These worked examples follow “Rechenmethoden der Quantentheorie, Siegfried Flügge, Springer, Berlin, 1965”. Library of Congress Catalog Card Number 65-24546, title-nr. 7288

Remark

The treatment of the quantum harmonic oscillator exceeds the scope of what can be expected of beginners. Nevertheless, beginners are also invited to read this text. They can learn from it how physicists proceed to adapt mathematics to the conditions of nature.

Hope I can help you with learning quantum mechanics.

Calculate energy values and eigenfunctions for the one-dimensional undamped harmonic oscillator.

In classical physics the undamped harmonic oscillator is defined by the equation of motion:

$$\ddot{x} + \omega \cdot x = 0$$

Alternatively, we can use the energy equation:

$$\frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 \cdot x^2 = E_{kin} + E_{pot} = E = const.$$

We have the potential:

$$V(x) = E_{pot} = -\frac{m}{2}\omega^2 \cdot x^2$$

Note: The potential is time-independent.

Note: The potential is negative because it is opposite to the direction of movement.

We use the shortcuts:

$$E = \frac{\hbar^2 \cdot k^2}{2m}, \qquad \lambda = \frac{m \cdot \omega}{\hbar}, \qquad \mu = \frac{k^2}{2 \cdot \lambda} = \frac{E}{\hbar \cdot \omega}$$

We check the units. This is not necessary but a good habit.

$$[E] = \frac{kg \cdot m^2}{s^2}$$

$$[\hbar] = \frac{kg \cdot m^2}{s}$$

$$[k^2] = \left[\frac{E \cdot m}{\hbar^2}\right] = \frac{kg \cdot m^2}{s^2} \cdot kg \cdot \frac{s^2}{kg^2 \cdot m^4} = \frac{1}{m^2}$$

$$[k] = \frac{1}{m}$$

$$[\lambda] = \left[\frac{m \cdot \omega}{\hbar}\right] = \frac{kg}{s \cdot \frac{kg \cdot m^2}{s}} = \frac{1}{m^2}$$

$$[\mu] = \left[\frac{k^2}{\lambda}\right] = \frac{1}{m^2 \cdot \frac{s^2}{m^2}} = 1, dimensionless$$

The Schrödinger equation for the one-dimensional case:

$$\frac{d^2}{dx^2}u(x) + \frac{2m}{\hbar^2}(E + V) \cdot u(x) = 0$$

We insert the definitions:

$$\frac{d^2}{dx^2}u(x) + \frac{2m}{\hbar^2}(E + V) \cdot u(x) = 0 \rightarrow$$

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

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

$$\frac{d^2}{dx^2}u(x) + (k^2 - \lambda^2 \cdot x^2) \cdot u(x) = 0$$

We use a new variable y:

$$y(x) \coloneqq \lambda \cdot x^2$$

Note: Here you find a short paper dealing with substitution: https://quantum-abc.de/var_substitution.pdf

Now the derivations change.

$$u(x) \rightarrow u\big(y(x)\big)$$

$\frac{du(x)}{dx} \rightarrow \frac{du(y(x))}{dy} \cdot \frac{dy(x)}{dx} =$ $\frac{du(y(x))}{dy} \cdot 2 \cdot \lambda \cdot x$	$\frac{d^2u(x)}{dx^2} = \frac{d}{dx}\left(\frac{du(y(x))}{dy} \cdot (2 \cdot \lambda \cdot x)\right) =$ $\left(\frac{d}{dx}\frac{du(y(x))}{dy}\right) \cdot (2 \cdot \lambda \cdot x) + \frac{du(y(x))}{dy} \cdot \frac{d}{dx}(2 \cdot \lambda \cdot x) =$ $\left(\frac{d}{dx}\frac{du(y(x))}{dy}\right) \cdot (2 \cdot \lambda \cdot x) + \frac{du(y(x))}{dy} \cdot 2 \cdot \lambda =$ $\left(\frac{d^2u(y(x))}{dy^2} \cdot \frac{dy(x)}{dx}\right) \cdot 2 \cdot \lambda \cdot x + \frac{du(y(x))}{dy} \cdot 2 \cdot \lambda =$ $\frac{d^2u(y(x))}{dy^2} \cdot 2 \cdot \lambda \cdot x \cdot 2 \cdot \lambda \cdot x + \frac{du(y(x))}{dy} \cdot 2 \cdot \lambda =$ $\frac{d^2u(y(x))}{dy^2} \cdot y \cdot 4 \cdot \lambda + \frac{du(y(x))}{dy} \cdot 2 \cdot \lambda$

We go back to the differential equation:

$$\frac{d^2}{dx^2}u(x) + (k^2 - \lambda^2 \cdot x^2) \cdot u(x) = 0 \rightarrow$$

$$\frac{d^2u(y(x))}{dy^2} \cdot y \cdot 4 \cdot \lambda + \frac{du(y(x))}{dy} \cdot 2 \cdot \lambda + (k^2 - \lambda^2 \cdot x^2) \cdot u(x) = 0$$

$$\frac{d^2u(y(x))}{dy^2} \cdot y \cdot 4 \cdot \lambda + \frac{du(y(x))}{dy} \cdot 2 \cdot \lambda + k^2 \cdot u(x) - \lambda^2 \cdot x^2 \cdot u(x) = 0$$

$$\frac{d^2u(y(x))}{dy^2} y \cdot + \frac{1}{2} \cdot \frac{du(y(x))}{dy} + \frac{k^2}{4 \cdot \lambda} \cdot u\big(y(x)\big) - \frac{y}{4} \cdot u\big(y(x)\big) = 0$$

$$\frac{d^2u(y(x))}{dy^2} y \cdot + \frac{1}{2} \cdot \frac{du(y(x))}{dy} + \frac{\mu}{2} \cdot u\big(y(x)\big) - \frac{\lambda \cdot x^2}{4} \cdot u\big(y(x)\big) = 0$$

$$\frac{d^2u(y(x))}{dy^2} \cdot y + \frac{1}{2} \cdot \frac{du(y(x))}{dy} + \left(\frac{\mu}{2} - \frac{y}{4}\right) \cdot u\big(y(x)\big) = 0$$

We try the ansatz:

$$u = f(y) \cdot e^{-\frac{1}{2}y}$$

We calculate the new derivations:

$\frac{du(y(x))}{dy} = \frac{d\left(f(y) \cdot e^{-\frac{1}{2}y}\right)}{dy} =$ $\left(\frac{df(y)}{dy}\right) \cdot e^{-\frac{1}{2}y} - \frac{1}{2}f(y) \cdot e^{-\frac{1}{2}y} =$ $\left(\left(\frac{df(y)}{dy}\right) - \frac{1}{2}f(y)\right) \cdot e^{-\frac{1}{2}y}$	$\frac{d^2u(y(x))}{dy^2} = \frac{d^2\left(f(y) \cdot e^{-\frac{1}{2}y}\right)}{dy^2} =$ $\frac{d}{dy}\left(\frac{d}{dy}\left(f(y) \cdot e^{-\frac{1}{2}y}\right)\right) =$ $\frac{d}{dy}\left(\left(\frac{d}{dy}f(y)\right) \cdot e^{-\frac{1}{2}y} - \frac{1}{2} \cdot f(y) \cdot e^{-\frac{1}{2}y}\right) =$ $\frac{d}{dy}\left(\left(\frac{df(y)}{dy} - \frac{1}{2} \cdot f(y)\right) \cdot e^{-\frac{1}{2}y}\right) =$ $\left(\left(\frac{d^2f(y)}{dy^2} - \frac{1}{2}\frac{df(y)}{dy}\right) - \frac{1}{2} \cdot \left(\frac{df(y)}{dy} - \frac{1}{2}f(y)\right)\right) \cdot e^{-\frac{1}{2}y} =$ $\left(\frac{d^2f(y)}{dy^2} - \frac{1}{2}\frac{df(y)}{dy} - \frac{1}{2}\frac{df(y)}{dy} + \frac{1}{4}f(y)\right) \cdot e^{-\frac{1}{2}y} =$ $\left(\frac{d^2f(y)}{dy^2} - \frac{df(y)}{dy} + \frac{1}{4}f(y)\right) \cdot e^{-\frac{1}{2}y}$

We rewrite the differential equation:

$$y \cdot \left(\frac{d^2f(y)}{dy^2} - \frac{df(y)}{dy} + \frac{1}{4} \cdot f(y)\right) \cdot e^{-\frac{1}{2}y} + \frac{1}{2} \cdot \left(\left(\frac{df(y)}{dy}\right) - \frac{1}{2} \cdot f(y)\right) \cdot e^{-\frac{1}{2}y} + \left(\frac{\mu}{2} - \frac{y}{4}\right) \cdot f(y) \cdot e^{-\frac{1}{2}y} = 0$$

$$\left(y \cdot \left(\frac{d^2f(y)}{dy^2} - \frac{df(y)}{dy} + \frac{1}{4} \cdot f(y)\right) + \frac{1}{2} \cdot \left(\left(\frac{df(y)}{dy}\right) - \frac{1}{2} \cdot f(y)\right) + \left(\frac{\mu}{2} - \frac{y}{4}\right) \cdot f(y)\right) \cdot e^{-\frac{1}{2}y} = 0$$

$$y \cdot \left(\frac{d^2f(y)}{dy^2} - \frac{df(y)}{dy} + \frac{1}{4} \cdot f(y)\right) + \frac{1}{2} \cdot \left(\left(\frac{df(y)}{dy}\right) - \frac{1}{2} \cdot f(y)\right) + \left(\frac{\mu}{2} - \frac{y}{4}\right) \cdot f(y) = 0$$

$$y \cdot \frac{d^2f(y)}{dy^2} - y \cdot \frac{df(y)}{dy} + y \cdot \frac{1}{4} \cdot f(y) + \frac{1}{2} \cdot \frac{df(y)}{dy} - \frac{1}{4} \cdot f(y) + \left(\frac{\mu}{2} - \frac{y}{4}\right) \cdot f(y) = 0$$

$$y \cdot \frac{d^2f(y)}{dy^2} - y \cdot \frac{df(y)}{dy} + \frac{1}{2} \cdot \frac{df(y)}{dy} + y \cdot \frac{1}{4} \cdot f(y) - \frac{1}{4} \cdot f(y) + \left(\frac{\mu}{2} - \frac{y}{4}\right) \cdot f(y) = 0$$

$$y \cdot \frac{d^2f(y)}{dy^2} + \frac{df(y)}{dy} \cdot \left(\frac{1}{2} - y\right) + y \cdot \frac{1}{4} \cdot f(y) - \frac{1}{4} \cdot f(y) + \left(\frac{\mu}{2} - \frac{y}{4}\right) \cdot f(y) = 0$$

$$y \cdot \frac{d^2f(y)}{dy^2} + \frac{df(y)}{dy} \cdot \left(\frac{1}{2} - y\right) + \left(y \cdot \frac{1}{4} - \frac{1}{4} + \frac{\mu}{2} - \frac{y}{4}\right) \cdot f(y) = 0$$

$$y \cdot \frac{d^2f(y)}{dy^2} + \frac{df(y)}{dy} \cdot \left(\frac{1}{2} - y\right) + \left(\frac{\mu}{2} - \frac{1}{4}\right) \cdot f(y) = 0$$

We remember the shortcuts:

$$E = \frac{\hbar^2 \cdot k^2}{2m}, \qquad \lambda = \frac{m \cdot \omega}{\hbar}, \qquad \mu = \frac{k^2}{2 \cdot \lambda} = \frac{E}{\hbar \cdot \omega}$$

We replace $\left(\frac{1}{4} - \frac{\mu}{2}\right)$ by a:

$$y \cdot \frac{d^2 f(y)}{dy^2} + \frac{df(y)}{dy} \cdot \left(\frac{1}{2} - y\right) - a \cdot f(y) = 0$$

This is a confluent hypergeometric equation.

Note: You may find additional information at:
https://encyclopediaofmath.org/wiki/Confluent_hypergeometric_function.

The confluent hypergeometric equation in its general form:

$$y \cdot \frac{d^2\omega}{dy^2} + \frac{d\omega}{dy} \cdot (b - y) - a \cdot \omega = 0$$

a and b are constants.

In our case we have $b = \frac{1}{2}$ and $a = \left(\frac{1}{4} - \frac{\mu}{2}\right)$.

The two linearly independent solutions are the Kummer series $\Phi(a, b, y)$ and $\Phi(a - b + 1, 2 - b, y)$ with the explicit representation:

Series one:

$$1 + \frac{a}{b} \cdot \frac{y}{1!} + \frac{a \cdot (a+1)}{b \cdot (b+1)} \cdot \frac{y^2}{2!} + \frac{a \cdot (a+1) \cdot (a+2)}{b \cdot (b+1) \cdot (b+2)} \cdot \frac{y^3}{3!} + \cdots$$

Series two:

$$1 + \frac{a + \frac{1}{2}}{2 - b} \cdot \frac{y}{1!} + \frac{\left(a + \frac{1}{2}\right) \cdot \left(a + \frac{3}{2}\right)}{(2-b) \cdot (3-b)} \cdot \frac{y^2}{2!} + \frac{\left(a + \frac{1}{2}\right) \cdot \left(a + \frac{3}{2}\right) \cdot \left(a + \frac{5}{2}\right)}{(2-b) \cdot (3-b) \cdot (4-b)} \cdot \frac{y^3}{3!} + \cdots$$

These series come to an end whenever one of the factors in the numerator becomes zero.

This happens if a becomes $0, -1, -2, -3, \ldots$ in the first series or $-\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots$ in the second series.

Note: You may find additional information at:

https://mathworld.wolfram.com/HypergeometricFunction.html

We calculate the energies that correspond to the values of a:

Case $a = 0$:

$$\frac{1}{4} - \frac{1}{2} \cdot \frac{E}{h} = 0 \rightarrow \frac{E}{h} = \frac{1}{2} \rightarrow E = \frac{h}{2}$$

The next cases are given by the Kummer series.

This behavior guarantees that the **Kummer series *one*** comes to an end:	This behavior guarantees that the **Kummer series *two*** comes to an end:
$\frac{1}{4}-\frac{1}{2}\cdot\frac{E}{h}=-1\rightarrow$ $\frac{5}{4}=\frac{1}{2}\cdot\frac{E}{h}\rightarrow$ $\frac{10}{4}=\frac{E}{h}\rightarrow$ $E=\frac{5}{2}\cdot h$ $\frac{1}{4}-\frac{1}{2}\cdot\frac{E}{h}=-2\rightarrow E=\frac{9}{2}\cdot h$ … and so on …	$\frac{1}{4}-\frac{1}{2}\cdot\frac{E}{h}=-\frac{1}{2}\rightarrow$ $\frac{3}{4}=\frac{1}{2}\cdot\frac{E}{h}\rightarrow$ $\frac{3}{2}=\frac{E}{h}\rightarrow$ $E=\frac{3}{2}\cdot h$ $\frac{1}{4}-\frac{1}{2}\cdot\frac{E}{h}=-\frac{3}{2}\rightarrow E=\frac{7}{2}\cdot h$ … and so on …

We get the energy levels of the harmonic oscillator:

$$E_n=h\cdot\left(n+\frac{1}{2}\right), n=0,1,2,\ldots$$

We go back to our differential equation:

$$y\cdot\frac{d^2f(y)}{dy^2}+\frac{df(y)}{dy}\cdot(b-y)-a\cdot f(y)=0$$

In our case we have $b=\frac{1}{2}$ and $a=\left(\frac{1}{4}-\frac{\mu}{2}\right)$.

The general solution may be written as:

$$f(y)=C_1\Phi\left(a,\frac{1}{2},y\right)+C_2\sqrt{y}\Phi\left(a+\frac{1}{2},\frac{3}{2},y\right)$$

We choose $a=-n$ and $C_2=0$. With this the eigenfunctions correspond to the according energy levels.	We choose $a+\frac{1}{2}=-n$ and $C_1=0$. With this the eigenfunctions correspond to the according energy levels.
We get the eigenfunctions: $u(y)=e^{-\frac{1}{2}y}\cdot\Phi\left(a,\frac{1}{2},y\right)$ Written with the original parameter x: $u(x)=e^{-\frac{1}{2}\lambda x^2}\cdot\Phi\left(a,\frac{1}{2},\lambda x^2\right)$	We get the eigenfunctions: $u(y)=e^{-\frac{1}{2}y}\cdot\sqrt{y}\cdot\Phi\left(a+\frac{1}{2},\frac{3}{2},y\right)$ Written with the original parameter x: $u(x)=e^{-\frac{1}{2}\lambda x^2}\cdot\sqrt{\lambda}\cdot x\cdot\Phi\left(a+\frac{1}{2},\frac{3}{2},\lambda x^2\right)$

We try to combine these two branches into a single notation by help of the Hermite polynomials.

We note that for any fitting value of $(a=-n)$ or $\left(a+\frac{1}{2}=-n\right)$ the series $\Phi(a,b,y)$ and $\Phi(a-b+1,2-b,y)$ build a polynomial in y.

We can transform these polynomials into the so-called Hermite polynomials:

$$H_{2n}(x) = (-1)^n \cdot \frac{(2n)!}{n!} \cdot \Phi\left(-a, \frac{1}{2}, x^2\right)$$

$$H_{2n+1}(x) = (-1)^n \cdot \frac{2 \cdot (2n+1)!}{n!} \cdot x \cdot \Phi\left(-a + \frac{1}{2}, \frac{3}{2}, x^2\right)$$

We get the sequence of the Hermite polynomials:

$H_0 = 1$	$H_1 = 2 \cdot x$	$H_2 = 4 \cdot x^2 - 2$
$H_3 = 8 \cdot x^3 - 12 \cdot x$	$H_4 = 16 \cdot x^4 - 48 \cdot x^2 + 12$	$H_5 = 32 \cdot x^5 - 160 \cdot x^3 + 120 \cdot x$

$$H_n = 2^n \cdot x^n \mp 1 \dots$$

The parameter n now gives the correct eigenfunctions, written with $\gamma \coloneqq \sqrt{\lambda} \cdot x$:

$$u_n(\gamma) = C_n \cdot e^{-\frac{1}{2}\gamma^2} \cdot H_n(\gamma)$$

The function $u_n(\gamma)$ is symmetric for $n = even$ and antisymmetric for $n = odd$ with respect to $\gamma = 0$ resp. $x = 0$. The number of zeros is equal to n.

We want to normalize the eigenfunctions:

$$\int_{-\infty}^{\infty} |u_n(\gamma)|^2 d\gamma = 1$$

$$C_n{}^2 \cdot \int_{-\infty}^{\infty} e^{-\gamma^2} \cdot |H_n(\gamma)|^2 d\gamma = 1$$

The Hermite polynomials are orthogonal: $H_n(x) \cdot H_m(\mathrm{x}) = 0$ for $m \neq n$.

We remember that $H_n(x)$ is a polynomial in x of grade n.

If we derivate $H_n(x)$ n-times, we will get the coefficient at $(x)^n$.

If we derivate $H_n(x)$ more than n-times, we will get zero.

We can produce the Hermite polynomials by repeatedly derivating the generating function:

$$H_n\big((\gamma)\big) = (-1)^n \cdot e^{\gamma^2} \cdot \frac{d^n}{d\gamma^n} e^{-\gamma^2}$$

Remark: Now comes a pretty crazy "trick".

We write $|u_n(\gamma)|^2 = u_n(\gamma) \cdot u_n(\gamma)$ such that we use one time the definition

$$u_n(\gamma) = C_n \cdot e^{-\frac{1}{2}\gamma^2} \cdot H_n(\gamma)$$

the other time the definition

$$u_n(\gamma) = C_n \cdot e^{-\frac{1}{2}\gamma^2} \cdot (-1)^n \cdot e^{\gamma^2} \cdot \frac{d^n}{d\gamma^n}\left(e^{-\gamma^2}\right)$$

We build the product:

$$u_n(\gamma) \cdot u_n(\gamma) =$$

$$C_n \cdot e^{-\frac{1}{2}\gamma^2} \cdot H_n(\gamma) \cdot C_n \cdot e^{-\frac{1}{2}\gamma^2} \cdot (-1)^n \cdot e^{\gamma^2} \cdot \frac{d^n}{d\gamma^n}\left(e^{-\gamma^2}\right) =$$

$$(-1)^n \cdot {C_n}^2 \cdot H_n(\gamma) \cdot \frac{d^n}{d\gamma^n}\left(e^{-\gamma^2}\right)$$

Substituting x by $\gamma \coloneqq \sqrt{\lambda} \cdot x$ leads to the normalizing integral:

$$\frac{1}{\sqrt{\lambda}} \cdot {C_n}^2 \cdot \int_{-\infty}^{\infty} H_n(\gamma) \cdot \frac{d^n}{d\gamma^n}\left(e^{-\gamma^2}\right) d\gamma = 1$$

If we integrate this by parts we will become a lot of products of the kind:

$$H_n(\gamma) \cdot H_1(\gamma), H_n(\gamma) \cdot H_2(\gamma), \ldots$$

All these products give zero because the Hermite polynomials are orthogonal.

Only the last integral "survives":

$$\frac{1}{\sqrt{\lambda}} \cdot {C_n}^2 \cdot \int_{-\infty}^{\infty} e^{-\gamma^2} \cdot \frac{d^n}{d\gamma^n}\left(H_n(\gamma)\right) d\gamma = 1$$

We use that derivating the Hermite polynomial H_n n-times gives:

$$\frac{d^n}{d\gamma^n} H_n = 2^n \cdot n!$$

We get:

$$\frac{1}{\sqrt{\lambda}} \cdot {C_n}^2 \cdot 2^n \cdot n! \cdot \int_{-\infty}^{\infty} e^{-\gamma^2} d\gamma = 1$$

$$\frac{1}{\sqrt{\lambda}} \cdot {C_n}^2 \cdot 2^n \cdot n! \cdot \sqrt{\pi} = 1$$

$${C_n}^2 = \frac{1}{2^n \cdot n!} \cdot \sqrt{\frac{\lambda}{\pi}}$$

Finally, we have the normalized eigenfunctions of the harmonic oscillator:

$$u_n(x) = \left(\frac{1}{2^n \cdot n!}\right)^{\frac{1}{2}} \cdot \left(\frac{\lambda}{\pi}\right)^{\frac{1}{4}} \cdot e^{-\frac{1}{2}\lambda x^2} \cdot H_n\left(\sqrt{\lambda} \cdot x\right)$$