Atoms

Box potential

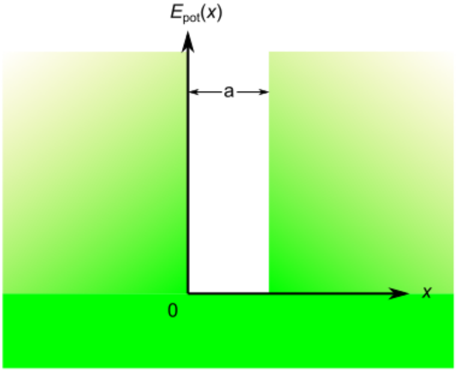
The Schrödinger equation as a wave equation

- Schrödinger equation
- Box potential
- Harmonic oscillator
- Orbital angular momentum
- Rotation of a diatomic molecule
- Schrödinger equation of the H-atom
- normal Zeeman effect
- Dia- and paramagnetism

Box potential 1

The one-dimensional box potential is defined as

$$E_{\text{pot}}(x) = 0 \quad \text{for} \quad 0 < x < a \quad \text{and} \quad E_{\text{pot}}(x) \to \infty \quad \text{else}$$



Box potential 1

Comment

A simple application of the Schrödinger equation is a particle that is trapped in an infinitely deep potential well.

The figure outlines the box potential in the one-dimensional case.

The particle can only move in an area between the coordinates $x = 0$ and $x = a$.

Outside these limits, the potential energy is infinite.

The particle can move freely within these limits.

Box potential 2

Schrödinger equation in the range $0 < x < a$

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

ansatz for the wave function

$$\underline{\psi = \varphi(x)e^{-iEt/\hbar}}$$

time independent Schrödinger equation

$$\boxed{E\varphi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}}$$

boundary conditions

$$\underline{\varphi(x=0) = \varphi(x=a) = 0}$$

Box potential 2 Comment 1

The Schrödinger equation can only be written down in the range between $x = 0$ and $x = \mathrm{a}$.

The potential energy is a constant in the range between $x = 0$ and $x = \mathrm{a}$, to which the value zero can be assigned.

The Hamilton operator only contains the kinetic energy and is not an explicit function of time.

The underlined approach can therefore be used and the time-independent Schrödinger equation results.

The solution to this differential equation is the complex exponential function, or the sine or cosine function.

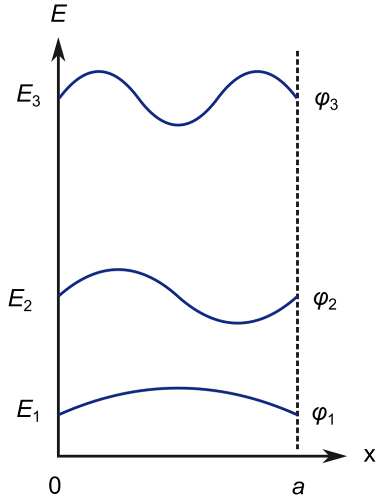
Box potential 2

Comment 2

The solution is determined by the boundary conditions underlined in red.

Since the potential energy at $x = 0$ and $x = a$ becomes infinitely large, the wave function must vanish there.

Box potential 3



solution of the Schrödinger equation

$$\boxed{\psi_n(x,t) = \psi_0 \sin(k_n x)\, e^{-iE_n t/\hbar}}$$

with $\varphi(x=a) = 0$

$$\underline{k_n a = n\pi}$$

and

$$\underline{k_n = n\frac{\pi}{a}} \quad und \quad n = 1, 2, \ldots$$

energy eigenvalues

$$\boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2}$$

Box potential 3 Comment 1

The formula outlined in red gives the solution of the Schrödinger equation.

With the sine function for the position-dependent part of the wave function, the boundary condition on the left edge of the potential well for $x = 0$ is automatically fulfilled.

The condition on the right edge of the potential well defines the wave number in the argument of the sine function.

With the boundary condition for $x = a$, the formula underlined in red results for the quantized wave number.

The wave number is an integral multiple of π/a.

The quantum number n can take the values 1, 2 etc..

Box potential 3 Comment 2

If the wave function is inserted into the Schrödinger equation, the formula outlined in red results for the energy eigenvalues.

It is the quantized kinetic energy of the particle.

The figure sketches the spatial part of the wave function.

The solutions of the Schrödinger equation for the box potential correspond to the standing waves of a vibrating string.

Since the kinetic energy of the particle increases when the quantum number increases, the derivation of the wave function according to the coordinate x must also assume larger numerical values.

Therefore, the number of nodes also increases as the quantum number n increases.

Box potential 4

normalization of the wave function

$$1 = \int_{x=0}^{a} \psi^* \psi dx = \int_{x=0}^{a} \psi_0^* \psi_0 \sin^2(k_n x) dx = \frac{a}{2} \psi_0^* \psi_0$$

normalized eigenfunctions of the box potential

$$\boxed{\psi_n(x,t) = \sqrt{\frac{2}{a}} \sin(k_n x)\, e^{-iE_n t/\hbar}}$$

Box potential 4 Comment

The square of the wave function can be normalized to one and indicates the probability of finding the particle.

The integral over the sine square results in the value $a / 2$ regardless of the wave number k_n.

The formula outlined in red gives the normalized eigenfunctions for a particle in the box potential.

Harmonic Oscillator

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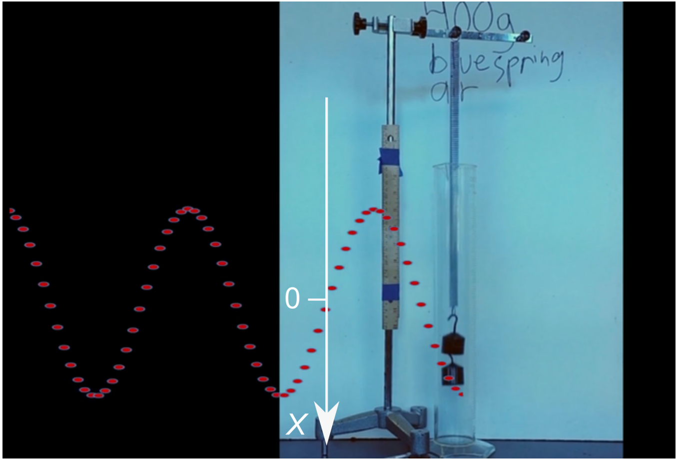
Harmonic oscillator 1



(UngedämpferOszillator.mp4)

Harmonic oscillator 1 Comment

The video shows a typical model of a harmonic oscillator: a mass attached to a spring.

The oscillation of the mass around the equilibrium position can be described by a sine function.

Harmonic oscillator 2

Newton's equation of motion

$$\boxed{m\ddot{x} = -Dx}$$

with the solution

$$\underline{x = x_0 \sin(\omega t + \varphi)}$$

The frequency of the oscillation is

$$\boxed{\omega = \sqrt{\frac{D}{m}}}$$

The potential energy is

$$\boxed{E_{pot}(x) = \frac{1}{2}Dx^2} \quad \rightarrow \quad F = -\frac{\partial E_{pot}(x)}{\partial x} = -Dx$$

Harmonic oscillator 2 Comment 1

The first equation outlined in red gives Newton's equation of motion for the mass m attached to the spring.

The force drives the mass back to the equilibrium position $x = 0$ and therefore takes on a negative sign.

The force is proportional to the distance to the equilibrium position. The constant of proportionality is the spring constant D.

The solution of Newton's equation of motion is, in agreement with the experiment, a sine function.

The second equation outlined in red gives the angular velocity of the oscillation.

Harmonic oscillator 2 Comment 2

The third equation outlined in red gives the potential energy stored in the spring.

The negative derivative of the potential energy gives the force acting on the mass and the force attempts to reduce the potential energy of the mass.

Harmonic oscillator 3

Hamilton function

$$\boxed{H = \frac{p^2}{2m} + \frac{1}{2}Dx^2}$$

Hamilton operator ($p \to \hat{p} = -i\hbar\frac{\partial}{\partial x}$)

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}Dx^2}$$

Harmonic oscillator 3 Comment

The total energy of the mass results from the sum of kinetic and potential energy.

The Hamilton function is found when the velocity is expressed by the momentum $v = p/m$.

The Hamilton function becomes the Hamilton operator when the momentum is replaced by the momentum operator.

Harmonic oscillator 4

Schrödinger equation ($i\hbar\partial_t\psi = \hat{H}\psi$)

$$\boxed{i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}Dx^2\right)\psi(x,t)}$$

ansatz for the solution

$$\underline{\psi(x,t) = \varphi(x)e^{-iEt/\hbar}}$$

time independent Schrödinger equation

$$\boxed{E\varphi(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}Dx^2\right)\varphi(x)}$$

Harmonic oscillator 4 Comment

The Schrödinger equation of the harmonic oscillator can be written down with the Hamilton operator.

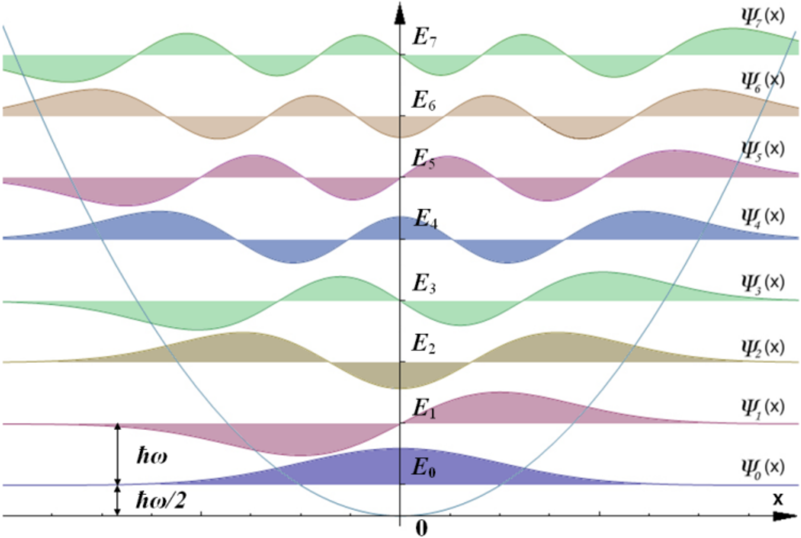
Since the Hamilton operator does not explicitly contain the time, the energy is conserved.

The solution is a standing wave.

The time dependence of the standing wave is determined by a harmonic oscillation with the angular velocity $\omega = E/\hbar$.

The spatial variation of the standing wave $\varphi(x)$ is determined by the time-independent Schrödinger equation, which is outlined in red in the last line.

Harmonic oscillator 5



Harmonic oscillator 5 Comment 1

The figure illustrates the solution of the Schrödinger equation for the harmonic oscillator.

The wave functions are reminiscent of the solution of the Schrödinger equation for a particle in the box potential.

In the ground state the wave function has no node.

The number of nodes increases from quantum state to quantum state. In the first excited state there is one node, in the second excited state there are two, etc.

With every further node the slope of the wave function increases and the kinetic energy of the particle increases accordingly.

Harmonic oscillator 5

Comment 2

As can be expected from the uncertainty relation, the energy in the ground state is not zero.

The energy would only be zero if the particle is at rest in the equilibrium position at $x = 0$.

But then its momentum would be zero, which in turn, because of the uncertainty relation, would mean that the spatial uncertainty diverges.

Hence the particle can never be at rest.

The energy increases from energy level to energy level by $\hbar\omega$.

Harmonic oscillator 6

The wave function of the groundstate is

$$\boxed{\varphi_0(x) = A_0 e^{-ax^2}}$$

with

$$a^2 = \frac{Dm}{4\hbar^2}$$

energy of the ground state

$$E_0 = \frac{1}{2}\hbar\sqrt{\frac{D}{m}} = \frac{1}{2}\hbar\omega$$

Harmonic oscillator 6 Comment

The wave function of the ground state is a Gaussian function.

If the Gaussian function is inserted into the Schrödinger equation, the parameter a and the energy of the ground state $\hbar\omega/2$ result.

Harmonic oscillator 7

The wave function of the first excited state has one node and is

$$\boxed{\varphi_1(x) = A_1 x e^{-ax^2}}$$

The energy of the first excited state is

$$E_1 = \frac{3}{2}\hbar\omega \quad \text{and} \quad a^2 = \frac{Dm}{4\hbar^2}$$

The wave function of the second excited state is

$$\boxed{\varphi_2(x) = A_2(1 - 4ax^2)e^{-ax^2}}$$

and the energy

$$E_2 = \frac{5}{2}\hbar\omega \quad \text{and} \quad a^2 = \frac{Dm}{4\hbar^2}$$

Harmonic oscillator 7 Comment

The wave function of the first excited state has a node at $x = 0$.

If the Gaussian function is multiplied by the coordinate x and inserted into the Schrödinger equation, the energy of the first excited state $E_1 = \frac{3}{2}\hbar\omega$ and the parameter a are obtained.

In the second excited state there are two nodes.

The ansatz for the second excited state consists of the Gaussian function which is multiplied by a quadratic polynomial.

The application of the Schrödinger equation gives the constants and the energy of the quantum state.

The same formula always results for the constant a.

Harmonic oscillator 8

The general formula for the energy is

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right)} \qquad \text{and} \qquad n = 0, 1, 2, \ldots$$

The general wave function is with $y = \sqrt{2a}\,x$

$$\underline{\varphi_n(x) = A_n f_n(y) e^{-y^2/2}}$$

A_n is the normalization constant and the $f_n(y)$ are Hermite polynomials

(https://en.wikipedia.org/wiki/Hermite_polynomials)

Harmonic oscillator 8 Comment

The formula outlined in red shows the energy values of the harmonic oscillator.

This is a very fundamental result, since many processes with small excitation energies can be traced back to harmonic oscillations.

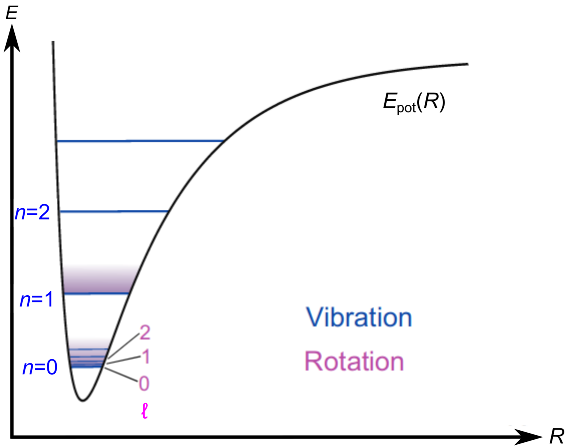
The formula underlined in red gives the general wave function of the harmonic oscillator.

This solution always results from the product of a Gaussian function and a polynomial.

The polynomials are the Hermite polynomials that can be looked up in tables.

Harmonic oscillator 9

potential energy and energy levels of a diatomic molecule



Harmonic oscillator 9

Comment 1

This figure contains a lot of information.

The black line shows the variation in potential energy in a diatomic molecule when the distance between the two atoms changes.

The potential energy increases very sharply when the atoms come very close.

Likewise, the potential energy increases when the distance between the atoms is increased.

In between is the equilibrium distance for which the potential energy is minimal.

In the vicinity of the equilibrium distance, the potential energy can be approximated by a parabola.

Harmonic oscillator 9 Comment 2

The energy of the oscillations is quantized and the figure shows the energy levels of the oscillation in blue.

In the case of the ideal harmonic oscillator, the distance between the energy levels is $\hbar\omega$.

Since the potential energy usually deviates from the simple square law of the harmonic oscillator, the distance between the energy levels decreases as the excitation energy increases.

A diatomic molecule can also rotate around its center of gravity.

The rotation is also quantized and is described by the quantum number $\ell = 0, 1, 2...$

Harmonic oscillator 9 Comment 3

The excitation energy of the rotation is very much smaller than the excitation energy of the vibrations.

The energy levels of the rotation are shown in pink for the ground state.

At the first excited energy level of the oscillation, the range of rotation is indicated by shading.

Harmonic oscillator 10

	$R_0\,(10^{-12}\,\text{m})$	$E_{0\to1}/hc\,(\text{cm}^{-1})$
H_2	74.16	4159
N_2	109.4	2330
O_2	120.7	1556
Li_2	267.3	246
NO	115.1	1876
HCl	127.4	2885

$$\lambda = 5\,\mu\text{m} \quad \rightarrow \quad \lambda^{-1} = 2000\,\text{cm}^{-1} \quad \text{and} \quad \boxed{E = \frac{hc}{\lambda}} \quad \rightarrow \quad E = 0.25\,\text{eV}$$

Harmonic oscillator 10 Comment

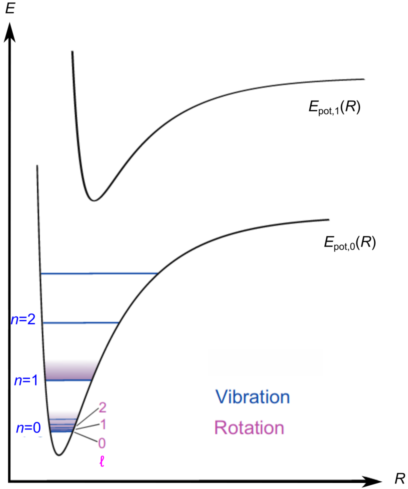
The table summarizes the equilibrium distances R_0 and excitation energies of some diatomic molecules. (for comparison: Bohr radius $a_\mathrm{B} = 0.529 \cdot 10^{-10}\,\mathrm{m} = 52.9 \cdot 10^{-12}\,\mathrm{m}$)

The energy is given in units of reciprocal centimeters.

Reciprocal centimeter is a unit of energy that is widely used in spectroscopy.

An example below the table shows how this unit works.

Harmonic oscillator 11



Energy scales of diatomic molecules

- electronic excitation

$$\Delta E = E_{\mathrm{pot},1} - E_{\mathrm{pot},0} \cong \mathrm{eV}$$

- oscillation

$$\Delta E_{\mathrm{vib}} \cong 0.1\,\mathrm{eV}$$

- rotation

$$\Delta E_{\mathrm{rot}} \cong \mathrm{meV}$$

Harmonic oscillator 11 Comment

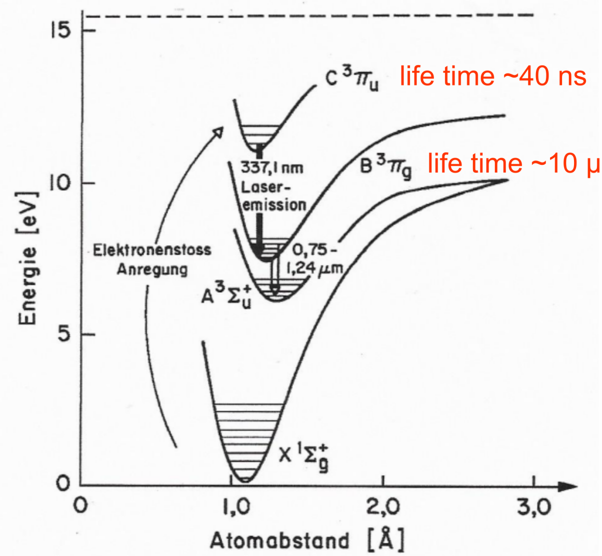
In addition to vibrations and rotations, the electron configuration of a diatomic molecule can also be excited.

In addition to the curve of the potential energy in the ground state of the electron configuration, the figure shows another curve for the potential energy $E_{\mathrm{pot},1}$ of an excited electron configuration.

The molecule can also vibrate and rotate when the electronic configuration is in an excited state.

The energy required to excite the electron configuration is much larger than the energy required to excite vibrations or rotations.

Harmonic oscillator 12



life time ~40 ns

life time ~10 µs

Harmonic oscillator 12 Comment 1

This figure shows the energy level scheme of the N_2 molecule.

The potential energy of the oscillation is shown for the ground state and three excited states of the electron configuration.

The electronic configuration is denoted by funny symbols: $X^1\Sigma_g^+$, $A^3\Sigma_u^+$, etc..

These symbols describe the symmetry properties of the electronic wave functions. The exact meaning is not important for my lecture (e.g. u and g denote the symmetry of the wave function (odd or even) with respect to an inversion at the center of the molecule.)

In addition, the energy levels due to the oscillations are shown.

Harmonic oscillator 12 Comment 2

In the 8th lecture it was shown that the emission of laser light can be stimulated when nitrogen molecules collide with electrons or other molecules in a gas discharge.

The laser transition occurs between the levels of the third and second electronically excited states.

The lifetime of the oscillation state of C $^3\pi_u$ is very short compared to the lifetime of the state B $^3\pi_g$, so that only short laser pulses can be generated in the UV through stimulated emission.

Orbital angular momentum

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Orbital angular momentum 0

Orbital angular momentum 0 Comment

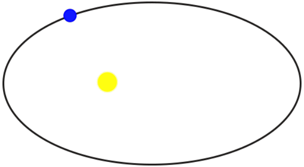
This picture illustrates the importance of angular momentum.

Without the angular momentum of the wheels, the motorcycles would simply fall to the side.

The angular momentum makes the motorcycles stable.

Orbital angular momentum 1

Johannes Kepler (1609): Planets move in elliptical orbits



Newton defines the orbital angular momentum

$$\underline{\vec{L} = \vec{r} \times \vec{p}}$$

Newton's mechanics: the angular momentum is conserved and perpendicular to the plane of the orbit of a planet

$$\boxed{\frac{d\vec{L}}{dt} = 0}$$

Orbital angular momentum 1 Comment 1

In 1609 Johannes Kepler published his findings on the movement of the planets.

Planets move in elliptical orbits around the sun.

A line segment joining a planet and the Sun sweeps out equal areas during equal intervals of time.

The squares (second powers) of the orbital times of two planets around the same central star behave like the cubes (third powers) of the major orbital half-axes.

Newtonian mechanics explains Kepler’s laws.

In particular, Newton defines the orbital angular momentum, which is indicated by the formula underlined in red.

Orbital angular momentum 1 Comment 2

According to its definition, the orbital angular momentum is perpendicular to the plane of the orbit and does not change during the movement of the planet.

With a central force such as gravitational force, the derivative of the orbital angular momentum with respect to time must always be zero.

The time derivative of the position vector gives the speed, which is parallel to the momentum, so that the cross product must be zero.

The time derivative of the momentum is the force that, due to the law of gravitation, is parallel to the position vector that connects the sun with the planet, so that the cross product must also be zero here.

Orbital angular momentum 2

According to the uncertainty relations, there can be no orbital plane for a quantum particle, i.e.

$$\frac{d\vec{L}}{dt} \neq 0$$

One can start the discussion of angular momentum in quantum physics with the uncertainty relation for the orbital angular momentum

$$\boxed{\Delta\varphi \Delta L_z \geq \frac{\hbar}{2}}$$

Orbital angular momentum 2 Comment

According to the uncertainty relations, a quantum particle cannot move in an orbital plane.

Hence the angular momentum in quantum physics cannot be independent of time.

A first access to the properties of the orbital angular momentum in quantum physics is provided by the uncertainty relation outlined in red.

Orbital angular momentum 3

uncertainty relation

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

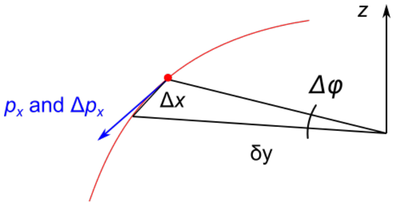
motion in the x-y plane

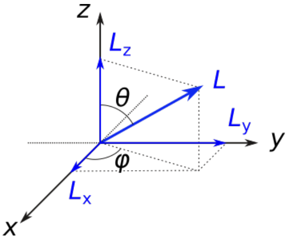
$$\frac{\Delta x}{r} r \Delta p_x \geq \frac{\hbar}{2}$$

With $\Delta x / r = \Delta \varphi$ and $r \Delta p_x = \Delta L_z$

$$\boxed{\Delta \varphi \Delta L_z \geq \frac{\hbar}{2}}$$

uncertainty relation of the angular momentum





Orbital angular momentum 3 Comment 1

I hope that the formulas and pictures on this page make the uncertainty principle for angular momentum plausible.

The first line shows the uncertainty relation for the x-component of the momentum.

The first figure on the right shows the momentum and the momentum uncertainty in the x-direction for a particle.

The distance of a point to the origin of the coordinates is denoted by r.

The quotient of the position uncertainty Δx and the distance r gives the uncertainty of the angle φ.

Orbital angular momentum 3 Comment 2

The product of the distance r and the uncertainty of the momentum Δp_x is the uncertainty of the orbital angular momentum in the z-direction.

The uncertainty in the angle $\Delta\varphi$ and the uncertainty in the z-component of the orbital angular momentum give the uncertainty relation of the z-component of the orbital angular momentum.

The second figure on the right shows the angular momentum vector.

The orientation of the angular momentum vector is determined by the angle φ and the angle θ.

Orbital angular momentum 3 Comment 3

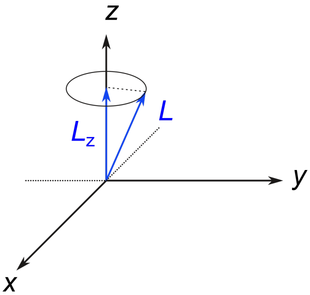
If the z-component of the angular momentum L_z has a fixed value, the angular φ is completely indeterminate.

If the angle φ cannot be determined because of the uncertainty relation, then the x- and y-components of the angular momentum can no longer be determined either.

Orbital angular momentum 4

When $\Delta L_z = 0$ follows $\Delta\varphi \to \infty$ and

L_x and L_y are not defined



it turns out that in addition to L_z also $|\vec{L}|$ can be fixed

Orbital angular momentum 4 Comment

If the z-component of the orbital angular momentum has a fixed value, i.e. the uncertainty ΔL_z is zero, then the uncertainty of the associated angle φ is infinite.

This means that it is no longer possible to assign fixed values to the x and y components of the orbital angular momentum.

As will be shown below, the length of the angular momentum vector is still defined.

The figure shows the vector representation of angular momentum in quantum physics.

The vector of the angular momentum lies on a conical surface around the z-axis.

However, the exact position of the angular momentum vector on this conical surface is not determined.

Orbital angular momentum 5

the operator of the orbital angular momentum

$$\vec{L} = \vec{r} \times \vec{p} \quad \rightarrow \quad \boxed{\hat{\vec{L}} = \vec{r} \times (-i\hbar)\nabla}$$

z-component of the angular momentum operator

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \quad \rightarrow \quad \boxed{\hat{L}_z = -i\hbar\frac{\partial}{\partial \varphi}}$$

compare

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \quad \rightarrow \quad \boxed{\Delta\varphi\Delta L_z \geq \frac{\hbar}{2}}$$

Orbital angular momentum 5 Comment 1

In classical mechanics, the orbital angular momentum is defined by the cross product of position and momentum vector.

The operator of the orbital angular momentum results when the momentum is replaced by the momentum operator.

The first equation outlined in red gives the angular momentum operator in Cartesian coordinates.

All properties of angular momentum can be determined by analyzing this operator.

However, this procedure leads to cumbersome calculations, which are not worth to be discussed in a lecture (for details see books of Quantum Mechanics).

Classical mechanics uses generalized coordinates adapted to the specific problem one wants to study.

Orbital angular momentum 5 Comment 2

For rotational problems usually the spherical coordinates r, θ, φ are used.

When spherical coordinates are used, the z component of the angular momentum operator is given by a formula which is quite similar to the formula of the momentum operator.

If one compares the uncertainty relations for momentum and orbital angular momentum, one recognizes that the coordinate x corresponds to the angle φ and the momentum p_x corresponds to the z-component of the orbital angular momentum L_z.

With simple replacement, the formula for the momentum operator results in the formula outlined in red for the z-component of the angular momentum operator.

This result can also be obtained if one strictly adheres to the rules of mathematics.

Orbital angular momentum 6

eigenvalue equation of $\hat{L}_z$

$$\hat{L}_z f(\varphi) = -i\hbar \frac{\partial}{\partial \varphi} f(\varphi) = \text{eigenvalue} \cdot f(\varphi)$$

eigenfunctions

$$\underline{f(\varphi) = e^{im\varphi}}$$

$$f(\varphi) = f(\varphi + 2\pi) \quad \rightarrow \quad m = 0, \pm 1, \pm 2, \ldots$$

Orbital angular momentum 6 Comment

The first line gives the formal definition of the eigenvalue equation.

The operator applied to the wave function gives the eigenvalue times the wave function.

The solution of this differential equation is simply the complex exponential function.

The quantum number m takes on the integer values $m = 0, \pm 1, \pm 2, ...$

This must be so, because adding a multiple of 2π to the argument of the complex exponential function, i.e. a rotation of 360° should not change the value of the function.

Orbital angular momentum 7

eigenvalue equation of $\hat{L}_z$

$$\boxed{\hat{L}_z f_m(\varphi) = m\hbar f_m(\varphi)}$$

quantum numbers of $\hat{L}_z$

$$m = 0, \pm 1, \pm 2, \ldots$$

eigenfunctions of $\hat{L}_z$

$$\underline{f_m(\varphi) = e^{im\varphi}}$$

eigenvalues of $\hat{L}_z$

$$\underline{L_z = m\hbar}$$

Orbital angular momentum 7 Comment

The slide summarizes the results.

The equation outlined in red gives the eigenvalue equation of $\hat{L}_z$.

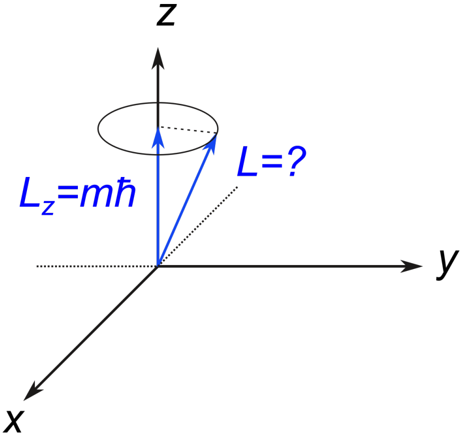
The quantum numbers of $\hat{L}_z$ are $m = 0, \pm 1, \pm 2, ...$

The eigenfunctions are the complex exponential functions and the eigenvalues of the z-component of the angular momentum are $m\hbar$.

If the z component of the angular momentum is conserved, it takes on the values $m\hbar$.

Orbital angular momentum 8

the length of the angular momentum vector



Orbital angular momentum 8 Comment

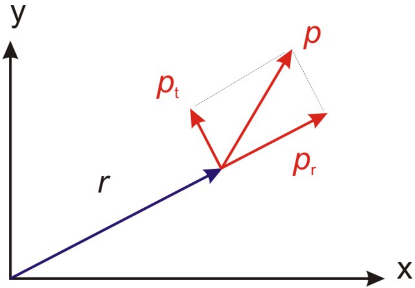
Only the z-component of the angular momentum operator has so far been determined by an eigenvalue equation.

The x and y components of the angular momentum operator cannot have fixed values.

What about the length of the angular momentum vector?

To find the eigenvalue equation for the absolute value of the angular momentum vector, I use a little trick.

Orbital angular momentum 9



$$\vec{L} = \vec{r} \times \vec{p} = \vec{r} \times \vec{p}_r + \vec{r} \times \vec{p}_t = r p_t \vec{e}_z$$

kinetic energy

$$E_{kin} = \frac{\vec{p}^{\,2}}{2m} = \frac{\vec{p}_r^{\,2}}{2m} + \frac{\vec{p}_t^{\,2}}{2m} = \frac{\vec{p}_r^{\,2}}{2m} + \frac{r^2 \vec{p}_t^{\,2}}{2mr^2} = \underline{\frac{\vec{p}_r^{\,2}}{2m} + \frac{\vec{L}^{\,2}}{2mr^2}}$$

Orbital angular momentum 9 Comment

The figure shows a particle moving in the xy-plane.

The momentum of the particle can be broken down into a component parallel to the position vector, which connects the particle with the origin of the coordinate system, and into a component perpendicular to the position vector.

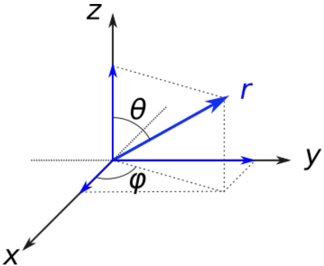
The angular momentum of the particle is perpendicular to the xy plane and is determined by the transverse momentum p_t.

The kinetic energy is proportional to the square of the momentum.

A small calculation shows that the kinetic energy is given by the kinetic energy in the radial direction and the kinetic energy of a rotation, which is proportional to the square of the angular momentum.

Orbital angular momentum 10

$$\boxed{\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m} = -\frac{\hbar^2\nabla^2}{2m}}$$



Laplace Operator in spherical coordinates (https://en.wikipedia.org/wiki/Laplace_operator)

$$\boxed{\begin{aligned}\nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\\ &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r^2}\right) + \frac{1}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}\end{aligned}}$$

Orbital angular momentum 10 Comment

The first formula outlined in red gives the Hamilton operator of the kinetic energy.

The Hamilton operator contains the square of Nabla, which is also known as the Laplace operator.

In the second area outlined in red, the first line specifies the Laplace operator in Cartesian coordinates.

The second line gives the Laplace operator in spherical coordinates.

Orbital angular momentum 11

Hamilton operator of the classical kinetic energy

$$\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m} = -\frac{\hbar^2 \nabla^2}{2m} \quad \text{and} \quad E_{kin} = \frac{\vec{p}_r^{\,2}}{2m} + \frac{\vec{L}^{\,2}}{2mr^2}$$

Laplace operator in spherical coordinates

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r^2}\right) + \frac{1}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}$$

operator of the square of the angular momentum

$$\boxed{\hat{\vec{L}}^2 = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}}$$

Orbital angular momentum 11 Comment

The first line gives the Hamilton operator of the kinetic energy and the decomposition of the kinetic energy into a radial component and a component that is related to the rotation of the mass *m*.

The second line gives the Laplace operator in spherical coordinates.

The comparison shows that the Hamilton operator of the kinetic energy can also be broken down into the radial contribution and a contribution that corresponds to a rotation.

The comparison results in the operator for the square of the orbital angular momentum, which is outlined in red in the bottom line.

Orbital angular momentum 12

eigenvalue equation of the square of the angular momentum

$$\boxed{\hat{\vec{L}}^2 Y_{\ell,m}(\theta,\varphi) = \ell(\ell+1)\hbar^2 Y_{\ell,m}(\theta,\varphi)}$$

the eigenfunctions are spherical harmonics $Y_{\ell,m}(\theta,\varphi)$

and the eigenvalues

$$\underline{L^2 = \ell(\ell+1)\hbar^2}$$

the quantum numbers ℓ and m are

$$\ell = 0, 1, 2, \ldots \quad \text{and} \quad |m| \leq \ell$$

Orbital angular momentum 12 Comment 1

The solutions to the eigenvalue equation for the angle-dependent part of the Laplace operator are known.

The equation outlined in red shows the eigenvalue equation for the square of the angular momentum.

The eigenfunctions are spherical harmonics, which will be discussed later.

The equation underlined in red gives the eigenvalues for the square of the angular momentum operator.

The eigenvalues are determined by the quantum number ℓ.

The quantum number ℓ takes on the values 0, 1, 2, etc.

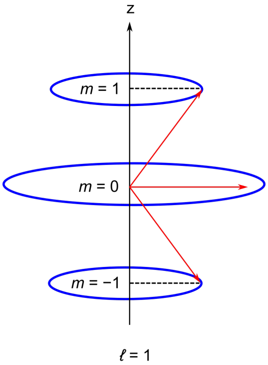
Orbital angular momentum 12 Comment 2

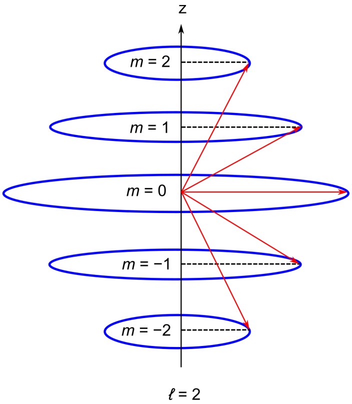
The spherical harmonics also depend on the quantum number m, since $\vec{L}^2$ contains the square of the z-component L_z.

The quantum number m takes the integer values between $-\ell$ and $+\ell$.

Orbital angular momentum 13

$$\boxed{\begin{aligned}\vec{L}^2 &= \ell(\ell+1)\hbar^2 \\ L_z &= m\hbar\end{aligned}}$$





Orbital angular momentum 13 Comment

The figure shows the vectors of angular momentum for the quantum number $\ell = 1$ and $\ell = 2$.

The length of the vector is $\hbar\sqrt{\ell(\ell + 1)}$.

The vectors lie on conical surfaces, the edge of which is indicated by the blue circles.

Due to the uncertainty relation for the angular momentum, it is not possible to define the orientation of the vectors more precisely.

Revision

Summary in Questions

1. Write down the Schrödinger equation of a particle in the box potential.
2. Sketch and explain the eigenfunctions of a particle in the box potential.
3. Write down the Schrödinger equation of a particle in the box potential.
4. Sketch and explain the eigenfunctions of a particle in the box potential.
5. Sketch the vector of the quantized angular momentum and justify the sketch.
6. Give the length of the z-component of the quantized angular momentum.
7. Give the length of the quantized angular momentum vector.
8. Give the eigenvalue equations of the angular momentum operator.