This paper deals with the time development by quantizing a classical system described with the Hamilton operator.

Related information you may find at:

http://scipp.ucsc.edu/~haber/ph215/TimeOrderedExp.pdf

Tutorium Quantenmechanik, J.-M. Schwindt, Springer, ISBN 978-3-642-37791-4. (… written in German…)

Hope I can help you with learning quantum mechanics.

Contents

Time independent Hamiltonian

We start with a classical system and its energy, E_{cl}. The Hamiltonian describes the energy.

$$i\hbar\frac{d}{dt}|v(t)\rangle = H|v(t)\rangle$$

By replacing the classical variables with quantum operators, we get the quantum Hamiltonian. The problem with this access is that the classical description may contain less information than the quantum mechanical. The replacement may be ambiguous.

An example that does not have this ambiguity is the time development of spin in an external magnetic field.

The Energy (classic):

$$E_{cl} = a \cdot \vec{s} \cdot \vec{B}$$

Note: a is a real constant, $\vec{s}$ is the spin of an electron, $\overline{B}$ the magnetic field.

If $a > 0$ we encounter a force that tries to orient the spin in the $-\vec{B}$-direction.

The Hamiltonian for this scenario is:

$$H = \frac{a\hbar}{2}\left(B_x\sigma_x + B_y\sigma_y + B_z\sigma_z\right)$$

Note: B_i are the components of the magnetic field, σ_i are 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 can write the Hamiltonian as one 2×2 complex valued matrix:

$$H = \frac{a\hbar}{2}\begin{pmatrix} B_z & B_x - i \cdot B_y \\ B_x + i \cdot B_y & -B_z \end{pmatrix}$$

Eigenvalues E_i of the operator H are the possible energies of the system:

$$H|v\rangle = E_i|E_i\rangle$$

Eigenvectors $|E_i\rangle$ are the possible states, building an orthonormal basis of the Hilbert space.

In case the time dependent state $|v(t)\rangle$ at time $t = 0$ is eigenvector of the time-independent Hamiltonian

$$|v(t = 0)\rangle = |E_i\rangle$$

then the Schrödinger equation

$$i\hbar\frac{d}{dt}|v(t)\rangle = H|v(t)\rangle$$

has a simple solution:

$$|v(t)\rangle = e^{-i\frac{E_i}{\hbar}t}|E_i\rangle$$

Up to a phase factor the state remains the same. The state is called stationary.

Note: This is valid for time independent Hamiltonian only.

In case $|v(t=0)\rangle$ is not stationary, we decompose it into the basis vectors $|E_i\rangle$:

$$|v(0)\rangle = \sum_{i=1}^{n} |E_i\rangle \langle E_i|v(0)\rangle$$

Note: Any vector can be decomposed with basis vectors. $|E_i\rangle$ build an orthonormal basis.

We remember:

$$|v(t)\rangle = e^{-i\frac{E_i}{\hbar}t}|E_i\rangle$$

We get:

$$|v(t)\rangle = \sum_{i=1}^{n} |E_i\rangle \langle E_i|v(t)\rangle = \sum_{i=1}^{n} |E_i\rangle \langle E_i|v(0)\rangle e^{-i\frac{E_i}{\hbar}t}$$

We use that the Hamiltonian operator H expressed in the orthonormal basis $\{|E_i\rangle\}$:

$$H = \begin{pmatrix} E_1 & 0 & 0 & \dots & 0 \\ 0 & E_2 & 0 & \dots & 0 \\ 0 & 0 & E_3 & \dots & 0 \\ \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & \dots & E_n \end{pmatrix}$$

For diagonal matrices holds:

$$e^{-i\frac{H}{\hbar}t} = e^{-\frac{i}{\hbar}\cdot\begin{pmatrix} E_1 & 0 & 0 & \dots & 0 \\ 0 & E_2 & 0 & \dots & 0 \\ 0 & 0 & E_3 & \dots & 0 \\ \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & \dots & E_n \end{pmatrix}\cdot t} = \begin{pmatrix} e^{-i\frac{E_1}{\hbar}t} & 0 & 0 & \dots & 0 \\ 0 & e^{-i\frac{E_2}{\hbar}t} & 0 & \dots & 0 \\ 0 & 0 & e^{-i\frac{E_3}{\hbar}t} & \dots & 0 \\ \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & \dots & e^{-i\frac{E_n}{\hbar}t} \end{pmatrix}$$

We chose the Hamiltonian for a constant magnetic field in z-direction:

$$H = \frac{a\hbar}{2}\begin{pmatrix} B_z & B_x - i\cdot B_y \\ B_x + i\cdot B_y & -B_z \end{pmatrix} \to \frac{a\hbar}{2}B_z\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Eigenvalues are:

$$E_1 = \frac{a\hbar B_z}{2}, E_2 = -\frac{a\hbar B_z}{2}$$

Eigenvectors are:

$$|E_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |z+\rangle, |E_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |z-\rangle$$

We check this:

$$\frac{a\hbar}{2}B_z\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{a\hbar}{2}B_z\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\frac{a\hbar}{2}B_z\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{a\hbar}{2}B_z\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The lower one E_2 is the ground energy and $|E_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ the ground state of the system.

We set $|v_1(t=0)\rangle = |E_1\rangle$, $|v_2(t=0)\rangle = |E_2\rangle$ and get the time dependent states:

$$|v_1(t)\rangle = e^{-i\frac{\frac{a\hbar B_z}{2}}{\hbar}t}|E_1\rangle = e^{-i\frac{aB_z}{2}t}|E_1\rangle \coloneqq e^{-i\omega t}|E_1\rangle$$

$$|v_2(t)\rangle = e^{i\omega t}|E_2\rangle$$

Note: $\omega = \frac{aB_z}{2}$

Note: $e^{-i\omega t}|E_1\rangle$ essentially is $|E_1\rangle$ up to a time dependent phase, the same holds for $e^{i\omega t}|E_2\rangle$.

What happens if e. g. we set $|v(t=0)\rangle = \frac{1}{\sqrt{2}}(|E_2 + E_2\rangle = |x+\rangle$?

We get:

$$|v(t)\rangle = e^{-i\frac{aB_z}{2}t}\frac{1}{\sqrt{2}}(|E_2 + E_2\rangle =$$

$$\frac{1}{\sqrt{2}}e^{-i\frac{aB_z}{2}t}\begin{pmatrix}1\\1\end{pmatrix} =;$$

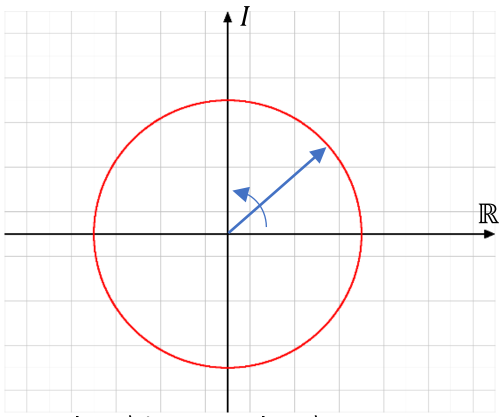
We replace the exponential of the diagonal matrix by the diagonal matrix of the exponentials:

$$\frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\frac{aB_z}{2}t} & 0\\ 0 & e^{i\frac{aB_z}{2}t}\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} =$$

$$\frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\frac{aB_z}{2}t}\\ e^{i\frac{aB_z}{2}t}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\omega t}\\ e^{i\omega t}\end{pmatrix} =$$

$$\frac{1}{\sqrt{2}}e^{-i\omega t}\begin{pmatrix}1\\ e^{2i\omega t}\end{pmatrix}$$

Note: $e^{-i\omega t}$ is a phase we ignore.



The expression

$$\begin{pmatrix}1\\ e^{2i\omega t}\end{pmatrix}$$

leads to a vector

$$\begin{pmatrix}1\\ z\end{pmatrix}$$

with z constantly varying between $1 \to i \to -1 \to -i \to 1$.

In other words: The state $|x+\rangle$ becomes $|y+\rangle$ becomes $|x-\rangle$ becomes $|y-\rangle$ becomes $|x+\rangle$ …

The spin is precessing round the z-axis, like in the classical case.

Time development operator

We remember time development from t_0 to t is performed by a unitary operator $e^{-i\frac{E_i}{\hbar}(t-t_0)}$:

$$|v(t)\rangle = e^{-i\frac{H}{\hbar}(t-t_0)}|v(t=0)\rangle$$

The unitary operator:

$$U(t,t_0) = e^{-i\frac{H}{\hbar}(t-t_0)}$$

We write this as:

$$|v(t)\rangle = U(t,t_0)|v(0)\rangle$$

The operator is unitary, the norm of the state vector doesn't change. If the state is normalized it stays normalized.

We call the operator $U(t,t_0)$ the time development operator or propagator.

We name two properties of $U(t,t_0)$:

$$U(t_2,t_0) = U(t_2,t_1)U(t_1,t_0)$$

$$U(t_0,t_0) = id$$

The first property results from the additivity of exponents, the second on from $e^0 = 1$.

Time dependent Hamiltonian

If the Hamiltonian is time dependent, we have no time-independent eigenvalues and eigenstates, but we claim that there must exist a unitary time-development operator $U(t,t_0)$.

To make the equations easier to read we use that we can choose any arbitrary t_0 and write $U(t)$ instead of $U(t,t_0)$.

We start with the Schroedinger equation:

$$i\hbar\frac{d}{dt}|v(t)\rangle = H(t)|v(t)\rangle$$

We insert the operator $U(t)$:

$$i\hbar\frac{d}{dt}U(t)|v(0)\rangle = H(t)U(t)|v(0)\rangle$$

We examine $i\hbar\frac{d}{dt}U(t)|v(0)\rangle$:

$$i\hbar\frac{d}{dt}U(t)|v(0)\rangle = i\hbar\left(\frac{d}{dt}U(t)\right)|v(0)\rangle + i\hbar U(t)\frac{d}{dt}\big(|v(0)\rangle\big) =$$

$$i\hbar\left(\frac{d}{dt}U(t)\right)|v(0)\rangle$$

Note: $|v(0)$ is constant.

We get a differential equation:

$$i\hbar \frac{d}{dt} U(t)|v(0)\rangle = H(t)U(t)|v(0)\rangle \rightarrow$$

$$i\hbar \frac{d}{dt} U(t) = H(t)U(t)$$

Differentiating an operator

In analogy to differentiating functions we differentiate an operator A:

$$\frac{d}{dt} A(t) = \lim_{\varepsilon \to 0} \frac{A(t+\varepsilon) - A(t)}{\varepsilon}$$

Operators are matrices, we apply the differentiating process to every element:

$$\frac{d}{dt} A(t) \rightarrow \frac{d}{dt} \left(A(t)_{ij}\right)$$

Note: the result depends on a chosen basis and changes if the basis changes.

Constant Hamiltonian

If the operator H is constant:

$$\frac{d}{dt} U(t) = \frac{1}{i\hbar} H \cdot U(t)$$

We get the solution:

$$U(t) = exp\left(\frac{1}{i\hbar} H \cdot t\right)$$

Time dependent but commuting Hamiltonians

Note: The Hamiltonian for a spin in a magnetic field fulfills this condition.

If operators $H(t)$ for different times t_1, t_2 are commuting, we get the solution:

$$\frac{d}{dt} U(t) = \frac{1}{i\hbar} H(t)U(t) \rightarrow$$

$$U(t) = exp\left(\frac{1}{i\hbar} \int_0^t H(\tau) d\tau\right)$$

Note: If and only if the operators $H(t)$ for different times t_1, t_2 are commuting, we get:

$$H(t) = \frac{d}{dt} \int_0^t H(\tau) d\tau$$

We will check this.

For reasons of simplicity, we substitute:

$$R(t) \coloneqq \frac{1}{i\hbar} \int_0^t H(\tau) d\tau$$

We differentiate with respect to time:

$$\dot{R}(t) \coloneqq \frac{1}{i\hbar} H(t)$$

The Hamiltonians $H(t), H(\tau)$ commute → $R(t)$ and $\dot{R}(t)$ commute:

$$\left[R(t), \dot{R}(t)\right] = \left[\frac{1}{i\hbar} H(t), \frac{1}{i\hbar} \int_0^t H(\tau) d\tau\right] =$$

$$\left(\frac{1}{i\hbar}\right)^2 \left(H(t) \int_0^t H(\tau) d\tau - \left(\int_0^t H(\tau) d\tau\right) H(t)\right) =$$

$$\left(\frac{1}{i\hbar}\right)^2 \left(\int_0^t H(t)H(\tau) d\tau - \int_0^t H(\tau)H(t) d\tau\right) =$$

$$\left(\frac{1}{i\hbar}\right)^2 \int_0^t H(t)H(\tau) - H(\tau)H(t) d\tau =$$

$$\left(\frac{1}{i\hbar}\right)^2 \int_0^t [H(t), H(\tau)] d\tau = 0$$

We rewrite the exponent by power series:

$$U = exp\big(R(t)\big) =$$

$$\frac{1}{0!} id + \frac{1}{1!} R(t) + \frac{1}{2!}\big(R(t)\big)^2 + \frac{1}{3!}\big(R(t)\big)^3 + \cdots$$

We derivate with respect to time:

$$\frac{d}{dt} U =$$

$$\frac{d}{dt}\left(\frac{1}{0!} id + \frac{1}{1!} R(t) + \frac{1}{2!}\big(R(t)\big)^2 + \frac{1}{3!}\big(R(t)\big)^3 + \frac{1}{4!}\big(R(t)\big)^4 + \cdots\right) =$$

$$\frac{1}{1!}\dot{R}(t) + \frac{1}{2!} 2R(t)\dot{R}(t) + \frac{1}{3!} 3\big(R(t)\big)^2 \dot{R}(t) + \frac{1}{4!} 4\big(R(t)\big)^3 \dot{R}(t) + \cdots =$$

$$\dot{R}(t)\left(\frac{1}{0!} + \frac{1}{1!} R(t) + \frac{1}{2!}\big(R(t)\big)^2 + \frac{1}{3!}\big(R(t)\big)^3 + \cdots\right) =$$

$$\dot{R}(t) exp\big(R(t)\big)$$

Result:

$$\frac{d}{dt} U = \dot{R}(t) exp\big(R(t)\big) \rightarrow$$

$$\frac{d}{dt} U = \frac{1}{i\hbar} H(t) exp\left(\frac{1}{i\hbar} \int_0^t H(\tau) d\tau\right)$$

with

$$H(t) = \frac{d}{dt}\int_{0}^{t} H(\tau)d\tau$$

In the end we get:

$$\frac{d}{dt}U = \frac{1}{i\hbar}H(t)U$$

We compare this with the solution of a constant Hamiltonian:

$$U(t) = exp\left(\frac{1}{i\hbar}H \cdot t\right)$$

The time development operator is essentially the same.

Not commuting Hamiltonians

For reason of completeness, now with the complete time-gap (t, t_0).

If the operators $H(t)$ for different times t_1, t_2 are not commuting, then $U(t, t_0)$ becomes:

$$U(t, t_0) = T\left\{exp\left(\frac{1}{i\hbar}\int_{t_0}^{t} H(\tau)d\tau\right)\right\}$$

T is the time-ordered exponential:

$$T\left\{exp\left(\frac{1}{i\hbar}\int_{t_0}^{t} H(\tau)d\tau\right)\right\} \coloneqq$$

$$id + \frac{1}{i\hbar}\int_{t_0}^{t} H(t_1)dt_1 + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} H(t_1)dt_1 \int_{t_0}^{t_1} H(t_2)dt_2 + \left(\frac{1}{i\hbar}\right)^3 \int_{t_0}^{t} H(t_1)dt_1 \int_{t_0}^{t_1} H(t_2)dt_2 \int_{t_0}^{t_2} H(t_3)dt_3 + \cdots$$

The term time-ordered refers to the fact that in the n-th term of the series we have a product $H(t_1)H(t_2)H(t_3) \cdot \ldots \cdot H(t_\mathrm{n})$ of non-commuting operators with integration ranges that force ordered times $t_1 \geq t_2 \geq \cdots \geq t_\mathrm{n}$.