

Via differential equations we chose a traditional access to quantum mechanics and the harmonic oscillator. We work in one dimension only.

This paper is based on "Hort-Thoma, Die Differentialgleichungen der Technik und Physik", Leipzig 1950.

Related information you may find at:

<https://ocw.mit.edu/courses/8-04-quantum-physics-i-spring-2016/pages/lecture-notes/>

Please refer to Part 2: Quantum Physics in One-dimensional Potentials, # 13 and 14/15.

Hope I can help you with learning quantum mechanics.

Note: the typo for the Greek letter ν and the letter v for speed are very similar. Therefore, throughout this text we will use ν for the Greek letter for frequency and \underline{v} for speed.

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Plane wave

For a plane wave in space holds the differential equation:

$$a^2 \Delta \psi(r, t) = \frac{\partial^2}{\partial t^2} \psi(r, t) \quad (1)$$

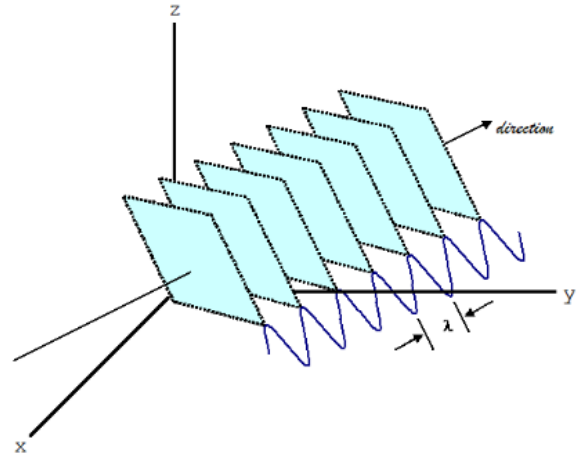
Note: Δ is the Laplace operator:

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Note: $\psi(r, t)$ is a function of space and time.

Note: Plane waves are an approximation based on radial waves if the distance to the origin of the wave is large compared to the wave length.

Note: When dealing with plane waves we always can orient the measuring system in a way that the wave propagates along one axis. The Laplace operator reduces to the partial derivatives along this axis.



Note: The vector pointing in the direction of the wave is called wave vector \vec{k} with magnitude:

$$|\vec{k}| = k = \frac{2\pi}{T} \cdot \frac{1}{c} = \frac{\omega}{c} = 2 \cdot \pi \cdot \nu \cdot \frac{1}{c} = \frac{2 \cdot \pi \cdot \nu}{\nu \cdot \lambda} = \frac{2 \cdot \pi}{\lambda}$$

Note: there are several ways to express k :

$$k = \frac{\omega}{c} \text{ or } k = \frac{2 \cdot \pi}{\lambda}$$

We orient our system in a way that the wave propagates along the x -axis.

The differential equation (1) then becomes:

$$a^2 \frac{\partial^2}{\partial x^2} \psi(x, t) = \frac{\partial^2}{\partial t^2} \psi(x, t) \quad (2)$$

We try the wave function:

$$\psi(x, t) = A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)\right)}$$

Note: A represents the amplitude, $-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)\right)$ the oscillation.

Note: If we fix position x , the oscillation is caused by changing in time.

Note: If we fix time t , the oscillation is caused by changing the position.

Note: Changing position can be done arbitrarily, changing in time not.

We check whether $\psi(x, t)$ is a solution to the differential equation (2):

$$a^2 \frac{\partial^2}{\partial x^2} \psi(x, t) = \frac{\partial^2}{\partial t^2} \psi(x, t)$$

| Left side: | Right side: |
|---|---|
| $a^2 \frac{\partial^2}{\partial x^2} \psi(x, t) = a^2 \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} \psi(x, t) \right) =$ $a^2 \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} \left(A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)} \right) \right) =$ $a^2 \frac{\partial}{\partial x} \left(\frac{i2\pi}{\lambda} \cdot A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)} \right) =$ $-\frac{4\pi^2 a^2}{\lambda^2} \left(A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)} \right) =$ $-\frac{4\pi^2 a^2}{\lambda^2} \psi(x, t)$ | $\frac{\partial^2}{\partial t^2} \psi(x, t) = \frac{\partial}{\partial t} \left(\frac{\partial}{\partial t} \psi(x, t) \right) =$ $\frac{\partial}{\partial t} \left(\frac{\partial}{\partial t} \left(A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)} \right) \right) =$ $\frac{\partial}{\partial t} \left(-\frac{i2\pi}{T} \cdot A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)} \right) =$ $-\frac{4\pi^2}{T^2} \cdot A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)} =$ $-\frac{4\pi^2}{T^2} \psi(x, t)$ |

We go back to the differential equation (2):

$$a^2 \frac{\partial^2}{\partial x^2} \psi(x, t) = \frac{\partial^2}{\partial t^2} \psi(x, t)$$

We insert our results:

$$-\frac{4\pi^2 a^2}{\lambda^2} \psi(x, t) = -\frac{4\pi^2}{T^2} \psi(x, t)$$

We get:

$$\frac{a^2 4\pi^2}{\lambda^2} = \frac{4\pi^2}{T^2} \rightarrow a^2 = \frac{\lambda^2}{T^2} \rightarrow a = \frac{\lambda}{T} = \lambda \nu$$

Note: a is the phase velocity of the plane wave.

Note: For an electromagnetic wave we have $c = \lambda \nu$ with c being the speed of light.

Note: The group velocity is the velocity of an envelope of the wave – e. g. a wave packet. For more information please see https://en.wikipedia.org/wiki/Group_velocity

Result: $\psi(x, t)$ is a solution to the differential equation (2):

$$\psi(x, t) = A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)}$$

Note: $\psi(x, t)$ is a complex function. We get the real part by calculating:

$$A \cdot \frac{e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)} + e^{i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)} \right)}{2}$$

De Broglie

De Broglie recognized an analogy between [Maupertuis'](#) principle, an integral over the generalized coordinates known as the abbreviated action or reduced action and [Fermat's](#) principle of least time.

| | |
|---|---|
| Maupertuis (particle): The variation of the path integral of the speed v of a particle vanishes: | Fermat (wave): The path light chooses between two points A and B is a minimum: |
| $\delta \int_A^B \underline{v} ds = 0$ | $\delta \int_A^B \frac{1}{u} du = 0$ |
| Note: \underline{v} is the speed of the particle | Note: $u = \lambda \cdot v$ is the phase velocity of the wave. |

De Broglie stated: The presence of a physically detectable space-time wave field is linked to the presence of a free material particle.

A particle with momentum p and energy E corresponds to a plane, monochromatic wave with wave number k and frequency ν , propagating in the direction of the momentum.

Note: For waves in x -direction we have $k = \frac{1}{\lambda}$.

| | |
|---|--|
| De Broglie: | Classic physics: |
| A particle with momentum p along the x -axis can be described as a plane wave: with wave number $k = \frac{p}{h}$ frequency $\nu = \frac{E}{h}$ wave length $\lambda = \frac{h}{p}$ | From (nonrelativistic) classic physics we use: energy: $E = \frac{p^2}{2m}$ speed: $\underline{v} = \frac{dE}{dp}$ |
| We can reorganize this: $k = \frac{p}{h} \rightarrow p = h \cdot k$ $\nu = \frac{E}{h} \rightarrow E = h \cdot \nu$ $\lambda = \frac{h}{p} \rightarrow p = \frac{h}{\lambda}$ | Note: for a free particle the kinetic energy is the total energy in nonrelativistic case. |

Note: h is the Planck constant. The unit of h is [energy · time].

Note: We are working in one dimension so we can omit vector notation: $\vec{p} = p$ etc.

Note: At this time the energy according to de Broglie is not quantized, despite the fact that we use Planck's constant, because ν is a real number. Quantization will become a result of the calculations below.

Note: In literature you find $k = \frac{2\pi}{\lambda}$. The factor 2π depends on the model the author is working with.

We combine de Broglie and classic:

$$E = h \cdot \nu = \frac{p^2}{2 \cdot m} = \frac{h^2}{2 \cdot m \cdot \lambda^2} \rightarrow \nu = \frac{h}{2 \cdot m \cdot \lambda^2}$$

Note: This is the de Broglie relation.

Nonrelativistic Schrödinger

We use the classic energy equation:

$$E = \frac{p^2}{2 \cdot m} \rightarrow E - \frac{p^2}{2 \cdot m} = 0$$

We rewrite by use of the de Broglie relation:

$$h \cdot \nu - \frac{h^2}{2 \cdot m \cdot \lambda^2} = 0 \rightarrow \nu - \frac{h}{2 \cdot m \cdot \lambda^2} = 0$$

We use the wave function:

$$\psi(x, t) = A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)\right)} \quad (3)$$

For this wave function holds:

| | |
|---|--|
| $-\frac{i}{2\pi} \cdot \frac{\partial}{\partial x} \psi(x, t) = \frac{1}{\lambda} \cdot \psi(x, t)$ $-\left(\frac{1}{2\pi}\right)^2 \cdot \frac{\partial^2}{\partial x^2} \psi(x, t) = \left(\frac{1}{\lambda}\right)^2 \cdot \psi(x, t)$ | $\frac{i}{2\pi} \cdot \frac{\partial}{\partial t} \psi(x, t) = \nu \cdot \psi(x, t)$ |
| We rewrite this in operator style: | |
| $\left(\frac{1}{\lambda}\right)^2 = -\left(\frac{1}{2\pi}\right)^2 \cdot \frac{\partial^2}{\partial x^2}$ | $\nu = \frac{i}{2\pi} \cdot \frac{\partial}{\partial t}$ |

We take the de Broglie relation (3):

$$\nu - \frac{h}{2 \cdot m} \cdot \frac{1}{\lambda^2} = 0$$

We insert ν and $\left(\frac{1}{\lambda}\right)^2$:

$$\frac{i}{2\pi} \cdot \frac{\partial}{\partial t} \psi(x, t) + \frac{h}{2 \cdot m} \cdot \left(\frac{1}{2\pi}\right)^2 \cdot \frac{\partial^2}{\partial x^2} \psi(x, t) = 0 \quad (4)$$

This is the nonrelativistic Schrödinger equation for a free particle moving in x -direction.

We can write this as a differential operator \hat{F} :

$$\hat{F} := \left(\frac{i}{2\pi} \cdot \frac{\partial}{\partial t} + \frac{h}{2 \cdot m} \cdot \left(\frac{1}{2\pi}\right)^2 \cdot \frac{\partial^2}{\partial x^2} \right)$$

$$\hat{F}\psi(x, t) = 0$$

$$\left(\frac{i}{2\pi} \cdot \frac{\partial}{\partial t} + \frac{h}{2 \cdot m} \cdot \left(\frac{1}{2\pi}\right)^2 \cdot \frac{\partial^2}{\partial x^2} \right) \psi(x, t) = 0$$

Note: The usage of the term operator is motivated by the aspect of eigenfunctions we need later.

Note: Together with:

$$\psi(x, t) = A \cdot e^{-i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)\right)}$$

we could also use:

$$\psi(x, t) = A \cdot e^{i\left(2\pi\left(\frac{t}{T} - \frac{x}{\lambda}\right)\right)}$$

This would represent a particle running into the opposite direction. From a classic point of view the energy of the particle is either positive or negative, depending on the direction it's moving. The absolute value of the energy is the same.

Particle in a potential

In classical physics we have the equation of motion:

$$m \cdot \frac{d^2}{dt^2} x(t) = F$$

If the force F is the result of a potential $U(x, t)$, we get:

$$F = -\frac{\partial}{\partial x} U(x, t)$$

Note: The potential might be time dependent.

We rewrite the equation of motion in the canonical Hamiltonian style:

$$\frac{dp}{dt} = -\frac{\partial}{\partial q} H(p, q, t)$$

$$\frac{dq}{dt} = \frac{\partial}{\partial p} H(p, q, t)$$

Note: the Hamiltonian corresponds to the total energy of the system.

Note: we often are interested in systems with constant energy in time.

Note: the canonical coordinate q in our example corresponds to the coordinate x .

In case the total energy of the system remains constant we get that the Hamiltonian depending on (p, q) is the total energy of the system, the sum of U potential and T kinetic energy:

$$H(p, q) = T + U$$

Note: classic $T = \frac{p^2}{2m}$

We use the momentum operator:

$$\hat{p} = -i\hbar \cdot \frac{\partial}{\partial x}$$

$$\hat{p}^2 = -\hbar^2 \cdot \frac{\partial^2}{\partial x^2}$$

Note: classic: $p \sim \dot{x}$

We rewrite the Hamiltonian as operator \hat{H} :

$$\hat{H} = \hat{T} + \hat{U}$$

We use:

$$\hat{T} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

Note: The potential operator \hat{U} multiplies the wave function by a value $U(x, t)$.

Note: The harmonic oscillator uses a potential depending on position x only, not on time t .

We can rewrite the Schrödinger equation in terms of the Hamiltonian operator:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + U \cdot \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t) \quad (5)$$

Note: This is the version of the nonrelativistic Schrödinger equation, extended by the potential energy.

Remark:

The basic idea of the wave-mechanical treatment is that the whole atom is treated as a generally very complicated vibrational state of an initially unspecified object according to the de Broglie relationships. Its stationary states are represented as possible vibrational forms in analogy to the natural vibrations of acoustic systems. The object itself does not need to have any real existence, it represents a mathematical tool for which, however, a clear interpretation can be given under certain conditions.

The Schrödinger equation is time-dependent:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + U \cdot \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t)$$

We separate time dependency by using:

$$\psi(x, t) = \chi(x) \cdot e^{-\frac{i}{\hbar} E \cdot t}$$

Note: We represent $\psi(x, t)$ as a vector $\chi(x)$, oscillating with $e^{-\frac{i}{\hbar} E \cdot t}$.

With this ansatz we rewrite the Schrödinger equation.

We note:

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = E \cdot \chi(x)$$

We rewrite the Schrödinger equation:

$$\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \chi(x) + (E - U) \cdot \chi(x) = 0$$

Remark:

This equation is to be solved in the entire range $-\infty < x < +\infty$ using a function that including its first derivative is continuous and must approach zero at the limits. This function has the property of yielding a physically meaningful solution only for certain energy values. These special values, for

which there are physically meaningful solutions, are the eigenvalues of the differential equation, and the corresponding solutions are the associated eigenfunctions.

The harmonic oscillator

The harmonic oscillator is a system that, when displaced from its equilibrium position, experiences a restoring force F proportional to the displacement $x(t)$.

In this case we have the potential energy U :

$$U = \frac{m \cdot \omega^2 \cdot x^2}{2}$$

The position is a function of time:

$$x(t) = A \cdot \sin(\omega \cdot t)$$

We use the time-independent Schrödinger equation:

$$\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \chi(x) + (E - U) \cdot \chi(x) = 0$$

We expand the potential energy U :

$$\begin{aligned} \frac{d^2}{dx^2} \chi(x) + \frac{2 \cdot m}{\hbar^2} \left(E - \frac{m \cdot \omega^2}{2} \cdot x^2 \right) \cdot \chi(x) &= 0 \\ \frac{d^2}{dx^2} \chi(x) + \left(\frac{2 \cdot m \cdot E}{\hbar^2} - \frac{m^2 \cdot \omega^2}{\hbar^2} \cdot x^2 \right) \cdot \chi(x) &= 0 \end{aligned}$$

This is a differential equation.

For easier manipulation we use:

$$\begin{aligned} E &= \hbar \cdot \omega \cdot \left(\lambda + \frac{1}{2} \right) \\ \xi &:= \sqrt{\frac{m \cdot \omega}{\hbar}} \cdot x \\ \xi^2 &= \frac{m \cdot \omega}{\hbar} \cdot x^2 \end{aligned}$$

Note: ξ is dimensionless.

Remark

The term $\left(\lambda + \frac{1}{2} \right)$ is somewhat mysterious and comes up in any literature dealing with this topic. Zwiebach (see the lecture notes) introduces it as a unit-free constant, needed to make calculations easier. Hört simply states this expression without any comment. I think that the problem lies in that this term is result of complex algebraic manipulation. I suggest that you follow the explanation, check that all is done correctly and trust that the energies of the quantum harmonic oscillator are quantized by $\hbar \cdot \omega \cdot \left(n + \frac{1}{2} \right)$. At the moment the following will be helpful: As λ is a real number you could set $\lambda = \frac{1}{2}$ and get $\left(\lambda + \frac{1}{2} \right) = 1$, the de Broglie relation.

λ later will become eigenvalue of eigenfunctions of differential equations resp. of operators.

We will need too:

$$x = \xi \cdot \sqrt{\frac{\hbar}{m \cdot \omega}}$$

$$x^2 = \xi^2 \cdot \frac{\hbar}{m \cdot \omega}$$

We calculate:

$$\frac{d^2}{dx^2} \chi(x) + \left(\frac{2 \cdot m \cdot E}{\hbar^2} - \frac{m^2 \cdot \omega^2}{\hbar^2} \cdot x^2 \right) \cdot \chi(x) = 0$$

$$\frac{d^2}{dx^2} \chi(x) + \left(\frac{2 \cdot m}{\hbar^2} \cdot \hbar \cdot \omega \cdot \left(\lambda + \frac{1}{2} \right) - \frac{m^2 \cdot \omega^2}{\hbar^2} \cdot \xi^2 \cdot \frac{\hbar}{m \cdot \omega} \right) \cdot \chi(x) = 0$$

$$\frac{d^2}{dx^2} \chi(x) + \left(\frac{2 \cdot m \cdot \omega}{\hbar} \cdot \left(\lambda + \frac{1}{2} \right) - \frac{m \cdot \omega}{\hbar} \cdot \xi^2 \right) \cdot \chi(x) = 0$$

$$\frac{d^2}{dx^2} \chi(x) - \frac{m \cdot \omega}{\hbar} \cdot (2 \cdot \lambda + 1 - \xi^2) \cdot \chi(x) = 0$$

Note: χ is a function of x . If we replace x by $\xi := c \cdot x$, the derivatives become:

$$\frac{d}{dx} \chi(x) \rightarrow \frac{d}{d\xi} \chi(\xi) \cdot \xi$$

$$\frac{d^2}{dx^2} \chi(x) \rightarrow \frac{d^2}{d\xi^2} \chi(\xi) \cdot \xi^2$$

In our case we get:

$$\frac{d^2}{dx^2} \chi(x) = \frac{d^2}{d\xi^2} \chi(\xi) \cdot \frac{m \cdot \omega}{\hbar}$$

We use this and get:

$$\frac{d^2}{dx^2} \chi(x) - \frac{m \cdot \omega}{\hbar} \cdot (2 \cdot \lambda + 1 - \xi^2) \cdot \chi(x) = 0 \rightarrow$$

Note: If we replace $\chi(x)$ by $\chi(\xi(x))$ the differential equation remains valid for $\chi(\xi)$.

$$\frac{d^2}{d\xi^2} \chi(\xi) \cdot \frac{m \cdot \omega}{\hbar} - \frac{m \cdot \omega}{\hbar} \cdot (2 \cdot \lambda + 1 - \xi^2) \cdot \chi(\xi) = 0$$

$$\frac{d^2}{d\xi^2} \chi(\xi) - (2 \cdot \lambda + 1 - \xi^2) \cdot \chi(\xi) = 0$$

In the limes $\xi \rightarrow \infty$ the dominant term will be:

$$\frac{d^2}{dx^2} \chi(x) - \xi^2 \cdot \chi(\xi) = 0$$

We use the ansatz:

$$\chi(\xi) = \varphi(\xi) \cdot e^{-\frac{\xi^2}{2}}$$

We calculate the derivatives.

$$\begin{aligned}\frac{d}{d\xi}\chi(\xi) &= \frac{d}{d\xi}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - \varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}} \\ \frac{d^2}{d\xi^2}\chi(\xi) &= \frac{d}{d\xi}\left(\frac{d}{d\xi}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - \varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}}\right) = \\ &= \frac{d^2}{d\xi^2}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - \frac{d}{d\xi}\varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}} - \left(\frac{d}{d\xi}\varphi(\xi) \cdot \xi + \varphi(\xi)\right) \cdot e^{-\frac{\xi^2}{2}} - \varphi(\xi) \cdot \xi^2 \cdot e^{-\frac{\xi^2}{2}} \\ &= \frac{d^2}{d\xi^2}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - \frac{d}{d\xi}\varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}} - \left(\frac{d}{d\xi}\varphi(\xi) \cdot \xi + \varphi(\xi)\right) \cdot e^{-\frac{\xi^2}{2}} + \varphi(\xi) \cdot \xi^2 \cdot e^{-\frac{\xi^2}{2}} = \\ &= \frac{d^2}{d\xi^2}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - 2 \cdot \frac{d}{d\xi}\varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}} - \varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} + \varphi(\xi) \cdot \xi^2 \cdot e^{-\frac{\xi^2}{2}}\end{aligned}$$

We insert into the differential equation:

$$\begin{aligned}\frac{d^2}{d\xi^2}\chi(\xi) - \xi^2 \cdot \chi(\xi) &= 0 \rightarrow \\ \frac{d^2}{d\xi^2}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - 2 \cdot \frac{d}{d\xi}\varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}} - \varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} + \varphi(\xi) \cdot \xi^2 \cdot e^{-\frac{\xi^2}{2}} - \xi^2 \cdot \chi(\xi) &= 0 \\ \frac{d^2}{d\xi^2}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - 2 \cdot \frac{d}{d\xi}\varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}} - \varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} + \varphi(\xi) \cdot \xi^2 \cdot e^{-\frac{\xi^2}{2}} - \xi^2 \cdot \varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} &= 0 \\ \frac{d^2}{d\xi^2}\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} - 2 \cdot \frac{d}{d\xi}\varphi(\xi) \cdot \xi \cdot e^{-\frac{\xi^2}{2}} - \varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} &= 0 \\ \left(\frac{d^2}{d\xi^2} - 2 \cdot \xi \cdot \frac{d}{d\xi}\right)\varphi(\xi) &= -2 \cdot \lambda \cdot \varphi(\xi)\end{aligned}$$

Note: We chose $-2 \cdot \lambda$ for better compatibility with the desired result. For $\lambda = -\frac{1}{2}$ we get back the original differential equation. What we hope to find are eigenfunctions of this operator with the values of λ being a set of discrete numbers.

The differential equation

$$\left(\frac{d^2}{d\xi^2} - 2 \cdot \xi \cdot \frac{d}{d\xi}\right)\varphi(\xi) = -2 \cdot \lambda \cdot \varphi(\xi) \quad (6)$$

looks like to be solvable by power series.

$$\varphi(\xi) = \sum_{i=0}^{\infty} A_i \xi^i$$

Note: we avoid negative exponentials because $\varphi(0)$ should be well defined.

We insert this ansatz into the differential equation:

$$\frac{d^2}{d\xi^2} \sum_{i=0}^{\infty} A_i \xi^i - (2 \cdot \xi) \cdot \frac{d}{d\xi} \sum_{i=0}^{\infty} A_i \xi^i = -2 \cdot \lambda \cdot \sum_{i=0}^{\infty} A_i \xi^i$$

We examine $\frac{d^2}{d\xi^2} \sum_{i=0}^{\infty} A_i \xi^i$:

$$\begin{aligned} \frac{d^2}{d\xi^2} \sum_{i=0}^{\infty} A_i \xi^i &= \frac{d^2}{d\xi^2} (A_0 \cdot \xi^0 + A_1 \cdot \xi^1 + A_2 \cdot \xi^2 + A_3 \cdot \xi^3 + A_4 \cdot \xi^4 + \dots) = \\ &= 2 \cdot 1 \cdot A_2 \cdot \xi^0 + 3 \cdot 2 \cdot A_3 \cdot \xi + 4 \cdot 3 \cdot A_4 \cdot \xi^2 + \dots = \\ &= \sum_{i=0}^{\infty} (i+2) \cdot (i+1) \cdot A_{i+2} \xi^i \end{aligned}$$

We examine $\frac{d}{d\xi} \sum_{i=0}^{\infty} A_i \xi^i$:

$$\begin{aligned} \frac{d}{d\xi} \sum_{i=0}^{\infty} A_i \xi^i &= \frac{d}{d\xi} (A_0 \xi^0 + A_1 \xi^1 + A_2 \xi^2 + A_3 \xi^3 + A_4 \xi^4 + \dots) \\ &= 1 \cdot A_1 \xi^0 + 2 \cdot A_2 \xi^1 + 3 \cdot A_3 \xi^2 + 4 \cdot A_4 \xi^3 + \dots = \\ &= \sum_{i=0}^{\infty} i \cdot A_{i+1} \xi^i \end{aligned}$$

We get:

$$(2 \cdot \xi) \cdot \left(\frac{d}{d\xi} \sum_{i=0}^{\infty} A_i \xi^i \right) = \sum_{i=0}^{\infty} 2 \cdot i \cdot A_{i+1} \xi^{i+1}$$

We insert into the differential equation:

$$\begin{aligned} \frac{d^2}{d\xi^2} \sum_{i=0}^{\infty} A_i \xi^i - (2 \cdot \xi) \cdot \frac{d}{d\xi} \sum_{i=0}^{\infty} A_i \xi^i &= -2 \cdot \lambda \cdot \sum_{i=0}^{\infty} A_i \xi^i \rightarrow \\ \sum_{i=0}^{\infty} (i+2) \cdot (i+1) \cdot A_{i+2} \xi^i - \sum_{i=0}^{\infty} 2 \cdot i \cdot A_{i+1} \xi^{i+1} &= -2 \cdot \lambda \cdot \sum_{i=0}^{\infty} A_i \xi^i \end{aligned}$$

We compare the coefficients at ξ^i :

$$(i+2) \cdot (i+1) \cdot A_{i+2} - 2 \cdot i \cdot A_{i+1} = -2 \cdot \lambda \cdot A_i$$

We get an equation for the coefficients:

$$\begin{aligned} (i+2) \cdot (i+1) \cdot A_{i+2} &= 2 \cdot (i-\lambda) \cdot A_i \\ A_{i+2} &= \frac{2 \cdot (i-\lambda)}{(i+2) \cdot (i+1)} \cdot A_i \end{aligned}$$

This is a recursive definition for A_i , starting with A_0 and A_1 .

Note: A_0 and A_1 remain undetermined. They are the integration constants:

$$A_0 = \varphi(0); A_1 = \frac{d}{d\xi} \varphi(0)$$

Note: We get two independent series for $A_{2,i}$ and $A_{2,i+1}$. Both series are never ending, thus not being acceptable candidates for energy eigenstates. We need to establish a condition the series terminate.

The power series for $\varphi(\xi)$:

$$\varphi(\xi) = \sum_{i=0}^{\infty} A_i \xi^i$$

with the recursive definition:

$$A_{i+2} = \frac{2 \cdot (i - \lambda)}{(i + 2) \cdot (i + 1)} \cdot A_i$$

comes to an end if $i = \lambda$.

The solution of

$$\frac{d^2}{d\xi^2} \chi(\xi) - (2 \cdot \lambda + 1 - \xi^2) \cdot \chi(x) = 0$$

declines according to:

$$\varphi(\xi) \cdot e^{-\frac{\xi^2}{2}} \tag{7}$$

Going back to the definition for the energy we replace λ by i resp. n :

$$E = \hbar \cdot \omega \cdot \left(n + \frac{1}{2} \right)$$

These are the quantized energies of the quantum harmonic oscillator. Condition (7) guarantees the functions and their derivatives will decline to zero for $x \rightarrow \pm\infty$.

$\varphi(\xi)$ will become the Hermite polynomials.

Visualization

Visualizing the wave functions for the harmonic oscillator needs the Hermite polynomials.

Note: for easier reading we replace ξ by x .

We go back to the differential equation (6):

$$\left(\frac{d^2}{dx^2} - 2 \cdot x \cdot \frac{d}{dx} \right) \varphi(x) = -2 \cdot \lambda \cdot \varphi(x)$$

This differential equation is solvable by the Hermite polynomials:

$$H_{n+2}(x) = 2 \cdot x \cdot H_{n+1}(x) - 2 \cdot (n + 1) \cdot H_n(x)$$

With $H_0(x) = 1$ and $H_1(x) = 2 \cdot x$ we get:

$$H_2(x) = 4 \cdot x^2 - 2$$

$$H_3(x) = 8 \cdot x^3 - 12 \cdot x$$

$$H_4(x) = 16 \cdot x^4 - 48 \cdot x^2 + 12$$

$$H_5(x) = 32 \cdot x^5 - 160 \cdot x^3 + 120 \cdot x$$

$$H_6(x) = 64 \cdot x^6 - 480 \cdot x^4 + 720 \cdot x^2 - 120$$

We will check

$$\left(\frac{d^2}{dx^2} - 2 \cdot x \cdot \frac{d}{dx}\right)\varphi(x) = -2 \cdot \lambda \cdot \varphi(x)$$

by an example:

$$H_5(x) = 32 \cdot x^5 - 160 \cdot x^3 + 120 \cdot x$$

$$\frac{d}{dx}H_5(x) = 160 \cdot x^4 - 480 \cdot x^2 + 120$$

$$\frac{d^2}{dx^2}H_5(x) = 640 \cdot x^3 - 960 \cdot x$$

$$\left(\frac{d^2}{dx^2} - 2 \cdot x \cdot \frac{d}{dx}\right)H_5(x) = -2 \cdot \lambda \cdot H_5(x) \rightarrow$$

$$640 \cdot x^3 - 960 \cdot x - 2 \cdot x \cdot (160 \cdot x^4 - 480 \cdot x^2 + 120) = -2 \cdot \lambda \cdot (32 \cdot x^5 - 160 \cdot x^3 + 120 \cdot x)$$

$$640 \cdot x^3 - 960 \cdot x - 320 \cdot x^5 + 960 \cdot x^3 - 240 \cdot x = -2 \cdot \lambda \cdot (32 \cdot x^5 - 160 \cdot x^3 + 120 \cdot x)$$

$$320 \cdot x^5 + 1600 \cdot x^3 - 1200 \cdot x = -2 \cdot \lambda \cdot (32 \cdot x^5 - 160 \cdot x^3 + 120 \cdot x)$$

Obviously $\lambda = -5$ fulfills the eigenvalue condition.

We plot the first few wave functions for the quantum harmonic oscillator up to $n = 6$:

$$\psi_n = H_n(x) \cdot e^{-\frac{x^2}{2}}$$

Note: These are the Hermite orthogonal functions. They build a complete, orthogonal basis of the space of possible functions for the quantum harmonic oscillator.

