangle$$

For Kronecker product holds a kind of distributive rule. Let A, B be two 2×2 matrices and u, v two 2×1 column vectors:

$$A \coloneqq \begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}, B \coloneqq \begin{pmatrix}b_{11} & ba_{12}\\ b_{21} & b_{22}\end{pmatrix}$$

$$u \coloneqq \begin{pmatrix}u_1\\ u_2\end{pmatrix}, v \coloneqq \begin{pmatrix}v_1\\ v_2\end{pmatrix},$$

$$u \otimes v = \begin{pmatrix}u_1\begin{pmatrix}v_1\\ v_2\end{pmatrix}\\ u_2\begin{pmatrix}v_1\\ v_2\end{pmatrix}\end{pmatrix} = \begin{pmatrix}u_1v_1\\ u_1v_2\\ u_2v_1\\ u_2v_2\end{pmatrix}$$

$$A \otimes B \coloneqq \begin{pmatrix}a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12}\\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22}\\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12}\\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22}\end{pmatrix},$$

To prove:

$$(A \otimes B)(u \otimes v) = (Au \otimes Bv)$$

Left side $(A \otimes B)(u \otimes v)$:

$$\begin{pmatrix}a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12}\\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22}\\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12}\\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22}\end{pmatrix}\begin{pmatrix}u_1v_1\\ u_1v_2\\ u_2v_1\\ u_2v_2\end{pmatrix} =$$

$$\begin{pmatrix}a_{11}b_{11}u_1v_1 + a_{11}b_{12}u_1v_2 + a_{12}b_{11}u_2v_1 + a_{12}b_{12}u_2v_2\\ a_{11}b_{21}u_1v_1 + a_{11}b_{22}u_1v_2 + a_{12}b_{21}u_2v_1 + a_{12}b_{22}u_2v_2\\ a_{21}b_{11}u_1v_1 + a_{21}b_{12}u_1v_2 + a_{22}b_{11}u_2v_1 + a_{22}b_{12}u_2v_2\\ a_{21}b_{21}u_1v_1 + a_{21}b_{22}u_1v_2 + a_{22}b_{21}u_2v_1 + a_{22}b_{22}u_2v_2\end{pmatrix}$$

Right side $(Au \otimes Bv)$:

$$Au = \begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}u_1\\ u_2\end{pmatrix} = \begin{pmatrix}a_{11}u_1 + a_{12}u_2\\ a_{21}u_1 + a_{22}u_2\end{pmatrix}$$

$$Bv = \begin{pmatrix}b_{11} & b_{12}\\ b_{21} & b_{22}\end{pmatrix}\begin{pmatrix}v_1\\ v_2\end{pmatrix} = \begin{pmatrix}b_{11}v_1 + b_{12}v_2\\ b_{21}v_1 + b_{22}v_2\end{pmatrix}$$

$$(Au \otimes Bv) = \begin{pmatrix}a_{11}u_1 + a_{12}u_2\\ a_{21}u_1 + a_{22}u_2\end{pmatrix} \otimes \begin{pmatrix}b_{11}v_1 + b_{12}v_2\\ b_{21}v_1 + b_{22}v_2\end{pmatrix} =$$

$$\begin{pmatrix} (a_{11}u_1 + a_{12}u_2)\begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \\ (a_{21}u_1 + a_{22}u_2)\begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1(b_{11}v_1 + b_{12}v_2) + a_{12}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{11}u_1(b_{21}v_1 + b_{22}v_2) + a_{12}u_2(b_{21}v_1 + b_{22}v_2) \\ a_{21}u_1(b_{11}v_1 + b_{12}v_2) + a_{22}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{21}u_1(b_{21}v_1 + b_{22}v_2) + a_{22}u_2(b_{21}v_1 + b_{22}v_2) \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1b_{11}v_1 + a_{11}u_1b_{12}v_2 + a_{12}u_2b_{11}v_1 + a_{12}u_2b_{12}v_2 \\ a_{11}u_1b_{21}v_1 + a_{11}u_1b_{22}v_2 + a_{12}u_2b_{21}v_1 + a_{12}u_2b_{22}v_2 \\ a_{21}u_1b_{11}v_1 + a_{21}u_1b_{12}v_2 + a_{22}u_2b_{11}v_1 + a_{22}u_2b_{12}v_2 \\ a_{21}u_1b_{21}v_1 + a_{21}u_1b_{22}v_2 + a_{22}u_2b_{21}v_1 + a_{22}u_2b_{22}v_2 \end{pmatrix}$$

Both sides are equal.

Lagrange equation:

The Lagrangian is kinetic energy minus potential energy:

$$L = E_{kin} - V(x)$$

For the potential of a harmonic oscillator:

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$$

We substitute:

$$x = x\sqrt{m}$$

$$\omega = \sqrt{\frac{k}{m}}$$

Note: ω will become the frequency of the harmonic oscillator.

The Lagrangian becomes:

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2$$

For a one-dimensional system (the harmonic oscillator) we have only one Lagrange equation:

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

We do partial differentiation:

$$\frac{\partial L}{\partial \dot{x}} = \dot{x}$$

This is called the canonical momentum conjugate to x. We complete:

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{d}{dt}\dot{x} = \ddot{x}$$

This is the right-hand side of the Lagrangian. We calculate the left side:

$$\frac{\partial L}{\partial x} = \frac{\partial}{\partial x}\left(\frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2\right) = -\omega^2 x$$

We write down the complete Lagrange equation:

$$-\omega^2 x = \ddot{x}$$

This differential equation is equivalent to $F = ma$ with the solution:

$$x = A\cos(\omega t) + B\sin(\omega t)$$

Lagrangian, harmonic oscillator and Lagrangian:

Kinetic and potential energy are $\frac{1}{2}m\dot{x}^2$ and $\frac{1}{2}kx^2$.

For convenience we aggregate the variable x to

$$x := \sqrt{m}x$$

and use a new variable, the frequency of the oscillator:

$$\omega = \sqrt{\frac{k}{m}}$$

With this the Lagrangian (kinetic energy minus potential energy):

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2$$

In this form, oscillators are distinguished from each other only by their frequency ω.

From the Lagrangian we can work out the equations of motion. We have a one-dimensional system with one Lagrangian:

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

Left side:

$$\frac{\partial L}{\partial x} = -\omega^2 x$$

Right side:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} =$$

$$\frac{d}{dt}\frac{\partial}{\partial \dot{x}}\left(\frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2\right) =$$

$$\frac{d}{dt}(\dot{x}) = \ddot{x}$$

We combine both results:

$$\ddot{x} = -\omega^2 x$$

This is a differential equation with the general solution:

$$x = A\,cos(\omega t) + B\,sin(\omega t)$$

Lagrangian, path integrals and Lagrangian:

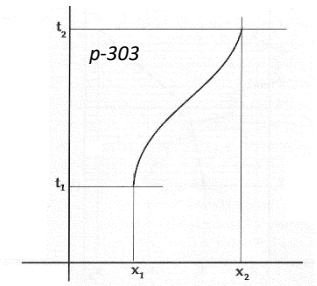
Prerequisite

For any integral over the position variable x we can insert the identity:

$$I = \int |x\rangle\langle x|\, dx$$

End prerequisite

Classical



According to the least action principle, classical trajectories are that of minimum action. Action is a technical term and stands for the integral of the Lagrangian between the end points of the trajectory.

For simple systems, the Lagrangian is kinetic energy minus potential energy. For a particle moving in one dimension, the action is:

$$A = \int_{t_1}^{t_2} L(x, \dot{x}) dt$$

We insert the Lagrangian:

$$A = \int_{t_1}^{t_2} \frac{1}{2} m\dot{x}^2 - \frac{1}{2} kx^2 dt$$

We search the path with the least action A by help of calculus procedures.

Quantum mechanical

The idea of well-defined trajectory between the two points makes no sense in quantum mechanics because of the uncertainty principle.

The global version of quantum mechanics asks: Given a particle starts at (x_1, t_1), what is the probability amplitude it will show up at (x_2, t_2)?

We call the amplitude $C_{1,2} \coloneqq C(x_1, t_1; x_2, t_2)$.

The initial state of the particle is:

$$|\psi(t_1)\rangle = |x_1\rangle$$

Over the time interval between t_1 and t_2 the state evolves to:

$$|\psi(t_2)\rangle = e^{-iH(t_2 - t_1)}|x_1\rangle$$

Note: we use units for which $\hbar = 1$.

We replace $(t_2 - t_1)$ by t. The probability amplitude to detect the particle at $|x_2\rangle$ is the inner product:

$$\langle x_2|\psi(t_2)\rangle = \left\langle x_2 \middle| e^{-iHt} \middle| x_1 \right\rangle$$

The process of quantization starts with splitting the time interval t into two smaller intervals of size $\frac{t}{2}$. The operator e^{-iHt} can be written as the product of two operators:

$$e^{-iHt} = e^{-iH\frac{t}{2}} e^{-iH\frac{t}{2}}$$

We integrate this via the help of the identity operator:

$$C_{1,2} = \int \left\langle x_2 \middle| e^{-iH\frac{t}{2}} \middle| x \right\rangle \left\langle x \middle| e^{-iH\frac{t}{2}} \middle| x_1 \right\rangle dx$$

The heart of this process is: the amplitude to go from x_1 to x_2 over the time interval t is an integral over an intermediate position x and is the product of two amplitudes.

We repeat this until we have time intervals of size ε (remember this process in calculus …). In the end, the amplitude is an integral over all possible paths between the end points. Feynman discovered that the amplitude for each path has a simple relation to an expression of classical mechanics, the action for that path.

The exact expression for the action A of each path is:

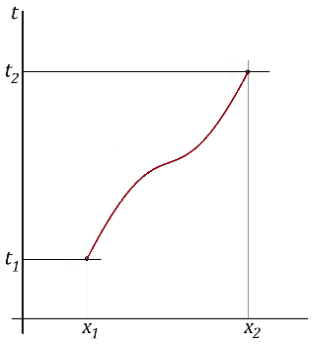
$$e^{i\frac{A}{\hbar}}$$

Feynman's formulation can be summarized by the equation:

$$C_{1,2} = \int_{paths} e^{i\frac{A}{\hbar}}$$

In quantum field theory this is the principal tool for formulating the laws of elementary particle physics.

Least action principle, classical physics:



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We search the path with the least action A by help of calculus procedures.

Linearity:

1.

Let $|A\rangle$, $|B\rangle$ and $|C\rangle$ be ket vectors, z a complex number, then:

1. Closure: the sum of two vectors is a vector:
   $|A\rangle + |B\rangle = |C\rangle$
2. Vector addition is commutative:
   $|A\rangle + |B\rangle = |B\rangle + |A\rangle$
3. Vector addition is associative:
   $\{\,|A\rangle + |B\rangle\,\} + |C\rangle = |A\rangle + \{\,|B\rangle + |C\rangle\,\}$
4. Existence of the 0:
   $|A\rangle + 0 = |A\rangle$
5. Existence of the inverse:
   $|A\rangle + (-|A\rangle) = 0$

6. Multiplication by a scalar produces a new vector:
   $|zA\rangle = z|A\rangle = |B\rangle$
7. Distributive property:
   $z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$
   $\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$

Axioms 6 and 7 taken together are often called *linearity*.

Note: for "ordinary" spatial vectors the multiplication with a complex number is not defined.

2.

An operator M acting on a ket $|A\rangle$ produces a new ket $|B\rangle$:

$$M|A\rangle = |B\rangle$$

For M to be a linear operator:

- $M|A\rangle = |B\rangle$ must hold for every ket $|A\rangle$
- $Mz|A\rangle = z|B\rangle$ for every complex number z
- $M\{|A\rangle + |B\rangle\} = M|A\rangle + M|B\rangle$

Linear motion (how to scatter wave packets):

Prerequisite

The quantum analog of Newton's equation for the time rate of change of momentum:

$$\frac{d}{dt}\langle P\rangle = -\langle\frac{dV}{dx}\rangle$$

Note: P momentum operator, V operator for potential Energy, $\langle\ \ \rangle$ the expectation value.

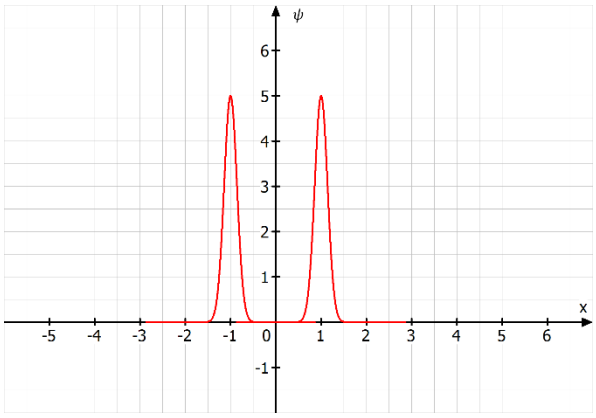
End prerequisite

The expectation value of the position operator X does not (always) follow the classical trajectory. It would if

$$\langle\frac{dV}{dx}\rangle = \frac{dV\langle x\rangle}{dx}$$

but this is not always true.

Imagine a wave packet $\psi(x)$ with bimodal shape:



The expectation value of $\psi(x)$ is zero because $\psi(x)$ is centered around the origin:

$$\langle x \rangle = 0$$

If we apply a force ($\frac{dV}{dx}$) of kind $F = x^2$ to this wave packet there is a difference between $\langle F(x) \rangle$ and $F(\langle x \rangle)$:

$$F(\langle x \rangle) = 0$$

$$\langle F(x) \rangle \neq 0$$

Quantum equation of motion looks classical if wave packets are coherent, well localized and the potential function $V(x)$ is smooth with respect to the size of the wave packets.

If this is not the case the wave packet will scatter, and the classical trajectory is lost.

Linear (Hermitian) operators:

A linear operator X acts on a function and gives a new function:

$$X\big(f(\dots)\big) = g(\dots)$$

X is said to be linear if:

$$X(f + g) = X(f) + X(g)$$

$$X(z \cdot f) = z \cdot X(f)$$

Note: z is a complex number.

We often work with the position operator X and the differentiation operator D.

The position operator X:

$$X\, f(x) \coloneqq x \cdot f(x)$$

The differentiation operator D:

$$D\, \psi(x) = \frac{d}{dx}\, \psi(x)$$

Both operators are linear.

An operator X is said to be Hermitian if it is identical with its transposed complex conjugated:

$$X = X^{\dagger}$$

An operator D is said to be anti-Hermitian, if:

$$D = -D^{\dagger}$$

By multiplying an anti-Hermitian operator with $-i$ it becomes Hermitian.

The position operator X is Hermitian.

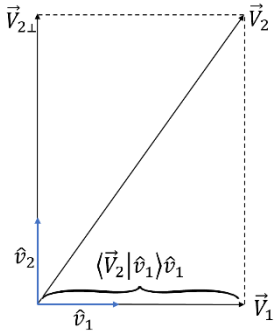
The differentiation operator D is anti-Hermitian. For later application we multiply D with $-\mathrm{i}\hbar$ to make it Hermitian.

Linear operators, eigenvalues and eigenvectors of linear operators:

A linear operator acting on a vector normally changes the direction of the vector.

Vectors that keep their direction are called eigenvectors. If length is not preserved, the eigenvector is multiplied by its eigenvalue, a (complex) number. If even the length of the vector is preserved, we call them eigenvector to eigenvalue 1.

Linear operators, the Gram-Schmidt procedure:



Given two vectors $\vec{V}_1$ and $\vec{V}_2$ in $\mathbb{R}^2$ that are not orthogonal.

We construct two orthonormal vectors, $\hat{v}_1$ and $\hat{v}_2$.

From $\vec{v}_1$ we get the unit vector $\hat{v}_1$:

$$\hat{v}_1 = \frac{\vec{v}_1}{|\vec{v}_1|}$$

We need the projection of $\vec{v}_2$ onto $\vec{v}_1$:

$$\langle\vec{v}_2|\hat{v}_1\rangle\hat{v}_1$$

We construct $\vec{v}_{2\perp}$:

$$\vec{v}_{2\perp} = \vec{v}_2 - \langle\vec{v}_2|\hat{v}_1\rangle\hat{v}_1$$

We build $\hat{v}_2$:

$$\hat{v}_2 = \frac{\vec{v}_{2\perp}}{|\vec{v}_{2\perp}|}$$

Vectors $\hat{v}_1$ and $\hat{v}_2$ are orthonormal.

Linear operators, Hermitian conjugation:

You take the matrix representing a linear operator M, transpose it $M \rightarrow M^T$ and complex conjugate the result $M^T \rightarrow (M^T)^*$.

$(M^T)^*$ is called the Hermitian conjugate to M, written as $M^\dagger$.

Note: an operator (a matrix) M that satisfies $M^\dagger M = I$ is called unitary.

Linear operators, Hermitian operators:

For Hermitian operators (and matrices) holds:

- Their eigenvalues all are real.
- Their eigenvectors form a complete set. Any vector the operator can generate can be expanded as a sum of its eigenvectors.
- If two eigenvectors have different eigenvalues, they are orthogonal.
- Two eigenvectors with equal eigenvalues can be orthogonalized (e.g. via the Gram-Schmidt procedure).

Linear operators, Machines and Matrices:

John Wheeler liked to call operators: machines with an input port and an output port. In the input port you insert a vector $|A\rangle$ and get back a vector $|B\rangle$ at the output port.

John Archibald Wheeler (July 9, 1911 – April 13, 2008) was an American theoretical physicist. He was largely responsible for reviving interest in general relativity in the United States after World War II.

Wheeler also worked with Niels Bohr in explaining the basic principles behind nuclear fission. Together with Gregory Breit, Wheeler developed the concept of the Breit–Wheeler process. He is best known for using the term "black hole" for objects with gravitational collapse already predicted during the early 20th century, for inventing the terms "quantum foam", "neutron moderator", "wormhole" and "it from bit", and for hypothesizing the "one-electron universe". *(Courtesy Wikipedia)*

Linear operators, observables and linear operators:

The principles of quantum mechanics involve the idea of an observable. They presuppose the existence of an underlying complex vector space whose vectors represent system states.

- Principle 1:
  the observable or measurable quantities of quantum mechanics are represented by linear, Hermitian operators L.
- Principle 2:
  the possible results of a measurement are the eigenvalues λ_i of the operator representing the observable. The eigenvalues λ_i corresponds with eigenvectors $|\lambda_i\rangle$.
  reformulated: if the system is in the eigenstate $|\lambda_i\rangle$, the result of a measurement is guaranteed to be λ_i.
- Principle 3:
  unambiguously distinguishable states are represented by orthogonal vectors.
- Principle 4:
  if $|A\rangle$ is the state-vector of a system, and the observable L is measured, the probability to observe value $|\lambda_i\rangle$ is:
  $$P(\lambda_i) = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$
  or equivalently:
  $$P(\lambda_i) = |\langle A|\lambda_i\rangle|^2$$
- Principle 5:
  The evolution of state-vectors with time is unitary.

Linear operators, outer product as linear operators:

Given the ket $|\psi\rangle$ and the bra $\langle\phi|$ we can form the outer product:

$$|\psi\rangle\langle\phi|$$

The outer product is not a number, it is a linear operator (a matrix).

We show this in matrix representation. Let $|\psi\rangle \coloneqq \begin{pmatrix} a \\ b \\ c \end{pmatrix}$ and $\langle\phi| = (d\ e\ f)$:

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix}(d\ e\ f) = \begin{pmatrix} ad & ae & af \\ bd & be & bf \\ cd & ce & cf \end{pmatrix}$$

Note: this looks similar to the tensor product.

The outer product $|\psi\rangle\langle\phi|$ acting on ket $|A\rangle$:

$$|\psi\rangle\langle\phi|A\rangle = |\psi\rangle z = z|\psi\rangle$$

As $\langle\phi|A\rangle$ is a (complex) number z, the result is proportional to $|\psi\rangle$.

The same goes for outer products acting on bra $\langle B|$:

$$\langle B|\psi\rangle\langle\phi| = z\langle\phi|$$

Linear operators, properties of linear operators:

- Linear operators give a unique output for every vector in the space:
$$M|A\rangle = |B\rangle$$
- A linear operator acting on a multiple of an input vector gives the same multiple of the output vector:
$$Mz|A\rangle = z|B\rangle$$
Note: z is a (complex) number.
- A linear operator M acting on a sum of vectors gives the sum of M acting on each vector:
$$M\{|A\rangle + |B\rangle\} = M|A\rangle + M|B\rangle$$

Linear operators, time-development operator:

Time-development of a quantum state $|\psi\rangle$ is written with a Hermitian time-development operator $U(t)$:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

and

$$\langle\psi(t)| = \langle\psi(0)|U^{\dagger}(t)$$

Suppose $|\psi(t)\rangle$ and $|\phi(t)\rangle$ are two distinguishable states. Therefore, they must be orthogonal:

$$\langle\psi(t)|\phi(t)\rangle = 0$$

Orthogonality is preserved for all times:

$$\langle\psi(t)|\phi(t)\rangle = \langle\psi(t)|U^{\dagger}(t)U(t)|\phi(0)\rangle$$

Consider an orthonormal basis of vectors $|i\rangle$ with $|\psi(0)\rangle$ and $|\phi(0)\rangle$ being members of this basis. Orthonormality is expressed:

$$\langle i|j\rangle = \delta_{ij}$$

Note: δ_{ij} is the Kronecker symbol.

We rewrite orthogonality:

$$\langle\psi(t)|\phi(t)\rangle = \langle i|U^{\dagger}(t)U(t)|j\rangle = \delta_{ij}$$

From this we could conclude that $U^{\dagger}(t)U(t)$ must be a diagonal matrix with all entries on the diagonal being 1 – the identity matrix. An operator U that satisfies this condition is called unitary.

In other words: time evolution in quantum mechanics is unitary.

Liouville's theorem:

In physics, Liouville's theorem, named after the French mathematician Joseph Liouville, is a key theorem in classical statistical and Hamiltonian mechanics. It asserts that the phase-space distribution function is constant along the trajectories of the system—that is that the density of system points in the vicinity of a given system point traveling through phase-space is constant with time. This time-independent density is in statistical mechanics known as the classical a priori probability. *(Courtesy Wikipedia)*

Locality:

Locality in the quantum field theorist's understanding means: it is impossible to send a signal faster than speed of light. In other words: an entangled system changes in one instant, even if it is spread out in space, but it is impossible to detect this change by measuring the subsystem you have in reach (and the information of the rest goes its way slowly by speed of light …)

Lowering operators (annihilation operators):

The Hamiltonian can be expressed in terms of the momentum operator P and position operator X:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2) = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{i\omega}{2}$$

Note: $\frac{i\omega}{2}$ is necessary because P and X do not commute.

$(P + i\omega X)$ is called the raising operator, $(P - i\omega X)$ the lowering operator, written as a^+ and a^-.

The raising operator a^+ shifts the energy level of the harmonic oscillator to the next possible higher level, the lowering operator a^- to the next possible lower level.

Applying the lowering operator to the ground level with Energy $E_0 = \frac{\omega\hbar}{2}$ annihilates this ground level. Symbolically this is expressed as

$$a^-|0\rangle = 0$$

with $|0\rangle$ representing the ground level state.

Machines, matrices and machines:

John Wheeler called operators: machines with an input port and an output port. In the input port you insert a vector $|A\rangle$ and get back a vector $|B\rangle$ at the output port.

We translate this in matrices acting on state vectors. A matrix acting on a vector $|A\rangle$ delivers a new vector $|B\rangle$.

Magnetic field, spin in magnetic field:

Prerequisite

The Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Let $|\psi(t)\rangle$ be a state vector and L an operator. The change of the expectation value of an operator L with time:

$$\frac{d}{dt}\langle\psi(t)|L|\psi(t)\rangle = -\frac{i}{\hbar}\langle[L,H]\rangle$$

Written in shorthand form:

$$\dot{L} = -\frac{i}{\hbar}\langle[L,H]\rangle$$

End prerequisite

When a classical spin (a charged rotor) is put into a magnetic field, it has an energy that depends on its orientation. It is proportional to the dot product of the spin and the magnetic field.

The quantum version of this:

$$H \sim \vec{\sigma} \cdot \vec{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$$

Note: σ_x, σ_y and σ_z represents the components of the spin operator.

The magnetic field lies along the z axis. We absorb all numerical constants without $\hbar$ into a single constant ω and get the quantum Hamiltonian:

$$H = \frac{\hbar\omega}{2}\sigma_z$$

We search how the expectation value of the spin changes with time, $\langle\sigma_x(t)\rangle$, $\langle\sigma_y(t)\rangle$ and $\langle\sigma_z(t)\rangle$. We use:

$$\langle\dot{\sigma_x}\rangle = -\frac{i}{\hbar}\langle\sigma_x, H\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i}{\hbar}\langle[\sigma_y, H]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i}{\hbar}\langle[\sigma_z, H]\rangle$$

We plug in the quantum Hamiltonian $H = \frac{\hbar\omega}{2}\sigma_z$ and get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i\omega}{2}\langle[\sigma_y, \sigma_z]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i\omega}{2}\langle[\sigma_z, \sigma_z]\rangle$$

We check this explicitly for $\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$ by using the Pauli-matrices:

$$[\sigma_x, \sigma_z] = \sigma_x\sigma_z - \sigma_x\sigma_z =$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} =$$

$$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} - \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = \begin{pmatrix}0 & -2\\ 2 & 0\end{pmatrix} =$$

$$-2i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = -2i\sigma_y$$

We get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle-2i\sigma_y\rangle = -\omega\langle\sigma_y\rangle$$

The results:

$$\langle\dot{\sigma_x}\rangle = -\omega\langle\sigma_y\rangle$$

$$\langle\dot{\sigma_y}\rangle = \omega\langle\sigma_x\rangle$$

$$\langle\dot{\sigma_z}\rangle = 0$$

In classical mechanics, the x and y components of angular momentum are precessing around the z axis.

In quantum mechanics the expectation values for $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ will be precessing, but each single measurement will always give +1 or -1. The expectation value for $\langle\sigma_z\rangle$ remains unchanged.

Mathematical concepts:

Complete sets of commutating variables:

In bigger quantum mechanical systems, we may have multiple observables that are compatible, their values can be known simultaneously. In these situations, we need multiple measurements to fully characterize the state of the system.

The logical chain is as follows:

One observable – one operator – one system of basis vectors.

Multiple observables – several operators – several systems of basis vectors.

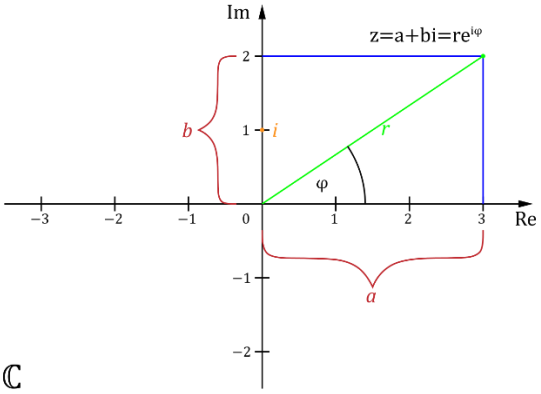
Multiple compatible observables (observables that can be measured parallel) – several commuting operators – several systems of basis vectors – the commutator of commuting operators destroying

the basis vectors – the commutator of commuting operators destroying every vector combined out of the basis system. This collection is called a complete set of commuting observables.

Mathematical concepts, complex numbers:

A complex number consists of a real part and an imaginary part. We can write it as $z = a + ib$ with $a, b \in \mathbb{R}$. The imaginary unit i has the property $i \cdot i = -1$ or $i^2 = -1$.

We can represent complex numbers by a plane with the horizontal real axis and the vertical imaginary axis. This is called the cartesian mode.



... graphic courtesy of Wikipedia ...

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A second way of representation describes a complex number by the angle it has with the real axis and its length resp. the absolute value. This is called the gaussian mode. In this mode we write a complex number as $r \cdot e^{i\varphi}$.

We can switch from one representation to the other:

Given $z = a + ib$: $\quad |z| \; or \; r = \sqrt{a^2 + b^2}$ $\qquad \varphi = \arccos\left(\frac{a}{r}\right)$ if $b \geq 0$

resp. $\qquad \varphi = -\arccos\left(\frac{a}{r}\right)$ if $b < 0$.

Given $z = re^{i\varphi}$: $\quad a = r \cdot \cos(\varphi)$ $\qquad b = r \cdot \sin(\varphi)$

or $\qquad z = r \cdot (\cos(\varphi) + i \cdot \sin(\varphi))$

Every complex number z has a complex conjugate number, marked as $\bar{z}$ or z^*. The complex conjugate switches the imaginary part to the opposite sign. $z = a + ib$ changes to $\bar{z} = a - ib$ and vice versa.

With this we get new formulas:

$$|z| = \sqrt{z\bar{z}}$$

$$re(z) \; or \; a = \frac{z + \bar{z}}{2}$$

$$im(z) \; or \; b = \frac{z - \bar{z}}{2}$$

Additions and subtraction of complex numbers are best performed with the cartesian representation.

$$(a + ib) + (c + id) = ac + ibd$$

Multiplication and division are best performed with the gaussian representation.

$$r_1 e^{i\varphi} \cdot r_2 e^{i\theta} = r_1 r_2 e^{i(\varphi + \theta)}$$

A number of the form $z = e^{i\varphi}$ has the absolute value 1: $\left|e^{i\varphi}\right| = \sqrt{e^{i\varphi}e^{-i\varphi}} = \sqrt{e^0} = \sqrt{1} = 1$. It is called a phase factor. No measurable quantity, no observable is sensitive to an overall phase-factor, so we can ignore it when specifying states.

Note: complex numbers often are used for "a trick" in calculations. With complex numbers you can transform a sum into a product: $(x + iy)(x - iy) = x^2 + y^2$.

Mathematical concepts, continuous function:

We begin by picking an observable L, with eigenvalues λ and eigenvectors $|\lambda\rangle$. Let $|\psi\rangle$ be a state-vector. Since the eigenvectors of a Hermitian operator form a complete orthonormal basis, the vector $|\psi\rangle$ can be expanded as $\sum_{i=1}^{n} \psi(\lambda_i)|\lambda_i\rangle$. The quantities $\psi(\lambda_i)$ are called the wave function in the L-basis of the system, so their actual form depends of the observable chosen.

Note: other observable – other wave functions, even it is the same state.

The eigenvectors are orthogonal to each other: $\langle\lambda_i|\lambda_j\rangle = \delta_{ij}$.

We can identify the wave functions with the inner product, the projections of the state-vector $|\psi\rangle$ onto the eigenvectors $|\lambda\rangle$: $\psi(\lambda) = \langle\lambda|\psi\rangle$.

You can think of the wave function in two ways. First of all, it is a set of components of the state-vector in a particular basis, the components forming a column vector:

$$\begin{pmatrix} \psi(\lambda_1) \\ \vdots \\ \psi(\lambda_n) \end{pmatrix}$$

You also can think of the wave function as a complex valued function of the discrete variable λ: $\psi(\lambda)$.

A single spin system has a two-dimensional space of state. The coordinates of a particle, moving on the x-axis can be found on any real value of x, the observable has an infinite number of possible values: $x \in \mathbb{R}$. The former discrete wave function $\psi(x_i)$ becomes a function of a continuous variable $\psi(x)$.

Mathematical concepts, continuous functions as vectors:

Let us consider the set of complex functions $\varphi(x)$ of a single variable x: $x \to \varphi(x)$ with $\varphi(x) \in \mathbb{C}$. With appropriate restrictions, functions like $\varphi(x)$ satisfy the mathematical axioms that define a vector space (algebraic structure) as there are:

1. Closure: $\varphi(x) + \theta(x) = \vartheta(x)$
2. Commutative property: $\varphi(x) + \theta(x) = \theta(x) + \varphi(x)$
3. Associative property: $\big(\varphi(x) + \theta(x)\big) + \vartheta(x) = \varphi(x) + (\theta(x) + \vartheta(x))$
4. Zero: $\varphi(x) + 0 = \varphi(x)$
5. Inverse: $\varphi(x) + (-\varphi(x)) = 0$
6. Multiplying property: $z\varphi(x) = \tau(x)$
7. Distributive properties:
    a. $z[\varphi(x) + \theta(x)] = z\varphi(x) + z\theta(x)$
    b. $[z + w]\,\varphi(x) = z\varphi(x) + w\varphi(x)$

All of this works with functions too so we can identify the functions $\varphi(x)$ with the ket-vectors $|\varphi\rangle$ in an abstract vector space. The corresponding bra vectors are $\varphi^*(x)$.

Continuous functions require:

a) Integrals replace sums
b) Probability densities replace probabilities
c) Dirac delta functions replace Kronecker deltas

a) Integrals replace sums:

the inner product $\langle\varphi|\theta\rangle$:

was: $\sum_{i,j}\varphi_i^*\theta_j\delta_{ij}$

is: $\int_{-\infty}^{\infty}\varphi^*(x)\theta(x)dx$

b) Probability densities replace probabilities:

was:

$|A\rangle$ state-vector, observable L, the probability to observe value λ_i: $P(\lambda_i)=\langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$

is:

probability density: $P(a,b)$: $\int_a^b P(x)dx=\int_a^b\varphi^*(x)\varphi(x)dx$

analog to the discrete case we define a normalization condition:

$$\int_{-\infty}^{\infty}\varphi^*(x)\varphi(x)dx=1$$

c) Dirac delta functions replace Kronecker deltas:

Consider a vector F_i in a discrete, finite dimensional space. $\sum_{i,j}\left(\delta_{ij}F_j\right)$ gives F_j because δ_{ij} is nonzero only for $i=j$.

The Dirac delta function performs this: $\delta(x-x')$ returns zero for all $x\neq x'$ and "∞" for $x=x'$:

$$\int_{-\infty}^{\infty}\delta(x-x')\,f(x')dx'=f(x)$$

Note: the Dirac delta function can be thought of as $\lim_{n\to\infty} ne^{-(nx)^2}$.

Mathematical concepts, continuous functions, integration by parts:

The rule for integration by parts:

$$\int_a^b FdG=FG|_a^b-\int_a^b GdF$$

We work with normalized functions that span the entire x-axis and go to zero at infinity, so the expression $FG|_a^b$ becomes zero. With this we get an expression that is often used in physics:

$$\int FdG=-\int GdF$$

Mathematical concepts, continuous functions, linear operators:

An operator L acting on wave functions is linear:

Additive: $L\big(\varphi(x)+\theta(x)\big)=L\varphi(x)+L\theta(x)$

Homogeny: $L\big(z\varphi(x)\big)=zL\varphi(x)$

Two examples:

a) The "multiply by x" operator with the symbol X: $X\varphi(x)=x\varphi(x)$ with $x\in\mathbb{R}$
b) The "differentiate" operator with the symbol D: $D\varphi(x)=\frac{d\varphi(x)}{dx}$

Both are linear operators.

Mathematical concepts, outer products:

Given the ket $|\psi\rangle$ and the bra $\langle\phi|$ we can form the outer product:

$$|\psi\rangle\langle\phi|$$

The outer product is not a number, it is a linear operator (a matrix).

We show this in matrix representation. Let $|\psi\rangle\coloneqq\begin{pmatrix}a\\b\\c\end{pmatrix}$ and $\langle\phi|=(d\ e\ f)$:

$$\begin{pmatrix}a\\b\\c\end{pmatrix}(d\ e\ f)=\begin{pmatrix}ad & ae & af\\ bd & be & bf\\ cd & ce & cf\end{pmatrix}$$

Note: this looks similar to the tensor product.

The outer product $|\psi\rangle\langle\phi|$ acting on ket $|A\rangle$:

$$|\psi\rangle\langle\phi|A\rangle=|\psi\rangle z=z|\psi\rangle$$

As $\langle\phi|A\rangle$ is a (complex) number z, the result is proportional to $|\psi\rangle$.

The same goes for outer products acting on bra $\langle B|$:

$$\langle B|\psi\rangle\langle\phi|=z\langle\phi|$$

Let $|\psi\rangle$ be a normalized ket with its corresponding bra $\langle\psi|$.

The outer product:

$$|\psi\rangle\langle\psi|$$

is called a projection operator.

Projection operators have the following properties:

- Projection operators are Hermitian (Hermitian matrix).
- The vector $|\psi\rangle$ is eigenvector of its projection operator with eigenvalue 1:
$$(|\psi\rangle\langle\psi|)|\psi\rangle=|\psi\rangle$$
- Any vector orthogonal to $|\psi\rangle$ is eigenvector with eigenvalue zero. Thus, the eigenvalues of $|\psi\rangle\langle\psi|$ are 0 with the exception of the eigenvector $|\psi\rangle$ itself that has eigenvalue 1.
- The square of a projection operator is the same as the projection operator itself:
$$|\psi\rangle\langle\psi|^{\,2}=|\psi\rangle\langle\psi|$$

- The trace Tr of a projection operator is 1 and has only one entry of value 1.
- If we add all the projection operators for a basis system, we obtain the identity operator:

$$\sum_i |i\rangle\langle i| = I$$

- The expectation value of any observable L in state $|\psi\rangle$ is given by:

$$\langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|\ L$$

Mathematical concepts, tensor products:

Let A and B be two 2×2 matrices: $A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{21} \end{pmatrix}$, $B \coloneqq \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{21} \end{pmatrix}$

The matrix version of the tensor product, sometimes called the Kronecker product:

$$A \otimes B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

We combine state vectors. The tensor product of the up and down state vectors:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We combine:

$$|uu\rangle = |u\rangle \otimes |u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

We combine operators. $\sigma_z \coloneqq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\tau_x \coloneqq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$:

$$\sigma_z \otimes \tau_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & -1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

We apply $\sigma_z \otimes \tau_x$ to $|ud\rangle$:

$$(\sigma_z \otimes \tau_x)|ud\rangle \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |uu\rangle$$

For tensor product holds a kind of distributive rule. Let A, B be two 2×2 matrices and u, v two 2×1 column vectors:

$$A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, B \coloneqq \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$u \coloneqq \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, v \coloneqq \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},$$

$$u \otimes v = \begin{pmatrix} u_1 \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \\ u_2 \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} u_1 v_1 \\ u_1 v_2 \\ u_2 v_1 \\ u_2 v_2 \end{pmatrix}$$

$$A \otimes B \coloneqq \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix},$$

To prove: $(A \otimes B)(u \otimes v) = (Au \otimes Bv)$

Left side $(A \otimes B)(u \otimes v)$:

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix} \begin{pmatrix} u_1 v_1 \\ u_1 v_2 \\ u_2 v_1 \\ u_2 v_2 \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11}u_1v_1 + a_{11}b_{12}u_1v_2 + a_{12}b_{11}u_2v_1 + a_{12}b_{12}u_2v_2 \\ a_{11}b_{21}u_1v_1 + a_{11}b_{22}u_1v_2 + a_{12}b_{21}u_2v_1 + a_{12}b_{22}u_2v_2 \\ a_{21}b_{11}u_1v_1 + a_{21}b_{12}u_1v_2 + a_{22}b_{11}u_2v_1 + a_{22}b_{12}u_2v_2 \\ a_{21}b_{21}u_1v_1 + a_{21}b_{22}u_1v_2 + a_{22}b_{21}u_2v_1 + a_{22}b_{22}u_2v_2 \end{pmatrix}$$

Right side $(Au \otimes Bv)$:

$$Au = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} a_{11}u_1 + a_{12}u_2 \\ a_{21}u_1 + a_{22}u_2 \end{pmatrix}$$

$$Bv = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix}$$

$$(Au \otimes Bv) = \begin{pmatrix} a_{11}u_1 + a_{12}u_2 \\ a_{21}u_1 + a_{22}u_2 \end{pmatrix} \otimes \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} =$$

$$\begin{pmatrix} (a_{11}u_1 + a_{12}u_2) \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \\ (a_{21}u_1 + a_{22}u_2) \begin{pmatrix} b_{11}v_1 + b_{12}v_2 \\ b_{21}v_1 + b_{22}v_2 \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1(b_{11}v_1 + b_{12}v_2) + a_{12}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{11}u_1(b_{21}v_1 + b_{22}v_2) + a_{12}u_2(b_{21}v_1 + b_{22}v_2) \\ a_{21}u_1(b_{11}v_1 + b_{12}v_2) + a_{22}u_2(b_{11}v_1 + b_{12}v_2) \\ a_{21}u_1(b_{21}v_1 + b_{22}v_2) + a_{22}u_2(b_{21}v_1 + b_{22}v_2) \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}u_1b_{11}v_1 + a_{11}u_1b_{12}v_2 + a_{12}u_2b_{11}v_1 + a_{12}u_2b_{12}v_2 \\ a_{11}u_1b_{21}v_1 + a_{11}u_1b_{22}v_2 + a_{12}u_2b_{21}v_1 + a_{12}u_2b_{22}v_2 \\ a_{21}u_1b_{11}v_1 + a_{21}u_1b_{12}v_2 + a_{22}u_2b_{11}v_1 + a_{22}u_2b_{12}v_2 \\ a_{21}u_1b_{21}v_1 + a_{21}u_1b_{22}v_2 + a_{22}u_2b_{21}v_1 + a_{22}u_2b_{22}v_2 \end{pmatrix}$$

Both sides are equal.

Mathematical concepts, vector spaces:

The space of states of a quantum system is a Hilbert vector space with either a finite or an infinite number of dimensions. It is composed of elements $|A\rangle$ called ket-vectors or just kets and their counterparts $\langle A|$, the complex conjugated and transposed version of $|A\rangle$. $\langle A|$ is called bra.

Note: the term vector and ket are used synonym.

The axioms for kets:

Let $|A\rangle$, $|B\rangle$ and $|C\rangle$ be vectors and z, w complex numbers, then:

1. Closure: the sum of two vectors is a vector:
   $|A\rangle + |B\rangle = |C\rangle$
2. Vector addition is commutative:
   $|A\rangle + |B\rangle = |B\rangle + |A\rangle$
3. Vector addition is associative:
   $\{|A\rangle + |B\rangle\} + |C\rangle = |A\rangle + \{|B\rangle + |C\rangle\}$
4. Existence of the 0:
   $|A\rangle + 0 = |A\rangle$
5. Existence of the inverse:
   $|A\rangle + (-|A\rangle) = 0$
6. Multiplication by a scalar produces a new vector:
   $|zA\rangle = z|A\rangle = |B\rangle$
7. Distributive property:
   $z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$
   $\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$

Axioms 6 and 7 taken together are often called *linearity*.

Ket $|A\rangle$ can be written as column vector:

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}$$

The corresponding bra $\langle A|$:

$$(\alpha_1^* \; \alpha_2^* \; \alpha_3^*)$$

If z is a complex number, then:

$$z|A\rangle \leftrightarrow \langle A|z^*$$

The dot product version, the inner product of bra and ket:

$$\langle B|A\rangle = z$$

Note: z is a complex number

The inner product is linear:

$$\langle C| \; \{|A\rangle + |B\rangle\} = \langle C|A\rangle + \langle C|B\rangle$$

Interchanging ket and bra corresponds to complex conjugation:

$$\langle B|A\rangle = \langle A|B\rangle^*$$

Note: $\langle A|A\rangle$ is always a real number.

A ket $|A\rangle$ is normalized:

$$\langle A|A\rangle = 1$$

Note: a spatial vector A of length 1 is called unit vector.

Two kets $|A\rangle$ and $|B\rangle$ are orthogonal:

$$\langle B|A\rangle = 0$$

Consider an orthonormal basis of kets labeled $|i\rangle$. The ket $|A\rangle$ can be written as:

$$|A\rangle = \sum_i \alpha_i |i\rangle$$

Analog to the spatial case we can express every ket as a sum of basis kets. The α_i are called the components of the ket.

Note: in quantum mechanics basis vectors generally are orthonormal:

$$\langle j|i\rangle = \delta_{ij}$$

To calculate the components, we take the inner product of both sides of $|A\rangle = \sum_i \alpha_i |i\rangle$ with a basis bra $\langle j|$:

$$\langle j|A\rangle = \sum_i \langle j|\alpha_i|i\rangle = \sum_i \alpha_i \langle j|i\rangle = \alpha_j$$

With this we can rewrite:

$$|A\rangle = \sum_i \alpha_i |i\rangle \rightarrow \sum_i \langle i|A\rangle\, |i\rangle = \sum_i |i\rangle\langle i|A\rangle$$

Note: $|i\rangle\langle i|$ is called the outer product, the sum over all i gives the identity matrix:

$$\sum_i |i\rangle\langle i| = I$$

Matrices:

Machines and matrices:

John Wheeler called operators: machines with an input port and an output port. In the input port you insert a vector $|A\rangle$ and get back a vector $|B\rangle$ at the output port.

We translate this in matrices acting on state vectors. A matrix acting on a vector $|A\rangle$ delivers a new vector $|B\rangle$.

Pauli matrices:

The Pauli matrices (operators):

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Any 2×2 Hermitian matrix L can be written as a sum of the Pauli matrices and the identity matrix I:

$$L = a\sigma_x + b\sigma_y + c\sigma_z + dI$$

Note: a, b, c, d are real numbers.

Building matrices from tensor product:

Prerequisite

To calculate the numerical values m_{jk} of a matrix M we use basis vectors $\langle j|$, $|k\rangle$:

$$m_{jk} = \langle j|M|k\rangle$$

The basis vectors of a single spin system in the up-down state in symbolic representation:

$$|uu\rangle, |du\rangle, |ud\rangle, |dd\rangle \text{ resp. } \langle uu|, \langle du|, \langle ud|, \langle dd|$$

The (Pauli) operator σ_z acts on the basis:

$$\sigma_z|uu\rangle = |uu\rangle, \qquad \sigma_z|ud\rangle = |ud\rangle, \qquad \sigma_z|du\rangle = -|du\rangle, \qquad \sigma_z|dd\rangle = -|dd\rangle$$

End prerequisite

Building a 4×4 matrix out of two 2×2 matrices via the tensor product:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \otimes \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} a\begin{pmatrix} e & f \\ g & h \end{pmatrix} & b\begin{pmatrix} e & f \\ g & h \end{pmatrix} \\ c\begin{pmatrix} e & f \\ g & h \end{pmatrix} & d\begin{pmatrix} e & f \\ g & h \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ae & af & be & bf \\ ag & ah & bg & bh \\ cd & cf & de & df \\ cg & ch & dg & dh \end{pmatrix}$$

We build the tensor product $\sigma_z \otimes I$:

$$\sigma_z \otimes I = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} 1\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 0\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ 0\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & -1\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

The operator σ_z (a short form of $\sigma_z \otimes I$) in the combined system can be represented by a 4×4 matrix.

We check this with the example $\sigma_z|du\rangle = -|du\rangle$.

$|du\rangle$ in vector representation:

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

σ_z resp. $\sigma_z \otimes I$:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$\sigma_z|du\rangle$:

$$\sigma_z|du\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = -\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = -|du\rangle$$

Matrix elements:

Let M be a 3×3 matrix:

$$M = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix}$$

The quantities m_{11} etc. are called the matrix elements.

Note: if M is an operator, it can be represented in more than one basis.

We can reproduce the matrix elements out of an operator by:

$$\langle k|M|j\rangle = m_{kj}$$

Note: the m_{kj} are complex numbers, their values changing with the basis $|j\rangle$, $\langle k|$ chosen.

Matrix multiplication:

In principle

Let M, N be two 3×3 matrices. The product $M \cdot N$:

$$M \cdot N = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \cdot \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} =$$

$$\begin{pmatrix} m_{11}n_{11} + m_{12}n_{21} + m_{13}n_{31} & m_{11}n_{12} + m_{12}n_{22} + m_{13}n_{32} & m_{11}n_{13} + m_{12}n_{23} + m_{13}n_{33} \\ m_{21}n_{11} + m_{22}n_{21} + m_{23}n_{31} & m_{21}n_{12} + m_{22}n_{22} + m_{23}n_{32} & m_{21}n_{13} + m_{22}n_{23} + m_{23}n_{33} \\ m_{31}n_{11} + m_{32}n_{21} + m_{33}n_{31} & m_{31}n_{12} + m_{32}n_{22} + m_{33}n_{32} & m_{31}n_{13} + m_{32}n_{23} + m_{33}n_{33} \end{pmatrix}$$

Multiplying a matrix M by a column vector $\vec{a}$:

$$M \cdot \vec{a} = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} =$$

$$\begin{pmatrix} m_{11}a_1 + m_{12}a_2 + m_{13}a_3 \\ m_{21}a_1 + m_{22}a_2 + m_{23}a_3 \\ m_{31}a_1 + m_{32}a_2 + m_{33}a_3 \end{pmatrix}$$

Multiplying a matrix M by a row vector $\vec{a}$:

$$\vec{a} \cdot M = (a_1\ a_2\ a_3) \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} =$$

$$(a_1m_{11} + a_2m_{21} + a_3m_{31} \quad a_1m_{12} + a_2m_{22} + a_3m_{32} \quad a_1m_{13} + a_2m_{23} + a_3m_{33})$$

Matrix notation, transposing in matrix notation:

For complex vector spaces

Switching from a $M|a\rangle$ to its corresponding $\langle a|M$ requests complex conjugation of the elements of the ket $|a\rangle$ and transposing and complex conjugation of the matrix M. The complex conjugate of a transposed matrix is called its Hermitian conjugate.

$$M \cdot |a\rangle = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} =$$

$$\begin{pmatrix} m_{11}a_1 + m_{12}a_2 + m_{13}a_3 \\ m_{21}a_1 + m_{22}a_2 + m_{23}a_3 \\ m_{31}a_1 + m_{32}a_2 + m_{33}a_3 \end{pmatrix}$$

Multiplying a matrix M by a bra $\langle a|$:

$$\langle a| \cdot M^\dagger = (a_1^* \;\; a_2^* \;\; a_3^*) \begin{pmatrix} m_{11}^* & m_{21}^* & m_{31}^* \\ m_{12}^* & m_{22}^* & m_{32}^* \\ m_{13}^* & m_{23}^* & m_{33}^* \end{pmatrix} =$$

$$(a_1^* m_{11}^* + a_2^* m_{12}^* + a_3^* m_{13}^* \quad a_1^* m_{21}^* + a_2^* m_{22}^* + a_3^* m_{23}^* \quad a_1^* m_{31}^* + a_2^* m_{32}^* + a_3^* m_{33}^*)$$

This might be puzzling in the beginning, so please remember:

$$M|A\rangle = |B\rangle \rightarrow \langle A|M^\dagger = \langle B|$$

Maximally entangled state:

Prerequisite

We have a single spin system in the up-down basis:

$$|\psi\rangle = \alpha|u\rangle + \beta|d\rangle$$

The wave function:

$$\psi(u) = \alpha \qquad \psi^*(u) = \alpha^*$$
$$\psi(d) = \beta \qquad \psi^*(d) = \beta^*$$

The density matrix:

$$\rho_{a'a} = \begin{pmatrix} \alpha^*\alpha & \alpha^*\beta \\ \beta^*\alpha & \beta^*\beta \end{pmatrix}$$

The density matrix describes the probability to change the system from one possible state into another. The probability for a state to change from $|u\rangle$ to $|u\rangle$ is $\alpha^*\alpha$ etc.

End prerequisite

Suppose we have a two-spin system, maximally entangled.

When Alice calculates the density matrix of her subsystem for the maximally entangled state, she finds:

$$\rho_{a'a} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

This means that Alice knows nothing about her system. The states $|u\rangle$ and $|d\rangle$ have a 50% chance. She cannot determine the state her subsystem is in. This is in contrast to a composite system in the product state. In this product state all of Alice's observations are described as if Bob and his system never existed. In this case the density matrix of Alice would have exactly one entry that is one, the rest equals zero – she can determine the state her system is in.

Note: the singlet state is maximally entangled:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$$

Maxwell's equations:

Quantum electrodynamic can be deduced from Maxwell's equations.

In particle physics, quantum electrodynamics (QED) is the relativistic quantum field theory of electrodynamics. In essence, it describes how light and matter interact and is the first theory where full agreement between quantum mechanics and special relativity is achieved. QED mathematically describes all phenomena involving electrically charged particles interacting by means of exchange of photons and represents the quantum counterpart of classical electromagnetism giving a complete account of matter and light interaction. *(courtesy Wikipedia)*

Mean value:

In quantum mechanics mean value or average value is called expectation value.

In statistics the mean value x is denoted by $\bar{x}$.

In quantum mechanics the mean value of the observable L is denoted by $\langle L \rangle$.

From a mathematical point of view, an average is defined by the equation

$$\langle L \rangle = \sum_i \lambda_i P(\lambda_i)$$

This is a weighted sum, weighted with the probability function P.

From an experimental point of view, we can identify $P(\lambda_i)$ as the fraction of observations whose result was λ_i. The greater the number of experiments, the better mathematical and experimental notions of probability and average will agree.

Let $|A\rangle$ be the normalized state of a quantum system.

We expand $|A\rangle$ in the orthonormal basis of eigenvectors of an observable L

$$|A\rangle = \sum_i \alpha_i \, |\lambda_i\rangle$$

and its counterpart:

$$\langle A| = \sum_i \langle \lambda_i | \alpha_i^*$$

We compute the quantity $\langle A|L|A\rangle$:

$$\langle A|L|A\rangle = \langle A|L| \textstyle\sum_i \alpha_i |\lambda_i\rangle =$$

$$\langle A| \textstyle\sum_i \alpha_i L \, |\lambda_i\rangle\rangle =$$

$$\langle A| \textstyle\sum_i \alpha_i \lambda_i \, |\lambda_i\rangle\rangle =$$

$$\langle \textstyle\sum_i \langle \lambda_i | \alpha_i^* \, | \sum_i \alpha_i \lambda_i \, |\lambda_i\rangle\rangle =$$

$$\sum_i \alpha_i^* \alpha_i \lambda_i \langle \lambda_i | \lambda_i \rangle =$$

$$\sum_i \alpha_i^* \alpha_i \lambda_i$$

Comparing this with the definition of an average $\langle L\rangle = \sum_i \lambda_i P(\lambda_i)$ we can identify:

$$P(\lambda_i) = \alpha_i^* \alpha_i$$

We get the result:

$$\langle L\rangle = \langle A|L|A\rangle$$

To get the mean value or average of an observable $\langle L\rangle$ we have to sandwich it between the bra and ket representation of the state-vector.

Measurables, states that depend on more than one measurable:

If there are multiple measurables, we need multiple measurements to fully characterize the state of a system. We start with a two-spin system and two operators (measurements) L and M.

If we measure both spins in a two-spin system, the systems winds up in a state that is simultaneously eigenvector of L and eigenvector of M.

Let λ_i, $|\lambda_i\rangle$ and μ_a, $|\mu_a\rangle$ be eigenvalues and eigenvectors of L and M, the eigenvectors building a basis. Leaving out the subscripts we write:

$$L|\lambda,\mu\rangle = \lambda|\lambda,\mu\rangle$$

$$M|\lambda,\mu\rangle = \mu|\lambda,\mu\rangle$$

We apply both operators:

$$ML|\lambda,\mu\rangle = M\lambda|\lambda,\mu\rangle = \mu\lambda|\lambda,\mu\rangle$$

$$LM|\lambda,\mu\rangle = L\mu|\lambda,\mu\rangle = \lambda\mu|\lambda,\mu\rangle = \mu\lambda|\lambda,\mu\rangle$$

We get:

$$ML|\lambda,\mu\rangle - LM|\lambda,\mu\rangle = [ML - LM]|\lambda,\mu\rangle = [M,L]|\lambda,\mu\rangle = 0$$

Result: if there is a complete basis of simultaneous eigenvectors of two observables, the two observables must commute and: if two observables commute, then there is a complete basis of simultaneous eigenvectors of the two observables.

In other words, the condition for two observables to be simultaneously measurable is that they commute.

Measurement:

Suppose we orient a spin in space and try to measure its value along the x axis and the y axis.

The spin observables are:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We try whether they commute:

$$[\sigma_x\sigma_y - \sigma_y\sigma_x] =$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} - \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} =$$

$$\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix} - \begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix} = \begin{pmatrix}2i & 0\\ 0 & -2i\end{pmatrix} =$$

$$2i\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = 2i\sigma_z$$

The important result: $[\sigma_x\sigma_y - \sigma_y\sigma_x] \neq 0$.

The same holds for any other combination of different directions. This tells us that no two spin components can simultaneously be measured.

Measurement, apparatus and measurement:

We use a single spin system and an apparatus A to measure the spin orientation. We take the basis states of the spin to be $|u\rangle$ and $|d\rangle$. The state of the apparatus (as complex it might be inside) is described by the basis states $|b\rangle$ for a blank state, $|+1\rangle$ for "detected up" and $|-1\rangle$ for "detected down".

From this we build a composite (tensor product) space of states with six basis vectors:

$$|u,b\rangle, |u,+1\rangle, |u,-1\rangle, |d,b\rangle, |d,+1\rangle, |d,-1\rangle$$

We assume the apparatus starts in the blank state and the spin starts in the up state. After the apparatus interacts with the spin, the final state is:

$$|u,+1\rangle$$

We write this as:

$$|u,b\rangle \rightarrow |u,+1\rangle$$

Similarly, starting with the spin in the down state (opposite to the direction of the apparatus) we get:

$$|d,b\rangle \rightarrow |d,-1\rangle$$

Assuming that the initial spin is oriented more general:

$$\alpha_u|u\rangle + \alpha_d|d\rangle$$

We include the apparatus as part of the system and get the initial state:

$$\alpha_u|u,b\rangle + \alpha_d|d,b\rangle$$

This is a completely unentangled state. We determine the final state after measurement:

$$\alpha_u|u,b\rangle + \alpha_d|d,b\rangle \rightarrow \alpha_u|u,+1\rangle + \alpha_d|d,-1\rangle$$

The final state is an entangled state. If $\alpha_u = -\alpha_d$, it is the maximally entangled singlet state.

We can look at the apparatus and tell what the spin state is. If the apparatus reads +1, the spin is up, and if it reads -1, the spin is $down$. The probability that the apparatus shows $+1$ is $\alpha_u^*\alpha_u$.

There might arise questions about wave functions and collapsing wave functions. Do not try to ask questions about the underlying reality. Quantum mechanics is a consistent calculus of probabilities for certain kinds of experiments. We use it and it works.

Measurement, collapse of the wave function and measurement:

Experimental physics measures observables. An experiment to measure L will have an unpredictable outcome, but after the measurement the system is left in an eigenstate of L corresponding to the outcome of the measurement.

This phenomenon is called the collapse of the wave function.

Suppose the state vector before the measurement:

$$\sum_j \alpha_j |\lambda_j\rangle$$

Randomly, with probability $|\alpha_j|^2$, the apparatus measures a value λ_j and leaves the system in a single eigenstate of L, namely $|\lambda_j\rangle$. The entire superposition of states collapses to a single term.

The system evolves one way between measurements and another way during a measurement.

Measurement, multiple measurements:

If there are multiple measurables, we need multiple measurements to fully characterize the state of a system. We start with a two-spin system and two operators (measurements) L and M.

If we measure both spins in a two-spin system, the systems winds up in a state that is simultaneously eigenvector of L and eigenvector of M.

Let λ_i, $|\lambda_i\rangle$ and μ_a, $|\mu_a\rangle$ be eigenvalues and eigenvectors of L and M, the eigenvectors building a basis. Leaving out the subscripts we write:

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We apply both operators:

$$ML|\lambda,\mu\rangle = M\lambda|\lambda,\mu\rangle = \mu\lambda|\lambda,\mu\rangle$$

$$LM|\lambda,\mu\rangle = L\mu|\lambda,\mu\rangle = \lambda\mu|\lambda,\mu\rangle = \mu\lambda|\lambda,\mu\rangle$$

We get:

$$ML|\lambda,\mu\rangle - LM|\lambda,\mu\rangle = [ML - LM]|\lambda,\mu\rangle = [M,L]|\lambda,\mu\rangle = 0$$

Result: if there is a complete basis of simultaneous eigenvectors of two observables, the two observables must commute and: if two observables commute, then there is a complete basis of simultaneous eigenvectors of the two observables.

In other words, the condition for two observables to be simultaneously measurable is that they commute.

Measurement, operators and measurement:

- Operators are the things we use to calculate eigenvalues and eigenvectors.
- Operators act on state-vectors, not on actual physical systems
- On operator acting on a state-vector produces a new state vector

There is a difference between “measuring an observable” and “operating with the corresponding operator on the state”.

Suppose we are interested in measuring an observable L. The state of the system before we do the measurement is $|A\rangle$. It is not correct to say that the measurement of L always changes the state to $l|A\rangle$ with l being a number.

We show this with an example.

We prepare the state $|r\rangle$ which is not eigenvector of σ_z. We can express the state $|r\rangle$ in terms of $|u\rangle$ and $|d\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

Acting on this state vector with σ_z:

$$\sigma_z|r\rangle = \frac{1}{\sqrt{2}}\sigma_z|u\rangle + \frac{1}{\sqrt{2}}\sigma_z|d\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

The measurement result would be either $+1$, leaving the system in state $|u\rangle$, or -1, leaving the system in state $|d\rangle$ – one of them.

The state after acting with the operator is a superposition of both states $|u\rangle$ and $|d\rangle$.

Measurement, states and measurement:

In the classical world, the state of a system can be determined by an experiment. A measurement shows the state of a system. In the quantum world, states and measurements are two different things. A measurement determines the state of a system.

Minimum-uncertainty wave packets:

Minimum-uncertainty wave packets are wave packets where $\Delta x \Delta p$ is equal to $\frac{\hbar}{2}$. In these cases, $\Delta x \Delta p$ is as small as quantum mechanics allows. They have the form of a Gaussian curve, and they are often called Gaussian wave packets. Over the time, they spread out and flatten.

The ground state of a harmonic oscillator is an example for a Gaussian wave packet.

Minus first law:

The minus first law says that information is never lost. If two identical isolated systems start out in different states, they stay in different states, they were in different states in the past and they will be in different states in the future. Distinctions are conserved.

In classical mechanics, this principle led to Hamilton's equations and Liouville's theorem.

In quantum mechanics it led to the principle of unitarity and the Schrödinger equation.

Minus first law, quantum version of the minus first law:

Let $|\psi(t)\rangle$ be the quantum state of a closed system at any time t. The system evolves by help of $U(t)$, acting on the state $|\psi(t)\rangle$ at time zero,

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

resp.

$$\langle\psi(t)| = \langle\psi(0)|U^{\dagger}(t)$$

Note: $U^{\dagger}$ is the Hermitian conjugated to U.

U is called the time-development operator for the system.

Two states $|\psi(t)\rangle$ and $|\phi(t)\rangle$ are distinguishable if they are orthogonal for all values of t:

$$\langle\psi(t)|\phi(t)\rangle = 0$$

We replace $\langle\psi(t)|$ and $|\phi(t)\rangle$:

$$\langle\psi(0)|U^{\dagger}(t)U(t)|\phi(0)\rangle = 0$$

To preserve orthogonality for all times:

$$U^{\dagger}(t)U(t) = I$$

An operator that satisfies this condition is called unitary. The evolution of state-vectors with time is unitary.

Mixed state:

Prerequisite

A projection operator is the outer product of any normalized ket $|\psi\rangle$ with its corresponding bra $\langle\psi|$:

$$|\psi\rangle\langle\psi|$$

Note: $|\psi\rangle\langle\psi|$ can be represented as a matrix by choosing a basis.

With this we can write the expectation value of an observable L

$$\langle L\rangle = \langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|\ L$$

or:

$$\langle L\rangle = Tr\ \rho L$$

Note: Tr is the trace of a matrix.

$|\psi\rangle\langle\psi|$ is called density matrix ρ.

A density matrix ρ can be the (normalized) sum of several projection operators.

With this we can rewrite:

$$\langle L\rangle = \sum_{a,a'} L_{a,a'}\rho_{a,a'}$$

End prerequisite

A mixed state is represented by a density matrix made of several projection operators. It is a matrix that has entries only on the diagonal, summing up to 1.

In contrast: a pure state is represented by a density matrix that has only one entry on its diagonal and this entry is 1.

Mixed states, composite system and mixed states:

We have a combined system and complete knowledge of its state:

$$\psi(a,b)$$

Alice is not interested in the combined system but wants to find out as much as she can about her subsystem A. She selects an observable L that belongs to A and does nothing to B when it acts.

The general rule for calculating the expectation value of L:

$$\langle L\rangle = \sum_{ab,a'b'} \psi^*(a'b')L_{a'b',ab}\,\psi(ab)$$

The observable L does nothing on system B:

$$\langle L\rangle = \sum_{ab,a'} \psi^*(a'b)L_{a',a}\,\psi(ab) = \sum_{ab,a'} L_{a,a'}\,\psi^*(a'b)\psi(ab)$$

This is similar to:

$$\langle L\rangle = \sum_{a,a'} L_{a,a'}\rho_{a,a'}$$

We can identify $\psi^*(a'b)\psi(ab) \approx \rho_{a,a'}$ and, by summing up over all b:

$$\rho_{a,a'} = \sum_{b} \psi^*(a'b)\psi(ab)$$

The kind of the density matrix $\rho_{a,a'}$ depends on how the combined system is build out of the two subsystems.

In case of a product state, ρ will have the form of a (single) projection operator. Alice's subsystem can be described like a stand-alone system, a pure state.

In case of an entangled state, ρ will be the sum of several projection operators. Despite the fact that Alice knows all about the combined state, she must describe her subsystem like a mixed state.

Mixed states, density matrices and mixed states:

There is a simple check whether a density matrix belongs to a pure state or a mixed state.

Pure state:

$$\rho^2 = \rho \text{ and } Tr(\rho^2) = 1$$

Mixed state:

$$\rho^2 \neq \rho \text{ and } Tr(\rho^2) < 1$$

Momentum:

Momentum, canonical momentum:

Classical part

Canonical Momentum: For a one-dimensional system (the harmonic oscillator) we have only one Lagrange equation:

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}$$

With partial differentiation we get:

$$\frac{\partial L}{\partial \dot{x}} = \dot{x}$$

This is called the canonical momentum conjugate to x.

The Hamiltonian for the Harmonic oscillator:

$$H = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega^2 x^2$$

We rewrite the Hamiltonian in terms of canonical momentum

$$p\frac{\partial L}{\partial \dot{x}} = \dot{x}$$

and get:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$$

Quantum mechanical part

We reinterpret p and x as momentum operator P and position operator X. P differentiates:

$$P|\psi(x)\rangle \to -i\hbar\frac{d}{dx}\psi(x)$$

X multiplies the wave function by x:

$$X|\psi(x)\rangle \to x(x)$$

With this we get the quantum mechanical Hamiltonian from the classical one:

$$H|\psi(x)\rangle \to -\frac{\hbar^2}{2}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}\omega^2 x^2\psi(x)$$

Note: we use partial derivatives because in general ψ also depends on the variable $time$ indicating that we describe the system at a fixed time.

Momentum, connection between quantum and classical physics:

Let f, g be two phase state functions of space and time, depending of canonical coordinates (q_i, p_i). The Poisson bracket $\{f, g\}$ in canonical coordinates (also known as Darboux coordinates):

$$\{f, g\} = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right)$$

The Poisson brackets of the canonical coordinates:

$$\{q_i, q_j\} = 0$$

$$\{p_i, p_j\} = 0$$

$$\{q_i, p_j\} = \delta_{ij}$$

We compare this with the quantum mechanical Hamiltonian, expressed in terms of momentum operator P and Position operator X. For this case the following holds:

$$XP\psi(x) = X\left(-i\hbar\frac{d\psi(x)}{dx}\right) = -i\hbar x\frac{d\psi(x)}{dx}$$

$$PX\psi(x) = P\big(x\psi(x)\big) = -i\hbar\psi(x) - i\hbar x\frac{d\psi(x)}{dx}$$

The commutator

$$[X,P]\psi(x) = XP\psi(x) - PX\psi(x) = i\hbar\psi(x)$$

or

$$[X,P] = i\hbar$$

The quantum mechanical commutator $[X,P] = i\hbar$ and the Poisson brackets $\{q_i, p_j\} = \delta_{ij}$ show the connection between quantum mechanics and classical mechanics.

Note: from $[X,P] = i\hbar$ we can derive the uncertainty relation $\Delta X \Delta P \geq \frac{\hbar}{2}$.

Momentum, eigenfunctions and momentum (harmonic oscillator):

The eigenfunctions of increasing energy levels oscillates more rapidly than the one below it. This corresponds to an increase in momentum.

Momentum, eigenvectors of momentum:

The momentum operator P:

$$P|\psi\rangle \rightarrow -i\hbar\frac{d}{dx}\psi(x)$$

An eigenvector of the momentum operator P with eigenvalue p:

$$P|\psi\rangle = p|\psi\rangle$$

We write this in wave functions:

$$-i\hbar\frac{d}{dx}\psi(x) = p\psi(x)$$

The solution:

$$\psi_p(x) = Ae^{\frac{ipx}{\hbar}}$$

Note: the subscript p is just a reminder that $\psi_p(x)$ is the eigenvector of P with the specific eigenvalue p. It is a function of x, but labeled by an eigenvalue of P.

With the appropriate normalizing we get:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}}e^{\frac{ipx}{\hbar}}$$

This represents the momentum eigenfunction in the position basis. It is a function of x, not an explicit function of p.

Momentum, forces and momentum:

Prerequisite

P is the momentum operator. In quantum mechanics holds that the average momentum equals the mass times the velocity:

$$\langle P\rangle = mv$$

The time derivative of the expectation value of any observable L is given by:

$$\frac{d}{dt}\langle P\rangle = \frac{i}{\hbar}\langle [H,P]\rangle$$

Note: H is the Hamiltonian.

The potential energy operator V acting on a wave function multiplies the wave function by the function $V(x)$:

$$V|\psi\rangle = V(x)\psi(x)$$

For the potential energy operator V holds the commutator relation:

$$[V,P] = i\hbar\frac{dV(x)}{dx}$$

We check this:

$$[V,P]\,\psi(x) =$$

$$V(x)\left(-i\hbar\frac{d}{dx}\right)\psi(x) - \left(-i\hbar\frac{d}{dx}\right)\big(V(x)\psi(x)\big) =$$

$$-i\hbar\left(V(x)\frac{d\psi(x)}{dx} - \left(\frac{dV(x)}{dx}\psi(x) + \frac{d\psi(x)}{dx}V(x)\right)\right) =$$

$$i\hbar\frac{dV(x)}{dx}\psi(x)$$

End prerequisite

As in classical mechanics the momentum of a particle is no longer conserved if forces act on the particle

$$\frac{dp}{dt} = F$$

or:

$$\frac{dp}{dt} = -\frac{\partial V}{\partial x}$$

We add $V(x)$ to the Hamiltonian:

$$H = \frac{P^2}{2m} + V(x)$$

We get the Schrödinger equation:

$$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

In general, multiplying by x and multiplying by a function of x are operations that commute:

$$[X,V(x)] = 0$$

We check the influence of the Potential P onto the quantum version of Newton's law:

$$\frac{dp}{dt} = F$$

We calculate the time derivative of the expectation value of P:

$$\frac{d}{dt}\langle P\rangle = \frac{i}{2m\hbar}\langle [P^2, P]\rangle + \frac{i}{\hbar}\langle [V, P]\rangle$$

The commutator of an operator with any power of itself is zero.

For the commutator $[V, P]$ we get:

$$[V, P] = i\hbar\frac{dV(x)}{dx}$$

Result:

$$\frac{d}{dt}\langle P\rangle = -\frac{dV(x)}{dx}$$

This is the quantum analog of Newton's equation for the time rate change of momentum.

Momentum, Heisenberg Uncertainty Principle and momentum:

Prerequisite

The Cauchy-Schwarz inequality:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

The commutator of momentum operator P and position operator X:

$$[X, P] = i\hbar$$

End prerequisite

Let $|\psi\rangle$ be any ket, A and B any two observables with expectation value zero.

We define $|X\rangle$ and $|Y\rangle$:

$$|X\rangle = A|\psi\rangle \text{ and } \langle X| = \langle\psi|A$$

$$|Y\rangle = iB|\psi\rangle \text{ and } \langle Y| = \langle\psi|(-iB)$$

We place $|X\rangle$ and $|Y\rangle$ into the Cauchy-Schwarz inequality:

$$2\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq |\langle\psi|AiB|\psi\rangle - \langle\psi|iBA|\psi\rangle| =$$

$$|\langle\psi|AB|\psi\rangle - \langle\psi|BA|\psi\rangle| = |\langle\psi|[AB]|\psi\rangle|$$

If A and B have expectation value zero, then $\langle A^2\rangle$ is the square of the uncertainty in A, $(\Delta\mathrm{A})^2$.

$\langle B^2\rangle$ the square of the uncertainty in B, $(\Delta\mathrm{B})^2$.

Note: by shifting A and B in an appropriate manner we can always fulfill that the shifted A and B have expectation value zero.

We rewrite:

$$2\sqrt{\langle A^2\rangle\langle B^2\rangle} = \Delta\mathrm{A}\Delta\mathrm{B}$$

We get:

$$\Delta A \Delta B \geq \frac{1}{2}|\langle\psi|[AB]|\psi\rangle|$$

The product of uncertainties cannot be smaller than half the magnitude of the expectation value of the commutator.

We apply this to the position operator X and the momentum operator P:

$$[\Delta X, \Delta P] \geq \frac{1}{2}|\langle\psi|[XP]|\psi\rangle| =$$

$$\frac{1}{2}|\langle\psi|i\hbar|\psi\rangle| = \frac{\hbar}{2}|\langle\psi|\psi\rangle| = \frac{\hbar}{2}$$

We get:

$$[\Delta X, \Delta P] \geq \frac{\hbar}{2}$$

This is the Heisenberg Uncertainty Principle.

Momentum, proposition for momentum:

A proposition is a statement that can be true or false. Propositions can be combined by classical logic. Elementary combinations are "and", "or" to give new propositions.

There is a difference between propositions in classical physics and quantum mechanics.

In classical physics holds: "A particle has position and momentum", meaning that position and momentum can be determined both exactly simultaneously, at least the order doesn't matter.

In quantum mechanics holds: "A particle has position or momentum", meaning that either the position or the momentum can be determined exactly – but not both simultaneously due to the Heisenberg Uncertainty Relation.

Momentum, velocity and momentum:

Prerequisite

In classical physics p is the momentum, x the position of a particle.

In quantum mechanics we use the momentum operator P and the position operator X and work with the averages (expectation values) $\langle P\rangle$ and $\langle X\rangle$.

For a free particle the Hamiltonian is the kinetic energy:

$$\frac{p^2}{2m}$$

The standard commutation relation:

$$[P, X] = -i\hbar$$

End prerequisite

In classical physics momentum is mass times velocity or:

$$v = \frac{p}{m}$$

In quantum mechanics we use the position operator $\langle X \rangle$ and work with the average position $\langle X \rangle = \langle \psi | X | \psi \rangle$:

$$v = \frac{d}{dt} \langle \psi | X | \psi \rangle$$

We express this in terms of wave functions:

$$v = \frac{d}{dt} \int \psi^*(x,t) \psi(x,t) dx$$

$\langle \psi | X | \psi \rangle$ varies with time according to the time-dependent Schrödinger equation.

The time-dependence of any observable L (the expectation value):

$$\frac{d}{dt} \langle L \rangle = \frac{i}{\hbar} \langle [H, L] \rangle$$

Note: $[H, L]$ is the commutator of the observable L with the Hamiltonian.

The Hamiltonian is the (kinetic) energy of the particle:

$$H = \frac{P^2}{2m}$$

We apply this to the velocity v:

$$v = \frac{d}{dt} \langle X \rangle = \frac{i}{\hbar} \langle [H, X] \rangle = \frac{i}{\hbar} \langle \left[\frac{P^2}{2m}, X \right] \rangle =$$

$$\frac{i}{2m\hbar} \langle [P^2, X] \rangle = \frac{i}{2m\hbar} \langle P[P, X] + [P, X]P \rangle =$$

$$\frac{i}{2m\hbar} \langle P(-i\hbar) + (-i\hbar)P \rangle = \frac{\langle P \rangle}{m}$$

We get

$$v = \frac{\langle P \rangle}{m}$$

or:

$$\langle P \rangle = mv$$

Momentum, wavelength and momentum:

Light of a given wavelength is composed of photons with momentum:

$$\lambda = \frac{2\pi\hbar}{p}$$

Momentum basis:

Prerequisite

The inner product of a position eigenvector $|x\rangle$ and a momentum eigenvector $|p\rangle$:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$

Please not the minus sign.

End prerequisite

The wave function gives the probability for finding a particle at position x:

$$P(x) = \psi^*(x)\psi(x)$$

As we will see, no experiment can determine both the position and the momentum of a particle simultaneously, analog to the impossibility to measure both the x and z component of a spin.

A momentum measurement will give p with probability $P(p)$:

$$P(p) = |\langle P|\psi\rangle|^2$$

$\langle P|\psi\rangle$ is called the wave function of $|\psi\rangle$ in the momentum representation. It is denoted by:

$$\tilde{\psi}(p) = \langle P|\psi\rangle$$

The state vector can be represented in two ways, the position basis or the momentum basis. Both wave functions, the position wave function $\psi(x)$ and the momentum wave function $\tilde{\psi}(p)$ represent exactly the same state-vector $|\psi\rangle$. The transformation between them is the Fourier transformation.

Given a basis of a phase state in basis vectors $|i\rangle$. We can rewrite the identity operator I in terms of the outer product:

$$I = \sum_i |i\rangle\langle i|$$

Because momentum and position are both Hermitian, the sets of vectors $|x\rangle$ and $|p\rangle$ each define basis vectors.

We replace the sum by an integral:

$$I = \int |x\rangle\langle x|\, dx$$

or

$$I = \int |p\rangle\langle p|\, dp$$

Suppose we know the wave function of the vector $|\psi\rangle$ in the position representation. By definition, it is equal to:

$$\psi(x) = \langle x|\psi\rangle$$

We build the wave function $\tilde{\psi}(p)$ in the momentum representation.

1. We use the definition of the momentum-representation wave function:
$$\tilde{\psi}(p) = \langle p|\psi\rangle$$
2. We insert the unit operator:
$$\tilde{\psi}(p) = \int \langle p|x\rangle\langle x|\psi\rangle \, dx$$
$\langle x|\psi\rangle$ is the wave function $\psi(x)$.
3. $\langle p|x\rangle$ is given by:
$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$
4. Result:
$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{ipx}{\hbar}} \psi(x) dx$$

By knowing $\psi(x)$ in the position representation we calculate the corresponding wave function in the momentum representation.

This works the other way around. We know the wave function in the momentum representation $\tilde{\psi}(p)$ and calculate the position representation:

1. We use the definition of the position-representation wave function:
$$\psi(x) = \langle x|\psi\rangle$$
2. We insert the unit operator:
$$\psi(x) = \int \langle x|p\rangle\langle p|\psi\rangle \, dp$$
$\langle p|\psi\rangle$ is the wave function $\tilde{\psi}(p)$.
3. $\langle x|p\rangle$ is given by:
$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$
4. Result:
$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{\frac{ipx}{\hbar}} \tilde{\psi}(p) dp$$

Position and momentum representation are reciprocal Fourier transforms of each other.

Momentum operator:

We have the differentiation operator D:

$$D = \frac{d}{dx}$$

Note: the differentiation operator in this form is not Hermitian.

We define the momentum operator P:

$$P = -i\hbar D = -i\hbar \frac{d}{dx}$$

Note: the momentum operator P is Hermitian.

Momentum representation of wave function:

Prerequisite

The inner product of a position eigenvector $|x\rangle$ and a momentum eigenvector $|p\rangle$:

$$\langle x|p\rangle = \langle p|x\rangle^*$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$

By help of the identity operator we can expand inner products:

$$I = \sum_i |i\rangle\langle i|$$

Note: $|i\rangle$ must be a complete set of basis vectors.

This works with integrals too:

$$I = \int |x\rangle\langle x|\, dx$$

$$I = \int |p\rangle\langle p|\, dp$$

Note: the eigenvectors of position operator X and momentum operator P define an appropriate basis.

End prerequisite

Suppose we know the wave function of the abstract vector $|\psi\rangle$ in position representation:

$$\psi(x) = \langle x|\psi\rangle$$

To know the wave function $\tilde{\psi}(x)$ in momentum representation we do the following steps.

1. We use the definition of the momentum-representation wave function:
   $$\tilde{\psi}(p) = \langle P|\psi\rangle = \langle p|\psi\rangle$$
   Note: P is the momentum operator, p is eigenvalue of $|\psi\rangle$.

2. We insert the unit operator:
   $$\tilde{\psi}(p) = \int \langle p|x\rangle\langle x|\psi\rangle\, dx$$
   $\langle x|\psi\rangle$ is just the wave function $\psi(x)$.

3. $\langle p|x\rangle$ is given by:
   $$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$

4. Result:
   $$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{ipx}{\hbar}} \psi(x) dx$$

By knowing $\psi(x)$ in the position representation we calculate the corresponding wave function in the momentum representation.

This works also the other way around. We know the wave function in the momentum representation $\tilde{\psi}(p)$ and calculate the position representation:

1. We use the definition of the position-representation wave function:
$$\psi(x) = \langle x|\psi\rangle$$
Note: X is the position operator, x is eigenvalue of $|\psi\rangle$.

2. We insert the unit operator:
$$\psi(x) = \int \langle x|p\rangle\langle p|\psi\rangle \, dp$$
$\langle p|\psi\rangle$ is just the wave function $\tilde{\psi}(p)$.

3. $\langle x|p\rangle$ is given by:
$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

4. Result:
$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{\frac{ipx}{\hbar}} \tilde{\psi}(p) dp$$

Position and momentum representation are reciprocal Fourier transforms of each other.

Multiplication:

Multiplication of column vector:

Multiplication of a column vector means “stretching” it by a (complex) number:

$$z\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} = \begin{pmatrix}z\cdot\alpha_1\\ z\cdot\alpha_2\end{pmatrix}$$

Multiplication of complex numbers:

In cartesian representation:

$$(a+ib)(c+id) = ac + aid + cib + i^2bd =$$

$$(ac - bd) + i(ad + cb)$$

Note: i is the imaginary unit.

In gaussian representation:

$$r_1 e^{i\varphi} \cdot r_2 e^{i\theta} = r_1 \cdot r_2 e^{i(\theta+\varphi)}$$

Note: multiplying a complex number with its complex conjugate always gives a positive real result.

$$(a+ib)(a-ib) = a^2 + b^2$$

$$re^{i\varphi} \cdot re^{-i\varphi} = r^2 e^{i(\varphi-\varphi)} = r^2 e^0 = r^2$$

Note: this is the square of the absolute value of the number.

Multiplication, matrix multiplication:

In principle

Let M, N be two 3×3 matrices. The product $M \cdot N$:

$$M \cdot N = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \cdot \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} =$$

$$\begin{pmatrix} m_{11}n_{11} + m_{12}n_{21} + m_{13}n_{31} & m_{11}n_{12} + m_{12}n_{22} + m_{13}n_{32} & m_{11}n_{13} + m_{12}n_{23} + m_{13}n_{33} \\ m_{21}n_{11} + m_{22}n_{21} + m_{23}n_{31} & m_{21}n_{12} + m_{22}n_{22} + m_{23}n_{32} & m_{21}n_{13} + m_{22}n_{23} + m_{23}n_{33} \\ m_{31}n_{11} + m_{32}n_{21} + m_{33}n_{31} & m_{31}n_{12} + m_{32}n_{22} + m_{33}n_{32} & m_{31}n_{13} + m_{32}n_{23} + m_{33}n_{33} \end{pmatrix}$$

Multiplying a matrix M by a column vector $\vec{a}$:

$$M \cdot \vec{a} = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} =$$

$$\begin{pmatrix} m_{11}a_1 + m_{12}a_2 + m_{13}a_3 \\ m_{21}a_1 + m_{22}a_2 + m_{23}a_3 \\ m_{31}a_1 + m_{32}a_2 + m_{33}a_3 \end{pmatrix}$$

Multiplying a matrix M by a row vector $\vec{a}$:

$$\vec{a} \cdot M = (a_1 \; a_2 \; a_3) \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} =$$

$$(a_1m_{11} + a_2m_{21} + a_3m_{31} \quad a_1m_{12} + a_2m_{22} + a_3m_{32} \quad a_1m_{13} + a_2m_{23} + a_3m_{33})$$

Multiplication, vector multiplication:

We can multiply a vector by a (complex) number:

$$z \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} z \cdot a \\ z \cdot b \\ z \cdot c \end{pmatrix}$$

We can build the inner product of two vectors:

$$(a \; b \; c) \cdot \begin{pmatrix} d \\ e \\ f \end{pmatrix} = ad + be + cf$$

The result of the inner product is a (complex) number.

We can build the outer product of two vectors:

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} (d \; e \; f) = \begin{pmatrix} ad & ae & af \\ bd & be & bf \\ cd & ce & cf \end{pmatrix}$$

The result of the outer product is a matrix.

Note: this is the tensor product.

Note: we can build inner and outer products of vectors of the same rank, the same dimension.

Near-singlet state:

We have a combined system of two spins, Alice and Bob. The near singlet state is a partially entangled state.

The state-vector:

$$\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$$

or in the extended form:

$$|near\ sing\rangle = 0|uu\rangle + \sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle + 0|dd\rangle$$

We have only one normalization condition:

$$\psi_{uu}^{*}\psi_{uu} + \psi_{ud}^{*}\psi_{ud} + \psi_{du}^{*}\psi_{du} + \psi_{dd}^{*}\psi_{dd} = 1$$

in this case reducing to:

$$\psi_{ud}^{*}\psi_{ud} + \psi_{du}^{*}\psi_{du} = 1$$

The density matrix for the full composite system: $\rho^2 = \rho, Tr(\rho^2) = 1.$

The density matrix for Alice's subsystem A: $\rho^2 \neq \rho, Tr(\rho^2) < 1$

We check the density matrix for Alice's subsystem:

The density matrix of Alice: $\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$

expanded a, a' (with $\psi^* = \psi$ due to all coefficients being real):

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = 0.6$$

$$\rho_{ud} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = 0$$

$$\rho_{du} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = 0$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = 0.4$$

gives Alice density matrix:

$$\rho := \begin{pmatrix} 0.6 & 0 \\ 0 & 0.4 \end{pmatrix}$$

The wave function is not factorized (partial entanglement): $\psi(a,b)$.

The expectation values:

$\langle\sigma_z\rangle = 0{,}2\ \langle\sigma_x\rangle = \langle\sigma_y\rangle = 0$

$\langle\tau_z\rangle = -0{,}2\ \langle\tau_x\rangle = \langle\tau_y\rangle = 0$

$\langle\tau_z\sigma_z\rangle = -1$

$\langle\tau_x\sigma_x\rangle = -2\sqrt{0{,}24}$

The correlation between the two systems: $\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = -0{,}96$

The main feature of a partially entangled state is that the composite system as a whole is fully characterized but there is no complete information about the subsystems.

Negation:

In formal logic a proposition is a statement that can be true or false. Any proposition can be negated, the truth-value (true or false) then is inverted.

Example: we have a die showing the number 4.

Proposition A: the die shows “4”.

The proposition is true.

The negated proposition $\bar{A}$: it is not true that the die shows “4”.

The negated proposition is false.

Note: in formal logic the negation often is written as $\neg A$.

Neutrino, moving at speed of light:

Prerequisite

The time-dependent Schrödinger equation:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

The momentum operator:

$$P = -i\hbar\frac{\partial}{\partial x}$$

Wave functions need to be normalized:

$$\int_{-\infty}^{\infty}\psi^*(x)\psi(x)dx = 1$$

End prerequisite

We start with a simple Hamiltonian, a fixed constant times the momentum operator P:

$$H = cP$$

We insert this Hamiltonian into the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = -ci\hbar\frac{\partial}{\partial x}|\psi\rangle$$

In terms of wave-functions:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -ci\hbar\frac{\partial\psi(x,t)}{\partial x}$$

Note: $\psi(x,t)$ is a function of both x and t.

We cancel the term $i\hbar$:

$$\frac{\partial\psi(x,t)}{\partial t} = -c\frac{\partial\psi(x,t)}{\partial x}$$

Any function of $(x-ct)$ is a solution.

We check this with an example:

$$\psi(x,t) \coloneqq (x-ct)^2$$

Left side:

$$\frac{\partial(x-ct)^2}{\partial t} = 2(x-ct)(-c) = -2c(x-ct)$$

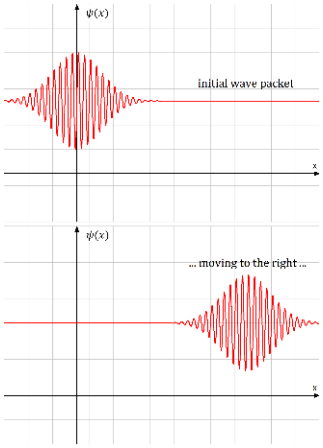
Right side:

$$-c\frac{\partial(x-ct)^2}{\partial x} = -2c(x-ct)$$

Both sides are equal. This may be enough for our quick check.

Any normalized function of this form solves the Schrödinger equation.

We look at the time evolution of $\psi(x-ct)$. How does a wave function $\psi(x-ct)$ evolve with time?



We start at time $t = 0$.

Our wave-function is a wave-packet localized on the x −axis.

As t increases the wave-packet is shifting to the right with uniform velocity c.

This description is pretty close to the correct description of a neutrino that moves immeasurably slower than the speed of light.

Newton's law classical:

The potential energy function is denoted by $V(x)$. In classical mechanics it is related to the forced on a particle by the equation:

$$F(x) = -\frac{\partial V}{\partial x}$$

We combine this with Newton's second law, $F = \dot{p}$:

$$\dot{p} = -\frac{\partial V}{\partial x}$$

Newton's law quantum mechanical:

Prerequisite

In quantum mechanics the time derivative of an operator L (L being any observable, H being the quantum Hamiltonian) is

$$\frac{dL}{dt} = -\frac{i}{\hbar}[L,H]$$

with $[L,H]$ being the commutator of L and H: $(LH - HL)$.

End prerequisite

In quantum mechanics we write the Hamiltonian. The potential energy $V(x)$ is replaced by the operator V that gets added to the Hamiltonian.

We use expectation values $\langle P\rangle$ instead of $P, \langle V\rangle$ instead of V and get the Hamiltonian:

$$H = \frac{\langle P^2\rangle}{2m} + \langle V\rangle$$

We take Newton's law again:

$$F = \dot{p}$$

We build the time derivative of the expectation value $\langle P\rangle$:

$$\frac{d\langle P\rangle}{dt} = -\frac{i}{\hbar}[\langle P\rangle, H] =$$

$$-\frac{i}{\hbar}\left[\langle P\rangle, \left(\frac{\langle P^2\rangle}{2m} + \langle V\rangle\right)\right] =$$

$$-\frac{i}{\hbar}\left(\langle P\rangle\left(\frac{\langle P^2\rangle}{2m} + \langle V\rangle\right) - \left(\frac{\langle P^2\rangle}{2m} + \langle V\rangle\right)\langle P\rangle\right) =$$

$$-\frac{i}{\hbar}\left(\frac{\langle P\rangle\langle P^2\rangle}{2m} + \langle P\rangle\langle V\rangle - \frac{\langle P^2\rangle\langle P\rangle}{2m} - \langle V\rangle\langle P\rangle\right) =$$

$$-\frac{i}{\hbar}(\langle P\rangle\langle V\rangle - \langle V\rangle\langle P\rangle) =$$

$$-\frac{i}{\hbar}[\langle P\rangle, \langle V\rangle] =^{(*)}$$

$$-\frac{i}{\hbar}(-i\hbar)\frac{d\langle V\rangle}{dx}$$

In summa:

$$\frac{d\langle P\rangle}{dt} = -\frac{d\langle V\rangle}{dx}$$

We have to show $(*)$:

$$[\langle P\rangle, \langle V\rangle] = -i\hbar\frac{d\langle V\rangle}{dx}$$

We check this:

$$[P, V]\,\psi(x) =$$

$$\left(-i\hbar\frac{d}{dx}\right)\big(V(x)\psi(x)\big) - V(x)\left(-i\hbar\frac{d}{dx}\right)\psi(x) =$$

$$-i\hbar\left(\left(\frac{dV(x)}{dx}\psi(x) + \frac{d\psi(x)}{dx}V(x)\right) - V(x)\frac{d\psi(x)}{dx}\right) =$$

$$-i\hbar\frac{dV(x)}{dx}\psi(x)$$

We have shown that

$$\frac{d\langle P\rangle}{dt} = -\frac{d\langle V\rangle}{dx}$$

This is the quantum analog of Newton's equation for the time rate change of momentum.

Nonlocality:

Of all the counterintuitive ideas quantum mechanics forces upon us, entanglement may be the hardest one to accept. There is no classical analog for this. The best way to come to terms with these issues is to internalize the mathematics.

Maybe we should follow Galileo Galilei who stated like this: do not ask questions why something is moving, better find out how it is moving. If you know the "how" you can predict the future. And he stated too: the book of nature is written in the language of mathematics.

Nonrelativistic free particles:

For a nonrelativistic free particle, the Hamiltonian is the kinetic energy (no potential):

$$H = \frac{p^2}{2m}$$

The left side of a time-dependent Schrödinger equation always is:

$$i\hbar\frac{\partial\psi}{\partial t} =$$

We replace the classical momentum by the quantum operator P. The operator P is defined as:

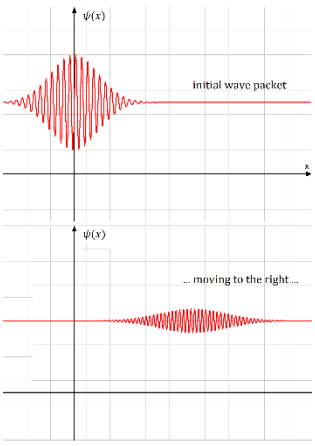
$$P = -i\hbar\frac{\partial}{\partial x}$$

The quantum mechanical Hamiltonian:

$$H = \frac{P^2}{2m} = \frac{-i\hbar}{2m}\frac{\partial^2}{\partial x^2}$$

We combine this to the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-i\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi$$



This is the traditional Schrödinger equation for an ordinary nonrelativistic free particle. Waves of different wavelength (and momenta) move with different velocities. Because of this the wave function does not maintain its shape. It tends to spread out and fall apart.

Normalizable functions:

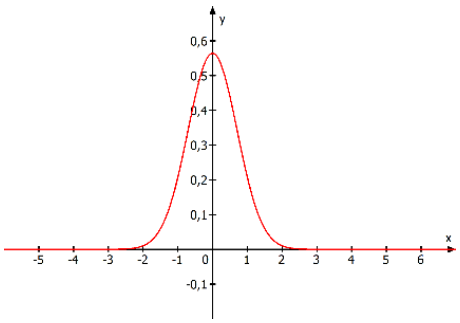
The integral over the probability density of a wave function must be 1:

$$\int_{-\infty}^{\infty}\psi^*(x)\psi(x)dx = 1$$

This requires the wave functions to come from ground and to go to ground.

An example are the gaussian functions:

$$f(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}$$



The integral:

$$\int_{-\infty}^{\infty} e^{-x^2} dx = 1$$

Normalization:

Normalization of near-singlet state:

The near-singlet state is a state of partial entanglement and has the state-vector $\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$.

The state-vector leads to the following wave-function:

$\psi_{uu} = 0|uu\rangle$ $\psi_{ud} = \sqrt{0.6}|ud\rangle$ $\psi_{du} = -\sqrt{0.4}|du\rangle$ $\psi = 0|dd\rangle$

As the values are all real, the complex conjugated are identical: $\psi_{uu} = {\psi^*}_{uu}$ etc.

Obviously, the wave function is normalized: $0^2 + \sqrt{0.6}^2 + (-\sqrt{0.4})^2 + 0^2 = 1$

$\psi(a,b)$ takes the form $\psi(a,b) = \psi_{ud} + \psi_{du} = \sqrt{0.6}|ud\rangle - \sqrt{0.4}|du\rangle$

and results in: $\psi_{uu} = 0,\ \psi_{ud} = \sqrt{0.6},\ \psi_{du} = -\sqrt{0.4},\ \psi_{dd} = 0$

Normalization of product state:

The product state is a state of independent subsystems and has a generalized state-vector $\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$.

The normalization conditions are $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$ and $\beta_u^*\beta_u + \beta_d^*\beta_d = 1$.

Normalization of singlet state:

The singlet state is a state of maximum entanglement and has the state-vector $\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$.

The state-vector leads to the following wave-function:

$\psi_{uu} = 0|uu\rangle$ $\psi_{ud} = \frac{1}{\sqrt{2}}|ud\rangle$ $\psi_{du} = -\frac{1}{\sqrt{2}}|du\rangle$ $\psi = 0|dd\rangle$

As the values are all real, the complex conjugated are identical: $\psi_{uu} = {\psi^*}_{uu}$ etc.

Obviously, the wave function is normalized: $0^2 + \frac{1}{\sqrt{2}}^2 + (-\frac{1}{\sqrt{2}})^2 + 0^2 = 1$

Normalized vector:

A vector V is normalized if its inner product with itself is 1:

$$\langle V|V\rangle = 1$$

Note: normalized vectors are sometimes called unit vectors.

not-rule:

In formal logic a proposition is a statement that can be true or false. Any proposition A can be negated by applying the logical not:

$$not\ A, \qquad \bar{A}, \qquad \neg A$$

The truth-value (true or false) then is inverted.

Example: we have a die showing the number 4.

Proposition A: the die shows "4".

The proposition is true.

The negated proposition $\bar{A}$: it is not true that the die shows "4".

The negated proposition is false.

Number operator:

The Hamiltonian expressed in terms of position operator X and momentum operator P:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2)$$

(*This is a classical as well as a quantum mechanical Hamiltonian, so it would be correct to use the classical lowercase symbols* p *and* x.)

The idea is to use the properties of X and P, especially the commutation relation $[X, P] = i\hbar$ to construct two (three) new operators, called creation (or raising) operator, annihilation (or lowering) operator and number operator.

The names are program. The raising operator shall produce a new eigenvector that has the next higher energy level, the lowering operator shall produce a new eigenvector that has the next lower energy level. The number operator returns the "number" of the energy level.

The construction process.

Using complex numbers, according to $a^2 + b^2 = (a + ib)(a - ib)$ we can split up the sum:

$$H \sim \frac{1}{2}(P + i\omega X)(P - i\omega X)$$

That is almost correct, because of the quantum mechanically behavior of X and P: they don't commute. The problems are the products PX and XP.

We expand:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + i\omega XP - i\omega PX - i^2\omega^2 X^2) =$$

$$\frac{1}{2}(P^2 + \omega^2 X^2) + \frac{1}{2} i\omega [X, P]$$

We know the value of the commutator: $[X, P] = i\hbar$ and get:

$$\frac{1}{2}(P + i\omega X)(P - i\omega X) = \frac{1}{2}(P^2 + \omega^2 X^2) - \frac{1}{2}\hbar\omega$$

Our correct Hamiltonian:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{1}{2}\hbar\omega$$

We define:

The lowering (or annihilating) operator:

$$a^- \coloneqq (P - i\omega X)$$

The raising operator:

$$a^+ \coloneqq (P + i\omega X)$$

The number operator is the product of both:

$$N \coloneqq a^+ a^-$$

Stated in terms of the number operator, the Hamiltonian becomes:

$$H = \hbar\omega(N + \frac{1}{2})$$

We call the states of the harmonic oscillator $|n\rangle$ instead of $|\psi_0\rangle$, $|\psi_1\rangle$, …

As the (excited) states $|n\rangle$ are eigenvectors of the number operator N, applying the number operator to the wave function of the n^{th} excited state gives back the eigenvalue n:

$$N|n\rangle = n|n\rangle$$

We check the number operator N acting on the ground state and the first excited state – it should give back the numbers 0 and 1 (this will become a little bit lengthy …)

The ground state:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

The number operator N:

$$(P + i\omega X)(P - i\omega X) =$$

$$PP - i\omega PX + i\omega XP + \omega^2 XX =$$

$$PP + i\omega(XP - PX) + \omega^2 XX =$$

$$PP + i\omega[X, P] + \omega^2 XX =$$

Note: the commutator $[X, P] = i\hbar$.

$$PP - \hbar\omega + \omega^2 XX$$

We need the details:

$$P = -i\hbar\frac{\partial}{\partial x}$$

$$X = x\cdot$$

$$PP = (-i\hbar)(-i\hbar)\frac{\partial^2}{\partial x^2} = -\hbar^2\frac{\partial^2}{\partial x^2}$$

$$XX = x^2$$

We apply the number operator to the wave function of the ground state:

$$\left(-\hbar^2\frac{\partial^2}{\partial x^2} - \hbar\omega + \omega^2x^2\right)e^{-\frac{\omega}{2\hbar}x^2}$$

We do this in parts:

First the derivation $-\hbar^2\frac{\partial^2}{\partial x^2}e^{-\frac{\omega}{2\hbar}x^2}$:

$$-\hbar^2\frac{\partial^2}{\partial x^2}e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-\hbar^2\frac{\partial}{\partial x}\frac{\partial}{\partial x}\left(e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$\hbar^2\frac{\partial}{\partial x}\left(\frac{\omega x}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$\hbar^2\left(\frac{\omega}{\hbar}e^{-\frac{\omega}{2\hbar}x^2} - \frac{\omega x}{\hbar}\frac{\omega x}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$\hbar^2\left(\frac{\omega}{\hbar}e^{-\frac{\omega}{2\hbar}x^2} - \frac{\omega^2x^2}{\hbar^2}e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$(\hbar\omega - \omega^2x^2)e^{-\frac{\omega}{2\hbar}x^2}$$

We add the rest:

$$(\hbar\omega - \omega^2x^2 - \hbar\omega + \omega^2x^2)e^{-\frac{\omega}{2\hbar}x^2} = 0$$

The number operator N applied to the ground state gives (correctly) 0. We try the same for the first excited state.

The first excited state:

$$\psi_1(x) = 2i\omega xe^{-\frac{\omega}{2\hbar}x^2}$$

The number operator N:

$$PP - \hbar\omega + \omega^2XX$$

We apply the number operator to the wave function of the first excited state:

$$\left(-\hbar^2\frac{\partial^2}{\partial x^2}-\hbar\omega+\omega^2x^2\right)2i\omega xe^{-\frac{\omega}{2\hbar}x^2}=$$

$$-2i\omega\hbar^2\frac{\partial^2}{\partial x^2}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right)-2i\hbar\omega^2xe^{-\frac{\omega}{2\hbar}x^2}+2i\omega^3x^3e^{-\frac{\omega}{2\hbar}x^2}=$$

We do this in parts:

First the derivation $-2i\omega\hbar^2\frac{\partial^2}{\partial x^2}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right)$:

$$-2i\omega\hbar^2\frac{\partial^2}{\partial x^2}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right)=$$

$$-2i\omega\hbar^2\frac{\partial}{\partial x}\frac{\partial}{\partial x}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right)=;$$

Deriving first time:

$$-2i\omega\hbar^2\frac{\partial}{\partial x}\left(e^{-\frac{\omega}{2\hbar}x^2}-\frac{\omega x^2}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}\right)=$$

$$-2i\omega\hbar^2\frac{\partial}{\partial x}\left(\left(1-\frac{\omega x^2}{\hbar}\right)e^{-\frac{\omega}{2\hbar}x^2}\right)=;$$

Deriving second time:

$$-2i\omega\hbar^2\left(-\frac{2\omega x}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}+\left(1-\frac{\omega x^2}{\hbar}\right)\left(-\frac{\omega x}{\hbar}\right)e^{-\frac{\omega}{2\hbar}x^2}\right)=$$

$$-2i\omega\hbar^2\left(-\frac{2\omega x}{\hbar}-\frac{\omega x}{\hbar}+\frac{\omega^2x^3}{\hbar^2}\right)e^{-\frac{\omega}{2\hbar}x^2}=$$

$$(4i\omega^2x\hbar+2i\omega^2x\hbar-2i\omega^3x^3)e^{-\frac{\omega}{2\hbar}x^2}=$$

$$(6i\omega^2x\hbar-2i\omega^3x^3)e^{-\frac{\omega}{2\hbar}x^2}$$

We add the rest:

$$(6i\omega^2x\hbar-2i\omega^3x^3-2i\omega^2\hbar x+2i\omega^3x^3)e^{-\frac{\omega}{2\hbar}x^2}=$$

$$4i\omega^2x\hbar e^{-\frac{\omega}{2\hbar}x^2}=;$$

We have been cheating a little bit – and will correct that. The raising operator and the lowering operator need a factor, the correct values are:

$$a^-=\frac{i}{\sqrt{2\omega\hbar}}(P-i\omega X)$$

$$a^+=\frac{-i}{\sqrt{2\omega\hbar}}(P+i\omega X)$$

This gives the correct number operator:

$$N = \frac{1}{2\omega\hbar}(P - i\omega X)(P + i\omega X)$$

We take the result above and divide it by $2\omega\hbar$:

$$\frac{4i\omega^2 x\hbar}{2\omega\hbar} e^{-\frac{\omega}{2\hbar}x^2} = 2i\omega x e^{-\frac{\omega}{2\hbar}x^2}$$

The number operator N applied to the first excited state $2i\omega x e^{-\frac{\omega}{2\hbar}x^2}$ gives correctly one time the first excited state.

For the calculation of the effect of the number operator to the ground state this was invisible due to $\frac{0}{2\omega\hbar} = 0$.

Observables:

Observables, complete set of commuting observables:

Two observables that commute have a complete basis of simultaneous eigenvectors. This can be expanded. One may need to specify a larger number of observables to completely label a basis of a state. Regardless of the number of observables needed, they must all commute among themselves. This is called a complete set of commuting observables.

The commutator of two observables is the zero operator.

Observables, composite observables:

We have a two-spin system, Alice and Bob, $\vec{\sigma}$ and $\vec{\tau}$. We are referring to the observable:

$$\vec{\sigma} \cdot \vec{\tau} = \sigma_x \tau_x + \sigma_y \tau_y + \sigma_z \tau_z$$

Neither Alice nor Bob can measure more than one component of the dot product of the operators.

Quantum mechanics insists that some kind of apparatus can be built to measure this observable.

A concrete example: Some atoms have spins that are described in the same way as electron spins. When two of these atoms are close to each other – for example, two neighboring atoms in a crystal lattice – the Hamiltonian will depend on the spins. In some situations, the neighboring spins' Hamiltonian is proportional to $\vec{\sigma} \cdot \vec{\tau}$. If this happens to be the case, then measuring $\vec{\sigma} \cdot \vec{\tau}$ is equivalent to measuring the energy of the atomic pair. This is a single measurement of the composite operator and does not entail measuring the individual components of either spin.

Observables, composite system:

In a product state of Alice and Bob, every prediction about Bob's half of the system is exactly the same as it would have been in the corresponding single-spin theory. The same goes for Alice.

For the example of a spin system this means that the expectation values of the components satisfy:

$$\langle \sigma_x \rangle^2 + \langle \sigma_y \rangle^2 + \langle \sigma_z \rangle^2 = 1$$

Measuring an isolated observable of a product state gives (at least for one direction) a certain result. Not all expectation values can be zero.

In an entangled state it could happen that:

$$\langle \sigma_x \rangle^2 = \langle \sigma_y \rangle^2 = \langle \sigma_z \rangle^2 = 0$$

In other words, measuring an isolated observable of an entangled state gives a completely uncertain result though the state-vector of the entangled state is as complete a description of a system as it is possible to make.

This is the true weirdness of entanglement, which so disturbed Einstein.

Observables, definition:

States in quantum mechanics are mathematically described as vectors in a vector space.

Physical observables – things that you can measure – are described by linear operators.

For example, we can make direct measurements of the coordinates of a particle; the energy, momentum, or angular momentum of a system; the electronic field at a point in space.

Observables are associated with a vector space, but they are not state vectors.

Observables, linear operators and observables:

The principles of quantum mechanics all involve the idea of an observable, and they presuppose the existence of an underlying complex vector space whose vectors represent system states.

An observable could also be called a measurable. It is something you can measure with a suitable apparatus. Please remember the principles of quantum mechanics:

- Principle 1: The observable or measurable quantities of quantum mechanics are represented by linear (Hermitian) operators L.
- Principle 2: The possible results of a measurement are the eigenvalues of the operator that represents the observable. We will call these eigenvalues λ_i. The state for which the result of a measurement is unambiguously λ_i is the corresponding eigenvector $|\lambda_i\rangle$.
- Principle 3: Unambiguously distinguishable states are represented by orthogonal vectors.
- Principle 4: If $|A\rangle$ is the state-vector of a system, and the observable L is measured, the probability to observe the value λ_i is:

$$P(\lambda_i) = |\langle A|\lambda_i\rangle|^2 = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$

Observables, multiple observables:

The physics of a single spin is extremely simple making it so attractive as an illustrative example. One property of a single spin is that its state can be fully specified by the eigenvalue of a single operator, say σ_z. If the value of σ_z is known, then no other observable – such as σ_y – can also be specified.

In more complicated systems, we may have multiple observables that are compatible, their values can be known simultaneously. Here are two examples:

- A particle moving in the three-dimensional space. All three spatial coordinates of a particle can be specified simultaneously.
- A system composed of two physically independent spins – a system of two qubits. We can measure one component of each spin simultaneous.

In these situations, we need multiple measurements to fully characterize the state of the system. For example, in our two-spin system, we measure each spin separately and associate these measurements with two different operators L and M.

Observations, collapse of the wave functions and observations:

The state-vector of a system evolves in a deterministic way according to the time-dependent Schrödinger equation. Measuring the observable L destroys the state-vector and leaves it in an eigenstate of L.

This is called the collapse of the wave function.

Suppose the state-vector before the measurement is:

$$\sum_j \alpha_j |\lambda_j\rangle$$

Randomly, with probability $|\alpha_j|^2$, the apparatus measures a value λ_j and leaves the system in the single eigenstate $|\lambda_j\rangle$. The superposition of states collapses to a single term.

Operator method:

Operator method, harmonic oscillator and operator method:

The Hamiltonian expressed in terms of momentum operator P and position operator X:

$$H = \frac{P^2 + \omega^2 X^2}{2}$$

We can transform this into:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{\omega\hbar}{2}$$

We define a complete set of commutating operators:

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

$$a^+ = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

$$N = a^+ a^-$$

The set is closing under commutation:

$$[a^-, a^+] = 1$$

$$[a^-, N] = a^-$$

$$[a^+, N] = -a^+$$

The operator a^+ is called raising operator. Instead of using the explicit energy states $|\psi_0\rangle$, $|\psi_1\rangle$ … we simply write $|n\rangle$. Given the eigenvector $|n\rangle$, we get:

$$a^+|n\rangle = |n+1\rangle$$

The operator a^- is called lowering or annihilating operator. Given the eigenvector $|n\rangle$, we get:

$$a^-|n\rangle = |n-1\rangle$$

The operator a^- applied to the ground state $|0\rangle$ annihilates it:

$$a^-|0\rangle = 0$$

The operator N is called the number operator. Given the eigenvector $|n\rangle$, we get:

$$N|n\rangle = n|n\rangle$$

With these operators we find the entire spectrum of harmonic oscillator energy levels:

$$E_n = \omega\hbar\left(\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\right)$$

Operator method, wave functions and operator method:

The ground state wave function:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

The lowering (or annihilating) operator:

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

The raising operator:

$$a^+ = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

This gives the number operator:

$$N = \frac{1}{2\omega\hbar}(P - i\omega X)(P + i\omega X)$$

The operators in detail:

$$P = -i\hbar\frac{\partial}{\partial x}\dots$$

$$X = x\cdot\dots$$

Acting with the lowering operator on the ground state wave function annihilates it:

$$a^-\psi_0(x) = 0$$

We check this, omitting the factor $\frac{i}{\sqrt{2\omega\hbar}}$:

$$a^-\psi_0(x) = (P - i\omega X)e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-i\hbar\frac{\partial}{\partial x}e^{-\frac{\omega}{2\hbar}x^2} - i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$i\omega x e^{-\frac{\omega}{2\hbar}x^2} - i\omega x e^{-\frac{\omega}{2\hbar}x^2} = 0$$

The lowering operator acting on the ground state wave function annihilates it.

Acting with the raising operator on the ground state wave function gives the first excited state:

$$a^+\psi_0(x) = \psi_1(x)$$

We check this, again omitting the factor $\frac{-i}{\sqrt{2\omega\hbar}}$:

$$(P + i\omega X)e^{-\frac{\omega}{2\hbar}x^2} =$$

$$-i\hbar\frac{\partial}{\partial x}e^{-\frac{\omega}{2\hbar}x^2} + i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$i\omega x e^{-\frac{\omega}{2\hbar}x^2} + i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$2i\omega x e^{-\frac{\omega}{2\hbar}x^2}$$

We get:

$$\psi_1(x) = 2i\omega x e^{-\frac{\omega}{2\hbar}x^2} = 2i\omega x \psi_0(x)$$

The important difference between $\psi_0(x)$ and $\psi_1(x)$ is the presence of the factor x in $\psi_1(x)$. This causes the wave function of the first excited state to have a zero, or node, at x=0. This is a pattern that continues going up the ladder: each successive excited state has an additional node.

Acting with the raising operator on the first excited state wave function gives the second excited state (and so on …):

$$a^+\psi_1(x) = \psi_2(x)$$

We check this, again omitting the factors $\frac{-i}{\sqrt{2\omega\hbar}}$ and $2i\omega$:

$$(P + i\omega X)xe^{-\frac{\omega}{2\hbar}x^2} =$$

$$-i\hbar\frac{\partial}{\partial x}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right) + i\omega x^2 e^{-\frac{\omega}{2\hbar}x^2} =;$$

The differentiation:

$$-i\hbar\frac{\partial}{\partial x}\left(xe^{-\frac{\omega}{2\hbar}x^2}\right) =$$

$$-i\hbar\left(e^{-\frac{\omega}{2\hbar}x^2} - \frac{\omega x^2}{\hbar}e^{-\frac{\omega}{2\hbar}x^2}\right) =$$

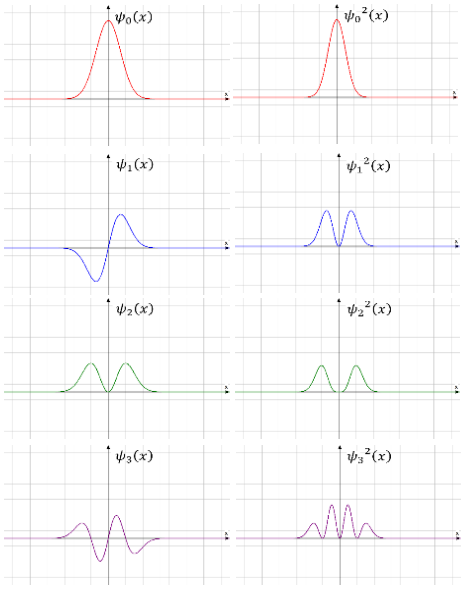
$$(-i\hbar + i\omega x^2)e^{-\frac{\omega}{2\hbar}x^2}$$

Adding the rest:

$$(-i\hbar + i\omega x^2)e^{-\frac{\omega}{2\hbar}x^2} + i\omega x^2 e^{-\frac{\omega}{2\hbar}x^2} =$$

$$i(-\hbar + 2\omega x^2)e^{-\frac{\omega}{2\hbar}x^2} = \psi_2(x)$$

The important difference between $\psi_1(x)$ and $\psi_2(x)$ is the raising power in x.



Result:

- Each eigenfunction is a polynomial in x, multiplied by $e^{-\frac{\omega}{2\hbar}x^2}$.
- Because the exponential goes faster to zero than any of these polynomials grow, each eigenfunction approaches zero asymptotically.
- Because the degree of each polynomial is one greater than the degree of the previous one, each eigenfunction has one more zero than the previous one.
- The polynomials are called the Hermite polynomials.
- The ground-state eigenfunction is symmetric in x.

Operator:

Operator, spin-operator, 3-vector operator:

The spin operator σ is neither a state-vector (a bra or a ket) nor a 3-vector. It has resemblance to a 3-vector because it is associated with a direction in space.

The spin operator σ is frequently used as though it were a simple 3-vector and is called a 3-vector operator.

There is a spin operator for each direction in which an apparatus measuring spin can be oriented.

The operator σ consist of the three components σ_x, σ_y and σ_z with the associated state-vectors:
$|left\rangle$ and $|right\rangle$ for σ_x
$|in\rangle$ and $|out\rangle$ for σ_y
$|up\rangle$ and $|down\rangle$ for σ_z

The components of the spin operator σ (or written as $\vec{\sigma}$) are represented by the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Note: i is the imaginary unit.

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Behaving like a 3-vector, the component of $\vec{\sigma}$ along any direction $\vec{n}$ is the dot-product of $\vec{\sigma}$ and $\vec{n}$:

$$\sigma_n = \vec{\sigma} \cdot \vec{n} = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z$$

Written in terms of the Pauli matrices this gives:

$$\sigma_n = n_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + n_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + n_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can combine this to a single matrix:

$$\sigma_n = \begin{pmatrix} n_z & (n_x - i n_y) \\ (n_x + i n_y) & -n_z \end{pmatrix}$$

If we find the eigenvectors and eigenvalues of σ_n, we will know the possible outcomes of a measurement along the direction of $\vec{n}$ with the corresponding probabilities. We have a complete picture of spin measurement in the three-dimensional space.

Operator, annihilation operator:

The lowering (or annihilating) operator is made out of the momentum operator P and the position operator X:

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

Applying the lowering operator to an excited state of the harmonic oscillator will give the next lower energy level. Applying the lowering operator to the ground state of the harmonic oscillator will give zero (annihilates that state).

Associated with the lowering operator is the raising operator that does exactly the opposite:

$$a^+ = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

Together they form the number operator:

$$N = a^+a^- = \frac{1}{2\omega\hbar}(P + i\omega X)(P - i\omega X)$$

The number operator, applied to an excited state, gives back a multiple of this state – the number of this state.

Operator, anti-Hermitian operator:

An operator (a matrix) L with $L^\dagger = L$ is called a Hermitian operator (a Hermitian matrix).

Note: $L^\dagger$ stands for the transposed and complex conjugated form of L.

An operator (a matrix) L with $L^\dagger = -L$ is called an anti-Hermitian operator (an anti-Hermitian matrix).

By multiplying an anti-Hermitian operator with either i or $-i$ make it Hermitian.

Note: operators that represent observables are Hermitian.

Operator, commutator and operator:

The commutator of two operators L and M:

$$[L, M] \coloneqq LM - ML$$

Note: as matrix multiplication is not commutative in general, the commutator of two operators generally will not be zero.

An operator always commute with itself:

$$[L, L] \coloneqq LL - LL = 0$$

If two operators do not commute, then there must be uncertainty in one or the other or both. The corresponding observables cannot be measured simultaneously exact.

For the position operator X and the momentum operator P holds:

$$[X, P] = i\hbar$$

The operators a^-, a^+ and N:

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

$$a^+ = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

$$N = a^+a^- = \frac{1}{2\omega\hbar}(P + i\omega X)(P - i\omega X)$$

The operators a^-, a^+ and N form a closed set, a kind of commutator algebra:

$$[a^-, a^+] = 1$$

$$[a^-, N] = a^-$$

$$[a^+, N] = -a^+$$

Operator, composite operator:

A composite operator can be made out of two operators by the tensor product. In this case the state is called a product state and can be handled as two independent states.

A composite operator can be made out of two operators by the dot-product. For a two-spin system:

$$\vec{\sigma} \cdot \vec{\tau} = \sigma_x \tau_x + \sigma_y \tau_y + \sigma_z \tau_z$$

Note: $\vec{\sigma}$ is not a vector but a 3-vector operator that behaves like a vector.

The value for the observable $\vec{\sigma} \cdot \vec{\tau}$ cannot be found by individual measurements because it is not possible to simultaneously measure the three components – they do not commute. Only one component can be simultaneously measured.

A situation like this occurs when two atoms in a crystal lattice are close to each other. The Hamiltonian will depend on the spins of these atoms. In some situations, the Hamiltonian of the neighboring spins is proportional to $\vec{\sigma} \cdot \vec{\tau}$. In this case, measuring $\vec{\sigma} \cdot \vec{\tau}$ is equivalent to measuring the energy of the atomic pair. It is a single measuring of the composite operator and does not entail measuring the individual components of either spin.

Operator, creation operator:

The creation (or raising) operator is made out of the momentum operator P and the position operator X:

$$a^+ = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

Applying the raising operator to a state of the harmonic oscillator will give the next higher energy level.

Associated with the raising operator is the lowering (annihilating) operator that does exactly the opposite:

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

Applying the lowering operator to the ground state of the harmonic oscillator will give zero (annihilates that state).

Together they form the number operator:

$$N = a^+ a^- = \frac{1}{2\omega\hbar}(P + i\omega X)(P - i\omega X)$$

The number operator, applied to an excited state, gives back a multiple of this state – the number of this state.

Operator, Hamiltonian operator:

The Hamiltonian operator represents the total energy of a system. In quantum mechanics, the Hamiltonian controls the time evolution of a system:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

This is the time-dependent Schrödinger equation.

To find $|\psi(t)\rangle$ we follow the recipe for a Schrödinger ket:

1. Derive, look up, guess, borrow or steal the Hamiltonian operator H for the system.
2. Prepare an initial state $|\psi(0)\rangle$.
3. Find the eigenvalues and eigenvectors of H by solving the time-independent Schrödinger equation:
   $$H|E_j\rangle = E_j|E_j\rangle$$
   You will get:
   $$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$$
   Note 1: E_j is eigenvalue to the eigenvector $|E_j\rangle$.
   Note 2: $H|E_j\rangle = E_j|E_j\rangle$ leads to a differential equation that determines $\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$.
4. Calculate the initial coefficients $\alpha_j(0) = \langle E_j|\psi(0)\rangle$.
5. Rewrite $|\psi(0)\rangle$ in terms of eigenvectors $|E_j\rangle$ and initial coefficients $\alpha_j(0)$:
   $$|\psi(0)\rangle = \sum_j \alpha_j(0)\,|E_j\rangle$$
6. Replace each $\alpha_j(0)$ with $\alpha_j(t)$ to capture its time-dependence. As the basis vectors $|E_j\rangle$ do not change, this leads to:
   $$|\psi(t)\rangle = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}\,|E_j\rangle$$

We can now predict the probabilities for each possible outcome of an experiment as a function of time, and we are not restricted to energy measurements. Suppose an observable, an operator L has eigenvalues λ_j and eigenvectors $|\lambda_j\rangle$. The probability for an outcome λ is:

$$P_\lambda(t) = |\langle\lambda|\psi(t)\rangle|^2$$

Operator, Hermitian operator:

Operators that represent observables are Hermitian:

- Since the result of an experiment must be a real number, the eigenvalues of the corresponding operator must be real.
- Eigenvectors that represent unambiguously distinguishable results have different eigenvalues and are orthogonal.

Operator, Identity operator:

The outer product of a normalized ket $|\psi\rangle$ with its corresponding bra $\langle\psi|$ is called a projection operator:

$$|\psi\rangle\langle\psi|$$

Note: this is a kind of tensor product.

If we add all the projection operators for a basis system, we obtain the identity operator:

$$\sum_i |i\rangle\langle i| = I$$

The expectation value of any observable L in state $|\psi\rangle$ is given by:

$$\langle L\rangle = \langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|L$$

Note: Tr is the trace of the projection operator.

Operator, linear operator:

A linear operator X acts on a function and gives a new function:

$$X\big(f(\dots)\big) = g(\dots)$$

X is said to be linear if:

$$X(f+g) = X(f) + X(g)$$

$$X(z\cdot f) = z\cdot X(f)$$

Note: z is a complex number.

Operator, measurement and operator:

Operator, misconception regarding operator:

Operator, state vector and operator:

The correspondence between operators and measurements is fundamental in quantum mechanics.

- Operators are the things we use to calculate eigenvalues and eigenvectors.
- Operators are “paper and pencil objects” acting on state-vectors, not on actual physical systems.
- Operators acting on a state-vector produce a new state-vector.

Physically:

There are two separate things: measuring an observable (in a laboratory with many devices) or operating with the corresponding operator on the state (with paper and pencil or computers).

Conceptually:

If the state of the system before the measurement is $|A\rangle$, it is not (always) correct to say that the measurement of the observable L changes the state to $l|A\rangle$.

We show this with a spin example.

The spin operator σ_z acting on the state $|u\rangle$ or the state $|d\rangle$:

$$\sigma_z|u\rangle = |u\rangle$$

$$\sigma_z|d\rangle = -|d\rangle$$

The operator σ_z changes the state $|u\rangle$ to $|u\rangle$ and the state $|d\rangle$ to $-|d\rangle$.

We try the state $|r\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

The spin operator σ_z acting on the state $|r\rangle$:

$$\sigma_z|r\rangle = \frac{1}{\sqrt{2}}\sigma_z|u\rangle + \frac{1}{\sqrt{2}}\sigma_z|d\rangle =$$

$$\frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

This time, the operator σ_z does not leave the state $|r\rangle$ intact but alters the state itself.

Any measurement result would be either $+1$ or -1, leaving the system in the state $|u\rangle$ or $|d\rangle$ but not in the superposition $\frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$.

Operator, momentum operator:

The differentiation operator D:

$$D \coloneqq \frac{d}{dx}$$

To make the differentiation operator Hermitian:

$$-iD \coloneqq -i\frac{d}{dx}$$

The momentum operator P:

$$P \coloneqq -i\hbar\frac{d}{dx}$$

The momentum operator P, in abstract vector notation:

$$P|\psi\rangle = p|\psi\rangle$$

Note: P is an operator, p is an eigenvalue, $|\psi\rangle$ is eigenvector to P with eigenvalue p.

The momentum operator P, acting on a wave function:

$$P\psi(x) = -i\hbar\frac{d\psi(x)}{dx}$$

In the case of an eigenequation we can write:

$$P\psi(x) = -i\hbar\frac{d\psi(x)}{dx} = p\psi(x)$$

Note: P is an operator, p is an eigenvalue, $\psi(x)$ is eigenfunction to P with eigenvalue p.

The eigenequation has the solution:

$$\psi_p(x) = Ae^{\frac{ipx}{\hbar}}$$

Note: the subscript p is a reminder that $\psi_p(x)$ is the eigenfunction (eigenvector) of P with the specific eigenvalue p. It is a function of x, labeled by an eigenvalue of P.

The constant A is not determined by the eigenvector equation but will be fixed by normalizing the wave function to unit probability.

Operator, number operator:

The Hamiltonian for the harmonic oscillator, expressed in terms of momentum operator P and position operator X:

$$H = \frac{P^2 + \omega^2 X^2}{2}$$

We can transform this:

$$H = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{\omega\hbar}{2}$$

From this we can define three new operators, the lowering operator a^-, the raising operator a^+ and the number operator N:

$$a^- = \frac{i}{\sqrt{2\omega\hbar}}(P - i\omega X)$$

$$a^+ = \frac{-i}{\sqrt{2\omega\hbar}}(P + i\omega X)$$

Note: the factor $\frac{\pm i}{\sqrt{2\omega\hbar}}$ coming out of historically reasons.

$$N = a^- a^+$$

The number operator, applied to an excited state, gives back a multiple of this state – the number of this state.

Operator, projection operator:

The outer product of a normalized ket $|\psi\rangle$ with its corresponding bra $\langle\psi|$ is called a projection operator:

$$|\psi\rangle\langle\psi|$$

Note: this is a kind of tensor product.

Properties of projection operators:

- Projection operators are Hermitian
- The vector $|\psi\rangle$ is eigenvector of its projection operator with eigenvalue 1:
  $$|\psi\rangle\langle\psi| \ |\psi\rangle = |\psi\rangle$$
- Any vector orthogonal to $|\psi\rangle$ is eigenvector with eigenvalue zero. Thus, the eigenvalues of $|\psi\rangle\langle\psi|$ are either zero or one, and there is only one eigenvector with eigenvalue 1, $|\psi\rangle$ itself.
- The square of a projection operator is the same as the projection operator itself:
  $$|\psi\rangle\langle\psi|^2 = |\psi\rangle\langle\psi|$$
- The trace of an operator or any square matrix is defined as the sum of its diagonal elements. We define the trace Tr of an operator L by using an appropriate basis $|i\rangle$:
  $$Tr = \sum_i \langle i|L|i\rangle$$
  This gives the sum of the diagonal elements of L.
  if we add all projection operators for a basis system, we obtain the identity operator I:
  $$\sum_i |i\rangle\langle i| = I$$

The expectation value of any observable L in state $|\psi\rangle$ is given by:

$$\langle L\rangle = \langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|L$$

Operator, spin operator:

The spin operators represent the components of a spin, σ_x, σ_y and σ_z.

The component σ_z

We begin with σ_z that has definite, unambiguous values for the states up and $down$, $|u\rangle$ and $|d\rangle$:

$$|u\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

$$|d\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

Note: these are the state vectors, not the orientation of spin in space.

Measurements will give $\sigma_z = \pm 1$.

We have three principles:

- Principle 1:
  Each component of σ is represented by a linear operator.
- Principle 2:
  The eigenvectors of σ_z are $|u\rangle$ and $|d\rangle$. The corresponding eigenvalues are $+1$ and -1. We express this with the equations:
  $$\sigma_z|u\rangle = |u\rangle$$
  $$\sigma_z|d\rangle = -|d\rangle$$
- Principle 3:
  States $|u\rangle$ and $|d\rangle$ are orthogonal to each other:
  $$\langle u|d\rangle = 0$$

From principle 2 we calculate the matrix representation of σ_z:

$$\sigma_z = \begin{pmatrix}(\sigma_z)_{11} & (\sigma_z)_{12}\\(\sigma_z)_{21} & (\sigma_z)_{22}\end{pmatrix}$$

$$\begin{pmatrix}(\sigma_z)_{11} & (\sigma_z)_{12}\\(\sigma_z)_{21} & (\sigma_z)_{22}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}$$

$$\begin{pmatrix}(\sigma_z)_{11} & (\sigma_z)_{12}\\(\sigma_z)_{21} & (\sigma_z)_{22}\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = -\begin{pmatrix}0\\1\end{pmatrix}$$

This gives the values for σ_z:

$$\sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$$

We repeat this for the other two components of spin, σ_x, and σ_y.

The component σ_x

The state vectors $right$, $|r\rangle$ and $left$, $|l\rangle$ expressed in terms of state vectors $|u\rangle$ and $|d\rangle$:

$$|r\rangle \coloneqq \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

$$|r\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$$|l\rangle \coloneqq \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

$$|l\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} - \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

Note: any spin state can be represented as a combination of the basis vectors $|u\rangle$ and $|d\rangle$.

We check whether those two vectors are orthogonal:

$$\langle r|l\rangle = \frac{1}{\sqrt{2}}(1\ 1)\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{2}(1\ 1)\cdot\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{2}\big(1\cdot 1 + 1\cdot(-1)\big) = 0$$

Note: the bra $\langle r|$ to the ket $|r\rangle$ is the complex conjugated, but as $|r\rangle$ is real it follows $\langle r^*| = \langle r|$.

The matrix representation of σ_x:

$$\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$$

We check the eigenvector property:

$$\langle\sigma_x|r\rangle = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 + 1\cdot 1\\1\cdot 1 + 0\cdot 1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$|r\rangle$ is eigenvector to the operator σ_x with eigenvalue 1.

$$\langle\sigma_x|l\rangle = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 + 1\cdot(-1)\\1\cdot 1 + 0\cdot(-1)\end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

$|l\rangle$ is eigenvector to the operator σ_x with eigenvalue -1.

The component σ_y

The state vectors in, $|i\rangle$ and out, $|o\rangle$ expressed in terms of state vectors $|u\rangle$ and $|d\rangle$:

$$|i\rangle \coloneqq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{i}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}$$

$$|o\rangle \coloneqq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} - \frac{i}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$$

Note: do not confuse the imaginary unit i with the state vector $|i\rangle$.

Note: any spin state can be represented as a combination of the basis vectors $|u\rangle$ and $|d\rangle$.

Both vectors are orthogonal to each other:

$$\langle i|o\rangle = \frac{1}{\sqrt{2}}(1\ (-i))\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = \frac{1}{2}(1\ (-i))\cdot\begin{pmatrix}1\\-i\end{pmatrix} =$$

$$\frac{1}{2}\big(1\cdot 1 + (-i)\cdot(-i)\big) = \frac{1}{2}(1 + i^2) = 0$$

Note: the bra $\langle i|$ to the ket $|i\rangle$ is the complex conjugated.

The matrix representation of σ_y:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

We check the eigenvector property:

$$\langle\sigma_y|i\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \cdot 1 - i^2 \\ i \cdot 1 + 0 \cdot i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$|i\rangle$ is eigenvector to the operator σ_y with eigenvalue 1.

$$\langle\sigma_y|o\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \cdot 1 + i^2 \\ i \cdot 1 + 0 \cdot (-i) \end{pmatrix} = -\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$|o\rangle$ is eigenvector to the operator σ_y with eigenvalue -1.

Conclusion

The matrix representations of the spin operators σ_x, σ_y and σ_z:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note: these are the Pauli matrices.

Note: the identity matrix is also a Pauli matrix.

The representation of the state vectors in the $up - down$ system:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|r\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |l\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$|i\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \qquad |o\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Operator, time development operator:

Operator, unitary operator:

The change of the state-vector with time:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

or

$$\langle\psi(t)| = \langle\psi(0)|U^\dagger(t)$$

Note: flipping from ket to bra needs Hermitian conjugation of the operator U.

U is called the time-development operator for the system.

$U(t)$ must fulfill the minus first law: the conservation of distinctions.

Two states are distinguishable if they are orthogonal. Being orthogonal, two different basis vectors (of an orthonormal basis) represent two distinguishable states.

Let $\psi(0)$ and $\phi(0)$ be two distinguishable states:

$$\langle\psi(0)|\phi(0)\rangle = 0$$

The conservation of distinctions implies that they will be orthogonal for all time:

$$\langle\psi(t)|\phi(t)\rangle = 0$$

We replace $\psi(t)$ and $\phi(t)$:

$$\langle\psi(0)U^\dagger(t)|U(t)\phi(0)\rangle = \langle\psi(0)|U^\dagger(t)U(t)|\phi(0)\rangle = 0$$

This only works if either $U^\dagger(t)U(t) = 0$ or $U^\dagger(t)U(t) = I$. We prefer the second case.

Let $|i\rangle$ build an orthonormal basis for the state in question:

$$\langle i|j\rangle = \delta_{ij}$$

Note: δ_{ij} is the Kronecker symbol.

We can express $\langle\psi(0)|U^\dagger(t)U(t)|\phi(0)\rangle$ in terms of basis vectors $|i\rangle$:

$$\langle i|U^\dagger(t)U(t)|j\rangle = \delta_{ij}$$

or

$$U^\dagger(t)U(t) = I$$

An operator U that satisfies $U^\dagger(t)U(t) = I$ is called unitary.

Operator, zero operator:

If an operator annihilates every member of a basis, it must also annihilate every vector in the vector space.

If two operators L and M are commuting:

$$LM - ML = 0$$

then the commutator:

$$[L, M] \coloneqq LM - ML$$

annihilates every vector in the vector space.

We call $[L, M]$ a zero operator.

Note: a zero operator is necessary if you want to handle operators with superstructures like field theory. There you need a zero element to properly define the (additive) inverse of an element. This zero element of the additive group must also be zero element of the multiplicative group and different to the 1-element (the identity matrix).

If two operators A and B are commuting, the commutator serves as this zero element.

Original Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

Note: H is the Hamiltonian.

The most famous example is the nonrelativistic Schrödinger equation for the wave function in position representation $|\psi(\vec{r},t)\rangle$ of a single particle subject to a potential $V(\vec{r},t)$ (e.g. electric Field):

$$i\hbar\frac{\partial}{\partial t}|\psi(\vec{r},t)\rangle = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right]\psi(\vec{r},t)$$

Note: ∇^2 is the Laplacian, representing the partial derivatives to every component of $\vec{r}$.

Original Schrödinger equation, nonrelativistic free particle:

Prerequisite

The momentum operator P:

$$P = -i\hbar\frac{\partial}{\partial x}$$

$$P^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

End prerequisite

For a nonrelativistic free particle, the kinetic energy is $\frac{1}{2}mv^2$.

We write the Hamiltonian in terms of momentum operator P:

$$H = \frac{P^2}{2m}$$

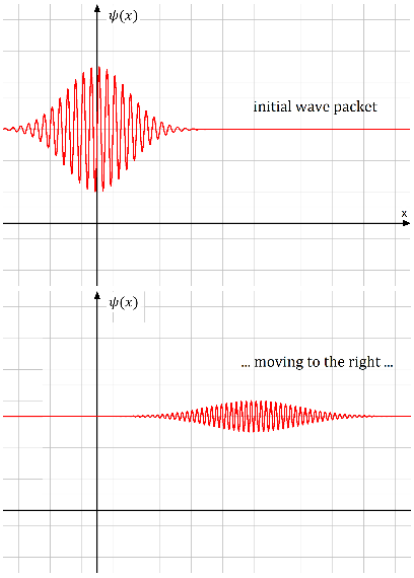
We take the original Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

We get:

$$i\hbar\frac{\partial\psi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(t)}{\partial x^2}$$

This is the traditional Schrödinger equation for a nonrelativistic free particle. It describes a wave packet (a particle) that tends to spread out and fall apart.



or rule:

In formal logic a proposition is a statement that can be $true = 1$ or $false = 0$. Any two propositions A and B can be combined by applying the logical or:

$$A\ or\ B, \qquad A \vee B$$

Note: in natural speech we often confuse the logical or with the logical XOR. The logical or is the inclusive version.

The combined proposition $A\ or\ B$ is false if both A and B are false.

We can show this with a truth-table:

A	B	$A\ or\ B$
0	0	0
0	1	1
1	0	1
1	1	1

Orthogonal basis vectors:

Normally for a vector space we chose a set of orthonormal basis vectors. They are mutually orthogonal to each other.

A vector space of dimension n has n orthonormal basis vectors.

Out of any set of vectors forming a basis for a vector space we can construct such an orthonormal set.

For a set of orthonormal basis vectors holds:

$$\langle i|j\rangle = \delta_{ij}$$

Note: δ_{ij} is the Kronecker delta.

For the case of a single spin system we found three pairs of mutually orthogonal (not orthonormal) basis vectors:

$$up \text{ and } down \text{ or } |u\rangle \text{ and } |d\rangle$$

$$right \text{ and } left \text{ or } |r\rangle \text{ and } |l\rangle$$

$$in \text{ and } out \text{ or } |i\rangle \text{ and } |o\rangle$$

note: the i in $|i\rangle$ does not stand for the imaginary unit.

Note: the directions are chosen with respect to the possible orientation of spin in space.

Orthogonal states:

Two states are (completely) distinguishable if they are orthogonal. Being orthogonal, two different basis vectors represent two distinguishable states. In other words, there is a precise experiment that can tell them apart, and therefore they are orthogonal:

$$\langle \psi(t)|\phi(t)\rangle = 0$$

Note: the minus first law requires the conservation of distinctions for all times.

For a single spin system, the basis vectors $|u\rangle$ and $|d\rangle$ are mutually orthogonal:

$$\langle u|d\rangle = 0$$

$$\langle d|u\rangle = 0$$

The physical meaning of this is that, if the spin is prepared up, then the probability to detect it $down$ is zero, and vice versa.

Two orthogonal states are physically distinct and mutually exclusive. This idea applies to all quantum systems.

Do not mistake the orthogonality of state-vectors for orthogonal directions in space.

Orthogonal state-vectors:

Physical distinct states are represented by orthogonal state-vectors. The inner product of two orthogonal state-vectors then is zero. If the inner product of two state-vectors is not zero, then the states are not distinguishable with certainty.

The inner product is sometimes called overlap.

Orthogonal vectors:

Two vectors A and B are said to be orthogonal if their inner product is zero:

$$\langle B|A\rangle = 0$$

This is the analog for the dot product of two spatial vectors being zero.

Basis vectors regularly are chosen to be orthogonal and normalized to one or shorter, to be orthonormal.

If λ_1 and λ_2 are unequal eigenvalues of a Hermitian operator, then the corresponding eigenvectors are orthogonal.

Unambiguously distinguishable states are represented by orthogonal vectors.

Orthonormal bases:

The maximum number of mutually orthonormal vectors is the dimension of the space. This holds for complex vector spaces too.

Out of orthonormal basis vectors every vector of the space can be constructed.

Note: in quantum mechanics we normally use orthonormal bases.

A vector has different representations in different (orthonormal) bases.

Let us consider a space of N dimensions and an orthonormal basis of ket-vectors $|i\rangle$, the label i running from 1 to N.

Any vector A can be written as a sum of basis vectors:

$$|A\rangle = \sum_i \alpha_i |i\rangle$$

Note: α_i are complex numbers called components of the vector.

Outer products:

The inner product of a bra $\langle\phi|$ and a ket $|\psi\rangle$ is a complex number z:

$$\langle\phi|\psi\rangle = z$$

The outer product of a bra $\langle\phi|$ and a ket $|\psi\rangle$ is a linear operator L:

$$|\psi\rangle\langle\phi| = L$$

Note: this is a kind of tensor product.

The outer product of a normalized ket $|\psi\rangle$ with its corresponding bra $\langle\psi|$ is called a Hermitian projection operator:

$$|\psi\rangle\langle\psi|$$

Overlap:

Sometimes the inner product of two states is called overlap. Overlap zero means that the corresponding states are physically distinct.

Assume a system has been prepared in state $|A\rangle$. Measuring the observable L will give one of the eigenvalues λ_i of the operator L with probability $P(\lambda_i)$.

The probability can be expressed in terms of the overlap of $|A\rangle$ and $|\lambda_i\rangle$:

$$P(\lambda_i) = |\langle A|\lambda_i\rangle|^2$$

or equivalently:

$$P(\lambda_i) = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$

Note: λ_i is the eigenvalue of the eigenvector$|\lambda_i\rangle$.

Parameters, counting parameters:

To define a direction in three-dimensional space it takes two angles – two parameters.

The general spin state is defined by two complex numbers α_u and α_d: four real parameters:

$$\alpha_u|u\rangle + \alpha_d|d\rangle$$

The general spin state has to be normalized, ${\alpha_u}^2 + {\alpha_d}^2 = 1$: minus one parameter.

The general spin does not depend on the overall phase factor: minus one parameter.

This leaves two real parameters to specify the state of a spin.

Note: a phase-factor is a complex number with length 1. For a phase-factor holds:

$$zz^* = 1$$

$$z = e^{i\varphi} \text{ or } z = \cos\varphi + i\sin\varphi$$

Partial derivatives, time and partial derivatives:

We have the position operator X and the momentum operator P:

$$X|\psi\rangle \rightarrow x\psi(x)$$

$$P|\psi\rangle \rightarrow -i\hbar\frac{d}{dx}\psi(x)$$

The position operator P multiplies the wave function with x, the momentum operator differentiates.

With this we write the quantum mechanical Hamiltonian:

$$H|\psi\rangle = -\frac{\hbar^2}{2}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}\omega^2x^2\psi(x)$$

We use partial derivatives because in general $\psi(x)$ also depends on another variable, $time$.

Time is not an operator and does not have the same status as x, but the state-vector changes with time, and we therefore treat time as a parameter. The partial derivative indicates that we are describing the system “at a fixed time”.

Particle dynamics:

Particle dynamics, example:

Prerequisite

The time-dependent Schrödinger equation:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

The momentum operator:

$$P = -i\hbar\frac{\partial}{\partial x}$$

Wave functions need to be normalized:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1$$

End prerequisite

We start with a simple Hamiltonian, a fixed constant times the momentum operator P:

$$H = cP$$

We insert this Hamiltonian into the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial|\psi\rangle}{\partial t} = -ci\hbar \frac{\partial}{\partial x}|\psi\rangle$$

In terms of wave-functions:

$$i\hbar \frac{\partial\psi(x,t)}{\partial t} = -ci\hbar \frac{\partial\psi(x,t)}{\partial x}$$

Note: $\psi(x,t)$ is a function of both x and t.

We cancel the term $i\hbar$:

$$\frac{\partial\psi(x,t)}{\partial t} = -c\frac{\partial\psi(x,t)}{\partial x}$$

Any function of $(x-ct)$ is a solution.

We check this with an example:

$$\psi(x,t) \coloneqq (x-ct)^2$$

Left side:

$$\frac{\partial(x-ct)^2}{\partial t} = 2(x-ct)(-c) = -2c(x-ct)$$

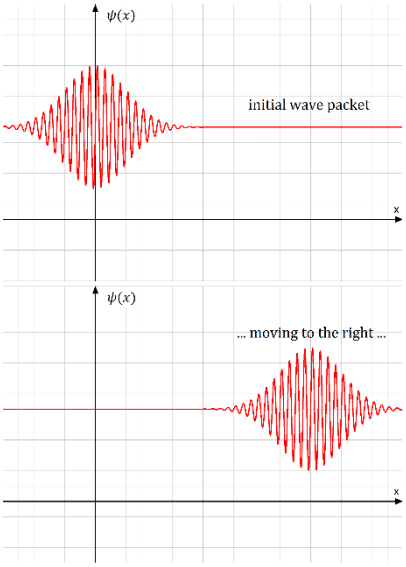
Right side:

$$-c\frac{\partial(x-ct)^2}{\partial x} = -2c(x-ct)$$

Both sides are equal. This may be enough for our quick check.

Any normalized function of this form solves the Schrödinger equation.

We look at the time evolution of $\psi(x-ct)$. How does a wave function $\psi(x-ct)$ evolve with time?



We start at time $t=0$.

Our wave-function is a wave-packet localized on the x −axis.

As t increases the wave-packet is shifting to the right with uniform velocity c.

This description is pretty close to the correct description of a neutrino that moves immeasurably slower than the speed of light. Our Hamiltonian would be a very good description of a neutrino.

With the wave function moving to the right with velocity c also the probability distribution does. That is the essential quantum mechanics of this system. The particle can only exist in a state where it moves at this velocity, it never can slow down or speed up.

We compare this with the classical description. With $H=cp$, the classical Hamiltonian:

$$\frac{\partial H}{\partial p}=\dot{x} \text{ and } \frac{\partial H}{\partial x}=-\dot{p}$$

We get:

$$\frac{\partial H}{\partial p}=\dot{x}=c \text{ and } \frac{\partial H}{\partial x}=-\dot{p}=0$$

The momentum is conserved, and the position moves with constant velocity c.

In other words, the expectation value of position behaves according to the classical equations of motion.

Particle dynamics, forces:

Prerequisite

In quantum mechanics the time derivative of an operator L (L being any observable, H being the quantum Hamiltonian) is

$$\frac{dL}{dt}=-\frac{i}{\hbar}[L,H]$$

with $[L,H]$ being the commutator of L and H: $(LH-HL)$.

We apply this to velocity:

$$v:=\frac{d\langle X\rangle}{dt}=-\frac{i}{2m\hbar}\langle[X,P^2]\rangle=\frac{\langle P\rangle}{m}$$

or

$$\langle P\rangle=mv$$

Note: X is the position operator, P the momentum operator, the Hamiltonian (forceless) $H=\frac{P^2}{2m}$.

The classical potential energy $V(x)$ becomes the quantum mechanical operator V.

The potential energy operator V acting on any wave function multiplies it by a function of x:

$$V|\psi\rangle \to V(x)\psi(x)$$

The commutator of the momentum operator P with the potential energy operator V:

$$[P,V] = -i\hbar\frac{dV}{dx}$$

We check this:

$$[P,V]\,\psi(x) =$$

$$\left(-i\hbar\frac{d}{dx}\right)\big(V(x)\psi(x)\big) - V(x)\left(-i\hbar\frac{d}{dx}\right)\psi(x) =$$

$$-i\hbar\left(\left(\frac{dV(x)}{dx}\psi(x) + \frac{d\psi(x)}{dx}V(x)\right) - V(x)\frac{d\psi(x)}{dx}\right) =$$

$$-i\hbar\frac{dV(x)}{dx}\psi(x)$$

End prerequisite

In classical mechanics the potential energy function is denoted by $V(x)$. It is related to the force on a particle:

$$F(x) = -\frac{\partial V}{\partial x}$$

In quantum mechanics we write the Hamiltonian. The potential energy $V(x)$ is replaced by the operator V that gets added to the Hamiltonian.

If forces are included, the momentum of a particle is not conserved. In Newton's laws of motions:

$$\frac{dp}{dt} = -\frac{\partial V}{\partial x}$$

The rules of quantization require us to add the operator V to the Hamiltonian:

$$H = \frac{P^2}{2m} + V$$

We check whether $\langle P\rangle = mv = m\langle\dot{X}\rangle$ still holds because we have a new term added to the Hamiltonian:

$$\dot{X} = \frac{dX}{dt} = -\frac{i}{\hbar}[X,H] =$$

$$-\frac{i}{\hbar}\left[X,\left(\frac{P^2}{2m}+V\right)\right] =$$

$$-\frac{i}{\hbar}\left(\frac{1}{2m}[X,P^2] + [X,V]\right)$$

For the additional commutator of X and V holds:

$$[X,V] = 0$$

because V multiplies by the wave function ψ by a function of x. Multiplying by x and by a function of x are operations that commute.

The additional term V has no effect on the velocity v.

What about the quantum version of Newton's law?

We take Newton's law again:

$$F = \dot{p}$$

We build the time derivative of the expectation value $\langle P \rangle$ with our new Hamiltonian:

$$\frac{d\langle P \rangle}{dt} = -\frac{i}{\hbar}[\langle P \rangle, H] =$$

$$-\frac{i}{\hbar}\left[\langle P \rangle, \left(\frac{\langle P^2 \rangle}{2m} + \langle V \rangle\right)\right] =$$

$$-\frac{i}{\hbar}\left(\langle P \rangle\left(\frac{\langle P^2 \rangle}{2m} + \langle V \rangle\right) - \left(\frac{\langle P^2 \rangle}{2m} + \langle V \rangle\right)\langle P \rangle\right) =$$

$$-\frac{i}{\hbar}\left(\frac{\langle P \rangle\langle P^2 \rangle}{2m} + \langle P \rangle\langle V \rangle - \frac{\langle P^2 \rangle\langle P \rangle}{2m} - \langle V \rangle\langle P \rangle\right) =$$

$$-\frac{i}{\hbar}(\langle P \rangle\langle V \rangle - \langle V \rangle\langle P \rangle) =$$

$$-\frac{i}{\hbar}[\langle P \rangle, \langle V \rangle] =^{(*)}$$

$$-\frac{i}{\hbar}(-i\hbar)\frac{d\langle V \rangle}{dx} = -\frac{d\langle V \rangle}{dx}$$

Result:

$$\frac{d\langle P \rangle}{dt} = -\frac{d\langle V \rangle}{dx}$$

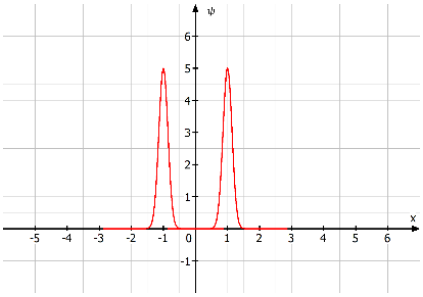
This is the quantum analog of Newton's equation for the time rate change of momentum for a particle under the influence of a potential V. The expectation value $\langle P \rangle$ changes according to the classical case.

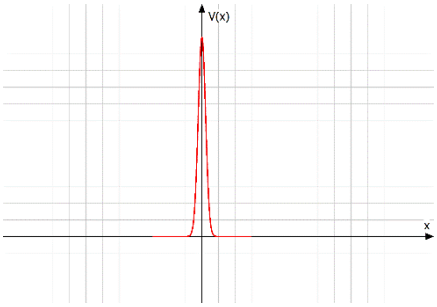
Particle dynamics, linear motion and classical limit:

The heart of the difference between quantum mechanics and classical physics can be expressed in the sentence: The average of a function $\langle f(x) \rangle$ (the expectation value of a function) is not the same as the function of the expectation value $f\langle x \rangle$.

In all cases where $\langle f(x) \rangle \sim f\langle x \rangle$ is valid, the quantum mechanical description can be replaced by a classical description. You can do classical physics and have no problems with uncertainty principle etc.

The picture shows a case in which $\langle f(x)\rangle \sim f\langle x\rangle$ is not valid. $f\langle x\rangle = f(0)$ but $\langle f(x)\rangle \neq f(0)$ for most functions f.





The second point of interest is the form of the potential.

If the potential in question is spiky it tends to cause the wave function to scatter and disintegrate – no classical behavior.

What physical situations lead to potentials that tend to break the wave function? Roughly speaking, if the features of the potential are shorter than the wavelength of the incoming particle, because then $\langle f(x)\rangle \sim f\langle x\rangle$ does not hold in the area of the potential – the classical limit is no longer valid.

Particle dynamics, nonrelativistic free particles:

Prerequisite

The quantum operator P:

$$P = -i\hbar\frac{\partial}{\partial x}$$

$$P^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

End prerequisite

For a nonrelativistic free particle, the kinetic energy is $\frac{1}{2}mv^2$.

We write the Hamiltonian in terms of momentum operator P:

$$H = \frac{P^2}{2m}$$

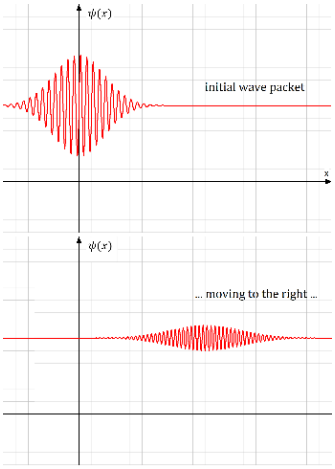
We take the original Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

We get:

$$i\hbar\frac{\partial\psi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(t)}{\partial x^2}$$

This is the traditional Schrödinger equation for a nonrelativistic free particle. It describes a wave packet (a particle) that tends to spread out and fall apart.



Particle dynamics, path integrals:

Prerequisite

For any integral over the position variable x we can insert the identity:

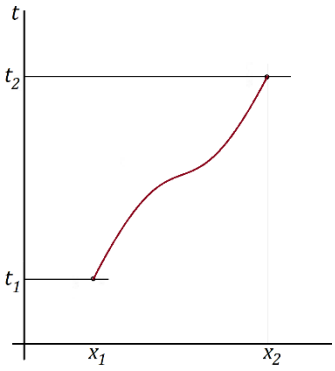
$$I = \int |x\rangle\langle x| \, dx$$

The Lagrangian $L(x, \dot{x})$ is kinetic energy minus potential energy:

$$\frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$$

End prerequisite

Classical



According to the least action principle, classical trajectories are that of minimum (stationary) action. Action is a technical term and stands for the integral of the Lagrangian between the end points of the trajectory.

For a particle moving in one dimension, the action is:

$$A = \int_{t_1}^{t_2} L(x, \dot{x})dt$$

We insert the Lagrangian:

$$A = \int_{t_1}^{t_2} \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 dt$$

We search the path with the least action A by help of calculus procedures.

Quantum mechanical

The idea of well-defined trajectory between the two points makes no sense in quantum mechanics because of the uncertainty principle.

The global version of quantum mechanics asks: Given a particle starts at (x_1, t_1), what is the probability amplitude it will show up at (x_2, t_2)?

We call the amplitude $C_{1,2} \coloneqq C(x_1, t_1; x_2, t_2)$.

The initial state of the particle is:

$$|\psi(t_1)\rangle = |x_1\rangle$$

Over the time interval between t_1 and t_2 the state evolves to:

$$|\psi(t_2)\rangle = e^{-iH(t_2 - t_1)}|x_1\rangle$$

Note: we use units for which $\hbar = 1$.

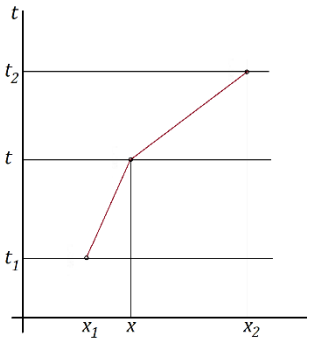
We replace $(t_2 - t_1)$ by t. The probability amplitude to detect the particle at $|x_2\rangle$ is the inner product:

$$\langle x_2|\psi(t_2)\rangle = \langle x_2|e^{-iHt}|x_1\rangle$$

The process of quantization starts with splitting the time interval t into two smaller intervals of size $\frac{t}{2}$.

The operator e^{-iHt} can be written as the product of two operators:

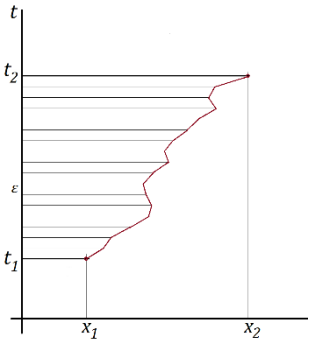
$$e^{-iHt} = e^{-iH\frac{t}{2}}e^{-iH\frac{t}{2}}$$



We integrate this via the help of the identity operator:

$$C_{1,2} = \int \left\langle x_2\left|e^{-iH\frac{t}{2}}\right|x\right\rangle \left\langle x\left|e^{-iH\frac{t}{2}}\right|x_1\right\rangle dx$$

The heart of this process is: the amplitude to go from x_1 to x_2 over the time interval t is an integral over an intermediate position x and is the product of two amplitudes.



We repeat this until we have time intervals of size ε (remember this process in calculus …). In the end, the amplitude is an integral over all possible paths between the end points. Feynman discovered that the amplitude for each path has a simple relation to an expression of classical mechanics, the action for that path.

The exact expression for the action A of each path is:

$$e^{i\frac{A}{\hbar}}$$

Feynman's formulation can be summarized by the equation:

$$C_{1,2} = \int_{paths} e^{i\frac{A}{\hbar}}$$

In quantum field theory this is the principal tool for formulating the laws of elementary particle physics.

Particle dynamics, quantization:

Quantum mechanics starts with a familiar classical system and quantizes it. Sometimes this works well, the quantum motion of electrons, quantum electrodynamics. Sometimes this works not so well like the quantization of general relativity. Some phenomena have no classical counterpart like the spin of a particle.

Particle dynamics, time-independent Schrödinger equation:

The time-independent Schrödinger equation essentially is the eigenvector equation for the Hamiltonian:

$$H|\psi\rangle = E|\psi\rangle$$

We write this in terms of the wave function $\psi(x)$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(t)}{\partial x^2} = E\psi(x)$$

We try the function:

$$\psi(x) = e^{\frac{ipx}{\hbar}}$$

We insert it into the Hamiltonian $H|\psi\rangle = E|\psi\rangle$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{\frac{ipx}{\hbar}} =$$

$$-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}e^{\frac{ipx}{\hbar}}\right) =$$

$$-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left(\frac{ip}{\hbar}e^{\frac{ipx}{\hbar}}\right) =$$

$$-\frac{\hbar ip}{2m}\frac{\partial}{\partial x}\left(e^{\frac{ipx}{\hbar}}\right) =$$

$$-\frac{\hbar ip}{2m}\frac{ip}{\hbar}e^{\frac{ipx}{\hbar}} =$$

$$\frac{p^2}{2m}e^{\frac{ipx}{\hbar}}$$

We get:

$$E = \frac{p^2}{2m}$$

E represents an energy eigenvalue of the Hamiltonian.

Particle dynamics, velocity and momentum:

Prerequisite

In statistics you get the expectation value of a continuous variable $\langle x\rangle$ by the integral over the probability density $f(x)$ multiplied by x:

$$\langle x\rangle = \int xf(x)dx$$

The commutator of momentum operator P and position operator X:

$$[X, P] = i\hbar$$

$$[X, P^2] = 2i\hbar P$$

End prerequisite

We will work with the connection between the quantum mechanical operator P and the classical notion of momentum $p = mv$.

The velocity of a quantum mechanical particle is the time derivative of the average position $\langle\psi|X|\psi\rangle$:

$$v = \frac{d\langle\psi|X|\psi\rangle}{dt}$$

We write this in terms of wave function:

$$v = \dot{x} = \frac{d}{dt}\int x\psi^*(x,t)\psi(x,t)dx$$

Instead of working through the time-dependent Schrödinger equation we use the quantum mechanical methods.

We replace the position x by the position operator X and use:

$$\frac{d\langle L\rangle}{dt} = -\frac{i}{\hbar}\langle[L,H]\rangle$$

We calculate:

$$\frac{d\langle X\rangle}{dt} = -\frac{i}{\hbar}\langle[X,H]\rangle =$$

$$-\frac{i}{2m\hbar}\langle[X,P^2]\rangle =$$

$$-\frac{2ii\hbar}{2m\hbar}\langle P\rangle =$$

$$\frac{\langle P\rangle}{m}$$

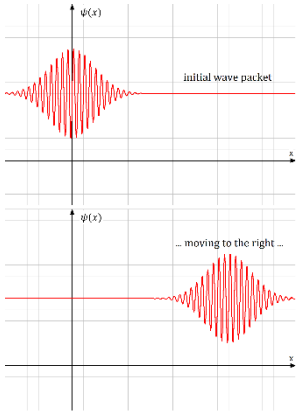
We get:

$$\langle\dot{X}\rangle = \frac{\langle P\rangle}{m}$$

We translate this into:

$$\langle P\rangle = mv$$

The average momentum equals mass times velocity. Let us suppose the wave function has the form of a packet. The expectation value of x will be approximately at the center of the packet. This center of the wave packet will travel according to the classical rule $p = mv$.



Particle, measuring moving particles in the three-dimensional space:

A basis of states for a particle moving in the three-dimensional space is specified by the position of the particle with three position coordinates: $|x,y,z\rangle$. All spatial coordinates can be simultaneously measured.

Particles:

Coordinates of particles:

Imagine a space where the coordinates of a particle lay along the x-axis on a finite number of coordinates $x_1, x_2, \ldots, x_n$. Then we could use a vector of n coordinates to describe possible positions of that particle and we could do matrix-based quantum mechanics.

A particle moving along the x-axis can be found at any real value of x, we must switch to wave functions to describe the system and expand the idea of vectors to include functions. Eigenvectors and eigenvalues will translate to eigenfunctions and eigenvalues, operators will become functions of functions.

With appropriate restrictions, functions like $\psi(x)$ satisfy mathematical axioms defining a vector space.

Particles, Heisenberg Uncertainty Principle and coordinates of particles:

Prerequisite

$[A, B]$ is the commutator of the operators A and B.

$\langle\psi|[A, B]|\psi\rangle$ gives the expectation value of the commutator of the operators A and B.

The value of the commutator $[X, P]$:

$$[X, P] = i\hbar$$

The momentum operator P in terms of wave functions:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

Note: $\psi_p(x)$ is the eigenfunction (eigenvector) of the momentum operator P with the specific eigenvalue p. It is a function of the position x and thus can be used to calculate the probability for finding the particle at position x, but it is labeled by an eigenvalue of P.

End prerequisite

The Heisenberg Uncertainty Principle puts a quantitative limit on the simultaneous uncertainties of two observables ΔA and ΔB:

$$\Delta A \Delta B \geq \frac{1}{2} |\langle\psi|[A, B]|\psi\rangle|$$

Note: if two operators commute, $[A, B] = 0$, then there is no uncertainty – both operators can be measured simultaneously exactly.

We take the position operator X and the momentum operator P:

$$\Delta X \Delta P \geq \frac{1}{2} |\langle\psi|[X, P]|\psi\rangle|$$

We use:

$$[X, P] = i\hbar$$

We get:

$$\Delta X \Delta P \geq \frac{1}{2} i\hbar$$

We will illustrate this.

The position operator X acting on a state $|\psi\rangle$:

$$X|\psi\rangle = x_0$$

Note: … via the help of the Dirac delta function $\delta(x - x_0)$.

In terms of wave functions, this becomes:

$$x\psi(x) = x_0\psi(x)$$

The wave function of an eigenstate of X is infinitely concentrated around some point x_0 on the x-axis. It is perfectly localized. We can measure the position with no uncertainty.

On the other hand, the momentum operator P in terms of (position) wave function:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

Note: this is a function of x, but it is labeled by an eigenvalue p of P.

We calculate the probability for a position x out of this wave function:

$$P(x) = \psi_p^*(x)\psi_p(x) =$$

$$\frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}} \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}} =$$

$$\frac{1}{2\pi} e^0 = \frac{1}{2\pi}$$

The result is a constant, independent from x. A state with definite momentum is completely uncertain in its position.

Particles, Hermitian operators and particles:

The distillation of many decades of experimental observation: about a particle on the x-axis we know either position x or momentum p.

The position of the particle is an observable, the Hermitian position operator X associated with it.

The momentum of the particle is an observable, the Hermitian momentum operator P associated with it.

The operators X and P do not commute:

$$[X, P] = i\hbar$$

Operators that do not commute gives observables that are not simultaneous exactly measurable.

Particles, Fourier transforms between position and momentum basis:

Prerequisite

We can write the identity operator I:

$$I = \sum_i |i\rangle\langle i|$$

Note: $|i\rangle$ are orthonormal basis vectors of a state. Because momentum and position are both Hermitian, the sets of vectors $|x\rangle$ and $|p\rangle$ each define such a set.

We replace summation with integration:

$I = \int |x\rangle\langle x| \; dx$ or $I = \int |p\rangle\langle p| \; dp$

The inner product of a position eigenvector $|x\rangle$ and a momentum eigenvector $|p\rangle$:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$

End prerequisite

We have two ways to represent a state-vector. One way is the position basis $\psi(x)$ and the other the momentum basis $\tilde{\psi}(p)$. Both represent exactly the same state-vector $|\psi\rangle$.

We search a transformation between these representation and find it in the Fourier transformation.

We start with the wave function in position representation:

$$\psi(x) = \langle x|\psi\rangle$$

We use the definition of the wave function in momentum representation:

$$\tilde{\psi}(p) = \langle p|\psi\rangle$$

We switch to continuous functions:

$$\tilde{\psi}(p) = \int \langle p|\psi\rangle \, dx =$$

$$\int \langle p|I|\psi\rangle \, dx =$$

$$\int \langle p|x\rangle\langle x|\psi\rangle \, dx =$$

$$\frac{1}{\sqrt{2\pi}} \int e^{-\frac{ipx}{\hbar}} \psi(x) \, dx$$

In the other direction we start with the wave function in momentum representation:

$$\tilde{\psi}(p) = \langle p|\psi\rangle$$

We use the definition of the wave function in position representation:

$$\psi(x) = \langle x|\psi\rangle$$

We switch to continuous functions:

$$\psi(x) = \int \langle x|\psi\rangle \, dp =$$

$$\int \langle x|I|\psi\rangle \, dp =$$

$$\int \langle x|p\rangle\langle p|\psi\rangle \, dp =$$

$$\frac{1}{\sqrt{2\pi}} \int e^{\frac{ipx}{\hbar}} \tilde{\psi}(p) \, dp$$

We compare our results:

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{ipx}{\hbar}} \psi(x)\, dx$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{\frac{ipx}{\hbar}} \tilde{\psi}(p)\, dp$$

Position and momentum representations are reciprocal Fourier transforms of each other.

Particles, state of particles:

In classical mechanics, for a particle of mass m moving along a one-dimensional axis x, the momentary state of the system is described by the pair (x, p). x is the location, p is the momentum. These two variables define the phase space of the system.

Given this, one might guess that the quantum state of a particle would be spanned by a basis of states labeled by position and momentum

$$|x, p\rangle$$

with the wave function:

$$\psi(x, p) = \langle x, p|\psi\rangle$$

This is not correct.

What we have is a wave function in the position representation $\psi(x)$ (resulting from the position operator X) and a wave function in the momentum representation $\tilde{\psi}(p)$ (resulting from the momentum operator P).

Both represent exactly the same state-vector $|\psi\rangle$.

Both are Fourier transforms of each other:

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{ipx}{\hbar}} \psi(x)\, dx$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{\frac{ipx}{\hbar}} \tilde{\psi}(p)\, dp$$

Particles, eigenvalues and eigenvectors of position:

The position operator X multiplies by x. What are possible outcomes of measuring X, and what are its eigenvalues and eigenvectors?

The eigen-equation for the operator X:

$$X|\psi\rangle = x_0|\psi\rangle$$

Note: X is the operator, x_0 is eigenvalue, $|\psi\rangle$ is eigenvector to the operator X.

In terms of wave functions:

$$x\psi(x) = x_0\psi(x)$$

The only function $\psi(x)$ that reproduces itself when multiplied by x is the Dirac delta function:

$$\psi(x) = \delta(x - x_0)$$

With the Dirac delta function, we get the inner product of a state $|\psi\rangle$ and a position eigenstate $|x_0\rangle$:

$$\langle x_0|\psi\rangle = \int_{-\infty}^{\infty} \delta(x - x_0)\psi(x)\, dx = \psi(x_0)$$

Because this is true for any x_0, we write:

$$\langle x|\psi\rangle = \psi(x)$$

This is the wave function in the position representation.

Particles, Momentum and its eigenvectors:

The momentum operator P:

$$P = -i\hbar\frac{d}{dx}$$

What are possible outcomes of measuring P, and what are its eigenvalues and eigenvectors?

The eigen-equation for the operator P:

$$P|\psi\rangle = p|\psi\rangle$$

Note: P is the operator, p eigenvalue, $|\psi\rangle$ eigenvector to the operator P.

In terms of wave functions:

$$-i\hbar\frac{d}{dx}\psi(x) = p\psi(x)$$

Solution:

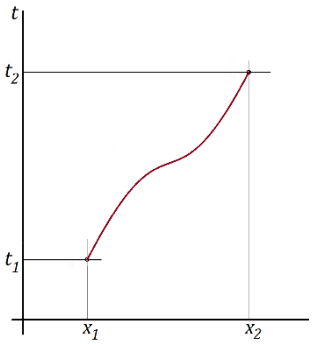
$$\psi_p(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{ipx}{\hbar}}$$

Note: the subscript p is a reminder that $\psi_p(x)$ is eigenvector of P with eigenvalue p. It is a function of x, but labeled by an eigenvalue of P.

This is the wave function in the momentum representation.

Path integrals:

Suppose a classical particle starts at position x_1 at time t_1 and arrives at position x_2 at time t_2. Action is a technical term, and it stands for the integral of the Lagrangian between the end points of the trajectory.



For simple (classic) systems, the Lagrangian is kinetic energy minus potential energy. For a particle moving in one dimension the action is:

$$A = \int_{t_1}^{t_2}\left(\frac{m\dot{x}^2}{2} - V(x)\right)dt$$

Under all possible paths the stationary ones (e.g. the minima, least action) are possible solutions.

In quantum mechanics the idea of a well-defined trajectory has its limits in the Heisenberg Uncertainty Principle. The quantum mechanical question is:

Given a particle starts at (x_1, t_1), what is the probability amplitude it will show up at (x_2, t_2)?

With the simplification $t_2 - t_1 = t$ we call the amplitude $C(x_1, x_2, t)$ resp. $C_{1,2}$.

The initial state of the particle is:

$$|\psi(t_1)\rangle = |x_1\rangle$$

The state evolves to:

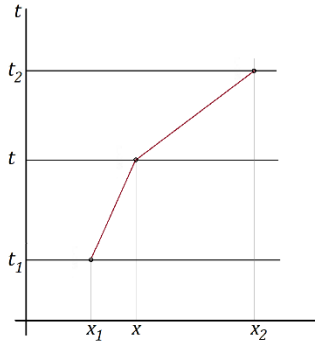
$$|\psi(t_2)\rangle = e^{-iHt}|x_1\rangle$$

Note: we use units with $\hbar = 1$.

The amplitude to detect the particle at $|x_2\rangle$ is the inner product of $|\psi(t_2)\rangle$ with $|x_2\rangle$:

$$C_{1,2} = \langle x_2|e^{-iHt}|x_1\rangle$$

Now we begin to break up the time interval t into smaller intervals of size $\frac{t}{2}$.



The operator e^{-iHt} can be written as:

$$e^{-iHt} = e^{-iH\frac{t}{2}}e^{-iH\frac{t}{2}}$$

We insert the identity operator:

$$I = \int |x\rangle\langle x|\ dx$$

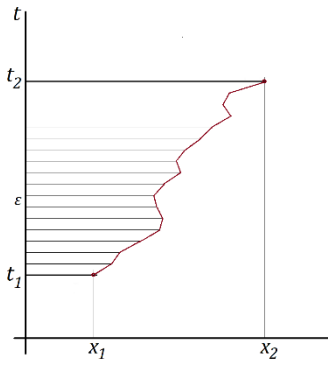
We rewrite the amplitude:

$$C_{1,2} = \int \left\langle x_2\middle|e^{-iH\frac{t}{2}}\middle|x\right\rangle \left\langle x\middle|e^{-iH\frac{t}{2}}\middle|x_1\right\rangle\ dx$$

The amplitude to go from x_1 to x_2 is the product of the amplitude to go from x_1 to x and the amplitude to go from x to x_2.

If we continue to divide into N time intervals of size ε, we have the product of many factors:

$$e^{-i\varepsilon H}$$



We define:

$$U(\varepsilon) = e^{-i\varepsilon H}$$

We write the entire product:

$$\langle x_2|U^N|x_1\rangle$$

We insert identity operators between each U and get the amplitude for the given path. In the limit of a large number of infinitesimal time intervals, the amplitude is an integral over all possible paths between the end points.

The elegant fact that Feynman discovered is that the amplitude for each path bears a simple relation to a familiar expression from classical mechanics – the action for that path.

The exact expression for each path is:

$$e^{i\frac{A}{\hbar}}$$

Note: A is the action for the individual path.

Feynman's formulation can be summarized:

$$C_{1,2} = \int_{paths} e^{i\frac{A}{\hbar}}$$

In quantum field theory it is the principal tool for formulating the laws of elementary particle physics.

Pauli matrices:

The Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The identity matrix is a Pauli matrix too.

Phase ambiguity, phase factor:

A complex number of the form $z = e^{i\theta}$ is called a phase-factor.

For phase-factors holds:

$$z^* z = 1$$

$$z = \cos(\theta) + i\, sin(\theta)$$

No measurable quantity is sensitive to the overall phase-factor, the orthogonality of states remains. Therefore we can ignore it when specifying states.

Photons:

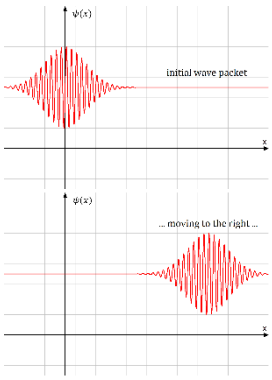
1.

Light of a given wavelength is composed of photons whose momentum is related to the wavelength:

$$\lambda = \frac{2\pi\hbar}{p}$$

2.

Photons can be represented by wave packets:



3.

The energy of an electromagnetic wave is quantized in indivisible units:

$$\frac{2\pi\hbar c}{\lambda}$$

Planck's constant:

$$\hbar = \frac{h}{2\pi} = 1{,}05457\ldots \times 10^{-34}\,\frac{kg\ m^2}{s}$$

Planck's constant seems so small because the units we use are anthropomorph – meaning they reflect us. A meter is used to measure rope or cloth, a second is about as long as a heartbeat. Planck's constant is so small because we are so big and slow. In many books about quantum mechanics units are used for which Planck's constant equals 1.

Poisson brackets, commutators and Poisson brackets:

Prerequisite

The time derivation of an operator L:

$$\frac{d}{dt}L = -\frac{i}{\hbar}[L, H]$$

End prerequisite

Given a phase space with two functions $f(p_i, q_i, t)$ and $g(p_i, q_i, t)$.

The Poisson bracket:

$$\{f, g\} = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right)$$

The Poisson brackets of the canonical coordinates are:

$$\{q_i, q_j\} = 0$$

$$\{p_i, p_j\} = 0$$

$$\{q_i, p_j\} = \delta_{ij}$$

This resembles a quantum mechanical commutator. The formal identification between them:

$$[L, H] \leftrightarrow i\hbar\{L, H\}$$

We use the time derivative of the operator L:

$$\frac{d}{dt}L = -\frac{i}{\hbar}[L, H]$$

We insert the Poisson brackets:

$$\frac{d}{dt}L = -\frac{i}{\hbar}i\hbar\{L, H\}$$

We get:

$$\frac{d}{dt}L = \{L, H\}$$

In fact, in the Poisson bracket formulation of classical mechanics we find:

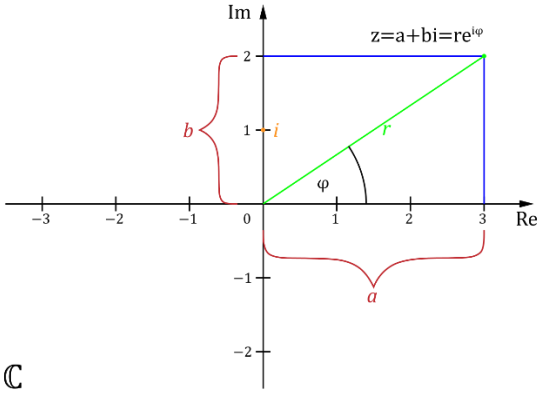
$$\dot{L} = \{L, H\}$$

Polarization vector:

The states of a spin are characterized by a polarization vector. Along that polarization vector the component of the spin is predictably +1.

Polar representation of complex number:

We can represent complex numbers by a plane with the horizontal real axis and the vertical imaginary axis. This is called the cartesian mode.



… graphic courtesy of Wikipedia …

$\mathbb{C}$

A second way of representation describes a complex number by the angle it has with the real axis and its length resp. the absolute value. This is called the Gaussian mode. In this mode we write a complex number as $r \cdot e^{i\varphi}$.

We can switch from one representation to the other:

Given $z = a + ib$: $\quad |z| \; or \; r = \sqrt{a^2 + b^2}$ $\qquad \varphi = \arccos\left(\frac{a}{r}\right)$ if $b \geq 0$

resp. $\qquad \varphi = -\arccos\left(\frac{a}{r}\right)$ if $b < 0$.

Given $z = re^{i\varphi}$: $\quad a = r \cdot \cos(\varphi)$ $\qquad b = r \cdot \sin(\varphi)$

or $\qquad z = r \cdot (\cos(\varphi) + i \cdot \sin(\varphi))$

Position:

Eigenvalues and eigenvectors of position:

Prerequisite

The inner product for continuous functions:

$$\langle \psi | \Phi \rangle = \int_{-\infty}^{\infty} \psi^*(x)\phi(x)\, dx$$

End prerequisite

Eigenvalues and eigenvectors of the position operator X.

The eigen-equation for the operator X:

$$X|\psi\rangle = x_0|\psi\rangle$$

Note: in this case $|\psi\rangle$ is eigenvector to the operator X with eigenvalue x_0.

Note: x_0 is a real number.

In terms of wave functions:

$$x\psi(x) = x_0\psi(x)$$

The function $\psi(x)$ that solves this equation is the Dirac delta function:

$$\delta(x - x_0)$$

The wave functions $\psi(x) = \delta(x - x_0)$ represent the state in which the particle is located at x_0.

The inner product of a state $|\psi\rangle$ and a position eigenstate $|x_0\rangle$:

$$\langle x_0|\psi\rangle$$

Note: as x_0 is a real number, $|x_0\rangle = \langle x_0|$.

We build the inner product in terms of wave functions:

$$\langle x_0|\psi\rangle = \int_{-\infty}^{\infty} \delta(x - x_0)\psi(x)\, dx = \psi(x_0)$$

The wave function $\psi(x)$ of a particle moving in the x-direction is the projection of a state-vector $|\psi\rangle$ onto the eigenvectors of position. $\psi(x)$ is the wave function in the position representation.

Proposition for position:

In formal logic following propositions are possible:

$A\ certain\ particle\ has\ position\ x.$

$A\ certain\ particle\ has\ momentum\ p.$

According to classical logic, propositions can be combined by the logical or resp. the logical and:

$$(A\ certain\ particle\ has\ position\ x)\ or\ (A\ certain\ particle\ has\ momentum\ p)$$

$$(A\ certain\ particle\ has\ position\ x)\ and\ (A\ certain\ particle\ has\ momentum\ p)$$

For classical physics both combinations are true.

For quantum mechanics only the first one is (always) true, because position and momentum cannot (always) be measured simultaneously.

Position representation of wave function:

Prerequisite

The inner product of a position eigenvector $|x\rangle$ and a momentum eigenvector $|p\rangle$:

$$\langle x|p\rangle = \langle p|x\rangle^*$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$

By help of the identity operator we can expand inner products:

$$I = \sum_i |i\rangle\langle i|$$

Note: $|i\rangle$ must be a complete set of basis vectors.

This works with integrals too:

$$I = \int |x\rangle\langle x|\, dx$$

$$I = \int |p\rangle\langle p|\, dp$$

Note: eigenvectors of position operator X and momentum operator P define an appropriate basis.

End prerequisite

Suppose we know the wave function of the abstract vector $|\psi\rangle$ in position representation:

$$\psi(x) = \langle x|\psi\rangle$$

To know the wave function $\tilde{\psi}(x)$ in momentum representation we do the following steps.

5. We use the definition of the momentum-representation wave function:
   $$\tilde{\psi}(p) = \langle P|\psi\rangle = \langle p|\psi\rangle$$
   Note: P is the momentum operator, p is eigenvalue of $|\psi\rangle$.

6. We insert the unit operator:
   $$\tilde{\psi}(p) = \int \langle p|x\rangle\langle x|\psi\rangle\, dx$$
   $\langle x|\psi\rangle$ is just the wave function $\psi(x)$.

7. $\langle p|x\rangle$ is given by:
   $$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}}$$

8. Result:
   $$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int e^{-\frac{ipx}{\hbar}} \psi(x) dx$$

By knowing $\psi(x)$ in the position representation we calculate the corresponding wave function in the momentum representation.

This works also the other way around. We know the wave function in the momentum representation $\tilde{\psi}(p)$ and calculate the position representation:

1. We use the definition of the position-representation wave function:
   $$\psi(x) = \langle X|\psi\rangle = \langle x|\psi\rangle$$
   Note: X is the position operator, x is eigenvalue of $|\psi\rangle$.

2. We insert the unit operator:
   $$\psi(x) = \int \langle x|p\rangle\langle p|\psi\rangle\, dp$$
   $\langle p|\psi\rangle$ is just the wave function $\tilde{\psi}(p)$.

3. $\langle x|p\rangle$ is given by:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}}$$

4. Result:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{\frac{ipx}{\hbar}} \tilde{\psi}(p) dp$$

Position and momentum representation are reciprocal Fourier transforms of each other.

Potential functions:

The potential energy function is denoted by $V(x)$.

In classical mechanics it is related to the force on a particle:

$$F(x) = -\frac{\partial V}{\partial x}$$

Combined with Newton's second law, $F = ma$:

$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

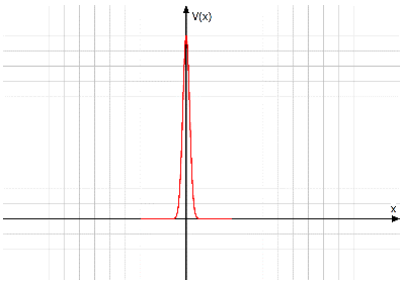
In quantum mechanics the potential energy function becomes an operator V that gets added to the Hamiltonian:

$$H = \frac{P^2}{2m} + V$$

The operator V acting on a wave function $\psi(x)$:

$$V|\psi\rangle \rightarrow V(x)\psi(x)$$

Potential functions, spiky potential functions:



Whether an experiment follows the rules of classical physics or quantum mechanics depends (among others) on the form of the potentials involved.

If a potential is "spiky" in relation to the other participant uncertainty in position, then the wave packet tends to scatter and break up.

If a potential is "smooth", the wave packet tends to remain and to show classical behavior.

Precession of spin in magnetic field:

Classical mechanics

The z component of the angular momentum is constant, the x and y components of the angular momentum are precessing.

We define the angular momentum L:

$$L = x\, p_y - y\, p_x$$

The Poisson brackets:

$$\{x, L_z\} = -y$$

$$\{y, L_z\} = x$$

$$\{z, L_z\} = 0$$

Quantum mechanics

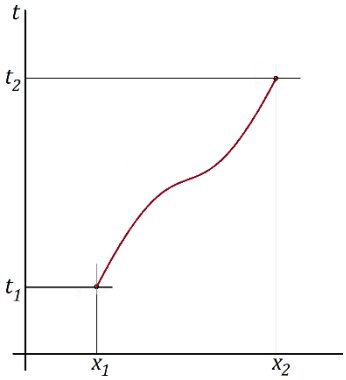
The expectation value for a σ_z measurement does not change with time, but the σ_x and σ_y expectation values do. Regardless, the result of each individual measurement is either $+1$ or -1.

$$\langle \dot{\sigma_x} \rangle = -\omega \langle \sigma_y \rangle$$

$$\langle \dot{\sigma_y} \rangle = \omega \langle \sigma_x \rangle$$

$$\langle \dot{\sigma_z} \rangle = 0$$

Principle of least/stationary action:



Suppose a classical particle starts at position x_1 at time t_1 and arrives at position x_2 at time t_2. Action is a technical term, and it stands for the integral of the Lagrangian between the end points of the trajectory.

For simple (classic) systems, the Lagrangian is kinetic energy minus potential energy. For a particle moving in one dimension the action is:

$$A = \int_{t_1}^{t_2} \left(\frac{m\dot{x}^2}{2} - V(x) \right) dt$$

Under all possible paths the stationary ones (e.g. the minima, least action) are possible solutions.

In quantum mechanics the idea of a well-defined trajectory has its limits in the Heisenberg Uncertainty Principle. The quantum mechanical question is:

Given a particle starts at (x_1, t_1), what is the probability amplitude it will show up at (x_2, t_2)?

With the simplification $t_2 - t_1 = t$ we call the amplitude $C(x_1, x_2, t)$ resp. $C_{1,2}$.

The initial state of the particle is:

$$|\psi(t_1)\rangle = |x_1\rangle$$

The state evolves to:

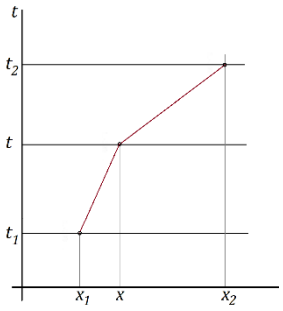
$$|\psi(t_2)\rangle = e^{-iHt}|x_1\rangle$$

Note: we use units with $\hbar = 1$.

The amplitude to detect the particle at $|x_2\rangle$ is the inner product of $|\psi(t_2)\rangle$ with $|x_2\rangle$:

$$C_{1,2} = \langle x_2 | e^{-iHt} | x_1 \rangle$$

Now we begin to break up the time interval t into smaller intervals of size $\frac{t}{2}$.



The operator e^{-iHt} can be written as:

$$e^{-iHt} = e^{-iH\frac{t}{2}}e^{-iH\frac{t}{2}}$$

We insert the identity operator:

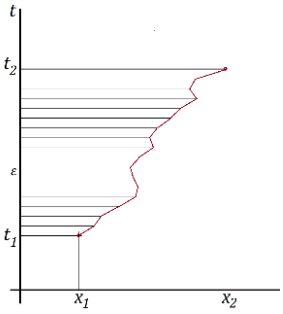
$$I = \int |x\rangle\langle x| \; dx$$

We rewrite the amplitude:

$$C_{1,2} = \int \left\langle x_2 \middle| e^{-iH\frac{t}{2}} \middle| x \right\rangle \left\langle x \middle| e^{-iH\frac{t}{2}} \middle| x_1 \right\rangle \; dx$$

The amplitude to go from x_1 to x_2 is the product of the amplitude to go from x_1 to x and the amplitude to go from x to x_2.

If we continue to divide into N time intervals of size ε, we have the product of many factors:



$$e^{-i\varepsilon H}$$

We define:

$$U(\varepsilon) = e^{-i\varepsilon H}$$

We write the entire product:

$$\langle x_2|U^N|x_1\rangle$$

We insert identity operators between each U and get the amplitude for the given path. In the limit of a large number of infinitesimal time intervals, the amplitude is an integral over all possible paths between the end points.

The elegant fact that Feynman discovered is that the amplitude for each path bears a simple relation to a familiar expression from classical mechanics – the action for that path.

The exact expression for each path is:

$$e^{i\frac{A}{\hbar}}$$

Note: A is the action for the individual path.

Feynman's formulation can be summarized:

$$C_{1,2} = \int_{paths} e^{i\frac{A}{\hbar}}$$

In quantum field theory it is the principal tool for formulating the laws of elementary particle physics.

Probability for experimental outcome:

1.

In the case of spin measurement, the measurements will always give either $+1$ or -1 as a result. Other probabilities we get as an average over a number of measurements, not directly as a result of one measurement.

2.

In classical physics you test two propositions A, B. Generally, the sequence has no influence on the result.

In quantum mechanics the sequence can be critical. If the two propositions are not simultaneously measurable, the sequence $A\ then\ B$ can give other results as $B\ than\ A$.

It seems that the logic foundation is different in quantum mechanics.

3.

Possible results of a measurement are the eigenvalues of the operator that represents the observable – the result of a measurement is guaranteed to be this.

If $|A\rangle$ is the state vector of a system, and the observable L is measured, the probability to observe value λ_i is:

$$P(\lambda_i) = |\langle A|\lambda_i\rangle|^2 = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$

Note: λ_i is eigenvalue of the operator L, $|\lambda_i\rangle$ eigenvector of the operator L.

4.

We calculate the average value, the expectation value of a measurement:

$$\langle L\rangle = \sum_i \lambda_i P(\lambda_i)$$

Note: this is the standard formula for an average value.

5.

In terms of wave functions the probability for an experiment to have outcome λ is:

$$P(\lambda) = \psi^*(\lambda)\psi(\lambda)$$

Note: $\psi(\lambda)$ is a complex valued function of the discrete variable λ.

Note: this works only for a discrete (finite dimensional) variable λ.

Probability for experimental outcome replaced by probability densities:

For a discrete variable λ the probability for an experiment to have outcome λ is:

$$P(\lambda) = \psi^*(\lambda)\psi(\lambda)$$

Note: $\psi(\lambda)$ is a complex valued function of the discrete variable λ.

For a continuous variable x, $P(x) = \psi^*(x)\psi(x)$ becomes the probability density.

As probability is defined by the integral over the probability density, the probability at exactly one point is zero.

We then can measure only the probability between two limits a and b:

$$P(a,b) = \int_a^b P(x)\,dx = \int_a^b \psi^*(\lambda)\psi(\lambda)\,dx$$

With this we can normalize the vector (wave function):

$$\int_{-\infty}^{\infty} \psi^*(\lambda)\psi(\lambda)\,dx = 1$$

Schrödinger ket and probability for experimental outcome:

1. Derive, look up, guess, borrow or steal the Hamiltonian operator H for the system.
2. Prepare an initial state $|\psi(0)\rangle$.
3. Find the eigenvalues and eigenvectors of H by solving the time-independent Schrödinger equation:

   $$H|E_j\rangle = E_j|E_j\rangle$$

   You will get:

   $$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$$

   Note 1: "E_j" is eigenvalue to the eigenvector $|E_j\rangle$.

   Note 2: $H|E_j\rangle = E_j|E_j\rangle$ leads to a differential equation that determines $\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$.

4. Calculate the initial coefficients $\alpha_j(0) = \langle E_j|\psi(0)\rangle$.
5. Rewrite $|\psi(0)\rangle$ in terms of eigenvectors $|E_j\rangle$ and initial coefficients $\alpha_j(0)$:

   $$|\psi(0)\rangle = \sum_j \alpha_j(0)\,|E_j\rangle$$

6. Replace each $\alpha_j(0)$ with $\alpha_j(t)$ to capture its time-dependence. As the basis vectors $|E_j\rangle$ do not change, this leads to:

   $$|\psi(t)\rangle = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}\,|E_j\rangle$$

We can now predict the probabilities for (any) experiment as a function of time. Suppose the observable (the operator) L has eigenvalues λ_i and eigenvectors $|\lambda_i\rangle$.

The probability for outcome λ is:

$$P_\lambda(t) = |\langle\lambda|\psi(t)\rangle|^2$$

Probability:

Entanglement and probability:

Prerequisite

We have an entangled two-spin system of Alice and Bob.

Alice's density matrix (a 2×2 matrix):

$$\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$$

This is purely a function of Alice variables a and a' because we have summed up over all b of Bob.

End prerequisite

We calculate the probability $P(a)$ that the system of Alice will be left in state a if a measurement is made.

We begin with $P(a,b)$, the probability that the combined system is in state $|ab\rangle$:

$$P(a,b) = \psi^*(a,b)\psi(a',b)$$

We sum over b and get the total probability for a:

$$P(a) = \sum_b \psi^*(a,b)\psi(a',b)$$

This is just a diagonal entry in the density matrix, so we can write:

$$P(a) = \rho_{a'a}$$

Wave function and probability:

The wave function $\psi(x)$ is used to determine the probability for finding a particle at position x:

$$P(x) = |\langle X|\psi\rangle|^2 = \langle X|\psi\rangle\langle\psi|X\rangle = \psi(x)\psi^*(x) = \psi^*(x)\psi(x)$$

The wave function $\tilde{\psi}(p)$ is used to determine the probability for finding a particle with momentum p:

$$P(p) = |\langle P|\psi\rangle|^2 = \langle P|\psi\rangle\langle\psi|P\rangle = \tilde{\psi}(p)\tilde{\psi}^*(p) = \tilde{\psi}^*(p)\tilde{\psi}(p)$$

$\psi(x)$ and $\tilde{\psi}(p)$ are reciprocal Fourier transforms of each other:

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}}\int e^{-\frac{ipx}{\hbar}}\psi(x)dx$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\int e^{\frac{ipx}{\hbar}}\tilde{\psi}(p)dp$$

Probability amplitude:

In a single spin system $|A\rangle$:

$$|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$$

α_u and α_d are the components of $|A\rangle$ along the basis directions $|u\rangle$ and $|d\rangle$.

The quantity ${\alpha_u}^*\alpha_u$ is the probability that a measurement of $\sigma_z = 1$.

The quantity ${\alpha_d}^*\alpha_d$ is the probability that a measurement of $\sigma_z = -1$.

The values α_u resp. α_d are called probability amplitudes. To compute the probabilities for up or $down$, their magnitudes must be squared:

$$P_u = \langle A|u\rangle\langle u|A\rangle = {\alpha_u}^*\alpha_u$$

$$P_d = \langle A|d\rangle\langle d|A\rangle = {\alpha_d}^*\alpha_d$$

Phase factors $e^{i\theta}$ change the probability amplitude, but not the probability:

$$\alpha_u \neq \alpha_u e^{i\theta}$$

$${\alpha_u}^*\alpha_u = {\alpha_u}^* e^{-i\theta}\alpha_u e^{i\theta} = {\alpha_u}^*\alpha_u e^{-i\theta}e^{i\theta} = {\alpha_u}^*\alpha_u$$

Probability density:

The probability density for finding a particle at position x:

$$P(x) = \psi^*(x)\psi(x)$$

This is combined with the normalization condition:

$$1 = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\,dx$$

The probability to find the particle anywhere on the x axis must be one.

A classical pure state is a special case of a probability density being nonzero at only one point. In the case above this would be the Dirac delta function that gives an "infinite" probability density at x_0 and zero elsewhere.

Probability density replacing probabilities:

For a discrete variable λ the probability for an experiment to have outcome λ is:

$$P(\lambda) = \psi^*(\lambda)\psi(\lambda)$$

Note: $\psi(\lambda)$ is a complex valued function of the discrete variable λ.

For a continuous variable x, $P(x) = \psi^*(x)\psi(x)$ becomes the probability density.

As probability is defined by the integral over the probability density, the probability at exactly one point is zero. We can measure only the probability between two limits a and b:

$$P(a,b) = \int_a^b P(x)\,dx = \int_a^b \psi^*(\lambda)\psi(\lambda)\,dx$$

With this we can normalize the vector (wave function):

$$\int_{-\infty}^{\infty} \psi^*(\lambda)\psi(\lambda)\,dx = 1$$

Probability distribution:

1.

If the probability distribution for an observable is a small, nice bell-shaped curve, then the expectation value is the value you expect to measure. It behaves like a classical one.

2.

Suppose you have a probability distribution $P(a,b)$ for two variables a and b.

If the variables are completely uncorrelated, then the probability distribution will factorize:

$$P(a,b) = P(a)P(b)$$

In terms of averages (of our two-spin system):

$$\langle\sigma_A\sigma_B\rangle = \langle\sigma_A\rangle\langle\sigma_B\rangle$$

3.

The mathematical indication of correlation is that the probability distribution does not factorize. In terms of averages:

$$\langle \sigma_A \sigma_B \rangle \neq \langle \sigma_A \rangle \langle \sigma_B \rangle$$

Probability distribution in classical mechanics:

In classical mechanics, the use of probability is always associated with an incompleteness of knowledge relative to all that could be known.

In classical mechanics, the complete knowledge of a system implies complete knowledge of every subsystem.

Particle dynamics and probability distribution:

In classical physics particles are moving.

In quantum mechanics probability distributions are moving (change their shape with time).

Uncertainty and probability distribution:

The uncertainty is the standard deviation.

Let A be an observable (operator) with eigenvalues a.

The expectation value of A:

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \sum_a a P(a)$$

We define the operator $\bar{A}$:

$$\bar{A} = A - \langle A \rangle I$$

The expectation value of $\bar{A}$ is zero.

The eigenvectors of $\bar{A}$ are the same as those of A. The eigenvalues are shifted:

$$\bar{a} = a - \langle A \rangle$$

The square of uncertainty or standard deviation of A:

$$(\Delta A)^2 = \sum_a \bar{a}^2 P(a) = \sum_a (a - \langle A \rangle)^2 P(a) = \langle \psi | \bar{A}^2 | \psi \rangle$$

If the expectation value of the operator A is zero, the square of the uncertainty is the average value of the operator A^2:

$$(\Delta A)^2 = \langle \psi | A^2 | \psi \rangle$$

Probability function:

An average is defined as a weighted sum:

$$\langle L \rangle := \sum_i \lambda_i P(\lambda_i)$$

Note: $P(\lambda_i)$ is the probability function.

$P(\lambda_i)$ is the fraction of observations whose result was λ_i.

Suppose the normalized state of a quantum system is $|A\rangle$. We expand $|A\rangle$ in the orthonormal basis of eigenvectors of L:

$$|A\rangle = \sum_i \alpha_i \, |\lambda_i\rangle$$

We calculate $\langle A|L|A\rangle$:

$$L|A\rangle = \sum_i L\alpha_i|\lambda_i\rangle = \sum_i \alpha_i L|\lambda_i\rangle = \sum_i \alpha_i\lambda_i|\lambda_i\rangle$$

$$\langle A|L|A\rangle = \sum_j \langle\lambda_j| \, \alpha_j{}^* \sum_i \alpha_i\lambda_i|\lambda_i\rangle =$$

$$\sum_{i,j} \langle\lambda_j| \, \alpha_j{}^*\alpha_i\lambda_i|\lambda_i\rangle =$$

$$\sum_{i,j} \alpha_j{}^*\alpha_i\lambda_i\langle\lambda_j|\lambda_i\rangle =$$

$$\sum_i \alpha_i{}^*\alpha_i\lambda_i$$

Note: $\langle\lambda_j|\lambda_i\rangle$ is the Kronecker delta δ_{ij}.

We get:

$$\langle A|L|A\rangle = \sum_i \alpha_i{}^*\alpha_i\lambda_i$$

We compare this with:

$$\langle L\rangle := \sum_i \lambda_i P(\lambda_i)$$

We get the average of an observable (an operator) L by sandwiching it between the bra and ket representations of the state-vector A:

$$\langle L\rangle = \langle A|L|A\rangle$$

The probability $P(\lambda_i) = \alpha_i{}^*\alpha_i$.

Product states:

The simplest type of state for a composite system (a two-spin system) is a product state. It consists of two independent spins.

The system of Alice:

$$\alpha_u|u\rangle + \alpha_d|d\rangle$$

The system of Bob:

$$\beta_u|u\rangle + \beta_d|d\rangle$$

Each state is normalized:

$$\alpha_u^* \alpha_u + \alpha_d^* \alpha_d = 1$$

$$\beta_u^* \beta_u + \beta_d^* \beta_d = 1$$

Note: without normalization no product state.

The product state describes the combined system:

$$|product\ state\rangle = \{\alpha_u|u\rangle + \alpha_d|d\rangle\} \otimes \{\beta_u|u\rangle + \beta_d|d\rangle\}$$

We expand this:

$$\alpha_u|u\rangle \otimes \beta_u|u\rangle + \alpha_u|u\rangle \otimes \beta_d|d\rangle + \alpha_d|d\rangle \otimes \beta_u|u\rangle + \alpha_d|d\rangle \otimes \beta_d|d\rangle$$

$$\alpha_u\beta_u(|u\rangle \otimes |u\rangle) + \alpha_u\beta_d(|u\rangle \otimes |d\rangle) + \alpha_d\beta_u(|d\rangle \otimes |u\rangle) + \alpha_d\beta_d(|d\rangle \otimes |d\rangle)$$

We get:

$$|product\ state\rangle = \alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

Note: $|u\rangle$ is a two-dimensional state vector. $|u\rangle \otimes |u\rangle$ resp. $|uu\rangle$ is a four-dimensional state vector.

Product states, correlation of product states:

Let us assume that A is an Alice observable and B is a Bob observable.

$\langle A\rangle$ is the expectation value of A, $\langle B\rangle$ is the expectation value of B and $\langle AB\rangle$ is the expectation value of the product.

If a combined state is a product state, the observables are independent:

$$\langle AB\rangle = \langle A\rangle\langle B\rangle$$

Correlation is defined as:

$$\langle AB\rangle - \langle A\rangle\langle B\rangle$$

In a product state, the correlation between two observables is zero:

$$\langle AB\rangle - \langle A\rangle\langle B\rangle = 0$$

Product states, counting parameters for product states:

To specify a product state (of two spins), we need four complex numbers $\alpha_u, \beta_u, \alpha_d, \beta_d$ or eight real numbers:

$$|product\ state\rangle = \alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

The normalization condition reduces this by two.

The overall phase have no physical significance, this reduces further by two.

There remains four real parameters to describe the combined system.

Note: this is valid only for product states. For entangled states we might need the full set of parameters.

Product states, density matrix and product states:

The eigenvector of a density matrix for a product state has exactly one nonzero eigenvalue, which equals 1. The eigenvector with this nonzero eigenvalue is the wave function of Alice's subsystem.

We try this for a product two-spin system of Alice and Bob.

The wave function of the combined system with $a = u, d$ and $b = u, d$ for each subsystem:

$$\psi(a, b) = \psi_{uu} + \psi_{ud} + \psi_{du} + \psi_{dd}$$

In terms of the subsystem values:

$$\alpha_u\beta_u + \alpha_u\beta_d + \alpha_d\beta_u + \alpha_d\beta_d$$

We have the normalization condition:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

$$\beta_u^*\beta_u + \beta_d^*\beta_d = 1$$

The density matrix of Alice:

$$\rho_{a,a'} = \sum_b \psi^*(a', b)\psi(a, b) =$$

$$\psi^*(a', u)\psi(a, u) + \psi^*(a', d)\psi(a, d)$$

Note: the right-hand index of ρ, that is, the a' index, corresponds to the complex conjugate state-vector $\psi^*(a', b)$ in the summation. This is a consequence of the convention:

$$L_{aa'} = \langle a|L|a'\rangle$$

We calculate each of the four possible terms:

$$\rho_{uu} = \psi^*(u, u)\psi(u, u) + \psi^*(u, d)\psi(u, d) =$$

$$\alpha_u^*\beta_u^*\alpha_u\beta_u + \alpha_u^*\beta_d^*\alpha_u\beta_d =$$

$$\alpha_u^*\alpha_u\beta_u^*\beta_u + \alpha_u^*\alpha_u\beta_d^*\beta_d =$$

$$\alpha_u^*\alpha_u(\beta_u^*\beta_u + \beta_d^*\beta_d) =$$

$$\alpha_u^*\alpha_u$$

$$\rho_{ud} = \psi^*(d, u)\psi(u, u) + \psi^*(d, d)\psi(u, d) =$$

$$\alpha_d^*\beta_u^*\alpha_u\beta_u + \alpha_d^*\beta_d^*\alpha_u\beta_d =$$

$$\alpha_u\alpha_d^*\beta_u^*\beta_u + \alpha_u\alpha_d^*\beta_d^*\beta_d =$$

$$\alpha_u\alpha_d^*(\beta_u^*\beta_u + \beta_d^*\beta_d) =$$

$$\alpha_u\alpha_d^*$$

$$\rho_{du} = \psi^*(u, u)\psi(d, u) + \psi^*(u, d)\psi(d, d) =$$

$$\alpha_u^*\beta_u^*\alpha_d\beta_u + \alpha_u^*\beta_d^*\alpha_d\beta_d =$$

$$\alpha_u^*\alpha_d\beta_u^*\beta_u + \alpha_u^*\alpha_d\beta_d^*\beta_d =$$

$$\alpha_u^*\alpha_d(\beta_u^*\beta_u + \beta_d^*\beta_d) =$$

$$\alpha_u^*\alpha_d$$

$$\rho_{dd} = \psi^*(d, u)\psi(d, u) + \psi^*(d, d)\psi(d, d) =$$

$$\alpha_d^*\beta_u^*\alpha_d\beta_u + \alpha_d^*\beta_d^*\alpha_d\beta_d =$$

$$\alpha_d^*\alpha_d\beta_u^*\beta_u + \alpha_d^*\alpha_d\beta_d^*\beta_d =$$

$$\alpha_d^*\alpha_d(\beta_u^*\beta_u + \beta_d^*\beta_d) =$$

$$\alpha_d^*\alpha_d$$

The density matrix for Alice:

$$\begin{pmatrix} \alpha_u^*\alpha_u & \alpha_u\alpha_d^* \\ \alpha_u^*\alpha_d & \alpha_d^*\alpha_d \end{pmatrix}$$

The diagonal of this matrix consists of real values.

The matrix is Hermitian.

The Trace of the matrix gives 1.

Note: any Hermitian matrix can be diagonalized.

We remember: The eigenvector of a density matrix for a product state has exactly one nonzero eigenvalue, which equals 1. The eigenvector with this nonzero eigenvalue is the wave function of Alice's subsystem.

We know the wave function of Alice's subsystem:

$$\psi_u + \psi_d \to \alpha_u|u\rangle + \alpha_d|d\rangle$$

The state-vector:

$$\begin{pmatrix} \alpha_u \\ \alpha_d \end{pmatrix}$$

The equation for the eigenvector/eigenvalue:

$$\begin{pmatrix} \alpha_u^*\alpha_u & \alpha_u\alpha_d^* \\ \alpha_u^*\alpha_d & \alpha_d^*\alpha_d \end{pmatrix}\begin{pmatrix} \alpha_u \\ \alpha_d \end{pmatrix} =$$

$$\begin{pmatrix} \alpha_u^*\alpha_u\alpha_u + \alpha_u\alpha_d^*\alpha_d \\ \alpha_u^*\alpha_d\alpha_u + \alpha_d^*\alpha_d\alpha_d \end{pmatrix} =$$

$$\begin{pmatrix} \alpha_u(\alpha_u^*\alpha_u + \alpha_d^*\alpha_d) \\ \alpha_d(\alpha_u^*\alpha_u + \alpha_d^*\alpha_d) \end{pmatrix} = \begin{pmatrix} \alpha_u \\ \alpha_d \end{pmatrix}$$

Result: $\begin{pmatrix} \alpha_u \\ \alpha_d \end{pmatrix}$ is eigenvector to the density matrix of Alice with eigenvalue 1.

Product states, density matrix test for entanglement and product states:

Suppose the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$. Then the composite wave function also is product of Bob's factor and Alice's factor:

$$\psi(a,b) = \vartheta(a)\theta(b)$$

Alice's density matrix:

$$\rho_{a'a} = \vartheta^*(a)\vartheta(a')\sum_b \theta^*(b)\theta(b)$$

As the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$, both Alice's and Bob's state separately are normalized, so:

$$\sum_b \theta^*(b)\theta(b) = 1$$

And Alice's density matrix becomes $\rho_{a'a} = \vartheta^*(a)\vartheta(a')$.

We prove a theorem about the eigenvalues of Alice's density matrix that is only true for product states but not for entangled states and thus can serve to identify them: for product states the density matrix of Alice or Bob has exactly one eigenvalue of value one.

The eigenvalue equation for Alice's matrix $\rho_{a'a}$:

$$\sum_a \rho_{a'a}\alpha_a = \lambda\alpha_a =$$

$$\sum_a \vartheta^*(a)\vartheta(a')\alpha_a = \vartheta(a')\sum_a \vartheta^*(a)\alpha_a$$

$\sum_a \vartheta^*(a)\alpha_a$ has the form of an inner product. If the column vector α is orthogonal to ϑ, then $\sum_a \vartheta^*(a)\alpha_a$ is zero giving an eigenvector with eigenvalue zero.

In a space state of dimension N we have $N-1$ vectors orthogonal to ϑ, so we have only one possible direction for an eigenvector with nonzero eigenvalue $\vartheta(a)$:

$\vartheta^*(a)\alpha_a = 0$ for all $\alpha_a \neq \vartheta(a)$ and 1 for $\alpha_a = \vartheta(a)$.

Alice's system is in a pure state, all of her observations are described as if Bob never existed.

In a maximally entangled system on the other hand Alice's density matrix is proportional to the unit matrix with all equal eigenvalues $\frac{1}{N}$:

$$\rho_{a'a} = \frac{1}{N}\delta_{a'a}$$

As the density matrix gives the probability for an outcome this means that every outcome has equal possibility.

For partial entanglement the weights of $\rho_{a'a}$ move from the equal distribution towards a concentration on a single value 1 on the diagonal of the density matrix.

Although in a maximum entangled state Alice can't predict the outcome of her experiments, she knows (after the experiment has been done) exactly about the relation between her and Bob's outcomes.

Product states, description of product states:

Given two states, $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$ and $|B\rangle = \beta_u|u\rangle + \beta_d|d\rangle$.

Each state is normalized: $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$ and $\beta_u^*\beta_u + \beta_d^*\beta_d = 1$

The product state describing the system is: $|product\ state\rangle = \{\alpha_u|u\rangle + \alpha_d|d\rangle\}\otimes\{\beta_u|u\rangle + \beta_d|d\rangle\}$.

Expanding and switching to composite notation gives:

$$|product\ state\rangle = \alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

This state vector of the combined system is automatically normalized too: $\alpha_u\beta_u + \alpha_u\beta_d + \alpha_d\beta_u + \alpha_d\beta_d = 1$.

The density matrix A as well as the density matrix B have exactly one nonzero eigenvalue 1, the eigenvector with this eigenvalue is the wave function of system A resp. B.

The wave function is factorized: $\psi(a)\psi(b)$.

The expectation values are: $\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$ and $\langle\tau_x\rangle^2 + \langle\tau_y\rangle^2 + \langle\tau_z\rangle^2 = 1$

The correlation between the two systems is zero: $\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = 0$

The main feature of a product state is that each subsystem behaves independently of the other.

Projection operator:

The outer product of a normalized ket $|\psi\rangle$ with its corresponding bra $\langle\psi|$ is called a projection operator:

$$|\psi\rangle\langle\psi|$$

Note: this is a kind of tensor product.

Properties of projection operators:

- Projection operators are Hermitian
- The vector $|\psi\rangle$ is eigenvector of its projection operator with eigenvalue 1:
$$|\psi\rangle\langle\psi| \ |\psi\rangle = |\psi\rangle$$
- Any vector orthogonal to $|\psi\rangle$ is eigenvector with eigenvalue zero. Thus, the eigenvalues of $|\psi\rangle\langle\psi|$ are either zero or one, and there is only one eigenvector with eigenvalue 1, $|\psi\rangle$ itself.
- The square of a projection operator is the same as the projection operator itself:
$$|\psi\rangle\langle\psi|^2 = |\psi\rangle\langle\psi|$$
- The trace of an operator or any square matrix is defined as the sum of its diagonal elements. We define the trace Tr of an operator L by using an appropriate basis $|i\rangle$:
$$Tr = \sum_i \langle i|L|i\rangle$$
This gives the sum of the diagonal elements of L.
if we add all projection operators for a basis system, we obtain the identity operator I:
$$\sum_i |i\rangle\langle i| = I$$

The expectation value of any observable L in state $|\psi\rangle$ is given by:

$$\langle L\rangle = \langle\psi|L|\psi\rangle = Tr\ |\psi\rangle\langle\psi|L$$

Propositions:

Classical propositions:

Formal logic means the classical logic that works with 1 and 0 resp. true and false.

A proposition can be true or false. Mathematical propositions can be equations like $2 + 3 = 5$. An equation like $2 \cdot x + 3 = 7$ is not a proposition but a propositional expression that becomes true or false depending on what you insert for the variable x.

If you concatenate propositions with "and" resp. the "or", the result follows rules. We must carefully distinguish between the $inclusive\ or$ we normally use when speaking and the $exclusive\ or$. The $exclusive\ or$ in formal logic is written as XOR.

Let A and B be propositions, then the truth values (A "or" B) are:

A	B	$A\ or\ B$
0	0	0
0	1	1
1	0	1
1	1	1

The truth values for (A "and" B):

A	B	$A\ and\ B$
0	0	0
0	1	0
1	0	0
1	1	1

Sometimes the logical connections are referred to as $+$ and $\cdot$:

A	B	$A+\ B$
0	0	0
0	1	1
1	0	1
1	1	1

Note that 1+1 gives 1 because "double true remains true".

A	B	$A \cdot B$
0	0	0
0	1	0
1	0	0
1	1	1

… perfect …

There is a special logical operator, the "not", that simply switches the truth value to its opposite:

A	$\neg A$
0	1
1	0

Classical computers work on basis of formal logic, computer memory consist of binary storage locations that only distinguish between 0 and 1 (and so does the processing unit too). That is pity because if we could isolate every single storage location perfectly then we would be able to store not only a binary digit but a real number (at least more than two different states).

In quantum mechanics often used is the orientation of a spin in space. This spin can be "up" or "down". We need a way to describe these. A simple variable with e.g. 1 for "spin up" and 0 for "spin down" is not sufficient, we use two variables for the orientation, one representing "up", the other "down".

As they are logically connected to each other, we write them as $\binom{a}{b}$.

$\binom{1}{0}$ defines the state with the spin-vector "up", $\binom{0}{1}$ the state with the spin-vector "down".

This fits with our formal logic. The proposition "the spin is up **or** down" is true for both combinations:

A	B	$A+\ B$
0	1	1
1	0	1

The proposition “the spin is up **and** down” is false for both combinations:

A	B	$A \cdot B$
0	1	0
1	0	0

We need a method to show that the positions “up” and “down” are mutually exclusive. We adopt the dot product: $\binom{a}{b} \cdot \binom{c}{d} = ac + bd$ and apply it: $\binom{1}{0} \cdot \binom{0}{1} = 1 \cdot 0 + 0 \cdot 1 = 0$.

We check another (“useless”) proposition: “The spin is up” and “the spin is up”. This is a true proposition. According the dot product $\binom{1}{0} \cdot \binom{1}{0} = 1 \cdot 1 + 0 \cdot 0 = 1$ delivers the “1” for “true”.

Unfortunately, things are a little bit more complicated in quantum mechanics. The result of measuring the spin gives either $\binom{1}{0}$ or $\binom{0}{1}$, the spin itself can take all combinations in between: $\alpha \binom{1}{0}$ and $\beta \binom{0}{1}$ with α and β being fractions between 0 and 1.

We standardize the notation for the spin positions: $\alpha \binom{1}{0}$ and $\beta \binom{0}{1}$ merge to $\binom{\alpha}{\beta}$. We check the proposition “the spin is $\binom{\alpha}{\beta}$” and “the spin is $\binom{\alpha}{\beta}$”, this should give $+1$ too. We test:

$$\binom{\alpha}{\beta} \cdot \binom{\alpha}{\beta} = \alpha \cdot \alpha + \beta \cdot \beta = \alpha^2 + \beta^2$$

As the result should be 1, we get a normalization condition: $\alpha^2 + \beta^2 = 1$.

Constantly writing terms like $\binom{1}{0}$ is cumbersome, therefore Dirac invented the symbol $|u\rangle$ for $\binom{1}{0}$ and $|d\rangle$ for $\binom{0}{1}$. He named this notation “ket”. Using kets instead of $\alpha \binom{1}{0}$ and $\beta \binom{0}{1}$ we can write more easily $\alpha|u\rangle + \beta|d\rangle$.

There will be a constant change between all possible notations, because for some problems special notation fits best.

Quantum propositions:

We take two composite propositions:

$$(1)\ the\ particle\ has\ position\ x\ \boldsymbol{and}\ momentum\ p$$

$$(2)\ the\ particle\ has\ position\ x\ \boldsymbol{or}\ momentum\ p$$

In classical logic both propositions are true.

In quantum mechanics proposition (1) cannot always be verified because measuring one component may destroy the other. It is not possible to always measure both simultaneously exact.

There seems to be a logical difference between classical and quantum concepts of the state of a system.

Pure states:

In a pure state the density matrix ρ corresponds to a single state, it is a projection operator that projects onto that state. A pure state represents the maximum amount of knowledge one can have of a quantum system.

A classical pure state is a special case of a probability density, in which the density matrix ρ has exactly one nonzero entry (on the diagonal).

Pure states, composite system and pure states:

We take a system composed of two parts, A and B, two spins or any other composite system. We suppose that Alice has complete knowledge of the state of the composed system, she knows the wave function $\psi(a, b)$.

We assume that Alice is not interested in B. Instead, she wishes to find out all about A without looking at B. She selects an observable (an operator) L that belongs to A, and does nothing to B when it acts.

She calculates the expectation value of L:

$$\langle L\rangle = \sum_{ab,a'b'} \psi^*(a'b')L_{a'b',ab}\psi(ab)$$

L belongs to A and acts trivially on the b-index ($b' = b$):

$$\langle L\rangle = \sum_{a,a',b} \psi^*(a'b)L_{a',a}\psi(ab) =$$

$$\sum_{a,a',b} L_{a',a}\psi(ab)\psi^*(a'b) =$$

Note: each summand is a (complex) number.

$$\sum_{a,a'} L_{a',a}\rho_{aa'}$$

with:

$$\rho_{aa'} = \sum_{b} \psi(ab)\psi^*(a'b)$$

Despite the fact that the composite system is described in a perfectly pure state, the subsystem A must be described by a mixed state.

Note: for a mixed or entangled state:

$$\rho^2 \neq \rho$$

$$Trace(\rho^2) < 1$$

Only in case of a product state ρ will have the form of a projection operator.

Note: for a product state:

$$\rho^2 = \rho$$

$$Trace(\rho^2) = Trace(\rho) = 1$$

Pure states, density matrices and pure states:

If the composite Alice-Bob system is in a product state, then Alice's or Bob's density matrix has one and only one eigenvalue equal to 1, and all the rest is zero. In this situation, both subsystems are in a pure state.

For pure states hold:

$$\rho^2 = \rho$$

meaning the matrix has a single entry "1" on the diagonal.

$$Trace(\rho^2) = 1$$

Quantization:

A well-known and well-trusted procedure to get the correct description for a free (one-dimensional) particle in terms of a quantum mechanical process is quantization.

1. Start with a classical system, use a set of coordinates x and momenta p.
   The coordinates and momenta come in pairs, x_i and p_i.
   The classical system also has a Hamiltonian, which is a function of all x_i and p_i.
2. Replace the classical phase space with a linear vector space. In the position representation, the space of states is represented by a wave function $\psi(x)$ that depends on the coordinates – in general, all of them.
3. Replace the x_i and p_i by the position operator X_i and the momentum operator P_i.
   Each X_i acts on the wave function by multiplying it with x_i.
   Each P_i acts on the wave function by differentiating to the coordinate i:
   $$P_i \to -i\hbar \frac{\partial}{\partial x_i}$$
4. The Hamiltonian becomes an operator that can be used in either the time-dependent or time-independent Schrödinger equation.
   The time-dependent equation tells us how the wave function changes with time.
   The time-independent form allows us to find the eigenvectors and eigenvalues of the Hamiltonian.

Note: Sometimes this procedure is successful, e.g. in fields ranging from the motion of particles to quantum electrodynamics.

Note: The spin of a particle has no real classical counterpart usable for this procedure.

Note: The quantization of general relativity has largely failed (date of this statement: 2020).

A paradigmatic example is the quantization of the harmonic oscillator.

Quantum abstractions:

Quantum abstractions are fundamentally different from classical ones.

The idea of a state in quantum mechanics is conceptually different from its classical counterpart.

States are represented by different mathematical objects and have a different logical structure.

States and measurements are two different things, and the relationship between them is subtle and nonintuitive.

Quantum field theory, path integrals and quantum field theory:

Feynman's path integral formulation is the principal tool for formulating the laws of elementary particle physics:

$$C_{1,2} = \int_{paths} e^{i\frac{A}{\hbar}}$$

Note: A is the action for the individual path. $C_{1,2}$ is the probability amplitude for a particle to transit from state 1 to state 2 and is the integral over all possible paths and their action A.

For reasons of completeness: The path integral formulation is a description in quantum mechanics that generalizes the action principle of classical mechanics. It replaces the classical notion of a single,

unique classical trajectory for a system with a sum, or functional integral, over an infinity of quantum-mechanically possible trajectories to compute a quantum amplitude. *(Courtesy Wikipedia)*

Quantum Hamiltonian:

$$H = \frac{P^2}{2m} + V(x)$$

P is the momentum operator:

$$P\psi = -i\hbar\frac{\partial\psi}{\partial x}$$

V is the operator of the potential energy:

$$V\psi = V(x)\psi(x)$$

We get the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(t)}{\partial x^2} + V(x)\psi$$

In terms of Energy:

$$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(t)}{\partial x^2} + V(x)\psi$$

Quantum mechanics:

Quantum mechanics as calculus of probabilities:

For practical reasons, we will adopt the following: Quantum mechanics is unavoidably unpredictable. Quantum mechanics is as complete a calculus of probabilities as is possible. The job of a physicist is to learn and use this calculus.

Classical mechanics vs. quantum mechanics:

Classical and quantum worlds have some important things in common. Quantum mechanics, however, is different in two ways:

1. Fundamentally different abstractions. The idea of a state in quantum mechanics is conceptually different from its classical counterpart. States are represented by different mathematical objects and have a different logical structure.
2. In the classical world one can perform an experiment to show the state of a system – the state of a system will not be altered by the experiment.
   In the quantum world, this is not true. States and measurements are two different things. Sometimes, measurements show the state of a system. Sometimes, measurements set the state of a system.

Conservation of energy and quantum mechanics:

For an observable (an operator) L:

$$\frac{d}{dt}L = -\frac{i}{\hbar}[L, H]$$

Note: $[L, H]$ is the commutator of the observable L with the Hamiltonian H.

Note: $[L, H] = LH - HL$

The Hamiltonian H is the energy of the system. The condition for the energy of the system to change:

$$\frac{d}{dt}H = -\frac{i}{\hbar}[H,H] = -\frac{i}{\hbar}(HH - HH) = 0$$

The energy of the system is conserved.

Fundamental theorem of quantum mechanics:

a) The eigenvectors of a Hermitian operator are a complete set.
   Any vector the operator can generate can be expanded as a sum of its eigenvectors.
b) If λ_1 and λ_2 are two unequal eigenvalues of a Hermitian operator, then the corresponding eigenvectors are orthogonal.
c) Even if two eigenvalues are equal, the corresponding eigenvectors can be chosen to be orthogonal.
   This situation is called degeneracy.

In toto: the eigenvectors of a Hermitian operator form an orthonormal basis.

For an explicit check of these conditions please see "*Eigenvectors of a Hermitian operator*".

Planck's constant and quantum mechanics:

Planck's constant h originally had a value of about $6.6 \times 10^{-34}\ \frac{kg \cdot m^2}{s}$. Usually it is used in form of $\hbar$:

$$\hbar \coloneqq \frac{h}{2\pi} = 1.054571726\ldots \times 10^{-34}\ \frac{kg \cdot m^2}{s}$$

As quantum mechanics is working with complex numbers and complex numbers are connected with sin and $cosin$, there often appears the value 2π. $\hbar$ prevents us from repeatedly writing 2π.

Max Karl Ernst Ludwig Planck, 1858 – 1947, was a German theoretical physicist whose discovery of energy quanta won him the Nobel Prize in Physics in 1918. Planck made many contributions to theoretical physics, but his fame as a physicist rests primarily on his role as the originator of quantum theory, which revolutionized human understanding of atomic and subatomic processes. *(Courtesy Wikipedia)*

Quantum mechanics, principles of quantum mechanics:

The principles of quantum mechanics all involve the idea of an observable, and they presuppose the existence of an underlying complex vector space whose vectors represent system states.

An observable could also be called a measurable. It is a thing that you can measure with a suitable apparatus.

- Principle 1: The observable or measurable quantities of quantum mechanics are represented by linear (Hermitian) operators L.
- Principle 2: The possible results of a measurement are the eigenvalues of the operator that represents the observable. We will call these eigenvalues λ_i. The state for which the result of a measurement is unambiguously λ_i is the corresponding eigenvector $|\lambda_i\rangle$.
  Results of a measurements is always a real number.
- Principle 3: Unambiguously distinguishable states are represented by orthogonal vectors.
- Principle 4: If $|A\rangle$ is the state-vector of a system, and the observable L is measured, the probability to observe the value λ_i is:
  $$P(\lambda_i) = |\langle A|\lambda_i\rangle|^2 = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$
- Principle 5: The evolution of state-vectors with time is unitary.

Principle one: observables are the "real" things, results of measurements. Operators are their theoretical counterpart, needed to compute probabilities for results of measurements.

Principle two defines the relation between the operator representing an observable and the possible numerical results of a measurement. The result of a measurement is always one of the eigenvalues of the corresponding operator.

Principle three requires physically distinct states to be represented by orthogonal state-vectors. Two states are physically distinct if there is a measurement that can tell them apart without ambiguity. The spin directions up and $down$ are an example. But you cannot unambiguously distinguish between the spin directions up and $left$. The inner product of two states is a measure of the inability to distinguish between them. Sometimes the inner product is called overlap – overlap zero means physically distinct states.

Principle four quantifies the results of possible measurements. If we assume that a system has been prepared in state $|A\rangle$, and subsequently measure the observable L, then the outcome will be one of the eigenvalues λ_i of the operator L:

$$P(\lambda_i) = |\langle A|\lambda_i\rangle|^2 = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle$$

Note: $|\lambda_i\rangle$ is eigenvector, λ_i eigenvalue. $P(\lambda_i)$ is the probability for outcome λ_i.

Principle five follows from the "minus first law", the conservation of distinctions. Distinguishable states are orthogonal to each other. Suppose that $|\psi(0)\rangle$ and $|\phi(0)\rangle$ are two distinguishable states. Therefore, they must have an orthogonal representation (no overlap):

$$\langle\psi(0)|\phi(0)\rangle = 0$$

The minus first law requires this to be true for all times:

$$\langle\psi(t)|\phi(t)\rangle = 0$$

We have a time-development operator $U(t)$.

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

$$\langle\psi(t)| = \langle\psi(0)|U^\dagger(t)$$

Note: $U^\dagger(t)$ is the Hermitian conjugated of $U(t)$.

$$|\phi(t)\rangle = U(t)|\phi(0)\rangle$$

We modify $\langle\psi(t)|\phi(t)\rangle = 0$ by the time-development operator:

$$\langle\psi(t)|\phi(t)\rangle = \langle\psi(0)|U^\dagger(t)U(t)|\phi(0)\rangle = 0$$

This requests $U^\dagger(t)U(t)$ to be the identity matrix (operator). An operator with this property is called unitary.

Quantum mechanics, 3-vector operators and quantum mechanics:

The spin operator σ is neither a state-vector (a bra or a ket) nor a spatial 3-vector. It has resemblance to a 3-vector because it is associated with a direction in space.

The spin operator σ is frequently used as though it were a simple 3-vector and is called a 3-vector operator.

There is a spin operator for each direction in which an apparatus measuring spin can be oriented.

The operator σ consist of the three components σ_x, σ_y and σ_z with the associated state-vectors $|left\rangle$ and $|right\rangle$ for σ_x,
$|in\rangle$ and $|out\rangle$ for σ_y
and
$|up\rangle$ and $|down\rangle$ for σ_z.

The components of the spin operator σ are represented by the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Note: i is the imaginary unit.

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Behaving like a 3-vector, the component of σ along any direction $\vec{n}$ is the dot-product of σ and $\vec{n}$:

$$\sigma_n = \vec{\sigma} \cdot \vec{n} = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z$$

Written in terms of the Pauli matrices this gives:

$$\sigma_n = n_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + n_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + n_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can combine this to a single matrix:

$$\sigma_n = \begin{pmatrix} n_z & (n_x - in_y) \\ (n_x + in_y) & -n_z \end{pmatrix}$$

If we find the eigenvectors and eigenvalues of σ_n, we will know the possible outcomes of a measurement along the direction of $\vec{n}$ with the corresponding probabilities. We have a complete picture of spin measurement in the three-dimensional space.

Quantum mechanics, measurement and operators:

- Operators are the things we use to calculate eigenvalues and eigenvectors.
- Operators act on state-vectors, not on actual physical systems
- On operator acting on a state-vector produces a new state vector

There is a difference between “measuring an observable” and “operating with the corresponding operator on the state”.

Suppose we are interested in measuring an observable L. The state of the system before we do the measurement is $|A\rangle$. It is not correct to say that the measurement of L always changes the state to $l|A\rangle$ with l being a number.

We show this with an example.

We prepare the state $|r\rangle$ which is not eigenvector of σ_z. We can express the state $|r\rangle$ in terms of $|u\rangle$ and $|d\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

Acting on this state vector with σ_z:

$$\sigma_z|r\rangle = \frac{1}{\sqrt{2}}\sigma_z|u\rangle + \frac{1}{\sqrt{2}}\sigma_z|d\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

The measurement result would be either $+1$, leaving the system in state $|u\rangle$, or -1, leaving the system in state $|d\rangle$ – one of them.

The state after acting with the operator is a superposition of both states $|u\rangle$ and $|d\rangle$.

Quantum mechanics, spin operators:

The spin operator σ is not a state-vector (bra or ket). It is not exactly a spatial 3-vector either, but it has a strong resemblance because it is associated with a direction in space.

We call it a 3-vector-operator.

A spin operator can only provide information about the spin component in a specific direction. To determine the direction of a spin we need a spin operator for each axis in space.

Quantum mechanics, spin operators, constructing spin operators:

The spin operators represent the components of a spin, σ_x, σ_y and σ_z.

The component $\boldsymbol{\sigma_z}$

We begin with σ_z that has definite, unambiguous values for the states up and $down$, $|u\rangle$ and $|d\rangle$:

$$|u\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

$$|d\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

Note: these are the state vectors, not the orientation of spin in space.

Measurements will give $\sigma_z = \pm 1$.

We have three principles:

- Principle 1:
  Each component of σ is represented by a linear operator.
- Principle 2:
  The eigenvectors of σ_z are $|u\rangle$ and $|d\rangle$. The corresponding eigenvalues are $+1$ and -1. We express this with the equations:
  $$\sigma_z|u\rangle = |u\rangle$$
  $$\sigma_z|d\rangle = -|d\rangle$$
- Principle 3:
  States $|u\rangle$ and $|d\rangle$ are orthogonal to each other:
  $$\langle u|d\rangle = 0$$

From principle 2 we calculate the matrix representation of σ_z:

$$\sigma_z = \begin{pmatrix}(\sigma_z)_{11} & (\sigma_z)_{12}\\(\sigma_z)_{21} & (\sigma_z)_{22}\end{pmatrix}$$

$$\begin{pmatrix}(\sigma_z)_{11} & (\sigma_z)_{12}\\ (\sigma_z)_{21} & (\sigma_z)_{22}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}$$

$$\begin{pmatrix}(\sigma_z)_{11} & (\sigma_z)_{12}\\ (\sigma_z)_{21} & (\sigma_z)_{22}\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = -\begin{pmatrix}0\\1\end{pmatrix}$$

This gives the values for σ_z:

$$\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

We repeat this for the other two components of spin, σ_x, and σ_y.

The component $\boldsymbol{\sigma_x}$

The state vectors $right$, $|r\rangle$ and $left$, $|l\rangle$ expressed in terms of state vectors $|u\rangle$ and $|d\rangle$:

$$|r\rangle \coloneqq \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

$$|r\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$$|l\rangle \coloneqq \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

$$|l\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} - \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

Note: any spin state can be represented as a combination of the basis vectors $|u\rangle$ and $|d\rangle$.

We check whether those two vectors are orthogonal:

$$\langle r|l\rangle = \frac{1}{\sqrt{2}}(1\ 1)\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{2}(1\ 1)\cdot\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{2}\big(1\cdot 1 + 1\cdot(-1)\big) = 0$$

Note: the bra $\langle r|$ to the ket $|r\rangle$ is the complex conjugated, but as $|r\rangle$ is real it follows $\langle r^*|$ = $\langle r|$.

The matrix representation of σ_x:

$$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

We check the eigenvector property:

$$\langle\sigma_x|r\rangle = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 + 1\cdot 1\\ 1\cdot 1 + 0\cdot 1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$|r\rangle$ is eigenvector to the operator σ_x with eigenvalue 1.

$$\langle\sigma_x|l\rangle = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\cdot 1 + 1\cdot(-1)\\ 1\cdot 1 + 0\cdot(-1)\end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

$|l\rangle$ is eigenvector to the operator σ_x with eigenvalue -1.

The component σ_y

The state vectors in, $|i\rangle$ and out, $|o\rangle$ expressed in terms of state vectors $|u\rangle$ and $|d\rangle$:

$$|i\rangle \coloneqq \frac{1}{\sqrt{2}}\binom{1}{0} + \frac{i}{\sqrt{2}}\binom{0}{1} = \frac{1}{\sqrt{2}}\binom{1}{i}$$

$$|o\rangle \coloneqq \frac{1}{\sqrt{2}}\binom{1}{0} - \frac{i}{\sqrt{2}}\binom{0}{1} = \frac{1}{\sqrt{2}}\binom{1}{-i}$$

Note: any spin state can be represented as a combination of the basis vectors $|u\rangle$ and $|d\rangle$.

Both vectors are orthogonal to each other:

$$\langle i|o\rangle = \frac{1}{\sqrt{2}}(1\ (-i)) \cdot \frac{1}{\sqrt{2}}\binom{1}{-i} = \frac{1}{2}(1\ (-i)) \cdot \binom{1}{-i} =$$

$$\frac{1}{2}\big(1 \cdot 1 + (-i) \cdot (-i)\big) = \frac{1}{2}(1 + i^2) = 0$$

Note: the bra $\langle i|$ to the ket $|i\rangle$ is the complex conjugated.

The matrix representation of σ_y:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

We check the eigenvector property:

$$\langle \sigma_y|i\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\binom{1}{i} = \frac{1}{\sqrt{2}}\binom{0 \cdot 1 - i^2}{i \cdot 1 + 0 \cdot i} = \frac{1}{\sqrt{2}}\binom{1}{i}$$

$|i\rangle$ is eigenvector to the operator σ_y with eigenvalue 1.

$$\langle \sigma_y|o\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\binom{1}{-i} = \frac{1}{\sqrt{2}}\binom{0 \cdot 1 + i^2}{i \cdot 1 + 0 \cdot (-i)} = -\frac{1}{\sqrt{2}}\binom{1}{-i}$$

$|o\rangle$ is eigenvector to the operator σ_y with eigenvalue -1.

Conclusion

The matrix representations of the spin operators σ_x, σ_y and σ_z:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note: these are the Pauli matrices.

The representation of the state vectors in the $up - down$ system:

$$|u\rangle = \binom{1}{0}, \qquad |d\rangle = \binom{0}{1}$$

$$|r\rangle = \frac{1}{\sqrt{2}}\binom{1}{1}, \qquad |l\rangle = \frac{1}{\sqrt{2}}\binom{1}{-1}$$

$$|i\rangle = \frac{1}{\sqrt{2}}\binom{1}{i}, \qquad |o\rangle = \frac{1}{\sqrt{2}}\binom{1}{-i}$$

Quantum mechanics, spin-polarization principle:

Any state of a single spin is an eigenvector of some component of the spin.

Given a state $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$, there exists some direction $\hat{n}$, such that:

$$\vec{\sigma} \cdot \vec{n}|A\rangle = |A\rangle$$

This means that for any spin state, there is some orientation of the measurement apparatus that it will constantly register $+1$ when measuring the spin.

In physics language we say that the states of the spin are characterized by a polarization vector. Along that polarization vector the component of the spin is predictably $+1$.

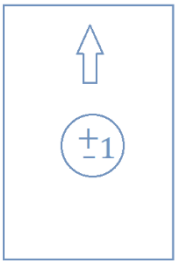
Note: for any state of a single spin system, the expectation values of all three components of σ sum to 1:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$$

Quantum simulation:

Imagine a computer game representing an entangled two-spin system for Alice and Bob on two terminals connected to a single computer. In its memory is stored the state-vector of the combined system, four complex numbers $\alpha_{uu}, \alpha_{ud}, \alpha_{du}, \alpha_{dd}$. The computer updates these numbers using the Schrödinger equation.

Each terminal shows a single spin of this two-spin system and an apparatus that can be used to measure the orientation of this single spin.



We assume that the terminals can access the central computer instantaneously but only to update the state-vector. No information exchange between Alice and Bob is possible.

This device can simulate the quantum mechanics of the two-spin system, as long as the connection of the terminals is online and works instantaneously.

As long as Alice and Bob cannot use it to instantaneously exchange other information, no locality-violating information exchange between them takes place.

Quantum spins:

1.

The isolated quantum spin is an example of the general class of simple systems we call qubits – quantum bits – that play the same role in the quantum world as logical bits play in defining the state of your computer.

2.

Measuring a spin in whatever direction gives the result $+1$ or -1. There is no more to know, or that can be known.

3.

Quantum spins can be simulated by classical computers.

Quantum states:

Along the x-axis and along the y-axis:

Prerequisite

We choose vectors $|u\rangle$ for up and $|d\rangle$ for $down$ as the two basis vectors along the z-axis and write any state as linear superposition of these two:

$$|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$$

$|A\rangle$ needs to be normalized:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

We name the vectors $|r\rangle$ for $right$, $|l\rangle$ for $left$ on the x-axis and $|i\rangle$ for in, $|o\rangle$ for out on the y-axis.

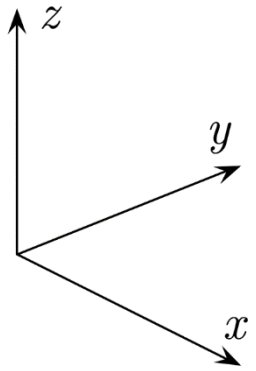
End prerequisite

Any spin state can be represented as a linear combination of the basis vectors $|u\rangle$ and $|d\rangle$.

If we prepare a spin along the x-axis and then measure in z-direction, there will be equal probabilities for up and $down$.

A vector $|r\rangle$ satisfying this rule:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$



We use that both vectors must be orthogonal:

$$\langle r|l\rangle = \langle l|r\rangle = 0$$

We get the vector $|l\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

With similar reasoning and evaluating more conditions, we get the vectors $|i\rangle$ and $|o\rangle$:

$$|i\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle$$

Note: i is the imaginary unit.

Note: all possible orientations are expressed in terms of up and $down$, the basis vectors in z-direction.

Quantum states, counting parameters:

The general spin state is defined by two complex numbers, α_u and α_d. This gives four real parameters.

The normalization condition: $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$ reduces the number of variables to three.

The physical properties of a state-vector do not depend on the overall phase-factor, this reduces the number of variables to two.

This is the same number of parameters to define a direction in a 3-dimensional space – two angles are needed.

Quantum states, incompleteness of quantum states:

We would not raise the question about hidden parameters. Quantum mechanics is a complete calculus of probabilities, and we use it.

Quantum states, representing spin states as column vectors:

We have the basis kets $|u\rangle$ and $|d\rangle$.

They are orthogonal:

$$\langle u|d\rangle = 0$$

We represent them as column vectors:

$$|u\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

$$|d\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

Note: as all spin directions can be expressed with kets $|u\rangle$ and $|d\rangle$, we can represent all spin states with these two vectors.

Quantum states, spin states:

Prerequisite

We have an apparatus $\mathcal{A}$ to measure the direction of a spin.

Note: measuring a spin means prepare the spin in this direction.

We can orient $\mathcal{A}$ into every possible direction in space.

If we express a state-vector A in a basis

$$|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$$

then the corresponding state-vector needs complex conjugated coefficients:

$$\langle A| = \langle u|\alpha_u^* + \langle d|\alpha_d^*$$

End prerequisite

If $\mathcal{A}$ is oriented along the z-axis, the two possible states that can be prepared correspond to $\sigma_z = \pm 1$. We call them up and $down$ and denote them by kets $|u\rangle$ and $|d\rangle$.

The space of states for a single spin has only two dimension.

We can write any state A:

$$|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$$

Mathematically, we can identify the components of $|A\rangle$ by the inner product:

$$\alpha_u = \langle u|A\rangle$$

$$\alpha_d = \langle d|A\rangle$$

The quantity $\alpha_u^*\alpha_u$ is the probability to measure $\sigma_z = 1$, $\alpha_d^*\alpha_d$ is the probability to measure $\sigma_z = -1$.

The values α_u and α_d itself are probability amplitudes.

The kets $|u\rangle$ and $|d\rangle$ are mutually orthogonal:

$$\langle u|d\rangle = \langle d|u\rangle = 0$$

Two orthogonal states are physically distinct and mutually exclusive. If the spin is in one of these states, it cannot be in the other one. This idea applies to all quantum systems.

Note: do not mistake the orthogonality of state-vectors for orthogonal directions in space. The directions up and $down$ are not orthogonal in space (they are antiparallel), their associated state-vectors are.

The normalization requirement:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

This means that the state-vector $|A\rangle$ is normalized:

$$\langle A|A\rangle = (\langle u|\alpha_u^* + \langle d|\alpha_d^*)(\alpha_u|u\rangle + \alpha_d|d\rangle) =$$

$$\langle u|\alpha_u^*\alpha_u|u\rangle + \langle u|\alpha_u^*\alpha_d|d\rangle + \langle d|\alpha_d^*\alpha_u|u\rangle + \langle d|\alpha_d^*\alpha_d|d\rangle =$$

$$\alpha_u^*\alpha_u\langle u|u\rangle + \alpha_u^*\alpha_d\langle u|d\rangle + \alpha_d^*\alpha_u\langle d|u\rangle + \alpha_d^*\alpha_d\langle d|d\rangle =$$

$$\alpha_u^*\alpha_u \cdot 1 + \alpha_u^*\alpha_d \cdot 0 + \alpha_d^*\alpha_u \cdot 0 + \alpha_d^*\alpha_d \cdot 1 =$$

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

This is a general principle of quantum mechanics: the state of a system is represented by a unit (normalized) vector in a vector space of states.

The squared magnitudes of the components of the state-vector (along particular basis vectors) represent the probabilities for experimental outcomes.

Quantum systems, combining quantum systems:

We have a composite system of two spins of Alice and Bob with the notation $|u\rangle$ … for both Alice's and Bob's system.

The notation $|uu\rangle$ … labels a single basis vector of the combined system, labeling the case that the spin of Alice is up and the spin of Bob is up etc.

Let M be a linear operator (a matrix) acting on the space of states of the composite system. As usual the matrix elements are constructed by sandwiching the operator between basis vectors:

$$\langle a'b'|M|ab\rangle = M_{a'b',ab}$$

The vectors $|ab\rangle$ build an orthonormal basis:

$$\langle ab|a'b'\rangle = \delta_{aa'}\delta_{bb'}$$

Note: this are two Kronecker deltas.

Any state in the composite system can be expanded as:

$$|\psi\rangle = \sum_{a,b} \psi(a,b)|ab\rangle$$

We make this explicit.

The basis vector for the $|u\rangle$ state of each Alice and Bob is $\binom{1}{0}$, equivalently the basis vector for the $|d\rangle$ state is $\binom{0}{1}$.

We combine by help of the tensor product.

$$|uu\rangle = |u\rangle \otimes |u\rangle =$$

$$\binom{1}{0} \otimes \binom{1}{0} =$$

$$\begin{pmatrix} 1\binom{1}{0} \\ 0\binom{1}{0} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

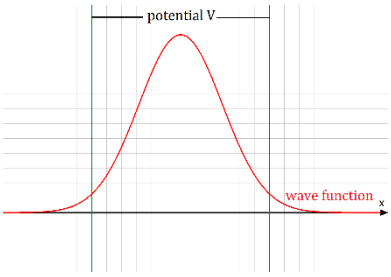
The basis vectors for the states $|uu\rangle, |ud\rangle, |du\rangle$ and $|dd\rangle$ are $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Obviously, the operator (the matrix) M must be a 4×4 matrix.

Combining quantum systems by help of the tensor product will give a product state meaning that both states of Alice and Bob can be treated as independent states, they are not entangled.

Quantum tunneling:

Consider the case that a wave function describes the position of a wave packet (a particle) within a potential.



Quantum mechanics only gives the probability for the position (with an average and an uncertainty).

There is a chance that the particle can be found outside of the potential, regardless how “high the walls” are.

This effect is called quantum tunneling and is completely unknown in classical physics.

Qubits:

The isolated quantum spin is an example of the general class of simple systems we call qubits.

They play the same role in the quantum world as logical bits play in the state of a computer.

Raising operator (creation operator):

The Hamiltonian can be expressed in terms of the operators P and X:

$$H = \frac{1}{2}(P^2 + \omega^2 X^2) = \frac{1}{2}(P + i\omega X)(P - i\omega X) + \frac{i\omega}{2}$$

Note: $\frac{i\omega}{2}$ is needed because P and X do not commute.

$(P + i\omega X)$ is called the raising operator, $(P - i\omega X)$ the lowering operator, written as a^+ and a^-.

The raising operator a^+ shifts the energy level of the harmonic oscillator to the next possible higher level, the lowering operator a^- to the next possible lower level.

Applying the lowering operator to the ground level with Energy $E_0 = \frac{\omega\hbar}{2}$ annihilates this ground level. Symbolically this is expressed as

$$a^-|0\rangle = 0$$

with $|0\rangle$ representing the ground level and 0 representing the number zero.

Real numbers, quantum mechanics and real numbers:

Real numbers play a special role in physics. The results of any measurements are real numbers.

We can put it in other words: observable quantities are equal to their own complex conjugates.

Quantum mechanical observables are represented by Hermitian operators. Hermitian operators are equal to their own transposed and complex conjugated:

$$H = H^\dagger$$

The connection is made by the fact that the eigenvectors of Hermitian operators (matrices) have real eigenvalues only.

We show this.

Let L be a Hermitian operator, $|\lambda\rangle$ an eigenvector with eigenvalue λ:

$$L|\lambda\rangle = \lambda|\lambda\rangle$$

Switching from the ket $L|\lambda\rangle$ to the bra needs Hermitian conjugation of the matrix (operator):

$$L|\lambda\rangle \leftrightarrow \langle\lambda|L^\dagger$$

The eigenvector relations remains valid but gives the complex conjugated eigenvalue:

$$\langle\lambda|L^\dagger = \langle\lambda|\lambda^*$$

For Hermitian operators holds:

$$L = L^\dagger$$

We combine this and get:

$$L|\lambda\rangle = \lambda|\lambda\rangle$$

$$\langle\lambda|L^\dagger = \langle\lambda|\lambda^*$$

We multiply the first one by $\langle\lambda|$ and the second one by $|\lambda\rangle$ and use $L = L^\dagger$:

$$\langle\lambda|L|\lambda\rangle = \langle\lambda|\lambda|\lambda\rangle = \lambda\langle\lambda|\lambda\rangle$$

$$\langle\lambda|L|\lambda\rangle = \langle\lambda|\lambda^*|\lambda\rangle = \lambda^*\langle\lambda|\lambda\rangle$$

We get:

$$\lambda^* = \lambda$$

For both equations to be true, λ must be a real value.

Reversibility:

Things are changing with time. Reversibility means that change can not only be described in the direction of future but also in the direction of past. An actual state has a predecessor and a follower. A good law describes both.

The quantum mechanical version of this is the minus first law: information is never lost. If two identical systems start out in different states, they stay in different states and they were in different states. The quantum version of this is called unitarity.

Row vectors, bras and row vectors:

Let z be a complex number, $|A\rangle$ any ket. The corresponding term to the product of z with $|A\rangle$:

$$z|A\rangle \leftrightarrow \langle A|z^*$$

Note: there is an implicit complex conjugation in switching from a ket $|A\rangle$ to its correspondent bra $\langle A|$ that might give some confusion in the beginning.

Let $|A\rangle$ be the column vector $\begin{pmatrix}\alpha_1\\ \vdots \\ \alpha_n\end{pmatrix}$, then the corresponding bra $\langle A|$ is $(\alpha_1^*, \dots, \alpha_n^*)$.

Schrödinger, Erwin:

Erwin Rudolf Josef Alexander Schrödinger 1887 – 1961 was a Nobel Prize-winning Austrian-Irish physicist who developed a number of fundamental results in quantum theory: the Schrödinger equation provides a way to calculate the wave function of a system and how it changes dynamically in time. *(Courtesy Wikipedia)*

There are (at least) two ways of thinking about quantum mechanics that go back to Heisenberg and Schrödinger. Heisenberg liked algebra, matrices, and, had he known what to call them, linear operators. Schrödinger thought in terms of wave functions and wave equations.

The two ways are not contradictory. Functions form a vector space and derivatives are operators.

Schrödinger equations:

The generalized or time-dependent Schrödinger equation:

$$\frac{\partial|\psi\rangle}{\partial t} = -iH|\psi\rangle$$

The time dependent Schrödinger equation describes the time-development of the state-vector. The essential ingredient is the Hamiltonian H, which in both classical and quantum mechanics represents the total energy of a system.

In the case of a nonrelativistic free particle we need a dimensional correction and get:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

Because the Hamiltonian of a nonrelativistic free particle is independent of the position, the Hamiltonian consists only of the momentum operator P:

$$H = \frac{P^2}{2m}$$
$$P = -i\hbar\frac{\partial}{\partial x}$$

and we get:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

This is the traditional Schrödinger equation for an ordinary nonrelativistic free particle.

Schrödinger, path integrals and Schrödinger equations:

In quantum field theory, the path integral formulation is the principal tool for formulating the laws of elementary particle physics. The Schrödinger equations and all the commutation relations of quantum mechanics can be derived from it.

Schrödinger, solving Schrödinger equations:

The time-dependent Schrödinger equation tells us how the state-vector of an undisturbed system changes with time:

$$\hbar\frac{\partial|\psi\rangle}{\partial t} = -iH|\psi\rangle$$

The time-independent Schrödinger equation, written with the Hamiltonian in ket-style is the eigenvalue equation:

$$H|E_j\rangle = E_j|E_j\rangle$$

Note: $|E_j\rangle$ is eigenvector, E_j eigenvalue of the operator H.

Let us suppose we have found all energy eigenvalues E_j and the corresponding eigenvectors $|E_j\rangle$. We use that information to solve the time-dependent Schrödinger equation by the fact that eigenvectors form an orthonormal basis. We expand the state-vector $|\psi\rangle$ in that basis:

$$|\psi(t)\rangle = \sum_j \alpha_j |E_j\rangle$$

Since the state-vector $|\psi\rangle$ changes with time and the basis vectors $|E_j\rangle$ do not, it follows that the coefficients α_j must depend on time:

$$\frac{\partial}{\partial t}|\psi(t)\rangle = \sum_j \dot{\alpha}_j(t)|E_j\rangle$$

We feed this back into the time-dependent Schrödinger equation $\hbar \frac{\partial|\psi\rangle}{\partial t} = -iH|\psi\rangle$ and get:

$$\hbar \sum_j \dot{\alpha}_j(t)|E_j\rangle = -iH|\psi\rangle$$

$$\sum_j \dot{\alpha}_j(t)|E_j\rangle = -\frac{i}{\hbar}H|\psi\rangle$$

$$\sum_j \dot{\alpha}_j(t)|E_j\rangle = -\frac{i}{\hbar}H\sum_j \alpha_j(t)|E_j\rangle$$

With $H|E_j\rangle = E_j|E_j\rangle$ we build the final result:

$$\sum_j \dot{\alpha}_j(t)|E_j\rangle = -\frac{i}{\hbar}\sum_j E_j\alpha_j(t)|E_j\rangle$$

The eigenvectors form an orthonormal basis therefore the equation must be valid for every coefficient:

$$\dot{\alpha}_j(t)|E_j\rangle = -\frac{i}{\hbar}E_j\alpha_j(t)|E_j\rangle$$

$$\left(\dot{\alpha}_j(t) + \frac{i}{\hbar}E_j\alpha_j(t)\right)|E_j\rangle = 0$$

$$\dot{\alpha}_j(t) + \frac{i}{\hbar}E_j\alpha_j(t) = 0$$

For each eigenvalue E_j we have the differential equation:

$$\dot{\alpha}_j(t) = -\frac{i}{\hbar}E_j\alpha_j(t)$$

The solution is:

$$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$$

We see that the real part is oscillating with the $\cos(-\frac{E_j}{\hbar}t)$. Oscillating frequency and energy are connected throughout quantum mechanics.

The factors $\alpha_j(0)$ are the values of the coefficients at time zero – the projections of the state-vector $|\psi\rangle$ at time zero on the eigenvectors:

$$\alpha_j(0) = \langle E_j|\psi(0)\rangle$$

We write the full solution of the time-dependent Schrödinger equation:

$$\psi(t) = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}|E_j\rangle =$$

$$\sum_j \langle E_j|\psi(0)\rangle e^{-\frac{i}{\hbar}E_j t}|E_j\rangle =$$

$$\sum_j |E_j\rangle\langle E_j|\psi(0)\rangle e^{-\frac{i}{\hbar}E_j t}$$

Note: $\langle E_j|\psi(0)\rangle$ is a (complex) number.

What we have is a description of a (time changing) state vector in terms of the energy basis vectors.

Schrödinger equations for time derivatives:

Suppose the state of a system at time t is represented by ket $|\psi\rangle$ and bra $\langle\psi|$.

The expectation value of the observable (the operator) L at time t:

$$\langle\psi(t)|L|\psi(t)\rangle$$

The expectation value changes with time:

$$\frac{d}{dt}\langle\psi(t)|L|\psi(t)\rangle = \langle\dot{\psi}(t)|L|\psi(t)\rangle + \langle\psi(t)|L|\dot{\psi}(t)\rangle$$

The Schrödinger equation in terms of kets and bras:

$$|\dot{\psi}\rangle = -\frac{i}{\hbar}H|\psi\rangle$$

and

$$\langle\dot{\psi}| = \frac{i}{\hbar}\langle\psi|H$$

We insert the Schrödinger equation in the time change of the expectation value:

$$\frac{d}{dt}\langle L\rangle = \frac{d}{dt}\langle\psi(t)|L|\psi(t)\rangle =$$

$$\frac{i}{\hbar}\langle\psi(t)H|L|\psi(t)\rangle - \frac{i}{\hbar}\langle\psi(t)|L|H\psi(t)\rangle =$$

$$\frac{i}{\hbar}\langle\psi(t)|HL|\psi(t)\rangle - \frac{i}{\hbar}\langle\psi(t)|LH|\psi(t)\rangle =$$

$$\frac{i}{\hbar}\langle\psi(t)|HL - LH|\psi(t)\rangle =$$

$$\frac{i}{\hbar}\langle\psi(t)|[H,L]|\psi(t)\rangle = \frac{i}{\hbar}\langle[H,L]\rangle$$

Note: $[H,L]$ is the commutator of the two operators H and L.

What we get is: the time change of the expectation value of the operator L is proportional to the expectation value of the commutator of this operator with the Hamiltonian:

$$\frac{d}{dt}\langle L\rangle = \frac{i}{\hbar}\langle[H,L]\rangle$$

Note: $[H,L] = -[L,H]$. With this we can write:

$$\frac{d}{dt}\langle L\rangle = -\frac{i}{\hbar}\langle[L,H]\rangle$$

Schrödinger ket:

1. Derive, look up, guess, borrow or steal the Hamiltonian operator H for the system.
2. Prepare an initial state $|\psi(0)\rangle$.
3. Find the eigenvalues and eigenvectors of H by solving the time-independent Schrödinger equation:

   $$H|E_j\rangle = E_j|E_j\rangle$$

   You will get:

   $$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$$

   Note 1: "E_j" is eigenvalue to the eigenvector $|E_j\rangle$.

   Note 2: $H|E_j\rangle = E_j|E_j\rangle$ leads to a differential equation that determines $\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}$.

4. Calculate the initial coefficients $\alpha_j(0) = \langle E_j|\psi(0)\rangle$.
5. Rewrite $|\psi(0)\rangle$ in terms of eigenvectors $|E_j\rangle$ and initial coefficients $\alpha_j(0)$:

   $$|\psi(0)\rangle = \sum_j \alpha_j(0)\,|E_j\rangle$$

6. Replace each $\alpha_j(0)$ with $\alpha_j(t)$ to capture its time-dependence. As the basis vectors $|E_j\rangle$ do not change, this leads to:

   $$|\psi(t)\rangle = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}\,|E_j\rangle$$

Sets, Boolean logic and sets:

Boolean logic is a formalized version of the classical logic of propositions – a logic that works with 1 and 0 resp. true and false.

A proposition can be true or false. Mathematical propositions can be equations like $2 + 3 = 5$. An equation like $2 \cdot x + 3 = 7$ is not a proposition but a propositional expression that becomes true or false depending on what you insert for the variable x.

If you concatenate propositions with "and" resp. the "or", the result follows rules. We must carefully distinguish between the $inclusive\ or$ we normally use when speaking and the $exclusive\ or$. The $exclusive\ or$ in formal logic is written as XOR.

Let A and B be propositions, then the truth values ($A\ or\ B$) are:

A	B	$A\ or\ B$
0	0	0
0	1	1
1	0	1
1	1	1

The truth values for ($A\ and\ B$):

A	B	$A\ and\ B$
0	0	0
0	1	0
1	0	0
1	1	1

Sometimes the logical connections are referred to as $+$ and $\cdot$:

A	B	$A+B$
0	0	0
0	1	1
1	0	1
1	1	1

Note that 1+1 gives 1 because "double true remains true".

A	B	$A\cdot B$
0	0	0
0	1	0
1	0	0
1	1	1

… perfect …

There is a special logical operator, the not ($\neg$) that simply switches the truth value to its opposite:

A	$\neg A$
0	1
1	0

Logical connections can be represented as intersections and combinations of sets, e.g. by a Venn diagram.

Simultaneous eigenvectors:

We have a two-spin system and measure with two different operators L and M.

If we measure both spins, the system winds up in a state that is simultaneously eigenvector of L and eigenvector of M.

L has eigenvectors $|\lambda_i\rangle$ with eigenvalues λ_i, M has eigenvectors $|\mu_a\rangle$ with eigenvalues μ_a.

We assume that there is a basis of state-vectors $|\lambda_i, \mu_a\rangle$ that are simultaneous eigenvectors of both observables: $L|\lambda_i, \mu_a\rangle = \lambda_i|\lambda_i, \mu_a\rangle$ and $M|\lambda_i, \mu_a\rangle = \mu_a|\lambda_i, \mu_a\rangle$.

Omitting the subscripts for better readability, we write

$$L|\lambda,\mu\rangle = \lambda|\lambda,\mu\rangle$$

$$M|\lambda,\mu\rangle = \mu|\lambda,\mu\rangle$$

In order to have a basis of simultaneous eigenvectors, the operators (the matrices) L and M must commute.

We apply both operators to any of the basis vectors:

$$LM|\lambda,\mu\rangle = L\mu|\lambda,\mu\rangle = \lambda\mu|\lambda,\mu\rangle$$

$$ML|\lambda,\mu\rangle = M\lambda|\lambda,\mu\rangle = \mu\lambda|\lambda,\mu\rangle$$

μ and λ are numbers that can be swapped:

$$LM|\lambda,\mu\rangle = ML|\lambda,\mu\rangle$$

$$(LM - ML)|\lambda,\mu\rangle = [L,M]|\lambda,\mu\rangle = 0$$

Because this is valid for all basis vectors:

$$[L,M] = 0$$

If an operator annihilates every basis vector, it annihilates every vector in that space – it is a zero operator.

Singlet state:

We have a system of two spins, σ and τ:

$$\vec{\sigma}\cdot\vec{\tau} = \sigma_x\tau_x + \sigma_y\tau_y + \sigma_z\tau_z$$

The most general vector in the composite space of states:

$$\psi_{uu}|uu\rangle + \psi_{ud}|ud\rangle + \psi_{du}|du\rangle + \psi_{dd}|dd\rangle$$

The $singlet$ state is a maximally entangled state:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

The singlet state is eigenvector of $\sigma\cdot\tau$:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

We apply $\vec{\sigma}\cdot\vec{\tau}$ to $|sing\rangle$:

$$\sigma_x\tau_x|sing\rangle = \sigma_x\tau_x\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle) = \sigma_x\frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle) = \frac{1}{\sqrt{2}}(|du\rangle - |ud\rangle) = -|sing\rangle$$

$$\sigma_y\tau_y|sing\rangle = \sigma_y\tau_y\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle) = \sigma_y\frac{1}{\sqrt{2}}(-i|uu\rangle - i|dd\rangle) = \frac{1}{\sqrt{2}}(|du\rangle - |ud\rangle) = -|sing\rangle$$

$$\sigma_z\tau_z|sing\rangle = \sigma_z\tau_z\frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle) = \sigma_z\frac{1}{\sqrt{2}}(-|ud\rangle - |du\rangle) = \frac{1}{\sqrt{2}}(-|ud\rangle + |du\rangle) = -|sing\rangle$$

We get:

$$\vec{\sigma} \cdot \vec{\tau}|sing\rangle = -3|sing\rangle$$

$|sing\rangle$ is eigenvector of $\vec{\sigma} \cdot \vec{\tau}$ with eigenvalue -3.

Singlet state, correlation:

The correlation between the two systems is -1:

$$\langle \sigma_z \tau_z \rangle - \langle \sigma_z \rangle \langle \tau_z \rangle = -1$$

Singlet state, density matrix:

For the composite system:

$$\rho^2 = \rho$$

$$Trace(\rho^2) = 1$$

For each subsystem (Alice and Bob): the density matrix is proportional to the unit matrix, having equal eigenvalues that add up to 1.

For the subsystems:

$$\rho^2 \neq \rho$$

$$Trace(\rho^2) < 1$$

Singlet state, description of singlet state:

The composite system as a whole is fully characterized. There is no information about Alice's and Bob's subsystem.

Singlet state, entanglement status of singlet state:

Fully entangled system.

Singlet state, expectation values:

For the subsystems:

$$\langle \sigma_x \rangle = \langle \sigma_y \rangle = \langle \sigma_z \rangle = 0$$

$$\langle \tau_x \rangle = \langle \tau_y \rangle = \langle \tau_z \rangle = 0$$

For the composite system:

$$\langle \tau_x \sigma_x \rangle = \langle \tau_y \sigma_y \rangle = \langle \tau_z \sigma_z \rangle = -1$$

Singlet state, normalization:

$$\psi_{uu}^* \psi_{uu} + \psi_{ud}^* \psi_{ud} + \psi_{du}^* \psi_{du} + \psi_{dd}^* \psi_{dd} = 1$$

Singlet state, state-vector:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

Singlet state, wave function:

$$\psi(a, b)$$

Note: the wave function is not factorized.

Space of states:

1.

The space of states of a quantum system is a complex Hilbert vector space.

2.

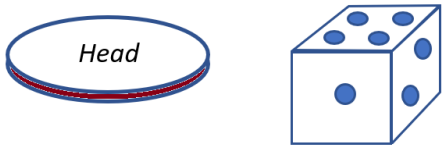
The space of states for a single spin has two dimensions. All possible spin states can be represented in a two-dimensional vector space.

The directions up and $down$ are not orthogonal in the spatial 3-dimensional space. Their associated state-vectors are.

3.

The space of states for a coin-die system has twelve dimensions:

		state labels of Bob					
		1	2	3	4	5	6
State labels of Alice	Head	H1	H2	H3	H4	H5	H6
	Tail	T1	T2	T3	T4	T5	T6



We give Alice the coin, Bob the die.

The system of Alice S_A (it is a quantum system) has two dimensions:

$$\alpha_h|H\rangle + \alpha_t|T\rangle$$

The system of Bob S_B (it is a quantum system too) has six dimensions:

$$\alpha_1|1\rangle + \alpha_2|2\rangle + \alpha_3|3\rangle + \alpha_4|4\rangle + \alpha_5|5\rangle + \alpha_6|6\rangle$$

The combined system S_{AB} (quantum) has twelve dimensions:

$$\alpha_h\alpha_1|H1\rangle + \alpha_h\alpha_2|H2\rangle + \alpha_h\alpha_3|H3\rangle + \alpha_h\alpha_4|H4\rangle + \alpha_h\alpha_5|H5\rangle + \alpha_h\alpha_6|H6\rangle + \alpha_t\alpha_1|T1\rangle + \alpha_t\alpha_1|T2\rangle + \alpha_t\alpha_1|T3\rangle + \alpha_t\alpha_1|T4\rangle + \alpha_t\alpha_1|T5\rangle + \alpha_t\alpha_1|T6\rangle$$

Note: $|H1\rangle$ etc. are the basis vectors of the combined system.

A superposition of two of these basis vectors might look like:

$$\alpha_h\alpha_3|H3\rangle + \alpha_h\alpha_4|H4\rangle$$

The space of states for a two-spin system has four dimensions:

	up	$down$	
up	$upup$	$updown$	
$down$	$downup$	$downdown$	

The system of Alice S_A (it is a quantum system) has two dimensions:

$$\alpha_u|u\rangle + \alpha_d|d\rangle$$

The system of Bob S_B (it is a quantum system too) has two dimensions:

$$\beta_u|u\rangle + \beta_d|d\rangle$$

The combined system S_{AB} (quantum) has four dimensions:

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

Note: these are the basis vectors of the combined system.

A superposition of two of these basis vectors might look like:

$$\alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle$$

4.

In a two-spin system we label the components of the spins of Alice $\sigma_x, \sigma_y, \sigma_z$ and Bob τ_x, τ_y, τ_z.

If we take the basis of the z-components up and $down$ we have the basis vectors:

$$|uu\rangle, |ud\rangle, |du\rangle, |dd\rangle$$

The vector $|ud\rangle$ is the state in which the Spin of Alice is up and the spin of Bob is $down$.

5.

The most general vector in the composite space of states:

$$\psi_{uu}|uu\rangle + \psi_{ud}|ud\rangle + \psi_{du}|du\rangle + \psi_{dd}|dd\rangle$$

Note: if ψ_{uu} etc. is used instead of $\alpha_u\beta_d$ etc. this indicates that we work with an entangled system and are not interested in the subsystems of Alice and Bob.

Entangled states in the case of two spins are the $singlet$ state and the $triplet$ states:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

$$|T_1\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$$

$$|T_2\rangle = \frac{1}{\sqrt{2}}(|uu\rangle + |dd\rangle)$$

$$|T_3\rangle = \frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle)$$

One fascinating feature of entangled states: an entangled state is a complete description of the combined system, but nothing is known about the individual subsystems.

6.

a) composite system
   If a composite system is in a product state, then the density matrix of Alice (or Bob) has one and only one eigenvalue equal to 1, the rest of the eigenvectors have eigenvalue zero. The eigenvector with the nonzero eigenvalue is the wave function of each subsystem.
   In this case we call the state of the subsystem a pure state.
   The subsystems are completely independent.
b) The opposite extreme of a pure state is a maximally entangled state. Nothing there is known about the subsystems, but we have complete knowledge of the combined system.

In this case, the density matrix for a subsystem is proportional to the unit matrix, all the entries on the main diagonal have the value $\frac{1}{N}$ with N being the dimension of the space of states.

7.

We can take the measuring apparatus $\mathcal{A}$ into account being a part of whole system.

The simplest way is to assign the states:

$$|b\rangle, \qquad |+1\rangle, \qquad |-1\rangle$$

The measuring apparatus can show a blank result $|b\rangle$ before the measurement is made and either $|+1\rangle$ or $|-1\rangle$ after the measurement of the spin is made. These states have to be combined with the states of the spin system.

8.

When the observables are discrete, we have a vector space of finite dimension – the spin with two dimensions, a (quantum) die with six dimensions and so on.

A particle along the x-axis has an infinite number of possible locations – the wave function becomes a function of a continuous variable. We have to expand the idea of vectors to include functions.

With appropriate restrictions, functions like $\psi(x)$ satisfy the mathematical axioms that define a vector space.

Vector space	Functions
Closure: the sum of two vectors is a vector: $\|A\rangle + \|B\rangle = \|C\rangle$	The sum of any two functions is a new function $\psi(x) + \phi(x) = \theta(x)$
Vector addition is commutative: $\|A\rangle + \|B\rangle = \|B\rangle + \|A\rangle$	The addition of two functions is commutative $\psi(x) + \phi(x) = \phi(x) + \psi(x)$
Vector addition is associative: $\{\|A\rangle + \|B\rangle\} + \|C\rangle = \|A\rangle + \{\|B\rangle + \|C\rangle\}$	The addition of functions is associative $\big(\psi(x) + \phi(x)\big) + \theta(x) = \psi(x) + \big(\phi(x) + \theta(x)\big)$
Existence of the 0: $\|A\rangle + 0 = \|A\rangle$	There is a unique zero-function $\psi(x) + 0(x) = \psi(x)$
Existence of the inverse: $\|A\rangle + (-\|A\rangle) = 0$	To every function there is an inverse function $\psi(x) + \big(-\psi(x)\big) = 0(x)$
Multiplication by a scalar produces a new vector: $\|zA\rangle = z\|A\rangle = \|B\rangle$	Multiplication by a scalar produces a new function(*) $z\psi(x) = \phi(x)$
Distributive property: $z\{\|A\rangle + \|B\rangle\} = z\|A\rangle + z\|B\rangle$ $\{z + w\}\|A\rangle = z\|A\rangle + w\|A\rangle$	Addition is distributive $z\{\psi(x) + \phi(x)\} = z\psi(x) + z\phi(x)$ $\{z + w\}\psi(x) = z\psi(x) + w\psi(x)$

(*) $z\psi(x) \neq \psi(zx)$ with the exception of rare cases.

9.

The classical phase space is the space of coordinates and momenta.

The quantum mechanical phase space is the linear vector space of states.

The change of states with time – classical – leads to Hamilton's equations and Liouville's(*) theorem.

The change of states with time – quantum mechanical – leads to the principle of unitarity and to the Schrödinger equations.

(*) for reasons of completeness: let ρ be the density matrix. The quantum mechanical version of Liouville's theorem is the von Neumann equation:

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H, \rho]$$

It resembles the time change of the expectation value of an observable (an operator).

Speed of light, particles moving at speed of light:

Prerequisite

The time-dependent Schrödinger equation:

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = H|\psi\rangle$$

The momentum operator:

$$P = -i\hbar \frac{\partial}{\partial x}$$

Wave functions need to be normalized:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1$$

End prerequisite

We start with a simple Hamiltonian, a fixed constant times the momentum operator P:

$$H = cP$$

We insert this Hamiltonian into the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = -ci\hbar \frac{\partial}{\partial x}|\psi\rangle$$

In terms of wave-functions:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -ci\hbar \frac{\partial \psi(x,t)}{\partial x}$$

Note: $\psi(x,t)$ is a function of both x and t.

We cancel the term $i\hbar$:

$$\frac{\partial \psi(x,t)}{\partial t} = -c\frac{\partial \psi(x,t)}{\partial x}$$

Any function of $(x - ct)$ is a solution.

We check this with an example:

$$\psi(x,t) \coloneqq (x - ct)^2$$

Left side:

$$\frac{\partial (x - ct)^2}{\partial t} = 2(x - ct)(-c) = -2c(x - ct)$$

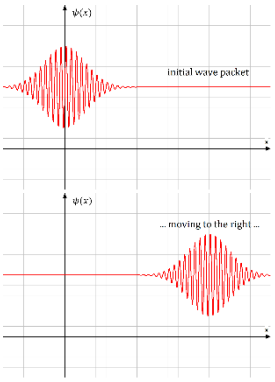
Right side:

$$-c\frac{\partial(x-ct)^2}{\partial x} = -2c(x-ct)$$

Both sides are equal. This may be enough for our quick check.

Any normalized function of this form solves the Schrödinger equation.

We look at the time evolution of $\psi(x-ct)$. How does a wave function $\psi(x-ct)$ evolve with time?



We start at time $t = 0$.

Our wave-function is a wave-packet localized on the x −axis.

As t increases the wave-packet is shifting to the right with uniform velocity c.

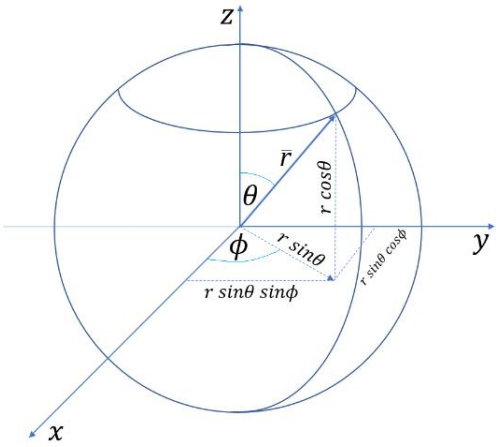
This description is pretty close to the correct description of a neutrino that moves immeasurably slower than the speed of light.

Spherical coordinates:

To define a direction in space we need two angles.

To define a vector in space we need additionally the length of this vector.

We can convert spherical coordinates into cartesian coordinates:



$$x = r\sin(\theta)\ \cos(\phi)$$

$$y = r\sin(\theta)\ sin(\phi)$$

$$z = r\ cos(\theta)$$

We can convert cartesian coordinates into spherical coordinates:

$$r = \sqrt{x^2+y^2+z^2}$$

$$\phi = arctan\left(\frac{y}{x}\right)$$

$$\theta = \arctan\left(\frac{\sqrt{x^2+y^2}}{z}\right)$$

Spin:

Spin, 3-vector operators and spin:

State-vectors e.g. $|u\rangle$ for “up” and $|d\rangle$ for “down” describe the state of a spin. They are part of a two-dimensional, complex-based vector-space.

The pauli-matrices σ_x, σ_y and σ_z are operators written as matrices:

$$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\ \sigma_y = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

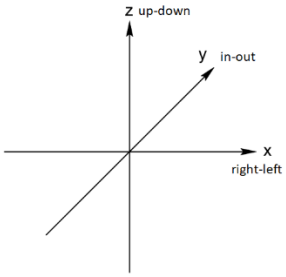
They act on state-vectors.

The vector $\vec{\sigma} \coloneqq \sigma_x + \sigma_y + \sigma_z$ is a 3-vector with the components σ_x, σ_y and σ_z and can be written as

$$\vec{\sigma} \coloneqq \begin{pmatrix} 1 & 1-i \\ 1+i & -1 \end{pmatrix}$$

Spin, spin along the x-axis and the y-axis:

Note: the names up-down, left-right, in-out refer to the spatial arrangement:



Note: the ordering z, y and x is due to the fact that we chose up-down as starting point, so the other pairs are derived from this.

The up and down state-vectors are $|u\rangle$ and $|d\rangle$, written as state-vectors:

$$|u\rangle \coloneqq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |d\rangle \coloneqq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The in and out state-vectors are $|i\rangle$ and $|o\rangle$. They are linear superpositions of $|u\rangle$ and $|d\rangle$:

$$|i\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle$$

Written as state-vectors:

$$|i\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{i}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

The right and left state-vectors are $|r\rangle$ and $|l\rangle$. They are linear superpositions of $|u\rangle$ and $|d\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

$$|l\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

Written as state-vectors:

$$|r\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|l\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Spin, density matrix for spin:

We have Alice with her single spin system. Her density matrix:

$$\rho_{aa'} = \psi^*(a')\psi(a)$$

In the σ_z-basis each index a and a' can take the values up and $down$.

The density matrix of Alice is a 2×2-matrix.

The density matrix for $|\psi\rangle = \alpha|u\rangle + \beta|d\rangle$:

$$\psi(u) = \alpha; \quad \psi^*(u) = \alpha^*$$

$$\psi(d) = \beta; \quad \psi^*(d) = \beta^*$$

$$\rho_{aa'} = \begin{pmatrix} \alpha\alpha^* & \alpha^*\beta \\ \alpha\beta^* & \beta\beta^* \end{pmatrix}$$

$$\rho_{a'a} = \begin{pmatrix} \alpha\alpha^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^* \end{pmatrix}$$

Spin, expectation values of spin:

We have a spin σ_n oriented with the angle θ in respect to the z-axis and work in the $up - down$ basis.

The expectation value of an observable (a measurement) L:

$$\langle L \rangle = \sum_i \lambda_i P(\lambda_i)$$

Note: this is a standard formula for an average value, the sum over all eigenvalues of the operator (the matrix) multiplied by the probability P.

If the angle between spin and x -axis is θ then the probability to get the result $+1$:

$$P(+1) = cos^2\frac{\theta}{2}$$

Analog:

$$P(-1) = sin^2\frac{\theta}{2}$$

We calculate the expectation value:

$$\langle \sigma_n \rangle = \sum_i \lambda_i P(\lambda_i) =$$

$$(+1)cos^2\frac{\theta}{2} + (-1)sin^2\frac{\theta}{2} =$$

$$cos^2\frac{\theta}{2} - sin^2\frac{\theta}{2} = \cos(\theta)$$

Note: regardless of the value of angle ϕ because we work in the $up - down$ basis.

Note: $\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$ for any orientation of the spin.

Spin, interaction with apparatus:

In contrast to classical physics the measurement of a spin is not a “measurement” that leaves the spin unchanged. The first interaction with the apparatus prepares the (floating) spin to one of the two possible directions up or $down$ (with respect to the orientation of the apparatus).

Subsequent measurements (with undisturbed spin) confirm that state.

If we rotate the apparatus after the preparation by e.g. 90° it starts to give randomly results of $+1$ or -1 with an average of zero but never the zero directly.

Spin in magnetic field:

Prerequisite

The Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Let $|\psi(t)\rangle$ be a state vector and L an operator. The change of the expectation value of an operator L with time:

$$\frac{d}{dt}\langle\psi(t)|L|\psi(t)\rangle = -\frac{i}{\hbar}\langle[L,H]\rangle$$

Written in shorthand form:

$$\dot{L} = -\frac{i}{\hbar}\langle[L,H]\rangle$$

End prerequisite

When a classical spin (a charged rotor) is put into a magnetic field, it has an energy that depends on its orientation. It is proportional to the dot product of the spin and the magnetic field.

The quantum version of this:

$$H \sim \vec{\sigma} \cdot \vec{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$$

Note: σ_x, σ_y and σ_z represents the components of the spin operator.

The magnetic field lies along the z axis. We absorb all numerical constants without $\hbar$ into a single constant ω and get the quantum Hamiltonian:

$$H = \frac{\hbar\omega}{2}\sigma_z$$

We search how the expectation value of the spin changes with time, $\langle\sigma_x(t)\rangle$, $\langle\sigma_y(t)\rangle$ and $\langle\sigma_z(t)\rangle$. We use:

$$\langle\dot{\sigma_x}\rangle = -\frac{i}{\hbar}\langle\sigma_x, H\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i}{\hbar}\langle[\sigma_y, H]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i}{\hbar}\langle[\sigma_z, H]\rangle$$

We plug in the quantum Hamiltonian $H = \frac{\hbar\omega}{2}\sigma_z$ and get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$$

$$\langle\dot{\sigma_y}\rangle = -\frac{i\omega}{2}\langle[\sigma_y, \sigma_z]\rangle$$

$$\langle\dot{\sigma_z}\rangle = -\frac{i\omega}{2}\langle[\sigma_z, \sigma_z]\rangle$$

We check this explicitly for $\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle[\sigma_x, \sigma_z]\rangle$ by using the Pauli-matrices:

$$[\sigma_x, \sigma_z] = \sigma_x\sigma_z - \sigma_x\sigma_z =$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} =$$

$$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} - \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = \begin{pmatrix}0 & -2\\ 2 & 0\end{pmatrix} =$$

$$-2i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = -2i\sigma_y$$

We get:

$$\langle\dot{\sigma_x}\rangle = -\frac{i\omega}{2}\langle -2i\sigma_y\rangle = -\omega\langle\sigma_y\rangle$$

The results:

$$\langle\dot{\sigma_x}\rangle = -\omega\langle\sigma_y\rangle$$

$$\langle\dot{\sigma_y}\rangle = \omega\langle\sigma_x\rangle$$

$$\langle\dot{\sigma_z}\rangle = 0$$

In classical mechanics, the x and y components of angular momentum are precessing around the z axis.

In quantum mechanics the expectation values for $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ will be precessing, but each single measurement will always give +1 or -1. The expectation value for $\langle\sigma_z\rangle$ remains unchanged.

Spin, number of distinct states for a Spin:

To define a direction in three-dimensional space it takes two angles – two parameters.

The general spin state is defined by two complex numbers α_u and α_d – four parameters:

$$\alpha_u|u\rangle + \alpha_d|d\rangle$$

The general spin state has to be normalized – minus one parameter.

The general spin does not depend on the overall phase-factor – minus one parameter.

This leaves two parameters to specify the state of a spin.

Spin components, simultaneous measurement of spin components:

Two operators can be simultaneously measured if they commute.

The commutator of two operators A and B (matrices):

$$[A, B] = AB - BA$$

The three spin components σ_x, σ_y and σ_z (the Pauli-matrices) in matrix representation:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We try whether σ_x and σ_y commute:

$$[\sigma_x, \sigma_y] = \sigma_x\sigma_y - \sigma_y\sigma_x =$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} =$$

$$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} =$$

$$2\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \neq 0$$

This holds for the other combinations too. It is not possible to measure two components of the spin simultaneously.

Spin operators:

The three spin operators (the Pauli-matrices):

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note: the 2×2 identity-matrix can be regarded as the fourth Pauli-matrix.

Spin operators, constructing spin operators:

The three principles of quantum mechanics:

- Principle 1: Each component of σ is represented by a linear operator (a matrix).
- Principle 2: The eigenvectors of σ_z are

  $$|u\rangle, up, \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

  and

  $$|d\rangle, down, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

  with the corresponding eigenvalues $+1$ and -1:

  $$\sigma_z|u\rangle = |u\rangle$$

$$\sigma_z|d\rangle = -|d\rangle$$

- Principle 3: states $|u\rangle$ and $|d\rangle$ are orthogonal to each other:

$$\langle u|d\rangle = 0$$

The eigenvector equation of σ_z:

$$\sigma_z|u\rangle = |u\rangle \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ c \end{pmatrix} \rightarrow a = 1$$

$$\sigma_z|d\rangle = -|d\rangle \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} b \\ d \end{pmatrix} \rightarrow d = -1$$

The operator σ_z:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We calculate the spin operators σ_x and σ_y.

The eigenvectors of σ_x are $|r\rangle$ and $|l\rangle$, $right$ and $left$.

The eigenvectors of σ_y are $|i\rangle$ and $|o\rangle$, in and out.

We express all eigenvectors by linear superpositions of $|u\rangle$ and $|d\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle \rightarrow |r\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$|l\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle \rightarrow |l\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$|i\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle \rightarrow |i\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle \rightarrow |o\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix}$$

Note: i is used in different meanings. $|i\rangle$ is the state vector along the y-axis. In $\frac{i}{\sqrt{2}}$, i is the imaginary unit.

The eigenvector equation of σ_x:

$$\sigma_x|r\rangle = |r\rangle \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\sigma_x|l\rangle = -|l\rangle \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = -\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

From $\sigma_x|r\rangle = |r\rangle$ we get:

$$\begin{pmatrix} \frac{a}{\sqrt{2}} + \frac{b}{\sqrt{2}} \\ \frac{c}{\sqrt{2}} + \frac{d}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

From $\sigma_x|r\rangle = -|l\rangle$ we get:

$$\begin{pmatrix} \frac{a}{\sqrt{2}} - \frac{b}{\sqrt{2}} \\ \frac{c}{\sqrt{2}} - \frac{d}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

We have four equations:

$$\frac{a}{\sqrt{2}} + \frac{b}{\sqrt{2}} = \frac{1}{\sqrt{2}} \rightarrow a + b = 1$$

$$\frac{c}{\sqrt{2}} + \frac{d}{\sqrt{2}} = \frac{1}{\sqrt{2}} \rightarrow c + d = 1$$

$$\frac{a}{\sqrt{2}} - \frac{b}{\sqrt{2}} = -\frac{1}{\sqrt{2}} \rightarrow a - b = -1$$

$$\frac{c}{\sqrt{2}} - \frac{d}{\sqrt{2}} = \frac{1}{\sqrt{2}} \rightarrow c - d = 1$$

From $a + b = 1$ and $a - b = -1$ we get $a = 0$ and $b = 1$.

From $c + d = 1$ and $c - d = 1$ we get $d = 0$ and $c = 1$.

The operator (the matrix) σ_x:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The eigenvector equation of σ_y:

$$\sigma_y|i\rangle = |i\rangle \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

$$\sigma_y|o\rangle = -|o\rangle \rightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix} = -\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

From $\sigma_y|i\rangle = |i\rangle$ we get:

$$\begin{pmatrix} \frac{a}{\sqrt{2}} + \frac{ib}{\sqrt{2}} \\ \frac{c}{\sqrt{2}} + \frac{id}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

From $\sigma_y|o\rangle = -|o\rangle$ we get:

$$\begin{pmatrix} \frac{a}{\sqrt{2}} - \frac{ib}{\sqrt{2}} \\ \frac{c}{\sqrt{2}} - \frac{id}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

We have four equations:

$$\frac{a}{\sqrt{2}} + \frac{ib}{\sqrt{2}} = \frac{1}{\sqrt{2}} \rightarrow a + ib = 1$$

$$\frac{c}{\sqrt{2}} + \frac{id}{\sqrt{2}} = \frac{i}{\sqrt{2}} \rightarrow c + id = i$$

$$\frac{a}{\sqrt{2}} - \frac{ib}{\sqrt{2}} = -\frac{1}{\sqrt{2}} \rightarrow a - ib = -1$$

$$\frac{c}{\sqrt{2}} - \frac{id}{\sqrt{2}} = \frac{i}{\sqrt{2}} \rightarrow c - id = i$$

From $a + ib = 1$ and $a - ib = -1$ we get $a = 0$ and $b = \frac{1}{i} = -i$.

From $c + id = i$ and $c - id = i$ we get $d = 0$ and $c = i$.

The operator (the matrix) σ_y:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Spin-Polarizing principle:

Any state of a single spin is eigenvector of some component of the spin. Given a state $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$ there exists some direction $\vec{n}$, such that $(\vec{\sigma}\cdot\vec{n})|A\rangle = |A\rangle$.

The states of a spin are characterized by a polarization vector, and along that polarization vector the component of the spin is predictably +1. This meets our expectations that the spin must have exactly one direction, even if we do not know it.

This means further that the expectation values of the components must sum up to 1:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$$

This is a kind of classical expectation and does not hold for entangled states.

Spin states:

Spin states as column vectors:

The spin states in z-direction are:

$$|u\rangle, up, \begin{pmatrix}1\\0\end{pmatrix}$$

and

$$|d\rangle, down, \begin{pmatrix}0\\1\end{pmatrix}$$

From this we can derive the spin states in y-direction and x-direction:

$$|r\rangle, right = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle \rightarrow |r\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}$$

$$|l\rangle, left = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle \rightarrow |l\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix}$$

$$|i\rangle, in = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle \rightarrow |i\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{i}{\sqrt{2}}\end{pmatrix}$$

$$|o\rangle, out = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle \rightarrow |o\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{i}{\sqrt{2}}\end{pmatrix}$$

Note: i is used in different meanings. $|i\rangle$ is the state vector along the y-axis. In $\frac{i}{\sqrt{2}}$, i is the imaginary unit.

The pairs are mutually orthogonal:

$$\langle u|d\rangle = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 0 + 0 = 0$$

$$\langle r|l\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix} = \frac{1}{2} - \frac{1}{2} = 0$$

$$\langle i|o\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{-i}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{i}{\sqrt{2}}\end{pmatrix} = \frac{1}{2} - \frac{1}{2} = 0$$

Note: if we change from the ket $|i\rangle$ to the bra $\langle i|$ we must complex conjugate the vector. The first two pairs $\langle u|d\rangle$ and $\langle r|l\rangle$ had only real coefficients making this invisible.

Spin states, representing spin states:

We chose $|u\rangle$ and $|d\rangle$ as basis vectors and write any state $|A\rangle$ as linear superposition:

$$|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$$

We get back the components α_u and α_d by:

$$\alpha_u = \langle u|A\rangle \text{ resp. } \alpha_u^* = \langle A|u\rangle$$

$$\alpha_d = \langle d|A\rangle \text{ resp. } \alpha_d^* = \langle A|d\rangle$$

The quantity $\alpha_u^*\alpha_u$ is the probability that the spin would be measured as $\sigma_z = +1$, spin up.

The quantity $\alpha_d^*\alpha_d$ is the probability that the spin would be measured as $\sigma_z = -1$, spin $down$.

The values α_u and α_d are the probability amplitudes. To measure the probabilities, they must be squared:

$$P_u = \langle A|u\rangle\langle u|A\rangle$$

$$P_d = \langle A|d\rangle\langle d|A\rangle$$

$|u\rangle$ and $|d\rangle$ are mutually orthogonal:

$$\langle u|d\rangle = \langle d|u\rangle = 0$$

The total probability for the spin:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

This is equivalent to the vector $|A\rangle$ being normalized:

$$\langle A|A\rangle = 1$$

Spring constant:

Graphic courtesy Wikipedia by Svjo

The force of a spring to an attached object:

$$F = -kx$$

This corresponds to a potential energy function:

$$V(x) = \frac{k}{2}x^2$$

The negative sign in the force tells us that the force acts opposite to the displacement x and pulls the mass back towards its origin.

This is important because almost any smooth function looks like a parabola close to a minimum of the function. The harmonic oscillator has a lot of applications in physics.

- If an atom situated in a crystal lattice is displaces slightly from its equilibrium position, it gets pushed back with an approximately linear restoring force.
- The electric current in a circuit of low resistance often oscillates with a characteristic frequency.
- If a water surface is disturbed, it sends out waves.
- A light wave or a radio wave oscillates.

Standard deviation:

The standard deviation is also called uncertainty.

Let A be an observable (operator) with eigenvalues a.

We begin with the expectation value (the average) of A:

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \sum_a aP(a)$$

To make calculations easier we define the operator $\bar{A}$:

$$\bar{A} = A - \langle A \rangle I$$

The operator $\bar{A}$ is centered around zero, meaning that the expectation value of $\bar{A}$ is zero.

The eigenvectors of $\bar{A}$ are the same as those of A because the basis is unaffected by this change.

The eigenvalues are shifted all:

$$\bar{a} = a - \langle A \rangle$$

The square of uncertainty or the square of standard deviation of A:

$$(\Delta A)^2 = \sum_a \bar{a}^2 P(a) = \sum_a (a - \langle A \rangle)^2 P(a) = \langle \psi | \bar{A}^2 | \psi \rangle$$

If the expectation value of the operator A is zero, the square of the uncertainty is easier to calculate, it is the average value of the operator A^2:

$$(\Delta A)^2 = \langle \psi | A^2 | \psi \rangle$$

State:

State of apparatus:

If the measuring apparatus (for spatial spin orientation) comes into play as a quantum system too, in the simplest description it has three states, a blank state and two outcome states with the following basis vectors: $|b\rangle$, $|(+1)\rangle$ and $|(-1)\rangle$.

The starting state at time 0 is always the blank state.

If we measure a single spin system $|u\rangle$ and $|d\rangle$ and form the tensor product with the states of the apparatus:

$$|u,b\rangle, |u,+1\rangle, |u,-1\rangle, |d,b\rangle, |d,+1\rangle, |d,-1\rangle$$

The composite system has six dimensions.

State, change over time:

Quantum mechanical time development is unitary.

Quantum systems change over time and follow the rule of the "minus first law" – distinctions are conserved. This leads to a unitary time-development operator $U(t)$:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

Note: $|\psi(0)\rangle$ stands for ψ at any time t_0.

A unitary operator (matrix) satisfies:

$$U^\dagger U = I$$

Note: $U^\dagger$ is the transposed and complex conjugated version of U.

Note: every unitary matrix is quadratic.

Examples of unitary matrices:

Example 1:

$$U \coloneqq \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

$$U^\dagger \coloneqq \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$$

$$U^\dagger U = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = \begin{pmatrix} -i^2 & 0 \\ 0 & -i^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Example 2:

$$U \coloneqq \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}$$

$$U^\dagger \coloneqq \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}$$

$$U^\dagger U = \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix} \cdot \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix} =$$

$$\frac{1}{4}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix} =$$

$$\frac{1}{4}\begin{pmatrix}(1-i)(1+i)+(1+i)(1-i) & (1-i)(1-i)+(1+i)(1+i)\\(1+i)(1+i)+(1-i)(1-i) & (1+i)(1-i)+(1-i)(1+i)\end{pmatrix}=$$

$$\frac{1}{4}\begin{pmatrix}2+2 & -2i+2i\\2i-2i & 2+2\end{pmatrix}=\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$$

State, maximally entangled state:

The opposite extreme of a pure state is a maximally entangled state. This is a complete description of the system as a whole, as complete as quantum mechanics allows, but nothing is known about either subsystem.

The state $|sing\rangle$ is a state of two maximally entangled spins of Alice and Bob.

When Alice calculates the density matrix $\rho_{aa'}$ for her subsystem (dimension 2), she gets:

$$\rho_{aa'}=\begin{pmatrix}\frac{1}{2} & 0\\0 & \frac{1}{2}\end{pmatrix}$$

All states have the same probability of $^1/_2$ – she knows nothing about her subsystem.

In general, the density matrix is proportional to the unit matrix:

$$\begin{pmatrix}\frac{1}{N} & 0\cdots & 0\\\vdots & \ddots & \vdots\\0 & \cdots 0 & \frac{1}{N}\end{pmatrix}$$

State, measurement and state:

In classical physics we perform an experiment to determine the state of a system.

In quantum mechanics we perform an experiment to set the state of a system – that is in general not correct but describes the relationship between state and measurement that are subtle and nonintuitive.

State, mixed state:

A mixed state is represented by a density matrix made of several projection operators. It is a matrix that has entries only on the diagonal, summing up to 1.

In contrast: a pure state is represented by a density matrix that has only one entry on its diagonal and this entry is 1.

State, near singlet state:

The near singlet state is a partially entangled state.

The state-vector:

$$\sqrt{0{,}6}|ud\rangle-\sqrt{0{,}4}|du\rangle$$

or in the extended form:

$$|nearsing\rangle=0|uu\rangle+\sqrt{0{,}6}|ud\rangle-\sqrt{0{,}4}|du\rangle+0|dd\rangle$$

We have only one normalization condition:

$$\psi_{uu}^{*}\psi_{uu} + \psi_{ud}^{*}\psi_{ud} + \psi_{du}^{*}\psi_{du} + \psi_{dd}^{*}\psi_{dd} = 1$$

in this case reducing to:

$$\psi_{ud}^{*}\psi_{ud} + \psi_{du}^{*}\psi_{du} = 1$$

The density matrix for the full composite system: $\rho^2 = \rho, Tr(\rho^2) = 1.$

The density matrix for Alice's subsystem A: $\rho^2 \neq \rho, Tr(\rho^2) < 1$

We check the density matrix for Alice's subsystem:

The density matrix of Alice: $\rho_{a'a} = \sum_b \psi^*(a,b)\psi(a',b)$

expanded a, a' (with $\psi^* = \psi$ due to all coefficients being real):

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = 0.6$$

$$\rho_{ud} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = 0$$

$$\rho_{du} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = 0$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = 0.4$$

gives Alice density matrix:

$$\rho := \begin{pmatrix} 0.6 & 0 \\ 0 & 0.4 \end{pmatrix}$$

The wave function is not factorized (partial entanglement): $\psi(a,b)$.

The expectation values:

$\langle\sigma_z\rangle = 0{,}2\ \langle\sigma_x\rangle = \langle\sigma_y\rangle = 0$

$\langle\tau_z\rangle = -0{,}2\ \langle\tau_x\rangle = \langle\tau_y\rangle = 0$

$\langle\tau_z\sigma_z\rangle = -1$

$\langle\tau_x\sigma_x\rangle = -2\sqrt{0{,}24}$

The correlation between the two systems: $\langle\sigma_z\tau_z\rangle - \langle\sigma_z\rangle\langle\tau_z\rangle = -0{,}96$

The main feature of a partially entangled state is that the composite system as a whole is fully characterized but there is no complete information about the subsystems.

State of a particle:

In classical physics we describe the state of the system by the pair (x,p), the coordinate x and the momentum p. Together with a potential V we can use Hamilton's equations to calculate position and momentum for all times – a flow through the phase space.

If we use the same approach for quantum mechanics, the quantum state of a particle would be spanned by a basis of states labeled by position and momentum:

$$|x,p\rangle$$

The corresponding wave function:

$$\psi(x,p) = \langle x,p|\psi\rangle$$

But:

$$\langle x,p|\psi\rangle \neq \langle p,x|\psi\rangle$$

Both observables position x and momentum p are not simultaneous measurable. This is the distillation of many decades of experimental observations and we had to find a mathematical framework confirming these results. We found it in terms of commutating operators (matrices) and their eigenvectors.

State, pure state:

In a pure state the density matrix ρ corresponds to a single state, it is a projection operator that projects onto that state. A pure state represents the maximum amount of knowledge one can have of a quantum system.

A classical pure state is a special case of a probability density, in which the density matrix ρ has exactly one nonzero entry (on the diagonal).

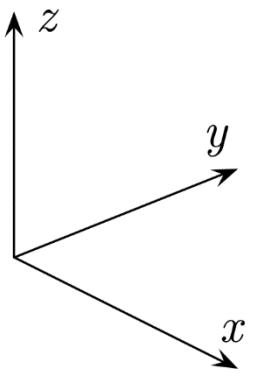
State, quantum state:

Any spin state can be represented as a linear combination of the basis vectors $|u\rangle$ and $|d\rangle$.

If we prepare a spin along the x-axis and then measure in z-direction, there will be equal probabilities for up and $down$.

A vector $|r\rangle$ satisfying this rule:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$



We use that both vectors must be orthogonal:

$$\langle r|l\rangle = \langle l|r\rangle = 0$$

We get the vector $|l\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

With similar reasoning and evaluating more conditions, we get the vectors $|i\rangle$ and $|o\rangle$:

$$|i\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle$$

Note: i is the imaginary unit.

Note: all possible orientations are expressed in terms of up and $down$, the basis vectors in z-direction.

State, in quantum mechanics:

In the classical world, the result of a measurement describes the state of a system – the system left unchanged.

In the quantum world, the measurement (sometimes) alters the system.

State, singlet state:

We have a system of two spins, σ and τ:

$$\vec{\sigma} \cdot \vec{\tau} = \sigma_x \tau_x + \sigma_y \tau_y + \sigma_z \tau_z$$

The most general vector in the composite space of states:

$$\psi_{uu}|uu\rangle + \psi_{ud}|ud\rangle + \psi_{du}|du\rangle + \psi_{dd}|dd\rangle$$

The $singlet$ state is a maximally entangled state:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

The singlet state is eigenvector of $\sigma \cdot \tau$:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

We apply $\vec{\sigma} \cdot \vec{\tau}$ to $|sing\rangle$:

$$\sigma_x \tau_x |sing\rangle = \sigma_x \tau_x \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle) = \sigma_x \frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle) = \frac{1}{\sqrt{2}}(|du\rangle - |ud\rangle) = -|sing\rangle$$

$$\sigma_y \tau_y |sing\rangle = \sigma_y \tau_y \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle) = \sigma_y \frac{1}{\sqrt{2}}(-i|uu\rangle - i|dd\rangle) = \frac{1}{\sqrt{2}}(|du\rangle - |ud\rangle) = -|sing\rangle$$

$$\sigma_z \tau_z |sing\rangle = \sigma_z \tau_z \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle) = \sigma_z \frac{1}{\sqrt{2}}(-|ud\rangle - |du\rangle) = \frac{1}{\sqrt{2}}(-|ud\rangle + |du\rangle) = -|sing\rangle$$

We get:

$$\vec{\sigma} \cdot \vec{\tau} |sing\rangle = -3|sing\rangle$$

$|sing\rangle$ is eigenvector of $\vec{\sigma} \cdot \vec{\tau}$ with eigenvalue -3.

States that depend on more than one measurable:

a) A particle moving in the 3-dimensional (spatial) space. A basis of states takes three position coordinates x, y and z, written in terms of kets:
$$|x, y, z\rangle$$
All spatial coordinates can simultaneously be specified.

b) A system of two physically independent spins, L and M, a system of two qubits. Each qubit L and M is characterized by the z-observable of the spin.
Quantum mechanics does not forbid simultaneous knowledge of these two observables.

c) A system of two maximally entangled spins. Quantum mechanics allows complete knowledge of the behavior of the entangled system, but nothing about the individual spins.

We will treat case b) in detail.

We measure each spin separately by associating the measurements with the operators (matrices) L and M.

To work with two different compatible operators L and M, we need two sets of labels for their basis vectors λ_i and μ_j.

We assume that we can produce a basis of state-vectors $|\lambda_i, \mu_j\rangle$ that are simultaneous eigenvectors of both observables (e.g. by help of the tensor product):

$$L|\lambda_i, \mu_j\rangle = \lambda_i|\lambda_i, \mu_j\rangle$$

$$M|\lambda_i, \mu_j\rangle = \mu_j|\lambda_i, \mu_j\rangle$$

Note: λ_i and μ_j are eigenvalues, $|\lambda_i, \mu_j\rangle$ is eigenvector of the combined system with $|\lambda_i\rangle$ and $|\mu_j\rangle$ being the constituents of each subsystem – no entanglement here.

In order to have a basis of simultaneous eigenvectors, the operators (matrices) L and M must commute

$$[L, M] := LM - ML = 0$$

because $LM|\lambda_i, \mu_j\rangle$ must give the same result as $ML|\lambda_i, \mu_j\rangle$.

Note: the operator $[L, M]$ is called the $zero\ operator$, the analogous to the zero vector. In mathematics, the zero vector is a special vector of a vector space, the defined neutral element with respect to vector addition. It is used to define some key terms of linear algebra.

State, triplet state:

In a system of two spins we have three triplet states:

$$|t_1\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$$

$$|t_2\rangle = \frac{1}{\sqrt{2}}(|uu\rangle + |dd\rangle)$$

$$|t_3\rangle = \frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle)$$

The triplet states are maximally entangled and cannot be written as product states.

The triplet states are eigenvectors to the operator $\vec{\sigma} \cdot \vec{\tau}$ with the same (degenerate) eigenvalue 1.

State, unambiguously distinct state:

Unambiguously distinguishable states are represented by orthogonal state vectors.

Two states are physically distinct if there is a measurement that can distinguish between them without ambiguity. In the basis system of eigenvectors of the appropriate operators their state vectors must be orthogonal.

State labels for the composite system:

We use two single spin system of Alice and Bob. The basis vectors in the system of Alice are $|u\rangle$ and $|d\rangle$, the basic vectors in the system of Bob are $|u\}$ and $|d\}$.

If we combine the two systems to one, we write $|ab\rangle$ to label a single basis vector of the combined system, in our case: $|uu\rangle$, $|ud\rangle$, $|du\rangle$ and $|dd\rangle$.

The corresponding bra to $|ab\rangle$ is $\langle a'b'|$.

In the combined system of Alice and Bob we have four basis vectors: $|uu\rangle$, $|ud\rangle$, $|du\rangle$ and $|dd\rangle$.

The basis vectors in the two-dimensional system of Alice are $|u\rangle$ and $|d\rangle$, the basic vectors in the two-dimensional system of Bob are $|u\}$ and $|d\}$. If we combine the two systems to one, we get a four-dimensional combined system with basis vectors $|uu\rangle$, $|ud\rangle$, $|du\rangle$ and $|dd\rangle$.

$|uu\rangle$ is one four-dimensional basis vector. The labelling $|uu\rangle$ etc. is chosen to indicate the origin: $|uu\rangle$ is composed out of $|u\rangle$ Alice and $|u\}$ Bob.

Example: consider a linear operator M acting on the space of states of the composite system of Alice and Bob. As usual, it can be represented as a matrix. The elements of the matrix can be extracted by sandwiching the operator between the basis vectors:

$$\langle a'b'|M|ab\rangle = M_{a'b',ab}$$

As basis vectors usually are orthonormal, this means that the inner product $\langle a'b'|ab\rangle$ gives the Kronecker delta:

$$\langle a'b'|ab\rangle = \delta_{aa'}\delta_{bb'}$$

With the basis vectors we can write any state vector in the composite system as:

$$|\psi\rangle = \sum_{a,b} \psi(a,b)|ab\rangle$$

For a product state of Alice and Bob this gives:

$$|\psi\rangle = \psi(u,u)|uu\rangle + \psi(u,d)|ud\rangle + \psi(d,u)|du\rangle + \psi(d,d)|dd\rangle$$

State of system, classical $vs.$ quantum physics:

Classical physics: a particle has position x and momentum p. Both can be measured simultaneously exact.

Quantum physics: a particle has position x or momentum p. Both can be measured simultaneously only with uncertainty.

Measuring the position uses the position operator X. Measuring the momentum uses the momentum operator P. Both can be simultaneous measured (exactly) only if the commutator of both operators is zero:

$$[X,P] \coloneqq XP - PX = 0$$

The commutator $[X,P] = i\hbar \neq 0$.

State vectors:

We have a single spin, knowing it is in the state $|u\rangle$ up or $|r\rangle$ $right$.

We can perform no single measurement that tells unambiguously the true state of the spin.

Single measuring σ_z will give $+1$ if the spin was up, but also $+1$ if the spin was $right$ with a chance of 50%.

For this reason, state $|u\rangle$ or $|r\rangle$ are said not to be physically distinguishable.

In contrast: if we know that the spin is either in state $|u\rangle$ (up) or $|d\rangle$ ($down$), a single measurement tells us unambiguously what state it is in: $+1$ up, -1 $down$.

For this reason, state $|u\rangle$ or $|d\rangle$ are said to be physically distinguishable.

We compare this with the result of the inner product:

$$|u\rangle \cdot |r\rangle \neq 0$$

$$|u\rangle \cdot |d\rangle = 0$$

The inner product is sometimes called $overlap$.

The inner product of two states is a measure of the inability to distinguish them with certainty.

Note: do not mix up state vectors with spatial directions of the spin in space. state vectors $|u\rangle$ and $|d\rangle$ are orthogonal, the spatial directions up and down are not.

State vectors, action of Hermitian operator on state vectors:

Prerequisite

Any state vector A can be written in the orthonormal basis of eigenvectors of a Hermitian operator L:

$$|A\rangle = \sum_i \alpha_i |\lambda_i\rangle$$

$$\langle A| = \sum_i \langle\lambda_i|\alpha_i^*$$

Note: $|\lambda_i\rangle$ resp. $\langle\lambda_i|$ are eigenvectors of the Hermitian operator L.

End prerequisite

Suppose the normalized state of a quantum system is $|A\rangle$. We expand $|A\rangle$ in the orthonormal basis of eigenvectors of the Hermitian operator L:

$$|A\rangle = \sum_i \alpha_i |\lambda_i\rangle$$

Note: $|\lambda_i\rangle$ are the eigenvectors of the operator L.

We let L act on the state $|A\rangle$:

$$L|A\rangle = \sum_i \alpha_i L|\lambda_i\rangle = \sum_i \alpha_i \lambda_i |\lambda_i\rangle$$

Note: λ_i are the eigenvalues of the eigenvectors $|\lambda_i\rangle$.

What we have so far is a new state vector A_L:

$$|A_L\rangle = \sum_i \alpha_i \lambda_i |\lambda_i\rangle$$

We take the inner product of $|A_L\rangle$ with $\langle A|$:

$$\langle A|A_L\rangle = \sum_i \langle\lambda_i|\alpha_i^* \sum_i \alpha_i \lambda_i |\lambda_i\rangle =;$$

As the $|\lambda_i\rangle$ build an orthonormal basis system, the double sum collapses via the Kronecker delta:

$$\sum_i \langle\lambda_i| \sum_i |\lambda_i\rangle = \delta_{ii}$$

Result:

$$\langle A|A_L\rangle = \sum_i \alpha_i^* \alpha_i \lambda_i \coloneqq \sum_i P_i \lambda_i$$

This is the statistical average.

In summa: to calculate the expectation value $\langle L\rangle$ (the average) of a Hermitian operator L, we "sandwich" the operator in between the normalized state vectors A of a quantum system.

$$\langle A|L|A\rangle = \langle L\rangle$$

State vectors, evolution of state vectors with time:

This is principle 5 of quantum mechanics: The evolution of state vectors with time is unitary.

Let us consider a closed system (no external forces etc.) and two distinguishable states ψ and θ that changes with time: $|\psi(t)\rangle$ and $|\theta(t)\rangle$.

The states at time t are given by some operation that we call $U(t)$, an operator acting on the states at time zero:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

$$\langle\psi(t)| = \langle\psi(0)|U^\dagger$$

$$|\theta(t)\rangle = U(t)|\theta(0)\rangle$$

U is called the time-development operator for the system.

Suppose $|\psi(0)\rangle$ and $|\theta(0)\rangle$ are two distinguishable states (in a closed system), then this must be valid for all times:

$$\langle\psi(0)|\theta(0)\rangle = \langle\psi(t)|\theta(t)\rangle = 0$$

We take a look at $\langle\psi(t)|\theta(t)\rangle$:

$$\langle\psi(t)|\theta(t)\rangle = 0 = \langle\psi(0)|U^\dagger(t)U(t)|\theta(0)\rangle$$

From this follows that $U^\dagger(t)U(t)$ must be the identity operator I:

$$U^\dagger(t)U(t) = I$$

An operator that satisfies $U^\dagger(t)U(t) = I$ is called unitary, therefore time evolution is unitary in quantum mechanics.

State vector of near singlet state:

The near-singlet state is a state of partial entanglement and has the state-vector $\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$ or in the extended form:

$$|nearsing\rangle = 0\big|uu\rangle + \sqrt{0{,}6}\big|ud\rangle + \left(-\sqrt{0{,}4}\right)|du\rangle + 0|dd\rangle$$

In contrast the singlet state is a state of complete entanglement and has the state vector $\frac{1}{\sqrt{2}}|ud\rangle - \frac{1}{\sqrt{2}}|du\rangle$ or in the extended form:

$$|sing\rangle = 0\left|uu\rangle + \frac{1}{\sqrt{2}}\right|ud\rangle + \left(-\frac{1}{\sqrt{2}}\right)|du\rangle + 0|dd\rangle$$

The singlet state is in an equilibrium concerning the weights of the basis vectors $|ud\rangle$ and $|du\rangle$, the near-singlet state is not.

State vectors, operators and state vectors:

1. Operators are used to calculate eigenvalues and eigenvectors.
2. Operators act on state-vectors, not on actual physical system.
3. When an operator acts on a state-vector, it produces a new state vector.

Note: measuring an observable is **not always** the same as operating with the corresponding operator on the state.

Example: if a spin is prepared in the right-state $|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$ and we act with the operator σ_z, the result would be the state-vector $\frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$.

The spin itself after the measurement in z-direction would be either up $|u\rangle$ or down $|d\rangle$.

State vectors, phase factor and state vectors:

A number of the form $z = e^{i\varphi}$ has the absolute value 1: $\left|e^{i\varphi}\right| = \sqrt{e^{i\varphi}e^{-i\varphi}} = \sqrt{e^0} = \sqrt{1} = 1$. It is called a phase factor.

No measurable quantity, no observable is sensitive to an overall phase-factor, so we can ignore it when specifying states.

State vectors, physical properties of state vectors:

To define a direction in three-dimensional space it takes two angles – two parameters.

The general spin state is defined by two complex numbers α_u and α_d: four real parameters:

$$\alpha_u|u\rangle + \alpha_d|d\rangle$$

The general spin state has to be normalized, ${\alpha_u}^2 + {\alpha_d}^2 = 1$: minus one parameter.

The general spin does not depend on the overall phase factor: minus one parameter.

This leaves two real parameters to specify the state of a spin.

State vector of product state:

Given two single spin states, $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$ and $|B\rangle = \beta_u|u\rangle + \beta_d|d\rangle$.

The product state describing the system:

$$|product\ state\rangle = \{\alpha_u|u\rangle + \alpha_d|d\rangle\}\otimes\{\beta_u|u\rangle + \beta_d|d\rangle\}$$

Note: $\otimes$ is the tensor product.

Expanding and switching to composite notation gives

$$|product\ state\rangle = \alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

The product state represents a classical system with complete knowledge about both subsystems and combined system.

State vector, representing spin states using state vectors:

We have a single spin system $|A\rangle$ and chose $|u\rangle$ and $|d\rangle$ as basis vectors. With this we can write any state $|A\rangle$ as linear superposition:

$$|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$$

We get back the components α_u and α_d by:

$$\alpha_u = \langle u|A\rangle \text{ resp. } \alpha_u^* = \langle A|u\rangle$$

$$\alpha_d = \langle d|A\rangle \text{ resp. } \alpha_d^* = \langle A|d\rangle$$

The quantity $\alpha_u^*\alpha_u$ is the probability that the spin would be measured as $\sigma_z = +1$, spin up.

The quantity $\alpha_d^*\alpha_d$ is the probability that the spin would be measured as $\sigma_z = -1$, spin $down$.

The values α_u and α_d are the probability amplitudes. To measure the probabilities, they must be squared:

$$P_u = \langle A|u\rangle\langle u|A\rangle$$

$$P_d = \langle A|d\rangle\langle d|A\rangle$$

$|u\rangle$ and $|d\rangle$ are mutually orthogonal:

$$\langle u|d\rangle = \langle d|u\rangle = 0$$

The total probability for the spin:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

This is equivalent to the vector $|A\rangle$ being normalized:

$$\langle A|A\rangle = 1$$

The state of a system is represented by a unit (normalized) vector in a space of states.

State vector of singlet state:

The singlet state is a state of complete entanglement and has the state vector $\frac{1}{\sqrt{2}}|ud\rangle - \frac{1}{\sqrt{2}}|du\rangle$ or in the extended form:

$$|sing\rangle = 0\left|uu\rangle + \frac{1}{\sqrt{2}}\right|ud\rangle + \left(-\frac{1}{\sqrt{2}}\right)|du\rangle + 0|dd\rangle$$

In contrast the near-singlet state is a state of partial entanglement and has the state-vector $\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$ or in the extended form:

$$|nearsing\rangle = 0\left|uu\rangle + \sqrt{0{,}6}\right|ud\rangle + \left(-\sqrt{0{,}4}\right)|du\rangle + 0|dd\rangle$$

The singlet state is in an equilibrium concerning the weights of the basis vectors $|ud\rangle$ and $|du\rangle$, the near-singlet state is not.

State vectors, time derivative of state vectors:

Prerequisite

Time evolution is unitary in quantum mechanics:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

If ε is very small, the unitary operator $U(\varepsilon)$ is close to the unit operator:

$$U(\varepsilon) = I - i\varepsilon H$$

Note: H is an observable with a complete set of eigenvectors and eigenvalues – the Hamiltonian.

End prerequisite

Time evolution of a state $\psi(t)$ can be written with the unitary time development operator $U(t)$:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

We begin with the infinitesimal case $t = \varepsilon$ and apply the time development operator:

$$|\psi(\varepsilon)\rangle = U(\varepsilon)|\psi(0)\rangle = (I - i\varepsilon H)|\psi(0)\rangle =$$

$$I|\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle = |\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle$$

We get:

$$|\psi(\varepsilon)\rangle = |\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle$$

We build the differential equation:

$$|\psi(\varepsilon)\rangle = |\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle$$

$$|\psi(\varepsilon)\rangle - |\psi(0)\rangle = -i\varepsilon H|\psi(0)\rangle$$

$$\frac{|\psi(\varepsilon)\rangle - |\psi(0)\rangle}{\varepsilon} = -\frac{i\varepsilon H|\psi(0)\rangle}{\varepsilon}$$

$$\frac{|\psi(\varepsilon)\rangle - |\psi(0)\rangle}{\varepsilon} = -iH|\psi(0)\rangle$$

This is the time derivative of the state vector ψ:

$$\frac{\partial|\psi(0)\rangle}{\partial t} = -iH|\psi(0)\rangle$$

We can replace $|\psi(0)\rangle$ by any fixed time $|\psi(t)\rangle$:

$$\frac{\partial|\psi(t)\rangle}{\partial t} = -iH|\psi(t)\rangle$$

What we got is the time-dependent Schrödinger equation.

State vectors, time evolution of state vectors:

Let $|\psi(t)\rangle$ be a quantum state, varying with time t.

Knowing the state at a specific time $t = 0$ we can use quantum equations of motion to calculate the state at any time by acting on $|\psi(0)\rangle$ with the time development operator $U(t)$:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

State vectors, wave functions and state vectors:

We have a basis of states for some quantum system with the orthonormal basis vectors $|\alpha_1\rangle$, $|\alpha_2\rangle$, … resp. $\langle\alpha_1|$, $\langle\alpha_2|$, …

$|\alpha_1\rangle$, $|\alpha_2\rangle$, … belongs to a complete set of commutating observables A_1, A_2, … with eigenvalues α_1, α_2, …

Any state vector $|\psi\rangle$ can be expanded in this basis:

$$|\psi\rangle = \sum_j \psi(\alpha_j)|\alpha_j\rangle$$

The quantities $\psi(\alpha_j)$ are the coefficients, each of them equal to the inner product of $|\psi\rangle$ with one of the basis vectors $\langle\alpha_j|$:

$$\psi(\alpha_j) = \langle\alpha_j|\psi\rangle$$

The set of coefficients $\psi(\alpha_j)$ is called the wave function of the system in the basis defined by the observables A_j.

Note: the probability for the commuting observables to have values α_1, α_2, …:

$$P(\alpha_j) = \psi^*(\alpha_j)\psi(\alpha_j)$$

Note: the total probability sums up to one:

$$\sum_j \psi^*(\alpha_j)\psi(\alpha_j) = 1$$

Statistical correlation:

In general: let $P(a, b)$ the probability distribution for two variables a and b.

If the variables are completely uncorrelated, the probability will factorize:

$$P(a, b) = P(a)P(b)$$

$$P(a, b) - P(a)P(b) = 0$$

In quantum mechanics

Let A and B be two observables (operators),
$\langle A\rangle$ the expectation value (average) of observable A,
$\langle B\rangle$ the expectation value (average) of observable B,
$\langle AB\rangle$ the expectation value (average) of the product of the operators A and B.

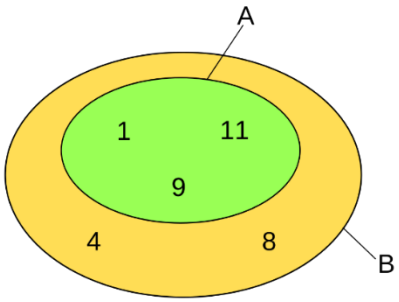
The two observables are correlated:

$$\langle AB\rangle = \langle A\rangle\langle B\rangle$$

$$\langle AB\rangle - \langle A\rangle\langle B\rangle = 0$$

Subset:

A is a proper subset of B. *(Graphic courtesy Wikipedia)*



Sums, integrals replacing sums:

Schematically:

$$\sum_i \rightarrow \int dx$$

The inner product discrete:

Let $|A\rangle$, $|B\rangle$ be two state vectors written in an orthonormal basis $|\lambda_i\rangle$:

$$|A\rangle = \sum_i \alpha_i |\lambda_i\rangle$$

$$|B\rangle = \sum_i \beta_i |\lambda_i\rangle$$

$$\langle A| = \sum_i \langle \lambda_i | \alpha_i^*$$

We build the inner product:

$$\langle A|B\rangle = \sum_i \langle \lambda_i|\alpha_i^* \cdot \sum_i \beta_i |\lambda_i\rangle = \sum_i \alpha_i^* \langle \lambda_i| \cdot \sum_i |\lambda_i\rangle \beta_i =;$$

The $|\lambda_i\rangle$ build an orthonormal basis, so the summation collapses to the Kronecker delta:

$$\sum_i \langle \lambda_i| \sum_i |\lambda_i\rangle = \delta_{ii}$$

We get:

$$\langle A|B\rangle = \sum_i \alpha_i^* \beta_i$$

The inner product continuous.

In the discrete case the α_i^* and β_i depend on the i basis vectors – in the continuous case they depend on the variable x.

The sum transforms into the integral:

$$\langle A|B\rangle = \int_{-\infty}^{\infty} \alpha^*(x)\beta(x)dx$$

Note: $\alpha^*(x)$ or $\alpha(x)$ and $\beta(x)$ then would be the corresponding wave functions to A and B.

Note: this works best if the wave functions A and B are normalized:

$$\int_{-\infty}^{\infty} \alpha^*(x)dx = 1$$

$$\int_{-\infty}^{\infty} \beta(x)dx = 1$$

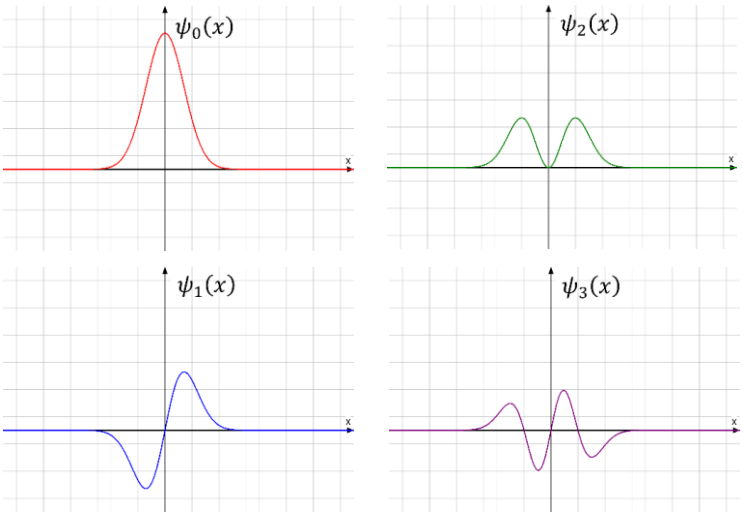
Symmetric eigenfunctions:

The eigenfunctions of the harmonic oscillator have a characteristic pattern.

Each eigenfunction is a polynomial in x multiplied by $e^{-\frac{\omega}{2\hbar}x^2}$.

The term $e^{-\frac{\omega}{2\hbar}x^2}$ makes these eigenfunctions normalizable.

The polynomial makes successive eigenfunctions alternate between being symmetric and antisymmetric.



Systems:

Systems, number of parameters characterizing systems:

The general state of a single spin system is defined by two complex numbers, α_u and α_d. This gives four real parameters.

The normalization condition: $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$ reduces the number of variables to three.

The physical properties of a state-vector do not depend on the overall phase-factor, this reduces the number of variables to two.

This is the same number of parameters needed to define a direction in a 3-dimensional space – two angles are needed.

Systems, combining quantum systems:

Prerequisite

We have two single spin systems of Alice and Bob with state vectors $|a\rangle$ for the system of Alice and $|b\rangle$ for the system of Bob (sometimes written as $|b\}$ to emphasize that they are not in the same space of states). Both systems are two-dimensional.

We can combine the two systems and get a four-dimensional system with basis vectors $|ab\rangle$.

End prerequisite

Let M be a linear operator (a matrix) acting on the space of states of a composite system made from two single spins.

M is a 4×4 matrix.

The matrix elements can be constructed by sandwiching the operator between basis vectors:

$$\langle a'b'|M|ab\rangle = M_{a'b',ab}$$

Note: $a'b'$ and ab each are a single index of the combined system, a single basis vector of an orthonormal basis:

$$\langle a'b'|ab\rangle = \delta_{a'a}\delta_{b'b} = \begin{cases} 1 \; if \; a' = a \; and \; b' = b \\ 0 \qquad\qquad else \end{cases}$$

Any state in the composite system can be expressed by help of the basis vectors:

$$|\psi\rangle = \sum_{a,b} \psi(a,b)|ab\rangle$$

Note: in the case of combining two single spin systems the wave function $\psi(a,b)$ has four components matching the four basis vectors $|ab\rangle$.

Tensor product of matrices:

Let A and B be two 2×2 matrices: $A \coloneqq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{21} \end{pmatrix}$, $B \coloneqq \begin{pmatrix} b_{11} & ba_{12} \\ b_{21} & b_{21} \end{pmatrix}$

The matrix version of the tensor product, sometimes called the Kronecker product:

$$A \otimes B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} =$$

$$\begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

Tensor product in composite form:

Let A and B two single spin systems, described each in the up and $down$ basis.

The tensor product of the up and down state vectors (for each subsystem):

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We combine by help of the tensor product:

$$|uu\rangle = |u\rangle \otimes |u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The same way the other combinations:

$$|ud\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |du\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } |dd\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

We combine operators. $\sigma_z \coloneqq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\tau_x \coloneqq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$:

$$\sigma_z \otimes \tau_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & -1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

We apply $\sigma_z \tau_x \coloneqq \sigma_z \otimes \tau_x$ to $|ud\rangle$:

$$\sigma_z \tau_x |ud\rangle = (\sigma_z \otimes \tau_x)|ud\rangle = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |uu\rangle$$

This result is according to the (short form) spin operation table, the operator σ_z etc. acting on the first index, the operator τ_x etc. acting on the second index:

	two-spin eigenvectors							
	$\|uu\rangle$		$\|ud\rangle$		$\|du\rangle$		$\|dd\rangle$
σ_z	$\|uu\rangle$		$\|ud\rangle$		$-\|du\rangle$		$-\|dd\rangle$
σ_x	$\|du\rangle$		$\|dd\rangle$		$\|uu\rangle$		$\|ud\rangle$
σ_y	$i\|du\rangle$		$i\|dd\rangle$		$-i\|uu\rangle$		$-i\|ud\rangle$
τ_z	$\|uu\rangle$		$-\|ud\rangle$		$\|du\rangle$		$-\|dd\rangle$
τ_x	$\|ud\rangle$		$\|uu\rangle$		$\|dd\rangle$		$\|du\rangle$
τ_y	$i\|ud\rangle$		$-i\|uu\rangle$		$i\|dd\rangle$		$-i\|du\rangle$

Test for entanglement:

prerequisite

Suppose the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$. Then the composite wave function also is product of Bob's factor and Alice's factor:

$$\psi(a,b) = \vartheta(a)\theta(b)$$

Alice's density matrix:

$$\rho_{a\prime a} = \vartheta^*(a)\vartheta(a')\sum_b \theta^*(b)\theta(,b)$$

As the state $|\psi\rangle$ is a product state of Bob's factor $|\theta\rangle$ and Alice's factor $|\vartheta\rangle$, both Alice's and Bob's state separately are normalized, so:

$$\sum_b \theta^*(b)\theta(,b) = 1$$

And Alice's density matrix becomes $\rho_{a\prime a} = \vartheta^*(a)\vartheta(a')$.

End prerequisite

We prove a theorem about the eigenvalues of Alice's density matrix that is only true for product states but not for entangled states and thus can serve to identify them: for product states the density matrix of Alice or Bob has exactly one eigenvalue of value one.

The eigenvalue equation for Alice's matrix $\rho_{a\prime a}$:

$$\sum_a \rho_{a'a}\alpha_a = \lambda\alpha_a =$$

$$\sum_a \vartheta^*(a)\vartheta(a')\alpha_a = \vartheta(a')\sum_a \vartheta^*(a)\alpha_a$$

$\sum_a \vartheta^*(a)\alpha_a$ has the form of an inner product. If the column vector α is orthogonal to ϑ, then $\sum_a \vartheta^*(a)\alpha_a$ is zero giving an eigenvector with eigenvalue zero.

In a space state of dimension N we have $N-1$ vectors orthogonal to ϑ, so we have only one possible direction for an eigenvector with nonzero eigenvalue $\vartheta(a)$:

$$\vartheta^*(a)\alpha_a = 0 \text{ for all } \alpha_a \neq \vartheta(a) \text{ and } 1 \text{ for } \alpha_a = \vartheta(a).$$

Alice's system is in a pure state, all of her observations are described as if Bob never existed.

In a maximally entangled system on the other hand Alice's density matrix is proportional to the unit matrix with all equal eigenvalues $\frac{1}{N}$:

$$\rho_{a'a} = \frac{1}{N}\delta_{a'a}$$

As the density matrix gives the probability for an outcome this means that every outcome has equal possibility.

For partial entanglement the weights of $\rho_{a'a}$ move from the equal distribution towards a concentration on a single value 1 on the diagonal of the density matrix.

Although in a maximum entangled state Alice can't predict the outcome of her experiments, she knows (after the experiment has been done) exactly about the relation between her and Bob's outcomes.

For reasons of completeness a worked-out example (this may become a little bit lengthy…)

The system of Alice:

$$|A\rangle = \sqrt{0{,}6}|u\rangle + \sqrt{0{,}4}|d\rangle = \begin{pmatrix}\sqrt{0{,}6}\\ \sqrt{0{,}4}\end{pmatrix}$$

The system of Bob:

$$|B\rangle = \sqrt{0{,}8}|u\rangle + \sqrt{0{,}2}|d\rangle = \begin{pmatrix}\sqrt{0{,}8}\\ \sqrt{0{,}2}\end{pmatrix}$$

Both states are normalized:

$$\sqrt{0{,}6}^2 + \sqrt{0{,}4}^2 = 1$$

$$\sqrt{0{,}8}^2 + \sqrt{0{,}2}^2 = 1$$

The wave function of Alice:

$$\chi(u) = \sqrt{0{,}6}$$

$$\chi(d) = \sqrt{0{,}4}$$

The wave function of Bob:

$$\phi(u) = \sqrt{0{,}8}$$

$$\phi(d) = \sqrt{0{,}2}$$

The probability for Alice to measure spin up:

$$\chi^*(u)\chi(u) = \sqrt{0{,}6}\cdot\sqrt{0{,}6} = 0{,}6$$

The probability for Alice to measure spin down:

$$\chi^*(d)\chi(d) = \sqrt{0{,}4}\cdot\sqrt{0{,}4} = 0{,}4$$

The probability for Bob to measure spin up:

$$\phi^*(u)\phi(u) = \sqrt{0{,}8}\cdot\sqrt{0{,}8} = 0{,}8$$

The probability for Bob to measure spin down:

$$\phi^*(d)\phi(d) = \sqrt{0{,}2} \cdot \sqrt{0{,}2} = 0{,}2$$

The two systems are combined by help of the tensor product:

$$\begin{pmatrix}\sqrt{0{,}6}\\ \sqrt{0{,}4}\end{pmatrix} \otimes \begin{pmatrix}\sqrt{0{,}8}\\ \sqrt{0{,}2}\end{pmatrix} = \begin{pmatrix}\sqrt{0{,}6}\begin{pmatrix}\sqrt{0{,}8}\\ \sqrt{0{,}2}\end{pmatrix}\\ \sqrt{0{,}4}\begin{pmatrix}\sqrt{0{,}8}\\ \sqrt{0{,}2}\end{pmatrix}\end{pmatrix} = \begin{pmatrix}\sqrt{0{,}6}\cdot\sqrt{0{,}8}\\ \sqrt{0{,}6}\cdot\sqrt{0{,}2}\\ \sqrt{0{,}4}\cdot\sqrt{0{,}8}\\ \sqrt{0{,}4}\cdot\sqrt{0{,}2}\end{pmatrix} = \begin{pmatrix}\sqrt{0{,}48}\\ \sqrt{0{,}12}\\ \sqrt{0{,}32}\\ \sqrt{0{,}08}\end{pmatrix}$$

We now „forget“ how this combined system was built and work with the wave function of the combined system:

$$\psi(ab) = \phi(a)\chi(b) = \phi(u)\chi(u) + \phi(u)\chi(d) + \phi(d)\chi(u) + \phi(d)\chi(d) =$$
$$\psi(uu) + \psi(ud) + \psi(du) + \psi(dd)$$

The wave function of the combined system in detail:

$$\psi(uu) = \sqrt{0{,}48}$$
$$\psi(ud) = \sqrt{0{,}12}$$
$$\psi(du) = \sqrt{0{,}32}$$
$$\psi(dd) = \sqrt{0{,}08}$$

The wave function of the combined system is normalized:

$$\psi^*(uu)\psi(uu) + \psi^*(ud)\psi(ud) + \psi^*(du)\psi(du) + \psi^*(dd)\psi(dd) = 1$$

The density matrix of Alice:

$$\rho_{a'a} = \sum\nolimits_b \psi^*(ab)\psi(a'b)$$

We expand this:

$$\rho_{uu} = \psi^*(uu)\psi(uu) + \psi^*(ud)\psi(ud)$$
$$\rho_{ud} = \psi^*(du)\psi(uu) + \psi^*(dd)\psi(ud)$$
$$\rho_{du} = \psi^*(uu)\psi(du) + \psi^*(ud)\psi(dd)$$
$$\rho_{dd} = \psi^*(du)\psi(du) + \psi^*(dd)\psi(dd)$$

With concrete values:

$$\rho_{uu} = \sqrt{0{,}48}\sqrt{0{,}48} + \sqrt{0{,}12}\sqrt{0{,}12} = 0{,}6$$
$$\rho_{ud} = \sqrt{0{,}32}\sqrt{0{,}48} + \sqrt{0{,}08}\sqrt{0{,}12} = \sqrt{0{,}1536} + \sqrt{0{,}0096} = \sqrt{0{,}24}\ (*)$$
$$\rho_{du} = \sqrt{0{,}48}\sqrt{0{,}32} + \sqrt{0{,}12}\sqrt{0{,}08} = \sqrt{0{,}1536} + \sqrt{0{,}0096} = \sqrt{0{,}24}$$
$$\rho_{dd} = \sqrt{0{,}32}\sqrt{0{,}32} + \sqrt{0{,}08}\sqrt{0{,}08} = 0{,}4$$

Note: $(*)$ numerical result, this ought to be proven mathematically.

The density matrix of Alice:

$$\rho_{a'a} = \begin{pmatrix} 0{,}6 & \sqrt{0{,}24} \\ \sqrt{0{,}24} & 0{,}4 \end{pmatrix}$$

The eigenvalue equation for Alice's density matrix:

$$det\begin{pmatrix} 0{,}6-\lambda & \sqrt{0{,}24} \\ \sqrt{0{,}24} & 0{,}4-\lambda \end{pmatrix} = 0$$

$$(0{,}6-\lambda)(0{,}4-\lambda) - 0{,}24 = 0$$

$$\lambda^2 - \lambda - 0{,}24 + 0{,}24 = 0$$

$$\lambda^2 - \lambda = \lambda(\lambda - 1) = 0$$

We have two eigenvalues, $\lambda_1 = 1$ and $\lambda_2 = 0$

The eigenvector equation for the eigenvalue $\lambda_1 = 1$:

$$\begin{pmatrix} 0{,}6 & \sqrt{0{,}24} \\ \sqrt{0{,}24} & 0{,}4 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}$$

$$0{,}6 \cdot x + \sqrt{0{,}24} \cdot y = x$$

$$\sqrt{0{,}24} \cdot x + 0{,}4 \cdot y = y$$

$$-0{,}4x + \sqrt{0{,}24}y = 0$$

$$\sqrt{0{,}24}x - 0{,}6y = 0$$

$$x = \frac{\sqrt{0{,}24}y}{0{,}4}$$

$$y = \frac{\sqrt{0{,}24}x}{0{,}6}$$

$$x = \frac{\sqrt{0{,}24} \cdot \frac{\sqrt{0{,}24}x}{0{,}6}}{0{,}4} = \frac{0{,}24}{0{,}24}x = x$$

$$y = \frac{\sqrt{0{,}24}}{0{,}6}x$$

The eigenvector for the eigenvalue 1:

$$\begin{pmatrix} 1 \\ \frac{\sqrt{0{,}24}}{0{,}6} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{\sqrt{0{,}24}}{\sqrt{36}} \end{pmatrix} = \begin{pmatrix} 1 \\ \sqrt{2/3} \end{pmatrix}$$

The eigenvector equation for the eigenvalue $\lambda_1 = 0$:

$$\begin{pmatrix} 0{,}6 & \sqrt{0{,}24} \\ \sqrt{0{,}24} & 0{,}4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$0{,}6 \cdot x + \sqrt{0{,}24} \cdot y = 0$$

$$\sqrt{0{,}24} \cdot x + 0{,}4 \cdot y = 0$$

$$x = -\frac{\sqrt{0{,}24}y}{0{,}6}$$

$$y = -\frac{\sqrt{0{,}24}x}{0{,}4}$$

$$x = \frac{\sqrt{0{,}24} \cdot \frac{\sqrt{0{,}24}x}{0{,}4}}{0{,}6} = \frac{0{,}24}{0{,}24}x \rightarrow x = x$$

$$y = -\frac{\sqrt{0{,}24}}{0{,}4}x$$

The eigenvector for the eigenvalue 0:

$$\begin{pmatrix} 1 \\ -\frac{\sqrt{0{,}24}}{0{,}4} \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{\sqrt{0{,}24}}{\sqrt{16}} \end{pmatrix} = \begin{pmatrix} 1 \\ -\sqrt{1{,}5} \end{pmatrix}$$

We check orthogonality:

$$\begin{pmatrix} 1 \\ \sqrt{2/3} \end{pmatrix} \begin{pmatrix} 1 \\ -\sqrt{1{,}5} \end{pmatrix} = 1 \cdot 1 - \sqrt{2/3} \cdot -\sqrt{1{,}5} = 0$$

Both eigenvectors are orthogonal. In contrast to the combined state we take the singlet state, a maximally entangled state and check this one.

The wave function for the singlet state:

$$\psi(uu) = 0$$

$$\psi(ud) = \frac{1}{\sqrt{2}}$$

$$\psi(du) = -\frac{1}{\sqrt{2}}$$

$$\psi(dd) = 0$$

The wave function of the singled state is normalized:

$$\psi^*(uu)\psi(uu) + \psi^*(ud)\psi(ud) + \psi^*(du)\psi(du) + \psi^*(dd)\psi(dd) = 1$$

The density matrix of Alice as part of the singlet state:

$$\rho_{a'a} = \sum_b \psi^*(ab)\psi(a'b)$$

We expand this:

$$\rho_{uu} = \psi^*(uu)\psi(uu) + \psi^*(ud)\psi(ud)$$
$$\rho_{ud} = \psi^*(du)\psi(uu) + \psi^*(dd)\psi(ud)$$
$$\rho_{du} = \psi^*(uu)\psi(du) + \psi^*(ud)\psi(dd)$$
$$\rho_{dd} = \psi^*(du)\psi(du) + \psi^*(dd)\psi(dd)$$

With concrete values:

$$\rho_{uu} = 0 + \frac{1}{2} = \frac{1}{2}$$
$$\rho_{ud} = 0$$
$$\rho_{du} = 0$$
$$\rho_{dd} = \frac{1}{2} + 0 = \frac{1}{2}$$

The density matrix of Alice:

$$\rho_{a'a} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

The eigenvalue equation for Alice's density matrix:

$$det \begin{pmatrix} 0{,}5 - \lambda & 0 \\ 0 & 0{,}5 - \lambda \end{pmatrix} = 0$$
$$(0{,}5 - \lambda)^2 = 0$$

We have one eigenvalue:

$$\lambda_{1/2} = 0{,}5$$

The eigenvector equation for the eigenvalue $\lambda_{1/2} = 0{,}5$:

$$\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{2} \begin{pmatrix} x \\ y \end{pmatrix}$$

Any vector fulfills this eigenvector equation. Obviously, we have neither an eigenvector to the eigenvalue one nor an eigenvector to the eigenvalue zero – the combined system is not a product system.

The density matrix of Alice shows complete uncertainty about the outcomes of her subsystem.

Time:

Time, change in expectation values over time:

Let L be an operator (a matrix), H be the quantum Hamiltonian.

The change of the expectation value (the average) of the operator L:

$$\frac{d}{dt}\langle L\rangle = \frac{i}{\hbar}\langle |H, L|\rangle$$

Note: $|H, L|$ is the commutator of the operators H and L:

$$|H, L| = HL - LH$$

Note: if the operators commute, $HL = LH$, the commutator is zero and there is no time change in the expectation value of the operator L.

Note: this is often written in the shorthand form:

$$\frac{d}{dt}L = \frac{i}{\hbar}|H, L|$$

Time, conservation of distinctions and time:

Principle five of quantum mechanics: The evolution of state-vectors with time is unitary.

Principle five of quantum mechanics follows from the "minus first law", the conservation of distinctions. Distinguishable states are orthogonal to each other.

Suppose $|\psi(0)\rangle$ and $|\phi(0)\rangle$ are two distinguishable states. Therefore, they must have an orthogonal representation (no overlap):

$$\langle\psi(0)|\phi(0)\rangle = 0$$

The minus first law requires this to be true for all times:

$$\langle\psi(t)|\phi(t)\rangle = 0$$

We have a time-development operator $U(t)$.

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

$$\langle\psi(t)| = \langle\psi(0)|U^{\dagger}(t)$$

Note: $U^{\dagger}(t)$ is the Hermitian conjugated of $U(t)$.

$$|\phi(t)\rangle = U(t)|\phi(0)\rangle$$

We modify $\langle\psi(t)|\phi(t)\rangle = 0$ by the time-development operator:

$$\langle\psi(t)|\phi(t)\rangle = \langle\psi(0)\big|U^{\dagger}(t)U(t)\big|\phi(0)\rangle = 0$$

This requests $U^{\dagger}(t)U(t)$ to be the identity matrix (operator):

$$U^{\dagger}U = I$$

An operator with this property is called unitary.

Note: if $|A\rangle$ and $|B\rangle$ are two distinct states and U is a unitary operator, then the inner product of $|A\rangle$ and $|B\rangle$ is the same as the inner product of $U|A\rangle$ and $U|B\rangle$. This is called the conservation of distinctions or the conservation of overlaps.

Time, determinism and time:

Time evolution of a state vector is deterministic in probability.

Let the state of a spin be $|r\rangle$.

The outcome of a measurement $\sigma_x = 1$.

The outcome of a measurement σ_z will be a series of -1 and 1, giving an average of 0.

Quantum evolution of states allows us to compute the probabilities of the outcomes of later experiments.

Time, time evolution operator:

Time evolution is unitary in quantum mechanics:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

$U(t)$ is a unitary operator.

For small times $t \coloneqq \varepsilon$ the unitary operator $U(\varepsilon)$ is close to the unit operator:

$$U(\varepsilon) = I - i\varepsilon H$$

$$U^\dagger(\varepsilon) = I + i\varepsilon H^\dagger$$

The unitary condition:

$$U^\dagger(\varepsilon)U(\varepsilon) = I$$

$$\left(I + i\varepsilon H^\dagger\right)(I - i\varepsilon H) = I$$

$$I^2 + Ii\varepsilon\left(H^\dagger - H\right) + \varepsilon^2 H^\dagger H = I$$

$$I + Ii\varepsilon\left(H^\dagger - H\right) + \varepsilon^2 H^\dagger H = I$$

We omit the second order in ε:

$$I + Ii\varepsilon\left(H^\dagger - H\right) = I$$

$$Ii\varepsilon\left(H^\dagger - H\right) = 0$$

$$H^\dagger - H = 0$$

$$H^\dagger = H$$

H is a Hermitian operator, an observable with a complete set of orthonormal eigenvectors and eigenvalues – the quantum Hamiltonian.

We begin with the infinitesimal case $t = \varepsilon$ and apply the time development operator:

$$|\psi(\varepsilon)\rangle = U(\varepsilon)|\psi(0)\rangle = (I - i\varepsilon H)|\psi(0)\rangle =$$

$$I|\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle = |\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle$$

We get:

$$|\psi(\varepsilon)\rangle = |\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle$$

We build the differential equation:

$$|\psi(\varepsilon)\rangle = |\psi(0)\rangle - i\varepsilon H|\psi(0)\rangle$$

$$|\psi(\varepsilon)\rangle - |\psi(0)\rangle = -i\varepsilon H|\psi(0)\rangle$$

$$\frac{|\psi(\varepsilon)\rangle - |\psi(0)\rangle}{\varepsilon} = -\frac{i\varepsilon H|\psi(0)\rangle}{\varepsilon}$$

$$\frac{|\psi(\varepsilon)\rangle - |\psi(0)\rangle}{\varepsilon} = -iH|\psi(0)\rangle$$

This is the time derivative of the state vector ψ:

$$\frac{\partial|\psi(0)\rangle}{\partial t} = -iH|\psi(0)\rangle$$

We can replace $|\psi(0)\rangle$ by any fixed time $|\psi(t)\rangle$:

$$\frac{\partial|\psi(t)\rangle}{\partial t} = -iH|\psi(t)\rangle$$

What we got is the time-dependent Schrödinger equation.

Time dependence:

1.

The time dependence of an observable is given by the commutator of the observable with the Hamiltonian,

$$\frac{d}{dt}L = \frac{i}{\hbar}|H, L|$$

or, in more elaborated writing:

$$\frac{d}{dt}\langle L\rangle = \frac{i}{\hbar}\langle|H, L|\rangle$$

Note: $\langle L\rangle$ and $\langle|H, L|\rangle$ are the expectation values (averages).

Note: $|H, L|$ is the commutator of the operators H and L:

$$|H, L| = HL - LH$$

Note: if the operators commute, $HL = LH$, the commutator is zero and there is no time change in the expectation value of the operator L.

2.

Let $|\psi(0)\rangle$ be an initial state at time $t = 0$.

Find the eigenvalues and eigenvectors of the Hamiltonian H by solving the time independent Schrödinger equation:

$$H|E_j\rangle = E_j|E_j\rangle$$

Note: E_j are the eigenvalues, $|E_j\rangle$ the according eigenvectors.

Calculate the initial coefficients:

$$\alpha_j(0) = E_j|\psi(0)\rangle$$

Rewrite $|\psi(0)\rangle$ in terms of eigenvectors $|E_j\rangle$ and initial coefficients $\alpha_j(0)$:

$$|\psi(0)\rangle = \sum_j \alpha_j(0)\,|E_j\rangle$$

Replace each $\alpha_j(0)$ with $\alpha_j(t)$:

$$|\psi(t)\rangle = \sum_j \alpha_j(t)\,|E_j\rangle$$

Replace $\alpha_j(t)$:

$$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j \cdot t}$$

We get the time dependence of the state $|\psi(t)\rangle$:

$$|\psi(t)\rangle = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j \cdot t}\,|E_j\rangle$$

Time dependent Schrödinger equation:

We get the time dependent Schrödinger equation of a state $|\psi(t)\rangle$ by applying the Hamiltonian to this state:

$$\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = -iH|\psi(t)\rangle$$

If we know the state vector at a specific time t, the equation gives what it will be next (and what it was before).

Particle dynamics and time dependent Schrödinger equation:

Let the Hamiltonian operator H be very simple, being a fixed constant times the momentum operator P:

$$H = cP$$

A classical physicist would use Hamilton's equations to describe a particle:

$$\frac{\partial H}{\partial p} = \dot{x}$$

and

$$\frac{\partial H}{\partial x} = -\dot{p}$$

Carrying out the partial derivatives with our simple Hamiltonian $H = cP$, these become

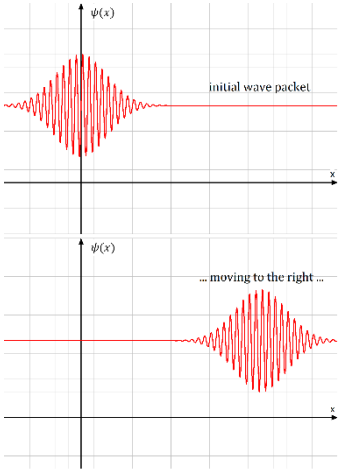
$$\frac{\partial H}{\partial p} = \dot{x} = c$$

and

$$\frac{\partial H}{\partial x} = -\dot{p} = 0$$

In the classical description of the particle, the momentum is conserved, and the particle moves with constant speed c.

In quantum mechanical description, the whole probability distribution and the expectation value move with velocity c – quantum mechanical and classical description match.



Solving the time dependent Schrödinger equation:

We get the time dependent Schrödinger equation of a state $|\psi(t)\rangle$ by applying the Hamiltonian to this state:

$$i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

This is the time dependent Schrödinger equation.

The Hamiltonian operator H represents the energy with eigenvalues E_j and eigenvectors $|E_j\rangle$:

$$H|E_j\rangle = E_j|E_j\rangle$$

Note: this is the time independent Schrödinger equation, used to find eigenvectors $|E_j\rangle$ and eigenvalues E_j.

Suppose we found all energy eigenvalues E_j and eigenvectors $|E_j\rangle$ of the time independent Schrödinger equation.

They form an orthogonal basis we can expand the state vector in:

$$|\psi\rangle = \sum_j \alpha_j |E_j\rangle$$

The basis vectors does not change with time but the α_j will:

$$|\psi(t)\rangle = \sum_j \alpha_j(t)|E_j\rangle$$

We feed this back into the time dependent Schrödinger equation $i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$:

$$i\hbar \sum_j \dot{\alpha}_j(t)|E_j\rangle = H \sum_j \alpha_j(t)|E_j\rangle =$$

$$\sum_j E_j \alpha_j(t)|E_j\rangle$$

We get:

$$i\hbar \sum_j \dot{\alpha}_j(t)|E_j\rangle - \sum_j E_j \alpha_j(t)|E_j\rangle = 0$$

$$\sum_j \left(i\hbar\dot{\alpha}_j(t) - E_j\alpha_j(t)\right)|E_j\rangle = 0$$

The eigenvectors $|E_j\rangle$ form an orthonormal basis, so the argument in the summation must be zero for every index j:

$$i\hbar\dot{\alpha}_j(t) - E_j\alpha_j(t) = 0$$

$$i\hbar\dot{\alpha}_j(t) = E_j\alpha_j(t)$$

$$\dot{\alpha}_j(t) = -\frac{i}{\hbar}E_j\alpha_j(t)$$

This is a differential equation with the solution:

$$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j \cdot t}$$

The factors $\alpha_j(0)$ are the values of the coefficients at time zero. We have:

$$|\psi(t)\rangle = \sum_j \alpha_j(t)|E_j\rangle = \sum_j \alpha_j(0)e^{-\frac{i}{\hbar}E_j \cdot t}|E_j\rangle$$

We get the values $\alpha_j(0)$ by the inner products of $|\psi\rangle$ with the basis eigenvectors:

$$\alpha_j(0) = \langle E_j|\psi(0)\rangle$$

The solution of the time dependent Schrödinger equation,

$$|\psi(t)\rangle = \sum_j \langle E_j|\psi(0)\rangle e^{-\frac{i}{\hbar}E_j \cdot t}|E_j\rangle$$

more elegant written as:

$$|\psi(t)\rangle = \sum_j |E_j\rangle\langle E_j|\psi(0)\rangle e^{-\frac{i}{\hbar}E_j \cdot t}$$

Time derivatives:

The time derivative of a state vector is its product with the Hamiltonian:

$$\frac{\partial|\psi\rangle}{\partial t} = -\frac{i}{\hbar}H|\psi\rangle$$

Note: this is the time dependent Schrödinger equation.

Note: the time dependent Schrödinger equation for a bra:

$$\frac{\partial\langle\psi|}{\partial t} = \frac{i}{\hbar}\langle\psi|H$$

Schrödinger equation for time derivatives:

Prerequisite

$[A, B]$ is the commutator of the operators (the matrices) A and B:

$$[A, B] = AB - BA$$

Note:

$$[A, B] = -[B, A]$$

If the commutator $[A, B]$ is zero, $AB = BA$, we say that the operators commute.

Note: every operator commutes with itself:

$$[A, A] = 0$$

End prerequisite

Let $\langle L \rangle$ be the expectation value of an observable at time t in a state represented by a ket $|\psi\rangle$ and a bra $\langle\psi|$:

$$\langle L \rangle = \langle \psi(t)|L|\psi(t)\rangle$$

We build the time derivative $\langle \dot{L} \rangle$:

$$\frac{d}{dt}\langle \psi(t)|L|\psi(t)\rangle = \langle \dot{\psi}(t)|L|\psi(t)\rangle + \langle \psi(t)|L|\dot{\psi}(t)\rangle$$

Note: L itself has no explicit time dependency.

We insert the bra and ket versions of the time dependent Schrödinger equation:

$$\frac{d}{dt}\langle \psi(t)|L|\psi(t)\rangle = \frac{i}{\hbar}(\langle \psi(t)|HL|\psi(t)\rangle - \langle \psi(t)|LH|\psi(t)\rangle) =$$

$$\frac{i}{\hbar}(\langle \psi(t)|[H, L]|\psi(t)\rangle)$$

We get:

$$\frac{d}{dt}\langle L \rangle = \frac{i}{\hbar}\langle H, L \rangle$$

Note: if the operators (the matrices) H and L commute, the expectation value of the observable L does not change with time.

Time development operator:

The quantum equation of time development:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

The operator U is called the time development operator for the system.

Note: instead of $\psi(0)$ we can choose any fixed time $\psi(t_0)$.

Conservation of distinctions and time development operator:

Principle five of quantum mechanics: The evolution of state-vectors with time is unitary.

This principle follows from the "minus first law", the conservation of distinctions.

Distinguishable states are orthogonal to each other.

Suppose $|\psi(0)\rangle$ and $|\phi(0)\rangle$ are two distinguishable states. Therefore, they must have an orthogonal representation (no overlap):

$$\langle\psi(0)|\phi(0)\rangle = 0$$

The minus first law requires this to be true for all times:

$$\langle\psi(t)|\phi(t)\rangle = 0$$

We have a time-development operator $U(t)$.

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

$$\langle\psi(t)| = \langle\psi(0)|U^{\dagger}(t)$$

Note: $U^{\dagger}(t)$ is the Hermitian conjugated of $U(t)$.

$$|\phi(t)\rangle = U(t)|\phi(0)\rangle$$

We modify $\langle\psi(t)|\phi(t)\rangle = 0$ by the time-development operator:

$$\langle\psi(t)|\phi(t)\rangle = \langle\psi(0)|U^{\dagger}(t)U(t)|\phi(0)\rangle = 0$$

This requests $U^{\dagger}(t)U(t)$ to be the identity matrix (operator):

$$U^{\dagger}U = I$$

An operator with this property is called unitary.

Note: if $|A\rangle$ and $|B\rangle$ are two distinct states and U is a unitary operator, then the inner product of $|A\rangle$ and $|B\rangle$ is the same as the inner product of $U|A\rangle$ and $U|B\rangle$. This is called the conservation of distinctions or the conservation of overlaps.

Time evolution:

In quantum mechanics, the Hamiltonian controls the time evolution of a system by the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\psi(t)}{\partial t} = H|\psi\rangle$$

Time evolution, determinism and time evolution:

In classical mechanics, there is no real difference between states and measurements. In quantum mechanics, the difference is profound.

Classical determinism allows us to predict the result of experiments. The quantum evolution of states allows us to compute the probabilities of the outcomes of later experiments.

Time independent Schrödinger equation:

The time-independent Schrödinger equation:

$$H|E_j\rangle = E_j|E_j\rangle$$

Note: H is the Hamiltonian, E_j the (energy) eigenvalue to the (energy) eigenvector $|E_j\rangle$.

We take a known particular value of energy E_j and calculate the ket-vector $|E_j\rangle$ that solves the equation or we search for eigenvectors $|E_j\rangle$ by trying arbitrary values of E_j.

Trace:

Trace of a density matrix:

Prerequisite

The trace of an operator L (a matrix that must be a square matrix) is defined as the sum of its diagonal elements. Let $|i\rangle$ and $\langle i|$ be a basis:

$$Tr\ L = \sum_i \langle i|L|i\rangle$$

End prerequisite

We have a single spin system of Alice in the $up - down$ basis:

$$|\psi\rangle = \alpha|u\rangle + \beta|d\rangle = \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix}$$

The wave function of Alice:

$$\psi(u) = \alpha;\ \psi^*(u) = \alpha^*;\ \psi(d) = \beta;\ \psi^*(d) = \beta^*$$

The density matrix of Alice:

$$\varrho_{a'a} = \begin{pmatrix}\alpha^*\alpha & \alpha^*\beta\\ \beta^*\alpha & \beta^*\beta\end{pmatrix}$$

$$\varrho_{uu} = \alpha^*\alpha$$

$$\varrho_{ud} = \alpha^*\beta$$

$$\varrho_{du} = \beta^*\alpha$$

$$\varrho_{dd} = \beta^*\beta$$

The $trace$ of the density matrix:

$$Tr\ \varrho_{a'a} = \varrho_{uu} + \varrho_{dd} = \alpha^*\alpha + \beta^*\beta$$

The trace of a density matrix is 1:

$$Tr(\varrho) = 1$$

The eigenvalues of a density matrix are all positive and lie between 0 and 1.

If one eigenvalue of a density matrix is 1, all others are zero.

For a pure state holds:

$$\varrho^2 = \varrho$$

$$Tr(\varrho^2) = 1$$

For a mixed or entangled state holds:

$$\varrho^2 \neq \varrho$$

$$Tr(\varrho^2) < 1$$

The trace of a product of two matrices A, B does not depend on their order of multiplication:

$$Tr(AB) = Tr(BA)$$

This is true even if:

$$AB \neq BA$$

Trace of a projection operator:

Prerequisite

A projection operator is the outer product of a normalized ket with its corresponding bra:

$$|\psi\rangle\langle\psi|$$

A projection operator projects a vector $|A\rangle$ onto the direction defined by $|\psi\rangle$:

$$|\psi\rangle\langle\psi|A\rangle = a|\psi\rangle$$

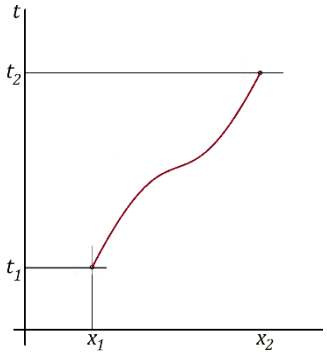
Note: a is a real number.

A projection operator is always a square matrix.

End prerequisite

The trace of a projection operator is 1.

Trajectories, path integrals and trajectories:



Suppose a classical particle starts at position x_1 at time t_1 and arrives at position x_2 at time t_2. Action is a technical term, and it stands for the integral of the Lagrangian between the end points of the trajectory.

For simple (classic) systems, the Lagrangian is kinetic energy minus potential energy. For a particle moving in one dimension the action is:

$$A = \int_{t_1}^{t_2} \left(\frac{m\dot{x}^2}{2} - V(x) \right) dt$$

Under all possible paths the stationary ones (e.g. the minima, least action) are possible solutions.

In quantum mechanics the idea of a well-defined trajectory has its limits in the Heisenberg Uncertainty Principle. The quantum mechanical question is:

Given a particle starts at (x_1, t_1), what is the probability amplitude it will show up at (x_2, t_2)?

With the simplification $t_2 - t_1 = t$ we call the amplitude $C(x_1, x_2, t)$ resp. $C_{1,2}$.

The initial state of the particle is:

$$|\psi(t_1)\rangle = |x_1\rangle$$

The state evolves to:

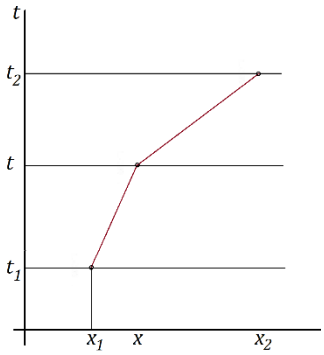
$$|\psi(t_2)\rangle = e^{-iHt}|x_1\rangle$$

Note: we use units with $\hbar = 1$.

The amplitude to detect the particle at $|x_2\rangle$ is the inner product of $|\psi(t_2)\rangle$ with $|x_2\rangle$:

$$C_{1,2} = \langle x_2|e^{-iHt}|x_1\rangle$$

Now we break up the time interval t into smaller intervals of size $\frac{t}{2}$.



The operator e^{-iHt} can be written as:

$$e^{-iHt} = e^{-iH\frac{t}{2}}e^{-iH\frac{t}{2}}$$

We insert the identity operator:

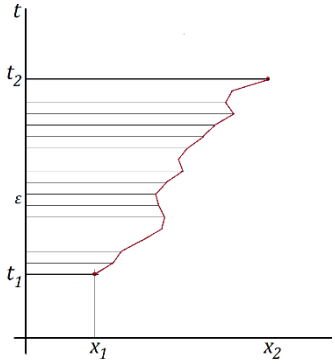
$$I = \int |x\rangle\langle x| \; dx$$

We rewrite the amplitude:

$$C_{1,2} = \int \left\langle x_2\middle|e^{-iH\frac{t}{2}}\middle|x\right\rangle \left\langle x\middle|e^{-iH\frac{t}{2}}\middle|x_1\right\rangle \; dx$$

The amplitude to go from x_1 to x_2 is the product of the amplitude to go from x_1 to x and the amplitude to go from x to x_2.

If we continue to divide into N time intervals of size ε, we have a product of many factors:



$$e^{-i\varepsilon H}$$

We define:

$$U(\varepsilon) = e^{-i\varepsilon H}$$

We write the entire product:

$$\langle x_2|U^N|x_1\rangle$$

We insert identity operators between each U and get the amplitude for the given path. In the limit of a large number of infinitesimal time intervals, the amplitude is an integral over all possible paths between the end points.

The elegant fact that Feynman discovered is that the amplitude for each path bears a simple relation to a familiar expression from classical mechanics – the action for that path.

The exact expression for each path is:

$$e^{i\frac{A}{\hbar}}$$

Note: A is the action for the individual path.

Feynman's formulation can be summarized:

$$C_{1,2} = \int_{paths} e^{i\frac{A}{\hbar}}$$

In quantum field theory it is the principal tool for formulating the laws of elementary particle physics.

Transposing:

In matrix notation, interchanging rows and columns is called transposing and indicated by a superscript T:

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & j \end{pmatrix}^T = \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & j \end{pmatrix}$$

Note: the diagonal remains unchanged.

A matrix needs not to be diagonal to transpose it:

$$\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}^T = \begin{pmatrix} a & d \\ b & e \\ c & f \end{pmatrix}$$

Triangle inequality:

For real vector spaces:

$$|\vec{X}||\vec{Y}| \geq |\vec{X} + \vec{Y}|$$

$$|\vec{X}||\vec{Y}| \geq \vec{X} \cdot \vec{Y}$$

Note: $\vec{X} \cdot \vec{Y}$ is the inner product, the dot product.

In squared form this is the Cauchy-Schwarz inequality:

$$|\vec{X}|^2 |\vec{Y}|^2 \geq |\vec{X} \cdot \vec{Y}|^2$$

For complex vector spaces:

Let $|X\rangle$ and $|Y\rangle$ be any two vectors in a complex vector space:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

This is the form of the Cauchy-Schwarz inequality that will lead to the uncertainty principle.

Triplet state:

Prerequisite

$\vec{\sigma}$ is the spin operator of Alice with the components σ_x, σ_y and σ_z according to three possible orientations of a single spin in space. $\vec{\tau}$ is the spin operator of Bob with components τ_x, τ_y and τ_z.

The effect of spin operators (matrices) on 2-Spin eigenvectors:

	two-spin eigenvectors							
	$\|uu\rangle$		$\|ud\rangle$		$\|du\rangle$		$\|dd\rangle$
σ_z	$\|uu\rangle$		$\|ud\rangle$		$-\|du\rangle$		$-\|dd\rangle$
σ_x	$\|du\rangle$		$\|dd\rangle$		$\|uu\rangle$		$\|ud\rangle$
σ_y	$i\|du\rangle$		$i\|dd\rangle$		$-i\|uu\rangle$		$-i\|ud\rangle$
τ_z	$\|uu\rangle$		$-\|ud\rangle$		$\|du\rangle$		$-\|dd\rangle$
τ_x	$\|ud\rangle$		$\|uu\rangle$		$\|dd\rangle$		$\|du\rangle$
τ_y	$i\|ud\rangle$		$-i\|uu\rangle$		$i\|dd\rangle$		$-i\|du\rangle$

End prerequisite

The triplet states for a combined spin system of Alice and Bob are maximally entangled states:

$$|T_1\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$$

$$|T_2\rangle = \frac{1}{\sqrt{2}}(|uu\rangle + |dd\rangle)$$

$$|T_3\rangle = \frac{1}{\sqrt{2}}(|uu\rangle - |dd\rangle)$$

The triplet states are eigenvectors of the operator (the matrix) $\vec{\sigma} \cdot \vec{\tau}$ with eigenvalue one:

$$\vec{\sigma} \cdot \vec{\tau}|T_1\rangle = |T_1\rangle$$

$$\vec{\sigma} \cdot \vec{\tau}|T_2\rangle = |T_2\rangle$$

$$\vec{\sigma} \cdot \vec{\tau}|T_3\rangle = |T_3\rangle$$

Note: if different eigenvectors have the same eigenvalue this is called degeneracy.

A worked-out example for $\vec{\sigma} \cdot \vec{\tau}|T_1\rangle = |T_1\rangle$:

$$\vec{\sigma} \cdot \vec{\tau} = \sigma_x\tau_x + \sigma_y\tau_y + \sigma_z\tau_z$$

$$\sigma_x\tau_x|T_1\rangle = \sigma_x\tau_x\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle) = \sigma_x\frac{1}{\sqrt{2}}(|uu\rangle + |dd\rangle) = \frac{1}{\sqrt{2}}(|du\rangle + |ud\rangle) = |T_1\rangle$$

$$\sigma_y\tau_y|T_1\rangle = \sigma_y\tau_y\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle) = \sigma_y\frac{1}{\sqrt{2}}(-i|uu\rangle + i|dd\rangle) = \frac{1}{\sqrt{2}}(|du\rangle + |ud\rangle) = |T_1\rangle$$

$$\sigma_z\tau_z|T_1\rangle = \sigma_z\tau_z\frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle) = \sigma_z\frac{1}{\sqrt{2}}(-|ud\rangle + |du\rangle) = \frac{1}{\sqrt{2}}(-|ud\rangle - |du\rangle) = -|T_1\rangle$$

Result:

$$\vec{\sigma} \cdot \vec{\tau}|T_1\rangle = \sigma_x\tau_x|T_1\rangle + \sigma_y\tau_y|T_1\rangle + \sigma_z\tau_z|T_1\rangle = |T_1\rangle + |T_1\rangle - |T_1\rangle = |T_1\rangle$$

$|T_1\rangle$ is eigenvector of $\vec{\sigma} \cdot \vec{\tau}$ with eigenvalue 1.

Truth-value:

Truth-value is a fundamental idea in Boolean logic. A proposition is either true or false – nothing in between:

$$The\ die\ shows\ the\ number\ three$$

is either true or false.

Propositions can be combined by the logical operators such as and, or, not.

The not operator applied to the proposition above would lead to something like:

$$It\ is\ not\ true\ that\ (The\ die\ shows\ the\ number\ three)$$

Two spins:

We need at least two single spins to work with combined and entangled systems. In quantum mechanics they are usually called the system of Alice and the one of Bob.

Two spins, entanglement for two spins:

Worked out example

We have a system of two spins of Alice and Bob in the state $|\psi\rangle$:

$$|\psi\rangle = 0 \cdot |uu\rangle + \frac{1}{\sqrt{2}}|ud\rangle + \frac{1}{\sqrt{2}}|du\rangle + 0 \cdot |dd\rangle$$

Note: $|uu\rangle$ etc. denote a single basis vector out of four basis vectors.

Note: the state is normalized.

Note: all coefficients are real.

Note: this is a fully entangled state, a triplet state.

For all possible inputs uu, ud, du, dd the values of the wave function:

$$\psi(uu) = 0$$

$$\psi(ud) = \frac{1}{\sqrt{2}}$$

$$\psi(du) = \frac{1}{\sqrt{2}}$$

$$\psi(dd) = 0$$

We are interested in Alice's subsystem only. We calculate her density matrix:

$$\varrho_{aa'} = \sum_b \psi^*(ab)\psi(a'b)$$

Note: a and b can take the values u and d.

We get the elements of the density matrix of Alice:

$$\varrho_{uu} = \psi^*(uu)\psi(uu) + \psi^*(ud)\psi(ud) = \frac{1}{2}$$

$$\varrho_{ud} = \psi^*(du)\psi(uu) + \psi^*(dd)\psi(ud) = 0$$

$$\varrho_{du} = \psi^*(uu)\psi(du) + \psi^*(ud)\psi(dd) = 0$$

$$\varrho_{dd} = \psi^*(du)\psi(du) + \psi^*(dd)\psi(dd) = \frac{1}{2}$$

The density matrix of Alice:

$$\varrho_{a\prime a} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

In general

An operator L acting on the subsystem of Alice only:

$$L_{a\prime b\prime ab} = \langle a'b'|L|ab\rangle$$

Note: this is the observable (the operator) written in the notation of the combined system.

As the operator acts only on the subsystem of Alice, we can filter out all elements that deals with the subsystem of Bob:

$$L_{a\prime b\prime ab} = L_{a\prime a}\delta_{b\prime b}$$

Note: the 4×4 matrix $L_{a\prime b\prime ab}$ is factored into a tensor product of two 2×2 matrices $L_{a\prime a}$ and $\delta_{b\prime b}$.

Note: $\delta_{b\prime b}$ is the 2×2 identity matrix, a kind of Kronecker delta.

We calculate the expectation value (the average) of L in the composite system:

$$\langle L\rangle = \langle\psi|L|\psi\rangle = \sum_{a,b,a',b\prime} \psi^*(a'b')L_{a\prime b\prime ab}\psi(ab)$$

The operator acts only on the subsystem of Alice and leaves the subsystem of Bob unchanged $L_{a\prime b\prime ab} = L_{a\prime a}\delta_{b\prime b}$:

$$\langle\psi|L|\psi\rangle = \sum_{a,b,a\prime} \psi^*(a'b)L_{a\prime a}\psi(ab)$$

We can pull out the sum over b:

$$\sum_b \psi^*(ab)\psi(a'b) \coloneqq \varrho_{a\prime a}$$

Note: this is the density matrix of the subsystem of Alice. It does not depend on any b-index since it has already been summed over b.

Note: this is purely a function of the variables of the subsystem of Alice.

We rewrite the expectation value (the average) of L:

$$\langle L \rangle = \sum_{a,a'} \varrho_{a'a} L_{aa'}$$

Note:

$$\sum_{a,a'} \varrho_{a'a} L_{aa'}$$

is a sum of diagonal matrix elements, the trace of the matrix ρL. The expectation value (the average) of the operator L can be written as a trace:

$$\langle L \rangle = Tr\ \rho L$$

Two state system:

We take a single spin with two states, either head up or $down$. We call σ a degree of freedom that can take two values.

State up:

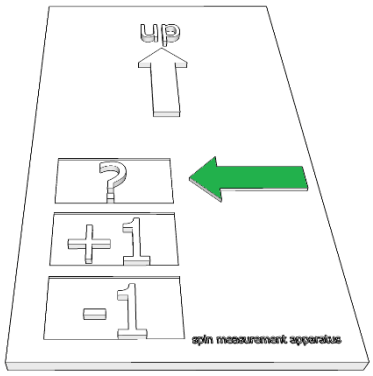
$$\sigma = +1$$

State $down$:

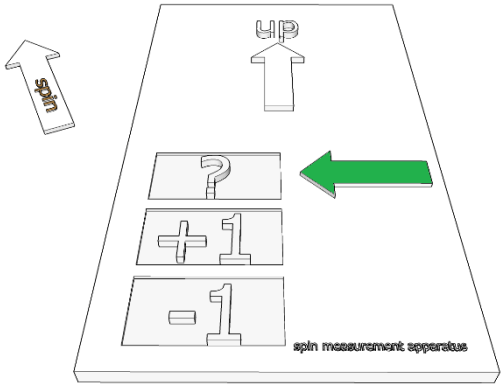
$$\sigma = -1$$

Note: this is called a qubit.

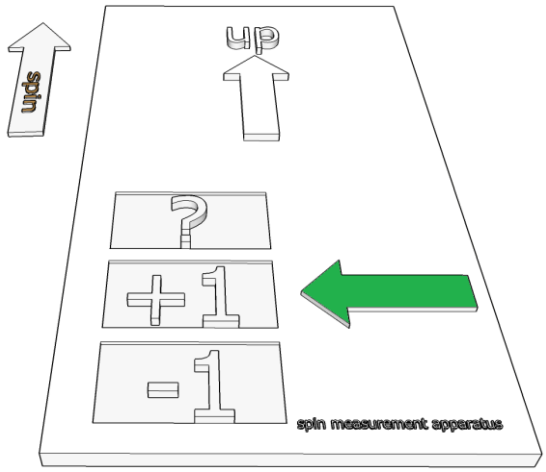
We have at hand an apparatus $\mathcal{A}$ to make measurements.



We orient the apparatus in z- direction and measure.



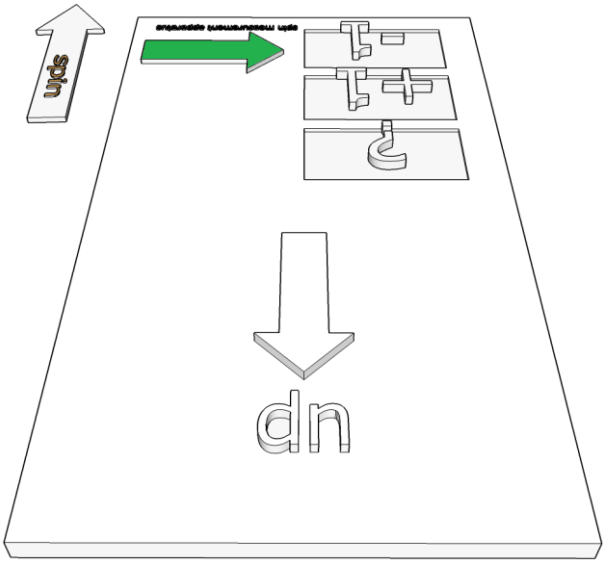
After the measurement the spin is oriented in z-direction, the apparatus shows the result $+1$.



Note: the first measurement changes the orientation of the spin.

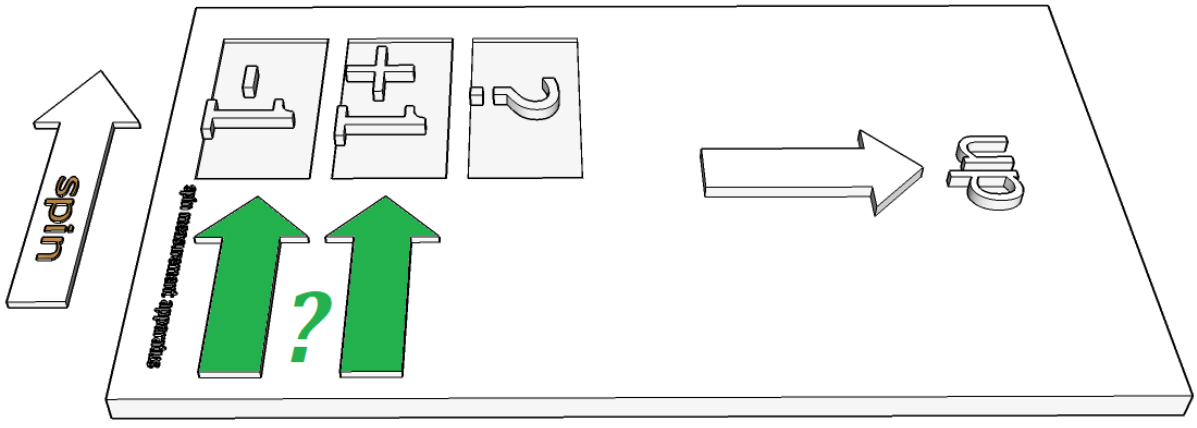
Any following measurement with the scene unchanged will repeat this value.

We turn the apparatus upside down (spin undisturbed) and measure again:



The result will be -1.

We turn the apparatus by 90° (spin undisturbed) and measure again:



The repeated experiments will give a random series of $+1$ and -1.

Instead of the classical result (the component of the spin along the x-axis with value zero) we get this zero as a statistical average of multiple measurements.

Quantum mechanical systems are not deterministic, but if we repeat an experiment many times, average quantities can follow the expectations of classical physics.

Uncertainty:

Uncertainty, definition of uncertainty:

Roughly speaking, the uncertainty is the standard deviation.

Let A be an observable (operator) with eigenvalues a.

The expectation value of A is the average:

$$\langle A\rangle = \langle\psi|A|\psi\rangle = \sum_a aP(a)$$

Note: a are the eigenvalues, $P(a)$ are the probabilities of each eigenvalue.

To make calculations easier we define the operator $\bar{A}$:

$$\bar{A} = A - \langle A\rangle I$$

The expectation value of $\bar{A}$ is zero.

The eigenvectors of $\bar{A}$ are the same as those of A but the eigenvalues are shifted:

$$\bar{a} = a - \langle A\rangle$$

The square of uncertainty or standard deviation of A:

$$(\Delta A)^2 = \sum_a \bar{a}^2 P(a) = \sum_a (a - \langle A\rangle)^2 P(a) = \langle\psi|\bar{A}^2|\psi\rangle$$

If the expectation value of the operator A already is zero, we need no shifting, the square of the uncertainty is the average value of the operator A^2:

$$(\Delta A)^2 = \langle\psi|A^2|\psi\rangle$$

Uncertainty, triangle inequality/Cauchy-Schwarz inequality and uncertainty:

The triangle inequality for **real** vectors:

$$|\vec{X}| + |\vec{Y}| \geq |\vec{X} + \vec{Y}|$$

squared:

$$\left(|\vec{X}| + |\vec{Y}|\right)^2 \geq |\vec{X} + \vec{Y}|^2$$

left side:

$$\left(|\vec{X}| + |\vec{Y}|\right)^2 = |\vec{X}|^2 + |\vec{Y}|^2 + 2|\vec{X}||\vec{Y}|$$

right side:

$$|\vec{X} + \vec{Y}|^2 = (\vec{X} + \vec{Y})(\vec{X} + \vec{Y}) = |\vec{X}|^2 + |\vec{Y}|^2 + 2(\vec{X} \cdot \vec{Y})$$

We get:

$$|\vec{X}||\vec{Y}| \geq |\vec{X} \cdot \vec{Y}|$$

Squared this is called the Cauchy-Schwarz inequality:

$$|\vec{X}|^2|\vec{Y}|^2 \geq |\vec{X} \cdot \vec{Y}|^2$$

The triangle inequality for **complex** valued vectors.

For complex vector spaces we get a more complicated form. We have to prove:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

We assume all vectors X and Y being nonzero.

Let λ be:

$$\lambda \coloneqq \frac{\langle X|Y\rangle}{\langle Y|Y\rangle} \rightarrow \langle X|Y\rangle = \lambda\langle Y|Y\rangle$$

Out of this definition we can conclude:

$$\langle Y|X\rangle = \overline{\langle X|Y\rangle} = \overline{\lambda\langle Y|Y\rangle} = \bar{\lambda}\langle Y|Y\rangle$$

We try:

$$0 \leq \langle X - \lambda Y|X - \lambda Y\rangle =$$

$$\langle X|X\rangle - \bar{\lambda}\langle X|Y\rangle - \lambda\langle Y|X\rangle + \lambda\bar{\lambda}\langle Y|Y\rangle =$$

$$\langle X|X\rangle - \bar{\lambda}\langle X|Y\rangle - \lambda\bar{\lambda}\langle Y|Y\rangle + \lambda\bar{\lambda}\langle Y|Y\rangle =$$

$$\langle X|X\rangle - \bar{\lambda}\langle X|Y\rangle =$$

$$|X|^2 - \frac{\overline{\langle X|Y\rangle}}{|Y|^2} \cdot \langle X|Y\rangle$$

Intermediate result:

$$0 \leq |X|^2 - \frac{\overline{\langle X|Y\rangle}}{|Y|^2} \cdot \langle X|Y\rangle$$

$$\frac{\overline{\langle X|Y\rangle}}{|Y|^2} \cdot \langle X|Y\rangle \leq |X|^2$$

$$\overline{\langle X|Y\rangle} \cdot \langle X|Y\rangle \leq |X|^2|Y|^2$$

$$|\langle X|Y\rangle|^2 \leq |X|^2|Y|^2$$

$$|\langle X|Y\rangle| \leq |X||Y|$$

We multiply the result by 2:

$$2|\langle X|Y\rangle| \leq 2|X||Y|$$

We get the following chain:

$$2|X||Y| \geq 2|\langle X|Y\rangle| = |\langle X|Y\rangle| + |\langle X|Y\rangle| =$$

$$|\langle X|Y\rangle| + |\langle Y|X\rangle| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

We get the form of the Cauchy-Schwarz inequality that is applicable for the uncertainty principle:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

Uncertainty principle, Heisenberg:

Classical physics: a particle has position x ***and*** momentum p.

Quantum mechanics: a particle has position x ***or*** momentum p.

Why? Because the momentum operator P and the position operator X do not commute. Observables belonging to operators that does not commute are not simultaneously measurable precisely.

Prerequisite

Let X and Y be vectors. The Cauchy-Schwarz inequality:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

End prerequisite

Let $|\psi\rangle$ be any normalized ket and let A and B be any two observables. Observables are always real. We define $|X\rangle$ and $|Y\rangle$:

$$|X\rangle = A|\psi\rangle \text{ and } \langle X| = \langle\psi|A$$

$$|Y\rangle = iB|\psi\rangle \text{ and } \langle Y| = \langle\psi| - iB$$

With these the Cauchy-Schwarz inequality becomes

$$\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq \frac{1}{2}|\langle\psi|AB|\psi\rangle - \langle\psi|BA|\psi\rangle|$$

or, written with the commutator:

$$\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq \frac{1}{2}|\langle\psi|[AB]|\psi\rangle|$$

For simplicity reasons let A and B have expectation values of zero. In that case, $\langle A^2\rangle$ is the square of the uncertainty in $A \coloneqq (\triangle A)^2$ and similar $B \coloneqq (\triangle B)^2$.

We get:

$$\sqrt{\langle A^2\rangle\langle B^2\rangle} \rightarrow \triangle A \triangle B$$

$$\triangle A \triangle B \geq \frac{1}{2}|\langle\psi|[AB]|\psi\rangle|$$

In plain words: the product of the uncertainties cannot be smaller than half the magnitude of the expectation value of the commutator.

If the commutator of A and B is not zero, both observables cannot simultaneous be certain.

Note: if A and B do not have expectation values of zero, we can shift them and build two new variables:

$$\bar{A} \coloneqq A - \langle A\rangle$$

$$\bar{B} \coloneqq B - \langle B\rangle$$

For these new variables hold:

$$\triangle A^2 = \langle \bar{A}^2 \rangle$$

$$\triangle B^2 = \langle \bar{B}^2 \rangle$$

$$[\bar{A}, \bar{B}] = [AB]$$

For the case of position operator X and momentum operator P we know that applying the commutator onto any wave function $\psi(x)$ gives:

$$[X, P]\psi(x) = i\hbar\psi(x)$$

We express this by writing:

$$[X, P] = i\hbar$$

The fact that X and P do not commute is the key to understanding that they are not simultaneously measurable. We insert them into

$$\triangle X \triangle P \geq \frac{1}{2}|\langle\psi|[XP]|\psi\rangle|$$

and get:

$$\triangle X \triangle P \geq \frac{1}{2}|\langle\psi|i\hbar|\psi\rangle| =$$

$$\frac{1}{2}|i\hbar\langle\psi|\psi\rangle| = \frac{1}{2}|i\hbar| = \frac{1}{2}\hbar$$

$$\triangle X \triangle P \geq \frac{1}{2}|i\hbar| = \frac{1}{2}\hbar$$

Remember $|\psi\rangle$ is normalized.

We got the Heisenberg Uncertainty Principle.

Unitarity:

Time development in quantum mechanics is unitary:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

The operator $U(t)$ is called the unitary time development operator for the system.

For a unitary operator (matrix) holds:

$$U^\dagger U = I$$

Note: $U^\dagger$ is the transposed and complex conjugated version of U.

For small time intervals ε the operator U is close to the identity operator I:

$$U(\varepsilon) = I - i\varepsilon H$$

U must be unitary:

$$U^\dagger(\varepsilon) = I + i\varepsilon H^\dagger$$

From the unitary condition for U and the small time-interval ε follows:

$$U^\dagger U = (I - i\varepsilon H)\left(I + i\varepsilon H^\dagger\right) = I^2 + i\varepsilon I H^\dagger - i\varepsilon I H + \varepsilon^2 H H^\dagger$$

We omit the second order in ε:

$$U^\dagger U = I \rightarrow$$

$$I = I + i\varepsilon H^\dagger - i\varepsilon H$$

$$0 = i\varepsilon H^\dagger - i\varepsilon H = i\varepsilon\left(H^\dagger - H\right)$$

We get that H must be unitary too:

$$H^\dagger = H$$

H will become the quantum Hamiltonian, a unitary operator.

Unitary evolution:

Suppose Alice and Bob have a (maybe entangled) system, one part of the system is here, the other part on Alpha Centaury.

The wave function for the combined system is $\psi(ab)$.

The complete description of the subsystem of Alice is contained in her density matrix:

$$\varrho_{aa'} = \sum_b \psi^*(a'b)\psi(ab)$$

The question is: can Bob with his subsystem do anything to instantly change the density matrix of Alice? According to the laws of quantum mechanics?

Whatever happens to the subsystem of Bob must be described by a unitary matrix $U_{bb'}$. It acts on the wave function ψ to produce an altered wave function $\psi_{altered}$:

$$\psi_{altered}(ab) = \sum_{b'} U_{bb'}\psi(ab')$$

The complex conjugated of $\psi_{altered}$ is:

$$\psi^*{}_{altered}(a'b) = \sum_{b''} \psi^*(a'b'')U^\dagger{}_{b''b}$$

Note: the primes added to avoid mixing the variables up.

We calculate the density matrix of Alice for the system after Bob acted on it.

Before:

$$\varrho_{aa'} = \sum_b \psi^*(a'b)\psi(ab)$$

After:

$$\varrho_{aa'} = \sum_{b,b',b''} \psi^*(a'b'')U^\dagger{}_{b''b}U_{bb'}\psi(ab')$$

The unitarian matrices combines to the unit matrix again:

$$U^{\dagger}{}_{b''b}U_{bb'} = \delta_{b''b'}$$

In the sum all indices are collapsing to b:

$$\varrho_{aa'} = \sum_{b} \psi^{*}(a'b)\psi(ab)$$

The action of Bob on his subsystem does not change the density matrix of Alice, her subsystem remains exactly as it was. This guarantees that no "faster-than-light" signal has been sent.

Unitary matrix:

For a unitary matrix (operator) holds:

$$U^{\dagger}U = I$$

Note: $U^{\dagger}$ is the transposed and complex conjugated version of U.

Time development in quantum mechanics is unitary:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

Unit matrix:

The unit matrix I is part of the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};\ I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Any 2×2 Hermitian matrix L can be written as a sum of these four matrices:

$$L = a\sigma_x + b\sigma_y + c\sigma_z + dI$$

Note: a, b, c, d are real numbers.

Unit matrix, density matrix and unit matrix:

We have a combined system, Alice and Bob, of two maximally entangled spins. If Alice calculates the density matrix for her subsystem:

$$\varrho_{aa'} = \frac{1}{N_A}\delta_{a'a}$$

All eigenvalues are equal, and given that they all sum to unity, each eigenvalue is equal to $\frac{1}{N_A}$ with N_A being the number of dimensions of the subsystem of Alice.

Every possible outcome is equally probable.

Unit (normalized) vector:

For normalized vectors $|A\rangle$ the inner product equals one:

$$\langle A|A\rangle = 1$$

For spatial vectors, normalized vectors are called unit vectors, vectors with length 1.

Unit vector, state of system and unit vector:

The state of a system is represented by a normalized vector in a vector space of states.

In a single spin system $|A\rangle = \begin{pmatrix}\alpha_u \\ \alpha_d\end{pmatrix}$, $\langle A| = (\alpha_u^* \ \alpha_d^*)$:

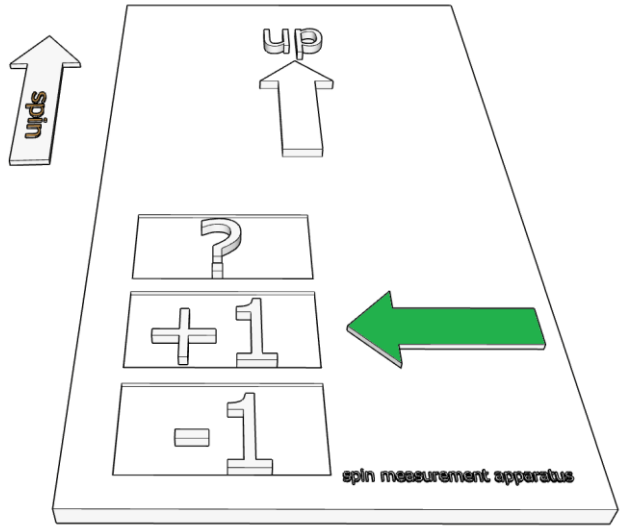
$$\langle A|A\rangle = (\alpha_u^* \ \alpha_d^*)\begin{pmatrix}\alpha_u \\ \alpha_d\end{pmatrix} = \alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

Up state:

We prepare a spin and orient the measuring apparatus along the z-axis.

The measurement will give the result $+1$, the spin is in the up-state, or -1, the spin is in the $down$-state.

The term up-state (and $down$-state) refers to the orientation of the spin relative to the apparatus.



Vector addition:

In quantum mechanics, a vector space is composed of kets (vectors) $|A\rangle, |B\rangle$:

$$|A\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

$$|B\rangle = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}$$

$$|A\rangle + |B\rangle = \begin{pmatrix} a_1 + b_1 \\ \vdots \\ a_n + b_n \end{pmatrix}$$

The corresponding bras $\langle A|, \langle B|$:

$$\langle A| = (a_1^*, \dots, a_n^*)$$

$$\langle B| = (b_1^*, \dots, b_n^*)$$

$$\langle A| + \langle B| = (a_1^* + b_1^*, \dots, a_n^* + b_n^*)$$

Note: a_1, a_n, b_1, b_n are complex numbers.

Note: there is an implicit conjugation in changing from ket to bra.

Vectors:

Vectors, basis vectors:

a) 3-vectors: a set of three mutually orthogonal unit vectors, e.g. $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ for the cartesian space.

b) $|u\rangle$ and $|d\rangle$ as a basis of the state of a spin.
Any state A can be written as $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$

c) If the state vector $|A\rangle$ is normalized, then $\langle A|A\rangle = 1$ or $\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$

d) $\alpha_u^* = \alpha_u = \alpha_d^* = \alpha_d = \frac{1}{\sqrt{2}}$ satisfies c)

e) If λ_1 and λ_2 are unequal eigenvalues of a Hermitian operator, then the corresponding eigenvectors are orthogonal, and all these eigenvectors can form a basis of the state space.

f) If λ_1 and λ_2 are equal eigenvalues of a Hermitian operator, then out of the corresponding eigenvectors can be chosen a pair of orthogonal vectors that are necessarily eigenvectors.

g) Orthogonal basis vectors represent two distinguishable states – for all times.

h) Every normalized state $|A\rangle$ of a quantum system can be expanded in the orthonormal basis of eigenvectors of L: $|A\rangle = \sum_i \alpha_i |\lambda_j\rangle$

i) The Hamiltonian applied to the energy eigenvectors of a state delivers the eigenvalues (the energy levels) of the system: $H|E_j\rangle = E_j|E_j\rangle$. Please not that $|E_j\rangle$ are the eigenvectors, E_j the eigenvalues resp. the energies.

j) The elements of a matrix M can be calculated by use of basis vectors: $m_{jk} = \langle j|M|k\rangle$ with $\langle j|$ and $|k\rangle$ representing the basis vectors. Note that $\langle j|$ is the complex conjugate to $|j\rangle$.

k) The basis vector for the $|u\rangle$ state is $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, the basis vector for the $|d\rangle$ state is $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

l) The basis vectors for the states $|uu\rangle, |ud\rangle, |du\rangle$ and $|dd\rangle$ are $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$.

Note that these are tensor product states.

m) The sum over the outer product of a set of basis vectors $|i\rangle$ and $\langle i|$ delivers the identity matrix:

$$\sum_i |i\rangle \langle i| = I$$

Note that I stands for the running index I and not the imaginary unit and that $\langle i|$ must be the complex conjugated of $|i\rangle$.

n) If the measuring apparatus (for spatial spin orientation) comes into play as a quantum system too, in the simplest description it has three states: a blank state and two outcome states with the following basis vectors: $|b\rangle, |(+1)\rangle$ and $|(-1)\rangle$. The starting state at time 0 is always the blank state.
Note that in the book these kets often are written as $|b\}, |+1\}$ and $|-1\}$ to make clear these are kets of the measuring system.

o) The quantum state of a particle spanned by position x and momentum p: $|x, p\rangle$
Note that the associated operators are X and P.

p) Because momentum and position are both Hermitian operators, the sets of $|x\rangle$ and $|p\rangle$ each define basis vectors.

Vectors, column vectors:

A column vector $|A\rangle$ (a ket) is a stack of complex numbers:

$$|A\rangle = \begin{pmatrix}a_1\\ \vdots \\ a_n\end{pmatrix}$$

We can add two kets:

$$|B\rangle = \begin{pmatrix}b_1\\ \vdots \\ b_n\end{pmatrix}$$

$$|A\rangle + |B\rangle = \begin{pmatrix}a_1 + b_1\\ \vdots \\ a_n + b_n\end{pmatrix}$$

We can multiply a ket with a complex number z:

$$z|A\rangle = z\begin{pmatrix}a_1\\ \vdots \\ a_n\end{pmatrix} = \begin{pmatrix}za_1\\ \vdots \\ za_n\end{pmatrix}$$

When working with single spin systems we use the kets $|u\rangle$ and $|d\rangle$, representing the two orthogonal states up and $down$ of a single spin:

$$|u\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

$$|d\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

Vectors, concept of vectors:

The space of states of a quantum system is a vector space, a mathematically construction that may or may not have anything to do with ordinary space (spatial vectors).

The vector space to define quantum mechanical states is called a Hilbert space with either a finite or an infinite number of dimensions.

The elements of the vector space are called ket vectors or kets $|A\rangle$.

Vectors, functions as vectors:

A single spin system can be described by a two-dimensional space of states:

$$|\psi\rangle = \alpha|u\rangle + \beta|d\rangle = \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix}$$

This is a discrete system.

Note: α and β are complex numbers.

A particle moving along the x-axis can be found at any real value of x.

For each value of x, $\psi(x)$ is a complex number.

This is a continuous system.

With appropriate restrictions, the functions $\psi(x)$ fulfill the mathematical axioms that define a vector space (Hilbert space):

1. The sum of any two functions is a function.
2. The addition of functions is commutative.
3. The addition of functions is associative.
4. There exists a zero function for addition.
5. There exists an inverse function for addition.
6. Multiplying a function by a complex number gives a new function and is linear.
7. The distributive property holds:
    a. $z[\varphi(x) + \theta(x)] = z\varphi(x) + z\theta(x)$
    b. $[z + w]\psi(x) = z\,\psi(x) + w\psi(x)$

Note: z and w are complex numbers.

With this we can identify functions $\psi(x)$ with ket-vectors $|\psi\rangle$.

The bra-vector $\langle\psi|$ corresponds to the complex conjugate function $\psi^*(x)$.

We have to replace:

a) Integrals replace sums,

$$\langle\psi|\theta\rangle = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx$$

our new inner product.

b) Probability densities replace probabilities. The probability of a continuous variable at exactly one point is zero, so we can only determine the probability that the variable is in between boundaries a and b:
$P(a,b) = \int_a^b P(x)dx = \int_a^b \psi^*(x)\psi(x)dx.$
$P(x)$ becomes a probability density.

c) For probability densities holds:

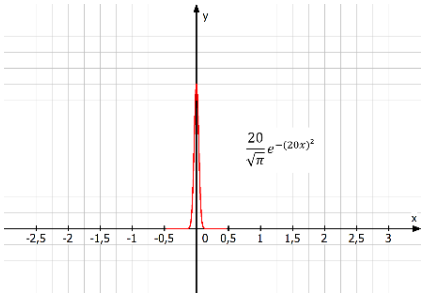
$$\int_{-\infty}^{\infty} P(x)dx = 1$$

d) Dirac delta functions replace Kronecker deltas.
The Kronecker delta satisfies:

$$\sum_j \delta_{ij} F_j = F_i$$

The Dirac delta functions $\delta(x - x')$ does the same job for integrals:

$$\int_{-\infty}^{\infty} \delta(x - x')F(x')dx' = F(x)$$



Note: the Dirac delta function can be approximated by e.g.:

$$\lim_{n\to\infty} \frac{n}{\sqrt{\pi}} e^{-(nx)^2}$$

Vectors, normalized vectors:

For normalized vectors $|A\rangle$ the inner product equals one:

$$\langle A|A\rangle = 1$$

For spatial vectors we say they have length 1.

Vectors, orthogonal vectors:

Two vectors $|A\rangle$, $|B\rangle$ are orthogonal if the inner product is zero:

$$\langle A|B\rangle = 0$$

Orthogonality of vectors has a special meaning in quantum mechanics.

Observables in quantum mechanics are represented by Hermitian operators (matrices).

The eigenvectors of a Hermitian operator (matrix) form a complete set and act as an orthogonal basis of the state.

If the eigenvalues of two eigenvectors are different, then the eigenvectors are orthogonal.

Even if two eigenvalues are equal, the corresponding eigenvectors can be chosen to be orthogonal by the Gram-Schmidt procedure.

Unambiguously distinguishable states are represented by orthogonal vectors.

Vectors, polarization:

The states of a spin are characterized by a polarization vector.

We have a single spin system. For any spin state, there is some orientation of the measuring apparatus $\mathcal{A}$ that will give the result $+1$ after measurement.

This is another way to express the spin-polarization principle:

Any state of a single spin is an eigenvector of some component of the spin.

Let $|A\rangle = \alpha|u\rangle + \beta|d\rangle$. There exists a direction $\vec{n}$:

$$\vec{\sigma} \cdot \vec{n} = |A\rangle$$

Note: $\vec{\sigma}$ is the spin operator, having a strong family resemblance with 3-vectors. We can use it as if it were a 3-vector.

The components of the spin operator are σ_x, σ_y and σ_z.

σ_x, σ_y and σ_z each are 2×2 matrices, the Pauli matrices.

Vectors, row vectors:

A column vector $|A\rangle$, a ket, is a stack of complex numbers:

$$|A\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

Its counterpart $\langle A|$, a bra, is a row of complex numbers:

$$\langle A| = (a_1^*, \dots, a_n^*)$$

Note: in quantum mechanics there is an implicit conjugation. $|A\rangle$ and $\langle A|$ are complex conjugated.

We can add two bras:

$$\langle B| = (b_1^*, \dots, b_n^*)$$

$$\langle A| + \langle B| = (a_1^* + b_1^*, \dots, a_n^* + b_n^*)$$

We can multiply a bra with a complex number z:

$$z\langle A| = \langle A|z = z(a_1^*, \dots, a_n^*) = (za_1^*, \dots, za_n^*)$$

Vectors, three-vectors (3-vectors):

Vectors in regular space, spatial vectors, are called 3-vectors.

For 3-vectors multiplication by complex numbers is not defined.

3-vectors form a real vector space, a spatial vector space.

Bras and kets form a complex vector space.

3-vectors are not rich enough to represent quantum states. For this we need bras and kets with complex valued components.

Vectors, unit-vectors:

For unit vectors $|A\rangle$ the inner product equals one:

$$\langle A|A\rangle = 1$$

For spatial vectors we say they have length 1.

Vector space:

In quantum mechanics, a vector space is made of bras $\langle A|$ and kets $|A\rangle$, it is a Hilbert space.

We use seven axioms to define a vector space. Let $|A\rangle, |B\rangle$ and $|C\rangle$ be vectors and z, w complex numbers, then:

1. Closure: the sum of two vectors is a vector:
   $|A\rangle + |B\rangle = |C\rangle$
2. Vector addition is commutative:
   $|A\rangle + |B\rangle = |B\rangle + |A\rangle$
3. Vector addition is associative:
   $\{|A\rangle + |B\rangle\} + |C\rangle = |A\rangle + \{|B\rangle + |C\rangle\}$
4. Existence of the 0:
   $|A\rangle + 0 = |A\rangle$
5. Existence of the inverse:
   $|A\rangle + (-|A\rangle) = 0$
6. Multiplication by a scalar produces a new vector:
   $|zA\rangle = z|A\rangle = |B\rangle$
7. Distributive property:
   $z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$
   $\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$

Axioms 6 and 7 taken together are often called *linearity*.

Note: spatial 3-vectors does not satisfy axiom 6, the multiplication of a 3-vector with a complex number is not defined.

Note: the bra corresponding to $z|A\rangle$ is $\langle A|z^*$.

Note: interchanging bra and ket corresponds to complex conjugation:

$$\langle A|B\rangle = \langle B|A\rangle^*$$

Note: there is an implicit complex conjugation when switching from $|A\rangle$ to $\langle A|$:

$$|A\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

$$\langle A| = (a_1^*, \dots, a_n^*)$$

We can write a ket $|A\rangle$ as a sum of basis vectors:

$$|A\rangle = \sum_i a_i |i\rangle$$

Note: $|i\rangle$ are the basis vectors.

Note: in quantum mechanics the basis is regularly an orthonormal basis.

Note: the a_i are complex numbers, the components of the vector.

We can calculate the components by taking the inner product with the basis bras $\langle j|$:

$$\langle j|A\rangle = \sum_i a_i \langle j|i\rangle$$

Note: we have an orthonormal basis, so $\langle j|i\rangle = \delta_{ji}$, the Kronecker delta. The sum collapses to one single term:

$$\langle j|A\rangle = a_j$$

The ket $|A\rangle$ is the sum of its projections onto the basis vectors:

$$|A\rangle = \sum_i |i\rangle\langle i|A\rangle$$

Vector space, axioms:

We use seven axioms to define a vector space. Let $|A\rangle, |B\rangle$ and $|C\rangle$ be vectors and z, w complex numbers, then:

1. Closure: the sum of two vectors is a vector:
   $|A\rangle + |B\rangle = |C\rangle$
2. Vector addition is commutative:
   $|A\rangle + |B\rangle = |B\rangle + |A\rangle$
3. Vector addition is associative:
   $\{|A\rangle + |B\rangle\} + |C\rangle = |A\rangle + \{|B\rangle + |C\rangle\}$
4. Existence of the 0:
   $|A\rangle + 0 = |A\rangle$
5. Existence of the inverse:
   $|A\rangle + (-|A\rangle) = 0$
6. Multiplication by a scalar produces a new vector:
   $|zA\rangle = z|A\rangle = |B\rangle$
7. Distributive property:
   $z\{|A\rangle + |B\rangle\} = z|A\rangle + z|B\rangle$
   $\{z + w\}|A\rangle = z|A\rangle + w|A\rangle$

Axioms 6 and 7 taken together are often called *linearity*.

Vector space, bras:

A complex vector space has a dual version, the complex conjugate vector space.

For every ket vector $|A\rangle$ there is a bra vector denoted by $\langle A|$.

Bra vectors satisfy the same axioms as ket vectors with two peculiarities:

- If z is a complex number, the bra corresponding to $z|A\rangle$ is $\langle A|z^*$.

If we write the ket $|A\rangle$ as

$$|A\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

then the corresponding bra is

$$\langle A| = (a_1^*, \ldots, a_n^*)$$

Vector space, column vectors:

Kets are identified with column vectors:

$$|A\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

Vector space, functions and vector space:

Functions satisfy the mathematical axioms that define a vector space:

1. The sum of any two functions is a function.
2. The addition of functions is commutative.
3. The addition of functions is associative.
4. There exists a zero function for addition.
5. There exists an inverse function for addition.
6. Multiplying a function by a complex number gives a new function and is linear.
7. The distributive property holds:
    a. $z[\varphi(x) + \theta(x)] = z\varphi(x) + z\theta(x)$
    b. $[z + w]\psi(x) = z\,\psi(x) + w\psi(x)$

With this we can identify functions $\psi(x)$ with ket-vectors $|\psi\rangle$. The bra-vector $\langle\psi|$ corresponds to the complex conjugate function $\psi^*(x)$.

Vector space, inner products:

We have kets $|A\rangle$, $|B\rangle$ and $|C\rangle$. For the inner product we need the bra versions $\langle B|$ and $\langle C|$. Remember that $\langle B|$ is complex conjugated:

$$\langle B|A\rangle$$

Inner products are linear:

$$\langle C|\,(\,|A\rangle + |B\rangle\,) = \langle C|A\rangle + \langle C|B\rangle$$

Interchanging bras and kets corresponds to complex conjugation:

$$\langle B|A\rangle = \langle A|B\rangle^*$$

The inner product in concrete representation:

$$|A\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

$$\langle B| = (b_1^*, \dots, b_n^*)$$

$$\langle B|A\rangle = (b_1^*, \dots, b_n^*)\begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} = (b_1^* a_1 + \cdots + b_n^* a_n)$$

Vector space, kets:

A ket is an element of a complex vector space:

$$|A\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

Note: a_i are complex numbers.

Note: the corresponding bra is

$$\langle A| = (a_1^*, \ldots, a_n^*)$$

Vector space, orthonormal bases:

A basis vector is a ket:

$$|i\rangle$$

We can break down a complex vector space by use of (normalized) orthogonal basis vectors. With these we can write any ket $|A\rangle$ as a sum of basis vectors:

$$|A\rangle = \sum_i a_i |i\rangle$$

Note: in quantum mechanics the basis is regularly an orthonormal basis.

Note: the a_i are complex numbers, the components of the vector.

We can calculate the components by taking the inner product with the basis bras $\langle j|$:

$$\langle j|A\rangle = \sum_i a_i \langle j|i\rangle$$

Note: we have an orthonormal basis, so $\langle j|i\rangle = \delta_{ji}$, the Kronecker delta. The sum collapses to one single term:

$$\langle j|A\rangle = a_j$$

The ket $|A\rangle$ is the sum of its projections onto the basis vectors:

$$|A\rangle = \sum_i |i\rangle\langle i|A\rangle$$

Vector space, tensor product as vector space:

A tensor product is a vector space for working with composite systems.

A product state is a state vector.

Most of the state vectors in the product space are not product states.

Vector space, triangle inequality and vector space:

We can derive from the triangle inequality

$$|\vec{X}| + |\vec{Y}| \geq |\vec{X} + \vec{Y}|$$

the form:

$$|\vec{X}||\vec{Y}| \geq |\vec{X} \cdot \vec{Y}|$$

This is true for vectors in any vector space, provided the length of a vector is defined as the square root of the inner product of the vector with itself.

Note: further processing gives:

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

This is the form of the Cauchy-Schwarz inequality that leads to the (Heisenberg) uncertainty principle.

Velocity, momentum and velocity:

Prerequisite

The quantum mechanical Hamiltonian for a nonrelativistic free particle:

$$H = \frac{P^2}{2m}$$

Note: P is the momentum operator.

The commutator of two operators (matrices):

$$[A, B] = AB - BA$$

The commutator of position operator X and momentum operator P:

$$[P, X] = -i\hbar$$

End prerequisite.

The velocity of a quantum mechanical particle:

$$v = \frac{d}{dt}\langle\psi|X|\psi\rangle = \frac{d}{dt}\langle X\rangle$$

Note: this is the time derivative of the average position $\langle X\rangle$.

The time derivative of an operator L is the expectation value of the commutator of the Hamiltonian H with the operator L:

$$\frac{d}{dt}\langle L\rangle = \frac{i}{\hbar}\langle[H, L]\rangle$$

We insert the quantum Hamiltonian:

$$v = \frac{d}{dt}\langle X\rangle = \frac{i}{\hbar}\langle[H, X]\rangle = \frac{i}{2m\hbar}\langle[P^2, X]\rangle =$$

$$\frac{i}{2m\hbar}\langle P[P, X] + [P, X]P\rangle =$$

$$\frac{i}{2m\hbar}\langle -Pi\hbar - i\hbar P\rangle = \frac{i}{2m\hbar}\langle -2i\hbar P\rangle =$$

$$\frac{\langle P\rangle}{m}$$

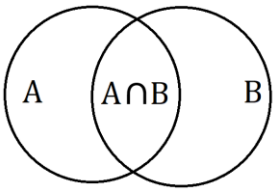
Result:

$$v = \frac{\langle P \rangle}{m} \quad resp. \ \langle P \rangle = mv$$

The center (average) of the wave packet travels according to the classical rule $p = mv$.

Venn diagram:

Venn diagrams are used to show combinations and intersections of subsets. The diagram shows the intersection of A and B, the logical and.



Wave functions:

Let L be an observable (a Hermitian operator) with eigenvalues λ and eigenvectors $|\lambda\rangle$.

The eigenvectors of a Hermitian operator form a complete orthonormal basis.

With this basis we can expand the vector $|\psi\rangle$:

$$|\psi\rangle = \sum_{\lambda} \psi(\lambda)|\lambda\rangle$$

Note: $\psi(\lambda)$ are called the wave function of the system and depend on the specific observable L we chose.

$\psi(\lambda)$ is the wave function in the L-basis.

For a different observable, the wave function will be different, even if we are working with the same state.

The basis vectors are orthonormal:

$$\langle\lambda_i|\lambda_j\rangle = \delta_{ij}$$

Note: δ_{ij} is the Kronecker delta.

We can identify the wave function $\psi(\lambda)$ in the L-basis with the inner products (the projection) of the state vector $|\psi\rangle$ onto the eigenvectors $|\lambda\rangle$:

$$\psi(\lambda) = \langle\lambda|\psi\rangle$$

The wave function $\psi(\lambda)$ is the set of components of the state vector in a particular basis:

$$\begin{pmatrix} \psi(\lambda_1) \\ \vdots \\ \psi(\lambda_n) \end{pmatrix}$$

In a more general way, the wave function is a function of a parameter λ that produces a complex number. It is a complex-valued function of the discrete variable λ.

In this scenario linear operators become operations that are applied to functions and give back new functions.

Wave functions, action of Hamiltonian on wave functions:

The action of the momentum operator P on a wave function $\psi(x)$:

$$P|\psi(x)\rangle \to -i\hbar\frac{\partial\psi(x)}{\partial x}$$

The action of the position operator X on a wave function $\psi(x)$:

$$X|\psi(x)\rangle \to x\psi(x)$$

The quantum mechanical Hamiltonian:

$$H = \frac{1}{2}P^2 + \omega^2 X^2$$

The quantum mechanical Hamiltonian acting on a wave function $\psi(x)$:

$$H|\psi(x)\rangle \to \frac{1}{2}\left(-i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial\psi(x)}{\partial x}\right)\right)+\frac{1}{2}\omega^2x^2\psi(x)$$

Note: we use partial derivatives because in general ψ depends on time too. We describe the system at a fixed time.

Wave functions, calculating density matrices and wave functions:

Suppose we know the wave function of a composite system:

$$\psi(a,b)$$

The probability that the system is in the state $|ab\rangle$:

$$P(a,b)=\psi^*(a,b)\psi(a,b)$$

To get the probability the subsystem being in the state a we sum over b:

$$P(a)=\sum_b\psi^*(a,b)\psi(a,b)$$

This is a diagonal entry in the density matrix:

$$P(a)=\rho_{aa}$$

Note: in a combined system of two spins, a,b can be either u or d.

A concrete example

We have a combined system of two spins (Alice and Bob) with the state vector:

$$|\psi\rangle=\frac{1}{5}(3|uu\rangle+4|ud\rangle)$$

The wave function:

$$\psi(u,u)=\frac{3}{5},\psi(u,d)=\frac{4}{5},\psi(d,u)=0,\psi(d,d)=0$$

The wave function is normalized:

$$\psi^*(u,u)\psi(u,u)+\psi^*(u,d)\psi(u,d)+\psi^*(d,u)\psi(d,u)+\psi^*(d,d)\psi(d,d)=$$

$$\frac{9}{25}+\frac{16}{25}+0+0=\frac{25}{25}=1$$

We calculate Alice's density matrix:

$$\rho_{uu}=\psi^*(u,u)\psi(u,u)+\psi^*(u,d)\psi(u,d)=\frac{3}{5}\cdot\frac{3}{5}+\frac{4}{5}\cdot\frac{4}{5}=\frac{9}{25}+\frac{16}{25}=\frac{25}{25}=1$$

$$\rho_{ud}=\psi^*(d,u)\psi(u,u)+\psi^*(d,d)\psi(u,d)=0\cdot\frac{3}{5}+0\cdot\frac{4}{5}=0$$

$$\rho_{du}=\psi^*(u,u)\psi(d,u)+\psi^*(u,d)\psi(d,d)=0$$

$$\rho_{dd}=\psi^*(d,u)\psi(d,u)+\psi^*(d,d)\psi(d,d)=0$$

The density matrix ρ of Alice:

$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

We calculate Bob's density matrix:

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(d,u)\psi(d,u) = \frac{3}{5}\cdot\frac{3}{5} + 0 = \frac{9}{25}$$

$$\rho_{ud} = \psi^*(u,d)\psi(u,u) + \psi^*(d,d)\psi(d,u) = \frac{4}{5}\cdot\frac{3}{5} + 0\cdot 0 = \frac{12}{25}$$

$$\rho_{du} = \psi^*(u,u)\psi(u,d) + \psi^*(d,u)\psi(d,d) = \frac{3}{5}\cdot\frac{4}{5} + 0\cdot 0 = \frac{12}{25}$$

$$\rho_{dd} = \psi^*(u,d)\psi(u,d) + \psi^*(d,d)\psi(d,d) = \frac{4}{5}\cdot\frac{4}{5} + 0 = \frac{16}{25}$$

The density matrix ρ of Bob:

$$\rho = \begin{pmatrix} \frac{9}{25} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{pmatrix}$$

Wave functions, collapse of wave functions:

We have a fresh quantum system, no previous measurement done.

An experiment to measure the observable L is done.

After the measurement the system is left in an eigenstate of L.

Let the state vector before the measurement be:

$$\sum_j \alpha_j |\lambda_j\rangle$$

After the measurement, with probability $|\alpha_j|^2$, the system is in the single eigenstate $|\lambda_j\rangle$.

The superposition of states collapses into a single term.

Note: subsequent measurements will reproduce this result.

Wave functions, entanglement and wave functions:

Entanglement is the quantum mechanical generalization of correlation.

Let $P(a,b)$ be the probability distribution for two variables a and b.

If the two variables are correlated (they depend from each other in some way):

$$P(a,b) \neq P(a)P(b)$$

If the two variables are uncorrelated (independent):

$$P(a,b) = P(a)P(b)$$

A concrete example

We have a combined system of two spins (Alice and Bob) with the state vector:

$$|\psi\rangle = \frac{1}{5}(3|uu\rangle + 4|ud\rangle)$$

The wave function:

$$\psi(u,u) = \frac{3}{5}, \psi(u,d) = \frac{4}{5}, \psi(d,u) = 0, \psi(d,d) = 0$$

We calculate Alice's density matrix:

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(u,d)\psi(u,d) = \frac{3}{5}\cdot\frac{3}{5} + \frac{4}{5}\cdot\frac{4}{5} = \frac{9}{25} + \frac{16}{25} = \frac{25}{25} = 1$$

$$\rho_{ud} = \psi^*(d,u)\psi(u,u) + \psi^*(d,d)\psi(u,d) = 0\cdot\frac{3}{5} + 0\cdot\frac{4}{5} = 0$$

$$\rho_{du} = \psi^*(u,u)\psi(d,u) + \psi^*(u,d)\psi(d,d) = 0$$

$$\rho_{dd} = \psi^*(d,u)\psi(d,u) + \psi^*(d,d)\psi(d,d) = 0$$

The density matrix ρ of Alice:

$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

We calculate Bob's density matrix:

$$\rho_{uu} = \psi^*(u,u)\psi(u,u) + \psi^*(d,u)\psi(d,u) = \frac{3}{5}\cdot\frac{3}{5} + 0 = \frac{9}{25}$$

$$\rho_{ud} = \psi^*(u,d)\psi(u,u) + \psi^*(d,d)\psi(d,u) = \frac{4}{5}\cdot\frac{3}{5} + 0\cdot 0 = \frac{12}{25}$$

$$\rho_{du} = \psi^*(u,u)\psi(u,d) + \psi^*(d,u)\psi(d,d) = \frac{3}{5}\cdot\frac{4}{5} + 0\cdot 0 = \frac{12}{25}$$

$$\rho_{dd} = \psi^*(u,d)\psi(u,d) + \psi^*(d,d)\psi(d,d) = \frac{4}{5}\cdot\frac{4}{5} + 0 = \frac{16}{25}$$

The density matrix ρ of Bob:

$$\rho = \begin{pmatrix} \frac{9}{25} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{pmatrix}$$

The probability for the combined system to be in the state $|uu\rangle$:

$$P(u,u) = \psi^*(u,u)\psi(u,u) = \frac{3}{5}$$

From the density matrices we extract the value $P_A(u)$ for the subsystem of Alice:

$$P_A(u) = \rho_{uu} = 1$$

The value $P_B(u)$ for the subsystem of Bob:

$$P_B(u) = \rho_{uu} = \frac{9}{25}$$

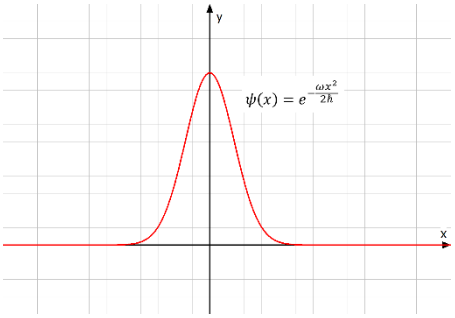
We get:

$$P(uu) \neq P_A(u)P_B(u)$$

$$\frac{3}{5} \neq \frac{9}{25}$$

The systems of Alice and Bob are not independent, they are entangled.

Wave functions, ground state:



Prerequisite

The time-independent Schrödinger equation:

$$H|\psi\rangle = E|\psi\rangle$$

Note: E is an energy eigenvalue.

The quantum mechanical Hamiltonian:

$$H|\psi(x)\rangle \rightarrow -\frac{\hbar^2}{2}\left(\frac{\partial}{\partial x}\left(\frac{\partial\psi(x)}{\partial x}\right)\right) + \frac{\omega^2 x^2}{2}\psi(x)$$

End prerequisite

The ground state wave function:

$$\psi(x) = e^{-\frac{\omega x^2}{2\hbar}}$$

It has no zeros and is the only energy eigenstate without nodes.

Concentrated near the origin it approaches fast to zero, so the probability density (the integral from $-\infty$ to ∞) exists.

We apply the Hamiltonian to this function.

We begin with the partial derivation:

$$-\frac{\hbar^2}{2}\left(\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}e^{-\frac{\omega x^2}{2\hbar}}\right)\right) \rightarrow$$

$$\frac{\hbar}{2}\left(\frac{\partial}{\partial x}\left(\omega x e^{-\frac{\omega x^2}{2\hbar}}\right)\right) \rightarrow$$

$$\frac{\hbar}{2}\left(\omega e^{-\frac{\omega x^2}{2\hbar}} - \frac{\omega^2 x^2}{\hbar}e^{-\frac{\omega x^2}{2\hbar}}\right) \rightarrow$$

$$\frac{\hbar\omega}{2}e^{-\frac{\omega x^2}{2\hbar}} - \frac{\omega^2 x^2}{2}e^{-\frac{\omega x^2}{2\hbar}}$$

We add the component of the position operator X:

$$\frac{\hbar\omega}{2}e^{-\frac{\omega x^2}{2\hbar}} - \frac{\omega^2 x^2}{2}e^{-\frac{\omega x^2}{2\hbar}} + \frac{\omega^2 x^2}{2}\psi(x) \rightarrow$$

$$\frac{\hbar\omega}{2}e^{-\frac{\omega x^2}{2\hbar}} - \frac{\omega^2 x^2}{2}e^{-\frac{\omega x^2}{2\hbar}} + \frac{\omega^2 x^2}{2}e^{-\frac{\omega x^2}{2\hbar}} \rightarrow$$

$$\frac{\hbar\omega}{2}e^{-\frac{\omega x^2}{2\hbar}}$$

Result:

$$H\big(\psi(x)\big) = \frac{\hbar\omega}{2}\psi(x)$$

The Hamiltonian applied to the ground state wave function gives back the wave function, multiplied with a factor $\frac{\hbar\omega}{2}$.

This is the ground state energy E_0.

Wave functions, locality and wave functions:

There exists the paradigmatic example of an entangled system of Alice and Bob, $\psi(ab)$. Alice may reside on Alpha Centauri, Bob in Palo Alto. What happens to the subsystem of Alice if Bob manipulates his part in Palo Alto?

Whatever Bob does to his system can be described by a unitary matrix $U_{bb'}$ (Bob's subsystem changing from the state b to the state b').

$U_{bb'}$ acts on the wave function and produces a new modified wave function:

$$\psi_{new}(ab) = \sum_{b'} U_{bb'}\,\psi(ab')$$

The complex conjugated of ψ_{new} is:

$$\psi^*{}_{new}(a'b) = \sum_{b''} \psi^*(a'b'')U^\dagger{}_{b''b}$$

Note: the primes added to avoid mixing the variables up.

We calculate the density matrix of Alice for the system after Bob acted on it.

Before the density matrix of Alice was:

$$\varrho_{aa'} = \sum_{b} \psi^*(a'b)\psi(ab)$$

After Bob's action the density matrix of Alice is:

$$\varrho_{aa'} = \sum_{b,b',b''} \psi^*(a'b'')U^\dagger{}_{b''b}U_{bb'}\psi(ab')$$

The unitarian matrices combines to the unit matrix again:

$$U^\dagger{}_{b''b}U_{bb'} = \delta_{b''b'}$$

In the sum all indices are collapsing to b:

$$\varrho_{aa'} = \sum_b \psi^*(a'b)\psi(ab)$$

The action of Bob on his subsystem does not change the density matrix of Alice, her subsystem remains exactly as it was.

Wave functions, momentum and wave functions:

We have the differentiation operator D:

$$D = \frac{d}{dx}$$

The momentum operator P:

$$P = -i\hbar D = -i\hbar \frac{d}{dx}$$

Note: the factor $-i$ is necessary to make the operator P Hermitian.

In terms of wave functions:

$$P\psi(x) = -i\hbar \frac{d\psi(x)}{dx}$$

In vector notation we have eigenvalues p and eigenvectors $|\psi\rangle$:

$$P|\psi\rangle = p|\psi\rangle$$

In terms of wave functions we use the momentum operator:

$$P = -i\hbar \frac{d}{dx}$$

We get the eigen equation:

$$-i\hbar \frac{d\psi(x)}{dx} = p\psi(x)$$

This is a differential equation:

$$\frac{d\psi(x)}{dx} = \frac{ip}{\hbar}\psi(x)$$

The solution to this differential equation:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{ip}{\hbar}x}$$

Note: the subscript p is a reminder that $\psi_p(x)$ is the eigenfunction (eigenvector) of P with the specific eigenvalue p. It is a function of x, labeled by an eigenvalue of P.

Note: $\psi_p(x)$ is a momentum eigenfunction in the position basis. It is a function of x, representing a momentum eigenstate.

Note: measurable quantities in physics are real values. The real part of $\psi_p(x)$ is a periodic function:

$$\cos\left(\frac{p}{\hbar}x\right)$$

The wavelength of this function:

$$\lambda = 2\pi\frac{\hbar}{p}$$

This is one aspect why wave functions are called wave functions.

Wave functions, momentum or position representation:

Prerequisite

Resolving the identity is a method to write the identity operator I:

$$I = \sum_i |i\rangle\langle i|$$

Note: $|i\rangle$ and $\langle i|$ are orthonormal basis vectors.

This method works in the case of integration too, either with the position representation

$$I = \int |x\rangle\langle x| dx$$

or with the momentum representation:

$$I = \int |p\rangle\langle p| dp$$

The inner product of a position eigenvector $|x\rangle$ and a momentum eigenvector $|p\rangle$ is symmetric:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ip}{\hbar}x}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ip}{\hbar}x}$$

End prerequisite

The wave function $\psi(x)$ of a particle moving in the x-direction is the projection of a state vector $|\psi\rangle$ onto the eigenvectors of position:

$$\langle X|\psi\rangle = \psi(x)$$

$\psi(x)$ is the wave function in position representation.

The probability to find a particle at position x:

$$P(x) = \psi^*(x)\psi(x)$$

The wave function $\tilde{\psi}(p)$ of a particle moving with momentum p is the projection of a state vector $|\psi\rangle$ onto the eigenvectors of momentum:

$$\langle P|\psi\rangle = \tilde{\psi}(p)$$

$\tilde{\psi}(p)$ is the wave function in momentum representation.

The probability to find a particle with momentum p:

$$P(p) = \tilde{\psi}^*(p)\tilde{\psi}(p)$$

Note: both wave functions $\psi(x)$ and $\tilde{\psi}(p)$ represent the same state vector $|\psi\rangle$.

If (x) and $\tilde{\psi}(p)$ represent the same state vector $|\psi\rangle$ there must be a possibility to transform them into each other – the Fourier transformation.

We begin with the wave function of the abstract state vector $|\psi\rangle$ in position representation:

$$\psi(x) = \langle X|\psi\rangle$$

We use the definition of the wave function in momentum representation:

$$\tilde{\psi}(p) = \langle P|\psi\rangle = \langle p|\psi\rangle$$

Note: p is an eigenvalue of P.

We insert the unit operator (position representation):

$$\tilde{\psi}(p) = \int \langle p|x\rangle\langle x|\psi\rangle dx$$

$\langle x|\psi\rangle$ is the wave function $\psi(x)$.

The inner product $\langle p|x\rangle$:

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-\frac{ip}{\hbar}x}$$

We get the wave function of momentum $\tilde{\psi}(p)$:

$$\tilde{\psi}(p) = \int \frac{1}{\sqrt{2\pi}} e^{-\frac{ip}{\hbar}x}\psi(x)dx = \frac{1}{\sqrt{2\pi}}\int e^{-\frac{ip}{\hbar}x}\psi(x)dx$$

This works the other way around too:

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\int e^{\frac{ip}{\hbar}x}\tilde{\psi}(p)dp$$

Momentum and position representation are reciprocal Fourier transforms of each other.

Wave function of near singlet state:

The near singlet state is a partially entangled state. The state-vector:

$$\sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle$$

or in the extended form:

$$|nearsing\rangle = 0|uu\rangle + \sqrt{0{,}6}|ud\rangle - \sqrt{0{,}4}|du\rangle + 0|dd\rangle$$

The wave function:

$$\psi_{uu} = 0 \quad \psi_{ud} = \sqrt{0{,}6} \quad \psi_{du} = -\sqrt{0{,}4} \quad \psi_{dd} = 0$$

Wave function, operator method and wave function:

Prerequisite

The lowering (annihilating) operator:

$$a^- = \frac{i}{\sqrt{2\pi\hbar}}(P - i\omega X)$$

The raising operator:

$$a^+ = \frac{-i}{\sqrt{2\pi\hbar}}(P + i\omega X)$$

Note: P is the momentum operator, X is the position operator:

$$P = -i\hbar\frac{d}{dx}$$

$$X = x$$

The ground state of the harmonic oscillator (a state vector):

$$|0\rangle$$

Note: this is not the zero vector. The ground state has the Energy $E_0 = \frac{\omega\hbar}{2}$.

End prerequisite

The annihilation (lowering) operator applied to the ground state "destroys" it:

$$a^-|0\rangle = 0$$

Note: $|0\rangle$ is the ground state, 0 is zero.

Written in terms of momentum operator P and position operator X:

$$\frac{i}{\sqrt{2\pi\hbar}}(P - i\omega X)\psi_0(x) = 0$$

Note: $\psi_0(x)$ is the ground state wave function we are searching for.

We divide by the constant factor:

$$(P - i\omega X)\psi_0(x) = 0$$

$$P\psi_0(x) - i\omega X\psi_0(x) = 0$$

$$-i\hbar\frac{d}{dx}\psi_0(x) = i\omega x\psi_0(x)$$

$$\frac{d}{dx}\psi_0(x) = -\frac{\omega x}{\hbar}\psi_0(x)$$

This is a first order differential equation with the solution:

$$\psi_0(x) = e^{-\frac{\omega}{2\hbar}x^2}$$

By applying the raising operator to the ground state wave function we get the wave function of the first excited state:

$$\psi_1(x) = a^+|0\rangle$$

Written in terms of momentum operator P and position operator X:

$$\frac{-i}{\sqrt{2\pi\hbar}}(P + i\omega X)\psi_0(x) = \psi_1(x)$$

Note: for better readability we omit the constant factor $\frac{-i}{\sqrt{2\pi\hbar}}$ and work with:

$$(P + i\omega X)\psi_0(x) = \psi_1(x)$$

We work with the left side of the equation and replace the operators:

$$i\left(-\hbar\frac{\partial}{\partial x} + \omega x\right)e^{-\frac{\omega}{2\hbar}x^2} =$$

$$i\hbar\frac{\omega x}{\hbar}e^{-\frac{\omega}{2\hbar}x^2} + i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$i\omega x e^{-\frac{\omega}{2\hbar}x^2} + i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$2i\omega x e^{-\frac{\omega}{2\hbar}x^2} =$$

$$2i\omega x\psi_0(x)$$

We multiply with the constant $\frac{-i}{\sqrt{2\pi\hbar}}$:

$$\frac{-i}{\sqrt{2\pi\hbar}}2i\omega x = \frac{2\omega}{\sqrt{2\pi\hbar}}x = \sqrt{\frac{2\omega^2}{\pi\hbar}}x$$

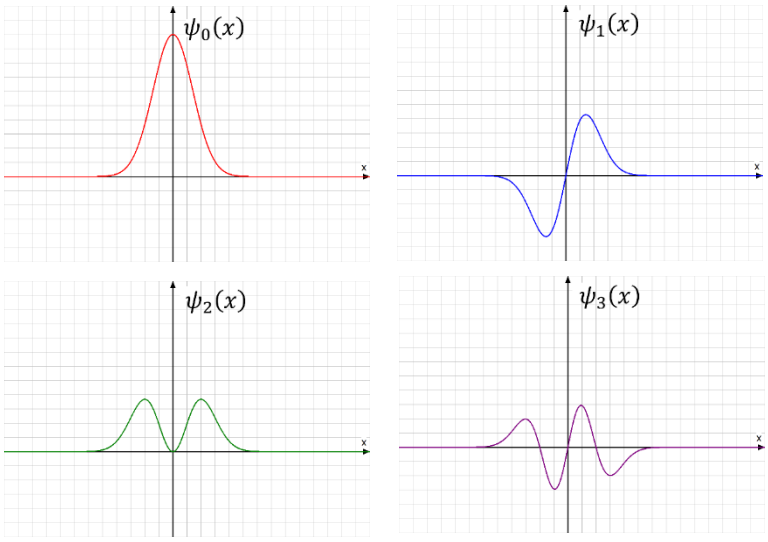
Result:

$$\psi_1(x) = \sqrt{\frac{2\omega^2}{\pi\hbar}}x\psi_0(x)$$

Applying the raising operator to the ground state we get the next excited state.

Note: an important difference between $\psi_0(x)$ and $\psi_1(x)$ is the presence of the factor x. The wave function of the first excited state has a zero, a node, at $x = 0$.

This continues going up the energy ladder, any successive excited state has on more node.



Wave function of product state:

The product state is a not entangled state, its two constituting states are independent, classical behavior.

The state-vector:

$$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$$

Note: the parameter α standing for Alice's subsystem, the parameter β for Bob's subsystem.

We have two normalization conditions:

$$\alpha_u^*\alpha_u + \alpha_d^*\alpha_d = 1$$

$$\beta_u^*\beta_u + \beta_d^*\beta_d = 1$$

The wave function is factorized:

$$\psi_{uu} = \alpha_u\beta_u \quad \psi_{ud} = \alpha_u\beta_d \quad \psi_{du} = \alpha_d\beta_u \quad \psi_{dd} = \alpha_d\beta_d$$

Wave function representing particles:

Let X be the position operator. The outcomes of measuring X must give the position of a particle.

X is an operator, we search for its eigenvalues and eigenvectors.

The eigen-equation for X:

$$X|\psi\rangle = x_0|\psi\rangle$$

Note: x_0 is eigenvalue to the eigenvector $|\psi\rangle$.

In terms of wave function this becomes:

$$x\psi(x) = x_0\psi(x)$$

We rewrite this:

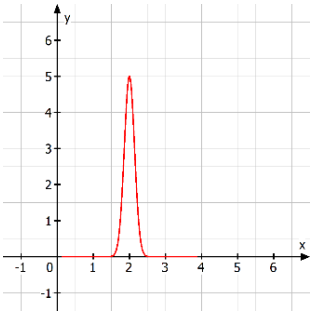
$$(x - x_0)\psi(x) = 0$$

What we need is a function that is zero for every $x \neq x_0$ and nonzero at a single point, the Dirac delta function $\delta(x - x_0)$.

Note: the Dirac delta function can be thought of as $\lim_{n\to\infty} ne^{-(n(x-x_0))^2}$.

The wave function $\psi(x) = \delta(x - x_0)$ represent the state in which the particle is located exactly at the point x_0 on the x-axis.

This fits into the intuitive picture that the wave function representing a particle at position x_0 must be zero everywhere except at x_0.



Wave function of singlet state:

In case of a two-spin system the maximum entangled state, the singlet state can be written as:

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle)$$

or in the extended form:

$$|sing\rangle = 0|uu\rangle + \frac{1}{\sqrt{2}}|ud\rangle - \frac{1}{\sqrt{2}}|du\rangle + 0|dd\rangle$$

The singlet state is a completely entangled state.

The wave function:

$$\psi_{uu} = 0 \quad \psi_{ud} = \frac{1}{\sqrt{2}} \quad \psi_{du} = -\frac{1}{\sqrt{2}} \quad \psi_{dd} = 0$$

Wave function, state vector and wave function:

a) A wave function is the collection of coefficients (components) that multiply the basis vectors in an eigenfunction expansion:

$$|\psi\rangle = \sum_j \alpha_j |\psi_j\rangle$$

Note: $|\psi_j\rangle$ are orthonormal eigenvectors of a Hermitian operator.
Note: for every index j (for every eigenvector) exists a coefficient α_j.
Note: the collection of coefficients α_j is the wave function.
Note: the relationship between the components often is cryptic (normalization constraints etc.)

b) In situations where the state vector is expressed as an integral, the wave function is a continuous function and needs to be properly defined.

Wavelength, momentum and wavelength:

Light of a given wavelength λ is composed of photons with momentum:

$$\lambda = \frac{2\pi\hbar}{p}$$

Photons with momentum p have wavelength:

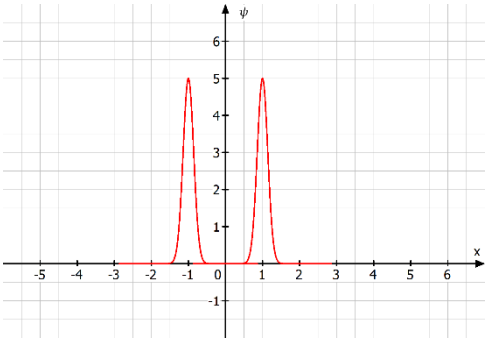
$$p = \frac{2\pi\hbar}{\lambda}$$

The product of wavelength and momentum:

$$\lambda p = 2\pi\hbar = const.$$

Wave packets:

Wave packets, bimodal wave packets:



Quantum equation of motion looks classical if the wave packets are unimodal (nice, centered single bump) or coherent and well localized.

If wave packets are bimodal (two-humped), it is not always true that the time rate of change of the momentum is the force evaluated at the expectation value of x:

$$\langle F(x)\rangle \neq F(\langle x\rangle)$$

This kind of wave packet tends to shatter more easily even if the potentials in question are smooth.

Wave packets, Gaussian or minimum uncertainty wave packets:

Gaussian wave packets are minimum uncertainty wave packets with $\Delta x \Delta p = \frac{\hbar}{2}$.

These wave packets have the form of a Gaussian curve. Over time, they spread out and flatten.

Note: the gaussian packet describes the probability distribution of the particle. The packet to spread out does not mean the particle itself in some sense is spreading out. The probability of finding the particle is spreading out.

Wave packets, moving at fixed speed:

We start with a simple Hamiltonian, a fixed constant times the momentum operator P:

$$H = cP$$

We insert this Hamiltonian into the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial|\psi\rangle}{\partial t} = -ci\hbar \frac{\partial}{\partial x}|\psi\rangle$$

In terms of wave-functions:

$$i\hbar \frac{\partial\psi(x,t)}{\partial t} = -ci\hbar \frac{\partial\psi(x,t)}{\partial x}$$

Note: $\psi(x,t)$ is a function of both x and t.

We cancel the term $i\hbar$:

$$\frac{\partial\psi(x,t)}{\partial t} = -c\frac{\partial\psi(x,t)}{\partial x}$$

Any function of $(x - ct)$ is a solution.

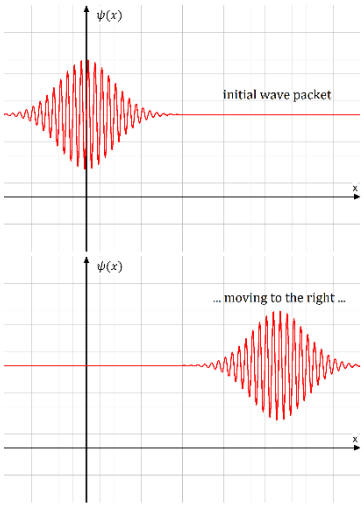
We look at the time evolution of $\psi(x - ct)$. How does a wave function $\psi(x - ct)$ evolve with time?

We start at time $t = 0$.

Our wave-function is a wave-packet localized on the x −axis.

As t increases the wave-packet is shifting to the right with uniform velocity c.

This description is pretty close to the correct description of a neutrino that moves immeasurably slower than the speed of light.

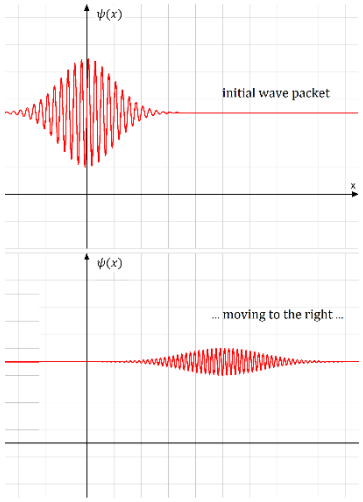


Wave packets for a nonrelativistic free particle:

The time dependent Schrödinger equation for a nonrelativistic free particle:

$$i\hbar\frac{\partial\psi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(t)}{\partial x^2}$$

In contrast to the wave particle of the simple Hamiltonian above, $H = cP$, waves of different wavelength move with different velocities, the wave function does not maintain its shape.



Wheeler, John:

John Archibald Wheeler (1911 – 2008) was an American theoretical physicist. He was largely responsible for reviving interest in general relativity in the United States after World War II. Wheeler also worked with Niels Bohr in explaining the basic principles behind nuclear fission. Together with Gregory Breit, Wheeler developed the concept of the Breit–Wheeler process. *(Courtesy Wikipedia)*

x-axis, spins along the x-axis:

We have a single spin system. We can represent the states $right$, $|r\rangle$ and $left$, $|l\rangle$ as a linear combination of the orthonormal basis vectors up, $|u\rangle$ and $down$, $|d\rangle$:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$$

$$|l\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

The corresponding bras:

$$\langle r| = \frac{1}{\sqrt{2}}\langle u| + \frac{1}{\sqrt{2}}\langle d|$$

$$\langle l| = \frac{1}{\sqrt{2}}\langle u| - \frac{1}{\sqrt{2}}\langle d|$$

Basis vectors must be orthogonal. We check:

$$\langle r|l\rangle = \left(\frac{1}{\sqrt{2}}\langle u| + \frac{1}{\sqrt{2}}\langle d|\right)\left(\frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle\right) =$$

$$\frac{1}{2}(\langle u|u\rangle - \langle u|d\rangle + \langle d|u\rangle - \langle d|d\rangle) =$$

$$\frac{1}{2}(1 - 0 + 0 - 1) = 0$$

Note: $|u\rangle$, $|d\rangle$ are orthonormal basis vectors.

The same holds for $\langle l|r\rangle$.

X-operator:

The position operator or X-operator (the matrix) has eigenvalues and eigenvectors, the observables.

The eigen-equation for the operator X:

$$X|\psi\rangle = x_0|\psi\rangle$$

Note: $|\psi\rangle$ is eigenvector to the operator X with eigenvalue x_0.

Note: x_0 is a real number, an observable or measurable.

y-axis, spins along the y-axis:

We have a single spin system. We can represent the states in, $|i\rangle$ and out, $|o\rangle$ along the y-axis as a linear combination of the orthonormal basis vectors up, $|u\rangle$ and $down$, $|d\rangle$:

$$|i\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle$$

$$|o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle$$

Note: i is the imaginary unit, $|i\rangle$ the state vector along the y-axis.

The corresponding bras:

$$\langle i| = \frac{1}{\sqrt{2}}\langle u| - \frac{i}{\sqrt{2}}\langle d|$$

$$\langle o| = \frac{1}{\sqrt{2}}\langle u| + \frac{i}{\sqrt{2}}\langle d|$$

Basis vectors must be orthogonal. We check:

$$\langle i|o\rangle = \left(\frac{1}{\sqrt{2}}\langle u| - \frac{i}{\sqrt{2}}\langle d|\right)\left(\frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle\right) =$$

$$\frac{1}{2}(\langle u|u\rangle - i\langle u|d\rangle - i\langle d|u\rangle - \langle d|d\rangle) =$$

$$\frac{1}{2}(1 - 0 + 0 - 1) = 0$$

Note: $|u\rangle$, $|d\rangle$ are orthonormal basis vectors.

The same holds for $\langle o|i\rangle$.

Zero function:

This is number 4 of the mathematical axioms defining a vector space:

1. The sum of any two functions is a function.
2. The addition of functions is commutative.
3. The addition of functions is associative.
4. **There exists a zero function for addition.**
5. There exists an inverse function for addition.
6. Multiplying a function by a complex number gives a new function and is linear.

There must be a function $g(x)$ such as:

$$f(x) + g(x) = f(x)$$

$g(x)$ is the zero function.

Zero operator:

A zero operator (a matrix) Z acting on any vector V of a space of states:

$$Z|V\rangle = |0\rangle$$

Example:

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$