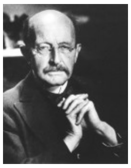
Birth of quantum physics



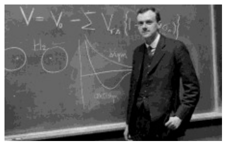
Max Planck
(1858-1947)

Niels Bohr
(1885-1962)

Erwin Schrödinger
(1887-1961)

Werner Heisenberg
(1901-1976)

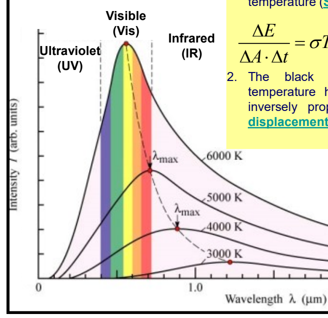
Wolfgang Pauli
(1900-1958)



Paul Dirac
(1902-1984)

Birth of quantum physics

Temperature (black body) radiation, thermal light sources



1. The total energy emitted from unit surface in unit time is directly proportional to the fourth power of the temperature (Stefan-Boltzmann law).

$$\frac{\Delta E}{\Delta A \cdot \Delta t} = \sigma T^4 \text{ where } \sigma = 5.67 \cdot 10^{-8}\,\mathrm{Wm^{-2}K^{-4}}$$

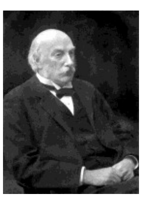
2. The black body radiation curve for different temperature has its peak at a wavelength that is inversely proportional to the temperature (Wien's displacement law).

$$\lambda_{max} T = 2.88 \cdot 10^{-3}\,\mathrm{mK}$$

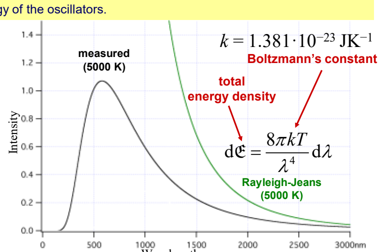
Birth of quantum physics

Temperature (black body) radiation, thermal light sources

- He studied black body radiation on the basis of classical mechanics.
- He considered the electromagnetic field to be a multitude of harmonic oscillators.
- The presence of light of the given ν frequency was interpreted by the excitation of the same frequency electromagnetic oscillator.
- He used the classical equipartition theorem ($\frac{1}{2}kT$ of energy for each degree of freedom) to calculate the average energy of the oscillators.



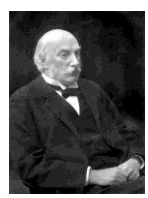
John William Strutt
(1842-1919)



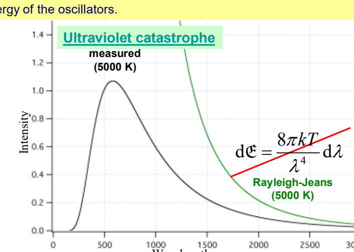
Birth of quantum physics

Temperature (black body) radiation, thermal light sources

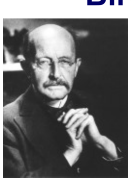
- He studied black body radiation on the basis of classical mechanics.
- He considered the electromagnetic field to be a multitude of harmonic oscillators.
- The presence of light of the given ν frequency was interpreted by the excitation of the same frequency electromagnetic oscillator.
- He used the classical equipartition theorem ($\frac{1}{2}kT$ of energy for each degree of freedom) to calculate the average energy of the oscillators.



John William Strutt
(1842-1919)



Birth of quantum physics



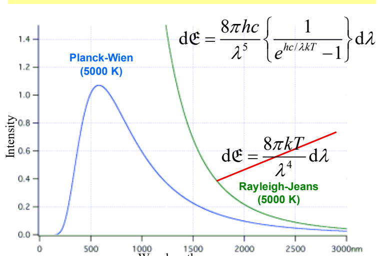
Max Planck
(1858-1947)

The quantum hypothesis

Planck: Small oscillators emitting radiation can only have energy values which is a multiple of a given energy dose. (The energy is quantized at a specified frequency and can be given as follows: $E = nh\nu$).

$h = 6.626 \cdot 10^{-34}\,\mathrm{Js}$, Planck's constant

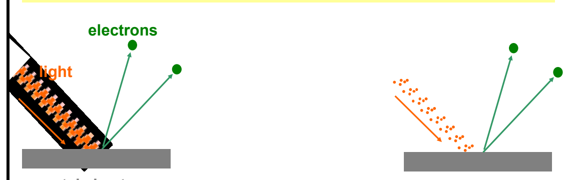
- The oscillators only excite the wall when they receive at least $h\nu$ (one photon) energy.
- Higher frequency oscillators do not have that much energy.



Birth of quantum physics

The photoelectric effect

- The photoelectric effect is the emission of electrons or other free charge carriers when light falls on a material. Electrons emitted in this manner are called photoelectrons. Their energy can be measured:
  - Electrons are dislodged only by the impingement of photons when those photons reach or exceed a threshold frequency (energy) characteristic to the metal.
  - Below that threshold, no electrons are emitted from the material regardless of the light intensity or the length of time of exposure to the light.
  - The kinetic energy of the emitted electrons is linearly dependent on the frequency of radiation, but does not depend on its intensity.
  - The number of emitted electrons depends on the intensity of the radiation.

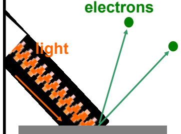


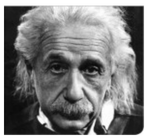
Birth of quantum physics

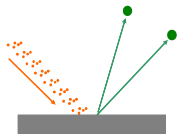
The photoelectric effect

- The photoelectric effect is the emission of electrons or other free charge carriers when light falls on a material. Electrons emitted in this manner are called photoelectrons. Their energy can be measured:
  - Electrons are dislodged only by the impingement of photons when those photons reach or exceed a threshold frequency (energy) characteristic to the metal.
  - Below that threshold, no electrons are emitted from the material regardless of the light intensity or the length of time of exposure to the light.
  - The kinetic energy of the emitted electrons is linearly dependent on the frequency of radiation, but does not depend on its intensity.
  - The number of emitted electrons depends on the intensity of the radiation.

$$\tfrac{1}{2} m_e v^2 = h\nu - E_{binding}$$




Albert Einstein
(1879-1955)



Birth of quantum physics

Compton effect

- He examined the scattering of X-rays on electrons.
  - The wavelength of the scattered radiation increases slightly.
  - The value of increase is a well-defined, single value.
  - The increase depends on the scattering angle, but does not depend on the wavelength of the incident radiation.

$d\lambda = \lambda_C(1-\cos\Theta)$ where $\lambda_C = 2.43$ pm

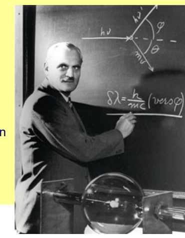
the Compton-wavelength of an electron

Photons have not only their energy but also momentum:

$$p = \frac{h\nu}{c} = \frac{h}{\lambda}$$

During the collisions, conservation of energy and conservation of momentum should be valid:

$$\lambda_C = \frac{h}{m_e c} = 2.426 \text{ pm}$$


Arthur Holly Compton
(1892-1962)

Birth of quantum physics

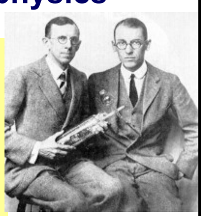
Electron diffraction

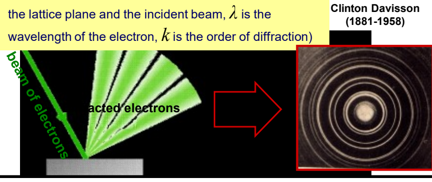
Clinton Davisson and **Lester Germer**

- guided a beam of electrons through a crystalline lattice.
  - They got a diffraction image.
  - When an electron beam is bent on polycrystalline material, then Debey-Scherrer rings will be in the deflection image of the interference enhancement sites.
  - The deflection image can be interpreted well on the basis of the Bragg equation describing the crystal diffraction:

$$2d\sin\Theta = k\lambda$$

(where d is the lattice constant, Θ is the angle between the lattice plane and the incident beam, λ is the wavelength of the electron, k is the order of diffraction)


Clinton Davisson (1881-1958) Lester Germer (1896-1971)



Birth of quantum physics

Electron diffraction

Clinton Davisson and **Lester Germer**

- guided a beam of electrons through a crystalline lattice.
  - They got a diffraction image.
  - When an electron beam is bent on polycrystalline material, then Debey-Scherrer rings will be in the deflection image of the interference enhancement sites.
  - The deflection image can be interpreted well on the basis of the Bragg equation describing the crystal diffraction:

$$2d\sin\Theta = k\lambda$$

(where d is the lattice constant, Θ is the angle between the lattice plane and the incident beam, λ is the wavelength of the electron, k is the order of diffraction)

Louis de Broglie:

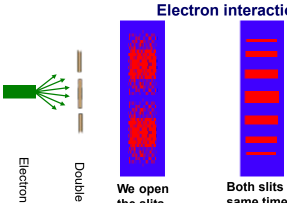
- He assigned a wavelength to each particle:

$$\lambda = \frac{h}{p}$$

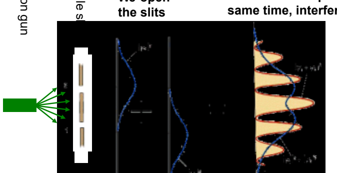

Louis de Broglie
(1892-1987)

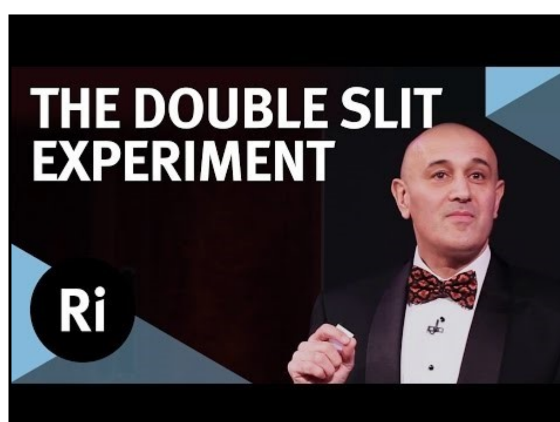
Birth of quantum physics

Electron interaction with matter



- Permanent intensity particle (e^-) source.
- The electron beam's intensity is so low that we do not have to consider the interaction of the particles (electrons).





Birth of quantum physics

Heisenberg's uncertainty principle

- It states that the more precisely the position of some particle is determined, the less precisely its momentum ($p = mv$) can be known, and *vice versa*. So, classical mechanical description (orbit definition) is not possible.
- Whatever method of measurement is chosen, the interaction between the measuring device and the particle in the measured characteristics causes some indeterminacy. The smaller the inprecision in one of the measured features, the greater the other.
- Mathematically:

$$\Delta x \Delta p_x \geq \tfrac{1}{2}\hbar \quad \text{where} \quad \hbar \ \ldots .05\cdot 10^{-34}\,\text{Js}$$

reduced Planck constant

Planck constant

- It does not have any particular effect on macroscopic bodies, but it does have an effect on atomic size particles.

Werner Heisenberg (1901-1976)

Birth of quantum physics

Heisenberg's uncertainty principle

- It states that the more precisely the position of some particle is determined, the less precisely its momentum ($p = mv$) can be known, and *vice versa*. So, classical mechanical description (orbit definition) is not possible.
- ~~Whatever method of measurement is chosen, the interaction between the measuring device and the particle in the measured characteristics causes some indeterminacy. The smaller the inprecision in one of the measured features, the greater the other.~~
- Mathematically:

$$\Delta x \Delta p_x \geq \tfrac{1}{2}\hbar \quad \text{where} \quad \hbar \ \ldots .05\cdot 10^{-34}\,\text{Js}$$

reduced Planck constant

Planck constant

- It does not have any particular effect on macroscopic bodies, but it does have an effect on atomic size particles.

$m = 1$ kg
$\Delta x = 10^{-4}$ m
↓
Uncertainty of speed:
$\Delta v \sim 10^{-30}$ m/s

$m_e = 9.1\cdot 10^{-31}$ kg
$\Delta x = 10^{-10}$ m
↓
Uncertainty of speed:
$\Delta v \sim 10^{6}$ m/s

Birth of quantum physics

Heisenberg's uncertainty principle

- It states that the more precisely the position of some particle is determined, the less precisely its momentum ($p = mv$) can be known, and *vice versa*. So, classical mechanical description (orbit definition) is not possible.
- ~~Whatever method of measurement is chosen, the interaction between the measuring device and the particle in the measured characteristics causes some indeterminacy. The smaller the inprecision in one of the measured features, the greater the other.~~
- Mathematically:

$$\Delta x \Delta p_x \geq \tfrac{1}{2}\hbar \quad \text{where} \quad \hbar \ \ldots .05\cdot 10^{-34}\,\text{Js}$$

reduced Planck constant

Planck constant

- It does not have any particular effect on macroscopic bodies, but it does have an effect on atomic size particles.

- No physical phenomenon can be represented with arbitrary precision as "classic point-like particle" or wave.
- The microscopic situation is best described by wave-particle duality, dealing with cases where neither the particle nor the wave property is a fully suitable approach.
- The uncertainty principle is sometimes mistakenly explained by the fact that the measurement of the particle location necessarily disrupts the momentum of the particle. The non-classical characteristics of quantum mechanical uncertainty measurements were clarified thanks to the Einstein-Podolsky-Rosen paradox.

Birth of quantum physics

Heisenberg's uncertainty principle

- **EPR (Einstein–Podolsky–Rosen) paradox**: is a thought experiment proposed by physicists Albert Einstein, Boris Podolsky and Nathan Rosen (EPR) that they interpreted as indicating that the explanation of physical reality provided by Quantum Mechanics was incomplete. In a 1935 paper titled Can Quantum-Mechanical Description of Physical Reality be Considered Complete?, they attempted to mathematically show that the wave function does not contain complete information about physical reality, and hence the Copenhagen interpretation is unsatisfactory; resolutions of the paradox have important implications for the interpretation of quantum mechanics.
- The work was done at the Institute for Advanced Study in 1934, which Einstein had joined the prior year after he had fled Nazi Germany.
- The essence of the paradox is that particles can interact in such a way that it is possible to measure both their position and their momentum more accurately than Heisenberg's uncertainty principle allows, unless measuring one particle instantaneously affects the other to prevent this accuracy, which would involve information being transmitted faster than light as forbidden by the theory of relativity ("spooky action at a distance"). This consequence had not previously been noticed and seemed unreasonable at the time; the phenomenon involved is now known as quantum entanglement..

Birth of quantum physics

The basics of quantum mechanics

Heisenberg's matrix mechanics

- The idea of *Einstein*'s theory of relativity is the starting point: in theory, only terms that represent observable physical quantities should be used. (The orbit of the electron in the atom is not such.)
- Instead of the orbit, the amplitudes of the Fourier series expansion of the location coordinates should be used. He figured out what algebraic rules these would have to meet to get the same results as the observations.
- *Max Born* and *Pascal Jordan* showed that Heisenberg's mathematical symbols used for the location coordinate and momentum of the electron are, in fact, matrices.
- *Heisenberg* published his results in July 1925. Einstein first did not believe it, and Bohr doubted is also but…
- *Pauli* calculated the energy eigenvalues of the hydrogen atom using the matrix mechanics.

Schrödinger's wave mechanics

- Based on the wave-particle duality concept introduced by *de Broglie*, he got a differential equation whose regular solutions give the energy eigenvalues of the atoms.
- He showed that the two types of mathematical descriptions (matrix mechanics and wave mechanics) are equivalent.
- *Paul Dirac* developed the mathematical theory of quantum mechanics based on state vectors and operators in Hilbert space. The essence of Dirac's discussion is that we assign an operator to every physical quantity and identify its own values with the values that can be measured quantitatively.

Equation of state

- The concept of movement is non-classical, instead of orbitals, works with the $\Psi(x,y,z,t)$ wave function.
- The probability that the particle is at moment t is in the small volume $\mathrm{d}V$ around (x,y,z) is:

$$\Psi^*(x,y,z,t)\Psi(x,y,z,t)\mathrm{d}V = |\Psi(x,y,z,t)|^2\,\mathrm{d}V$$

- The probability of the particle being present in the finite V volume:

$$\int_V \Psi^*(x,y,z,t)\Psi(x,y,z,t)\mathrm{d}V \quad \text{or} \quad \int_V \Psi^*\Psi\mathrm{d}V$$

- Integrated into the full space: $\int \Psi^*\Psi\mathrm{d}V = 1$

This is ensured by normalization.

Max Born (1882-1970)

- **The equation of motion of quantum mechanics (equation of state or Schrödinger equation)** on a particle moving in conservative field is:

$$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t} \ldots \frac{\hbar}{2\mu} \ldots, y, z)\Psi \quad \text{where} \quad \Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Laplace-operátor

nabla

potential energy

mass of particle

immaginary unit = $\sqrt{-1}$

Equation of state

- When $\Psi(x,y,z,0)$ is known, the value of $\Psi(x,y,z,t)$ can be calculated using the Schrödinger equation.
- The Schrödinger equation can be extended to the event when the test particle interacts in time.
- The Schrödinger equation is an axiom.

- **The equation of motion of quantum mechanics (equation of state or Schrödinger equation)** on a particle moving in conservative field is:

$$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t} \quad \frac{\hbar}{2\mu} \quad (x,y,z)\Psi$$

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

Laplace-operátor

nabla

potential energy

mass of particle

immaginary unit = $\sqrt{-1}$

Stationary Schrödinger equation

- The solution of the state equation gives a time-dependent residence probability.
- The probability of electron residence in an atom free of external force (stationary state of electron) is independent of time.

$$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t} \quad \frac{\hbar}{2\mu}$$ and $\Psi(x,y,z,t)=\Psi(x,y,z)T(t)$

$$\frac{1}{T}\left(-\frac{\hbar}{\mathrm{i}}\frac{}{dt}\right) \quad \frac{}{\Psi}\left(\frac{\hbar}{2\mu}\right)$$

This is only true for all variable values if both sides are constant (E, total energy of the particle). $E = E_{kinetic} + V$

- So, the **stationary Schrödinger equation** is:

$$-\frac{\hbar}{2\mu} \quad \Psi = E\Psi$$

- Calculation of residence probability: $\Psi^*\Psi = \Psi^*\Psi$

Free particle

- The simplest quantum mechanical object, but in reality it is only valid for a short time.
- It does not interact with other physical objects, its potential energy is constant.
- The **stationary Schrödinger equation of the free particle** in 1D:

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} = -\alpha^2\Psi \quad \text{where } \alpha^2 = \frac{2\mu E}{\hbar}$$

- The solution of the equation:

$$\Psi(x) = N\mathrm{e}^{\mathrm{i}\alpha x}, \text{ and since } T(t) = \mathrm{e}^{-\frac{\mathrm{i}Et}{\hbar}}$$

constant independent of place

For the full wave function of the stationary state:

$$\Psi(x,t) = \Psi(x)T(t) = N\mathrm{e}^{\mathrm{i}\left(\alpha x - \frac{Et}{\hbar}\right)} = N\left[\cos\left(\alpha x - \frac{Et}{\hbar}\right) + \mathrm{i}\sin\left(\alpha x - \frac{Et}{\hbar}\right)\right]$$

- The Ψ function describes a a wave that is periodic both in **space and time**, for which:

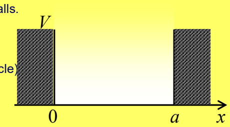
$$\lambda = \frac{2\pi\hbar}{\sqrt{2\mu E}} \quad \frac{\hbar}{p_x} \quad p_x$$ (de Broglie equation), and $E = \frac{2\pi\hbar}{T}$ (Planck)

wavelength — momentum = $\sqrt{2\mu E}$ — period — frequency = $1/T$

- For the free particle in stationary state, $\Psi^*\Psi = N^*N$

Particle in a box

- The particle moves inside a box with impenetrable walls.
- At the walls, the potebtial is infinite, the particle wave function in the range of ((∞,0) and (a,+∞) is zero.



- The Schrödinger equation (same as for the free particle)

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} = -\alpha^2\Psi \quad \text{where } \alpha^2 = \frac{2\mu E}{\hbar}$$

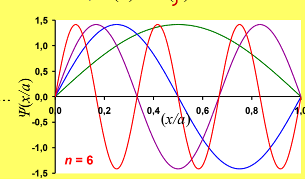
General solution: $\Psi(x) = A\sin(\alpha x) + B\cos(\alpha x)$ — $B = 0$

Boundary condition (from the continuity of wave function): $\Psi(0) = \Psi(a) = 0$ — $\alpha a = n\pi$

Normalization: $A^2\int_0^a \sin^2(\alpha x)\mathrm{d}x = 1$

$$E_n = \frac{n^2\pi^2\hbar}{2\mu a^2} \quad \text{where } n = 1,2,3\ldots$$

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$



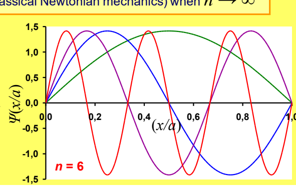
Particle in a box

- The wavelength assigned to the "wave-like" residence probability: $\lambda = \frac{2a}{n}$
- The energy of a particle in a box can only assume discrete values in a stationary state (quantized).
- n: quantum number
- The lowest energy state is the ground state, from which it can be excited to the higher energy excited state.
- Residence probability: $w = \frac{x_2 - x_1}{a}$ (classical Newtonian mechanics) when $n \longrightarrow \infty$

Bohr correspondence principle

$$E_n = \frac{n^2\pi^2\hbar}{2\mu a^2} \quad \text{where } n = 1,2,3\ldots$$

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$



Particle in a box

2D box

- Stationary Schrödinger equation for 2D:

$$-\frac{\hbar}{2\mu}\left(\frac{}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right) = E\Psi$$

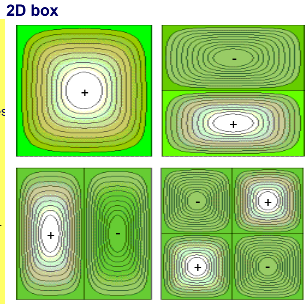
- In the case of 2D, there are two n values (n_1 and n_2) to be taken into account.
- Separation of variables:

$$\Psi(x,y) = X(x)Y(y)$$

$$-\frac{\hbar}{2\mu}\left(\frac{}{\mathrm{d}x^2} + X\frac{\mathrm{d}^2Y}{\mathrm{d}y^2}\right) = EXY$$

- Solution:

$$E = E^X + E^Y = -\frac{\hbar}{2\mu}\left(\frac{}{\mathrm{d}x^2} + \frac{\mathrm{d}^2Y}{\mathrm{d}y^2}\right)$$



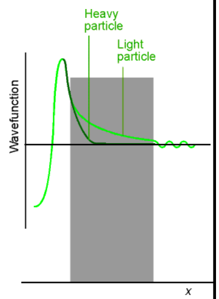
Particle in a box

Tunneling effect

- If the potential energy of the particle enclosed in the box does not become infinite at the walls of the box, then the wave function of this place will not be reduced to a sudden zero.
- In the case of thin walls (where the potential energy is again zero after finite distance) the exponential decrease of the wave function stops on the other side of the wall, and the oscillation usual inside the box follows.
- The particle can be found outside the walls of the box, although - according to the classic mechanics – it has not enough energy to escape.
- Inside the potential barrier:

$V > 0$ and

$$\frac{d^2\Psi}{dx^2} = \frac{2\mu(V-E)\Psi}{\hbar}$$



- The solution of the equation:

$$\Psi = Ae^{\kappa x} + Be^{-\kappa x} \quad \text{where} \quad \kappa = \left\{\frac{2\mu(V-E)\Psi}{\hbar}\right\}^{1/2}$$

Harmonic oscillator

Classical mechanics

- Body on a spring, linear force law.

$$F_x = -kx$$

- Equation of motion (Newton's second law):

$$\mu\frac{d^2x}{dt^2} = -kx$$

- Solution: $x(t) = A\sin(\omega t + \alpha)$

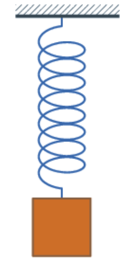
initial phase
angular frequency

where $\omega = \sqrt{\frac{k}{\mu}} = 2\pi\nu = \frac{2\pi}{T}$

amplitude

$$A = \sqrt{\frac{2E}{k}} = \sqrt{\frac{\mu|v|^2 + kx^2}{k}}$$

speed of particles

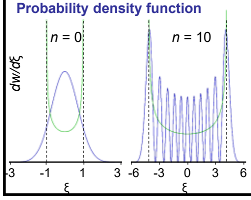


Harmonic oscillator

n	$H_n(\xi)$
0	1
1	2ξ
2	$4\xi^2 - 2$
3	$8\xi^3 - 12\xi$
4	$16\xi^4 - 48\xi^2 + 12$

Bohr correspondence principle

Probability density function



Quantum mechanics

- Stationary Schrödinger equation:

$$-\frac{\hbar}{2\mu\, dx^2} + \tfrac{1}{2}kx^2\Psi = E\Psi$$

Boundary condition: $\Psi \to 0$, if $x \to \pm\infty$
General solution
Normalization

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar \quad \tfrac{1}{2})h\nu$$

$$\Psi_n(\xi) = \left(\frac{\sqrt{\beta/\pi}}{2^n n!}\right)^{1/2} H_n(\xi)e^{-\xi^2/2}$$

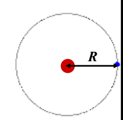
Hermite polynomial

where $\beta = \frac{\mu\omega}{\hbar}$, $\xi = \sqrt{\beta}x$ and $n = 0,1,2\ldots$

Circular motion in quantum mechanics

- Initial form of the stationary Schrödinger equation (now for 2D motion):

$$-\frac{\hbar}{2\mu}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right) = E\Psi$$



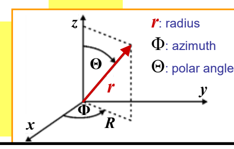
Introducing angular coordinates (movement only in the xy plane):

$$-\frac{\hbar}{2\mu}\left(\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial\Psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\Psi}{\partial\Phi^2}\right) = E\Psi$$

As $r = R =$ constants:

$$-\frac{\hbar}{2\mu}\left(\frac{\Psi}{R^2\,\partial\Phi^2}\right) = E\Psi \quad \text{or} \quad \frac{\partial^2\Psi}{\partial\Phi^2} = -\frac{2\mu ER^2}{\hbar}\Psi$$

Condition: $\Psi(\Phi) = \Psi(\Phi + 2\pi)$



Circular motion in quantum mechanics

$$-\frac{\hbar}{2\mu}\left(\frac{\Psi}{R^2\,\partial\Phi^2}\right) = E\Psi \quad \text{or} \quad \frac{\partial^2\Psi}{\partial\Phi^2} = -\frac{2\mu ER^2}{\hbar}\Psi$$

Condition: $\Psi(\Phi) = \Psi(\Phi + 2\pi)$

- Solution: $\Psi(\Phi) = Ne^{im\Phi} = N[\cos(m\Phi) + i\sin(m\Phi)]$

Stationary energy values and wave function:

$$E_m = \frac{m^2\hbar}{2\Theta} \quad \text{where } m = 0, \pm1, \pm2\ldots$$

$$\Psi_m(\Phi) = \left(\frac{1}{2\pi R}\right)^{1/2} e^{im\Phi}$$

- If a given energy value is possible by more than one wave functions (state), degeneracy is said to appear.
- All $m \neq 0$ energy values have a degeneracy of two.
- Both in classical and quantum mechanics: $E = \frac{L_z^2}{2\Theta}$

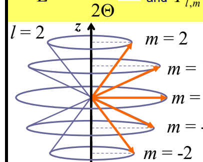
angular momentum in direction z: $L_z = m\hbar$

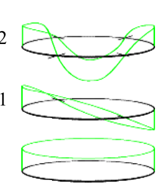
Circular motion in quantum mechanics

Motion on the surface of a sphere

- The full, three-dimensional form of the stationary Schrödinger equation.
- Two quantum numbers ($l = 0,1,2\ldots$ and $m = -l, (-l+1)\ldots0\ldots(l-1), l$) appear in the solution:

$$E = \frac{l(l+1)\hbar}{2\Theta} \quad \text{and} \quad \Psi_{l,m} = N_{l,m}P_l^{|m|}(\cos\Theta)e^{im\Phi}$$





For each energy value, there are $(2l + 1)$ wave functions.

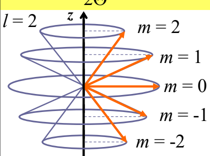
Circular motion in quantum mechanics

Motion on the surface of a sphere

- The full, three-dimensional form of the stationary Schrödinger equation.
- Two quantum numbers ($l = 0,1,2\ldots$ and $m = -l,(-l+1)\ldots0\ldots(l-1),l$) appear in the solution:

$$E = \frac{l(l+1)\hbar}{2\Theta} \quad \text{and} \quad \Psi_{l,m} = N_{l,m}P_l^{|m|}(\cos\Theta)\mathrm{e}^{im\Phi}$$

associated Legendre polynomial



$$P_l^{|m|}(\xi) = \left(2^l l!\right)^{-1}\left(1-\xi^2\right)^{|m|/2}\frac{d^{l+|m|}}{d\xi^{l+|m|}}\left(\xi^2-1\right)^l$$

- If a given energy value is possible by more than one wave functions (state), degeneracy is said to appear.
- All $m \neq 0$ energy values have a degeneracy of two.
- Both in classical and quantum mechanics: $E = \frac{L_z^2}{2\Theta}$ angular momentum in direction z: $L_z = m\hbar$

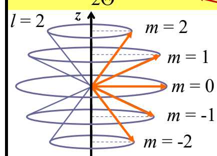
Circular motion in quantum mechanics

Motion on the surface of a sphere

- The full, three-dimensional form of the stationary Schrödinger equation.
- Two quantum numbers ($l = 0,1,2\ldots$ and $m = -l,(-l+1)\ldots0\ldots(l-1),l$) appear in the solution:

$$E = \frac{l(l+1)\hbar}{2\Theta} \quad \text{and} \quad \Psi_{l,m} = N_{l,m}P_l^{|m|}(\cos\Theta)\mathrm{e}^{im\Phi}$$

normalized spherical functions



l	m	$\Psi_{l,m}$
0	0	$(1/4\pi)^{1/2}$
1	1	$(3/8\pi)^{1/2}\sin\Theta\exp(i\Phi)$
1	0	$(3/4\pi)^{1/2}\cos\Theta$
1	-1	$(3/8\pi)^{1/2}\sin\Theta\exp(-i\Phi)$
2	2	$(5/32\pi)^{1/2}\sin^2\Theta\exp(2i\Phi)$
2	1	$(5/8\pi)^{1/2}\cos\Theta\sin\Theta\exp(i\Phi)$
2	0	$(5/16\pi)^{1/2}(3\cos^2\Theta-1)$
2	-1	$(5/8\pi)^{1/2}\cos\Theta\sin\Theta\exp(i\Phi)$
2	-2	$(5/32\pi)^{1/2}\sin^2\Theta\exp(-2i\Phi)$

Variational principle

Approximate solution of the stationary Schrödinger equation

- It is used if
  - a quantum mechanical problem cannot be solve exactly,
  - information of limited precision is useful.
- It is used for finding the ground state.
- Stationary Schrödinger equation: $H\Psi = E\Psi$

where $H = -\frac{\hbar}{2\mu} \ldots (x,y,z)$ (Hamilton operator)

In the ground state: $H\Psi_0 = E_0\Psi_0$

After re-arrangement and integration:

$$E_0 = \frac{\int \Psi_0^* H \Psi_0 \mathrm{d}V}{\int \Psi_0^* \Psi_0 \mathrm{d}V}$$

- If he exact wave function of the ground state is unknown, the exact energy cannot be found with this formula, but a suitable probe function Ψ can be selected:

$$E = \frac{\int \Psi^* H \Psi \mathrm{d}V}{\int \Psi^* \Psi \mathrm{d}V}$$

If $\Psi \approx \Psi_0$, then most probably $E \approx E_0$.

It can be proved that E obtained by any probe function Ψ cannot be lower than E_0.

Schrödinger's cat

- Schrödinger's cat is a thought experiment, sometimes described as a paradox, devised by Austrian physicist Erwin Schrödinger in 1935.
- It illustrates what he saw as the problem of the Copenhagen interpretation of quantum mechanics applied to everyday objects.
- In the Copenhagen interpretation, a system stops being a superposition of states and becomes either one or the other when an observation takes place.
- Thought experiment: A cat is penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a Geiger counter, there is a tiny bit of radioactive substance, so small, that perhaps in the course of the hour one of the atoms decays, but also, with equal probability, perhaps none; if it happens, the counter tube discharges and through a relay releases a hammer that shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The first atomic decay would have poisoned it. The psi-function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts.
- This thought experiment makes apparent the fact that the nature of measurement, or observation, is not well-defined in this interpretation. The experiment can be interpreted to mean that while the box is closed, the system simultaneously exists in a superposition of the states "decayed nucleus/dead cat" and "undecayed nucleus/living cat", and that only when the box is opened and an observation performed does the wave function collapse into one of the two states.
- However, Niels Bohr never had in mind the observer-induced collapse of the wave function, as he did not regard the wave function as physically real, but a statistical tool; thus, Schrödinger's cat did not pose any riddle to him.

Schrödinger's cat

Experimental tests:

- https://www.scientificamerican.com/article/bringing-schrodingers-quantum-cat-to-life/
-

Possible practical application: quantum computing

- Quantum computing is the use of quantum-mechanical phenomena such as superposition and entanglement to perform computation. A quantum computer is used to perform such computation, which can be implemented theoretically or physically. A quantum computer with a given number of qubits is fundamentally different from a classical computer composed of the same number of classical bits. For example, representing the state of an n-qubit system on a classical computer requires the storage of 2^n complex coefficients, while to characterize the state of a classical n-bit system it is sufficient to provide the values of the n bits, that is, only n numbers. Although this fact may seem to indicate that qubits can hold exponentially more information than their classical counterparts, care must be taken not to overlook the fact that the qubits are only in a probabilistic superposition of all of their states.

Schrödinger's cat