

1 The Photon

c $\left[\frac{\text{m}}{\text{s}}\right]$	speed of light
h $\left[\frac{\text{m}^2 \text{kg}}{\text{s}}\right]$	planc's constant
e [C]	electorn charge
m_e [kg]	electron mass
k_B $\left[\frac{\text{m}^2 \text{kg}}{\text{s}^2 \text{K}}\right]$	bolzmann constant
ϵ_0 $\left[\frac{\text{F}}{\text{m}}\right]$	vacuum permittivity

$$c = 2.998 \cdot 10^8 \left[\frac{\text{m}}{\text{s}}\right]$$

$$h = 6.626 \cdot 10^{-34} \left[\frac{\text{m}^2 \text{kg}}{\text{s}}\right]$$

$$\hbar = \frac{h}{2\pi}$$

$$e = 1.602 \cdot 10^{-19} \text{ [C]}$$

$$m_e = 9.109 \cdot 10^{-31} \text{ [kg]}$$

$$k_B = 1.381 \cdot 10^{-23} \left[\frac{\text{m}^2 \text{kg}}{\text{s}^2 \text{K}}\right]$$

$$\epsilon_0 = 8.854 \cdot 10^{-12} \left[\frac{\text{F}}{\text{m}}\right]$$

$$1 \text{ [eV]} = 1.602 \cdot 10^{-19} \text{ [J]}$$

1.1 Photon & Electron

λ [m], ν $\left[\frac{1}{\text{s}}\right]$	Wavelength, Freq.
k	Wavenumber
E [J]	Energy
\vec{F}_c [N]	Coulomb Force

$$\lambda = \frac{c}{\nu} \quad \nu = \frac{c}{\lambda} \quad \omega = 2\pi\nu$$

$$k = \frac{2\pi\nu}{c}$$

$$E = h \cdot \nu = \hbar \cdot \omega$$

$$\left|\vec{F}_c\right| = \frac{Q_1 \cdot Q_2}{4\pi\epsilon_0 r^2}$$

1.2 Photoelectric effect

V [V]	Voltage
ϕ_0 [eV]	Work function
I [A]	Photo-current
n $[\text{m}^{-3}]$	Volume density of electrons
A $[\text{m}^2]$	Area
v $\left[\frac{\text{m}}{\text{s}}\right]$	velocity of electrons

$$h\nu - \phi_0 = \frac{1}{2}mv^2 = eV$$

$$V(\nu) = \frac{h}{e}\nu - \frac{\phi_0}{e}$$

$$I = nAve$$

1.3 Blackbody Radiation

L [m]	length of blackbody cube	k_i	wave constants
E_x	Electric field in x-direction	$\langle E \rangle$	Average Energy
N	Number of states	D	Density of states
u	Blackbody radiation	I	Power radiated

$$E_x(x, y, z) = E_{0x} \cos(k_x x) \sin(k_y y) \sin(k_z z)$$

$$k_x = n \frac{\pi}{L} \quad k_y = m \frac{\pi}{L} \quad k_z = l \frac{\pi}{L} \quad k = \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$$N(k) = \frac{1}{3\pi^2} k^3 L^3 \quad D(k) = \frac{k^2}{\pi^2}$$

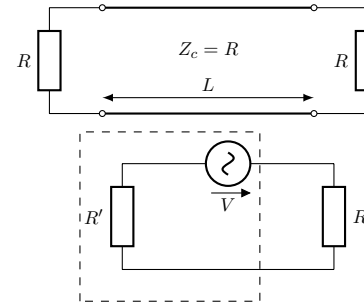
$$u(\omega) = \frac{\omega^2}{\pi^2 c^3} \cdot \frac{\hbar \omega}{\exp\left(\frac{\hbar \omega}{kT}\right) - 1} d\omega \quad u(\nu) = \frac{8\pi h \nu^3}{c^3 \left(\exp\left(\frac{h\nu}{kT}\right) - 1\right)} d\nu$$

$$I(\omega) = c \cdot u(\omega)$$

Equipartition-Theorem: Each degree of Freedom has an energy of kT

1.4 Johnson-Noise

This is the noise created in a one-dimensional circuit (like a coax-cable).

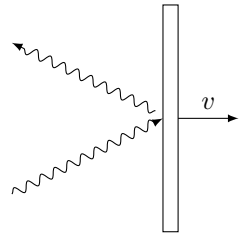


$\langle V^2 \rangle$	Noise Voltage
$\Delta\nu$	Bandwidth

$$E = E_0 \cdot \sin(k_x \cdot x)$$

$$\langle V^2 \rangle = 4R \cdot k_B T \cdot \Delta\nu$$

1.5 Momentum of a photon



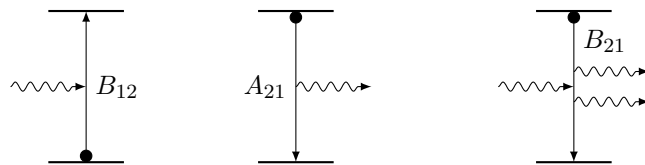
$$p \left[\frac{\text{kg m}}{\text{s}} \right] \quad \text{momentum}$$

$$p_{\text{absorbing}} = \frac{h\nu}{c} = m \cdot v$$

$$p_{\text{reflecting}} = 2 \cdot \frac{h\nu}{c}$$

$$p = \sqrt{2m_e e \Delta V}$$

1.6 Absorption, spontaneous and stimulated emission



absorption spontaneous emission stimulated emission

n_1 Number of electrons in the lower energy state

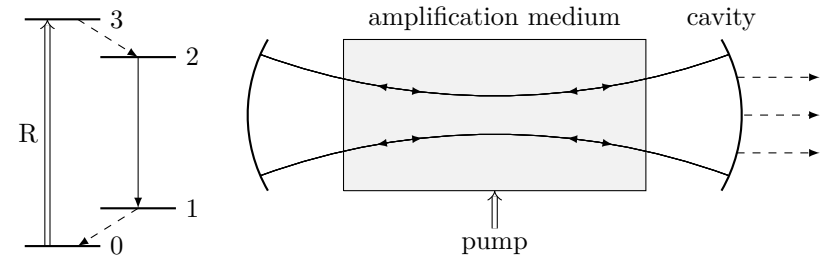
n_2 Number of electrons in the higher energy state

$$\frac{dn_2}{dt} = \underbrace{n_1 \cdot u(\nu) \cdot B_{12}}_{\text{absorption}} - \underbrace{n_2 \cdot u(\nu) \cdot B_{21}}_{\text{stimulated emission}} - \underbrace{n_2 \cdot A_{21}}_{\text{spontaneous emission}}$$

$$\frac{n_2}{n_1} = e^{-\frac{h\nu}{k_B T}} = \frac{u(\nu) B_{12}}{u(\nu) B_{21} + A_{21}}$$

$$B_{21} = B_{12} = B \quad A_{21} = \frac{8\pi h \nu^3}{c^3}$$

1.7 Laser-optical amplification



Electrons are excited from the ground state “0” to the level “3” by pumping through incoherent radiation. The electrons then fall onto a long-lived state n_2 (State “2”) from level “3”. The pumping can be done either optically by shining a strong incoherent light or by passing a current. It is also assumed that the lower state is quickly emptied by a fast process with lifetime τ_1 . As a result, the population in state “2” is:

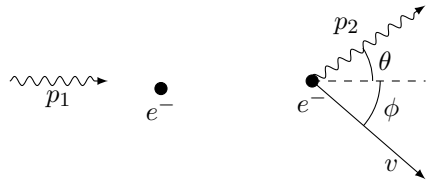
$$n_2 = \frac{R}{A_{21}} \quad \text{whereas} \quad n_1 \approx 0 \quad \text{because} \quad A_{21} < \frac{1}{\tau_1}$$

We have therefore a population inversion between the two states. The likelihood of a stimulated emission process is larger than the one of absorption. If we enclose the system in an optical cavity, we can achieve self-sustained oscillation at the frequency ν .

2 Wave mechanics

	frequency	wavelength	momentum	energy
Particle		$\lambda_b = \frac{h}{p}$	$p = mv$	$E = \frac{1}{2}mv^2$
Wave	ω	$\lambda = \frac{2\pi c}{\omega}$	$p = \frac{\hbar \omega}{c}$	$E = \hbar \omega$

2.1 Compton Scattering

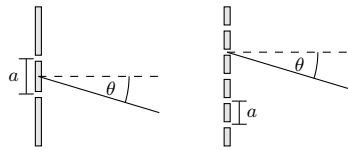


$$p_1 = \frac{h\nu_1}{c} \quad p' = \frac{h\nu_2}{c}$$

$$\nu_2 = \nu_1 - \frac{P_e^2}{2m_e h}$$

$$\lambda_2 - \lambda_1 = \frac{h}{m_e c} (1 - \cos \theta);$$

2.2 Double Slit and Bragg Diffraction

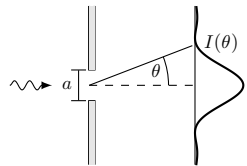


Constructive $\sin \theta = \frac{n\lambda}{a}$

Destructive $\sin \theta = \frac{(n + \frac{1}{2})\lambda}{a}$

$n \in \mathbb{Z}$

2.3 Single slit and uncertainty relation



$$I(\theta) = I_0 \frac{\sin^2 \theta}{\theta^2} \quad \sin \theta = \frac{\lambda}{a}$$

$$\Delta x \Delta p \geq \hbar \quad \Delta t \Delta E \geq \hbar \quad (E = \hbar \omega)$$

2.4 Bohr-Sommerfeld quantisation

Every single particle must satisfy the following equation. The quantized energy levels below relate to the hydrogen atom

p	Momentum of particle	$\int_{length} p \cdot ds = n \cdot h \quad n \in \mathbb{N}$
E_n	Energy of the nth state	$E_n = -\frac{Z^2}{n^2} \cdot \frac{m_e e^4}{8\epsilon_0^2 h^2} = -\frac{Z^2}{n^2} \cdot E_{ry}$
E_{ry}	Rydberg Energy	$r_n = \frac{n^2}{Z} \cdot \frac{2\epsilon_0 h}{m_e e^2} = \frac{n^2}{Z} \cdot a_0$
a_0	Bohr-radius	$E_{ry} = 13.6 \text{ [eV]}$
Z	Number of protons	$a_0 = 5.292 \cdot 10^{-11} \text{ [m]}$

3 Quantum Mechanics

3.1 Wave function

$$\psi(\mathbf{x}, t) : \mathbb{R}^4 \rightarrow \mathbb{C} \quad \iiint |\psi(\mathbf{x}, t)|^2 d^3 r = 1$$

$$\psi(\mathbf{x}, t) = a\psi_1(\mathbf{x}, t) + b\psi_2(\mathbf{x}, t), \quad |a|^2 + |b|^2 = 1$$

3.2 The Schrödinger equation

$$V(\mathbf{x}, t) \quad \text{potential} \quad \left| \begin{array}{l} m \\ \text{mass} \end{array} \right.$$

$$i\hbar \cdot \frac{\partial \Psi}{\partial t}(\mathbf{x}, t) = -\frac{\hbar^2}{2m} \cdot \nabla^2 \Psi(\mathbf{x}, t) + V(\mathbf{x}, t) \Psi(\mathbf{x}, t)$$

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

$$\Psi = A \cdot e^{i(\mathbf{k}\mathbf{x} - \omega t)} \quad \mathbf{k} = [k_x \quad k_y \quad k_z], \quad \mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$E = \omega \hbar = \frac{\hbar^2 k^2}{2m}, \quad k^2 = |\mathbf{k}|^2$$

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 |r|}$$

3.2.1 Phase and Group Velocity

The phase velocity v_φ describes how fast the phase of the wave moves forward. The group velocity v_g describes how fast the energy is moving forward.

$$v_\varphi = \frac{\omega}{k} \quad v_g = \frac{\partial \omega}{\partial k}$$

For a particle wave, the phase velocity v_φ is half the group velocity v_g

$$v_\varphi \cdot 2 = v_g$$

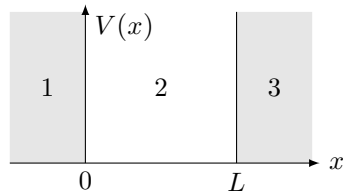
3.2.2 Stationary (Time independent) States

In a stationary state, the wave function is a product of a function $\varphi(\mathbf{x})$ independent of time and a function $\chi(t)$ independent of space.

$$\begin{aligned}\Psi_n(\mathbf{x}, t) &= \psi_n(\mathbf{x}) \cdot \chi_n(t) = \psi_n(\mathbf{x}) \cdot e^{-i \frac{E_n}{\hbar} t} \\ -\frac{\hbar^2}{2m} \nabla^2 \psi_n(\mathbf{x}) + V(\mathbf{x}) \psi_n(\mathbf{x}) &= \psi_n(\mathbf{x}) \cdot E_n \\ \iiint |\Psi|^2 d^3 \mathbf{x} &= \iiint |\psi|^2 d^3 \mathbf{x} = 1 \\ \Psi(\mathbf{x}, t) &= \sum a_n \psi_n(\mathbf{x}) \cdot e^{-i \frac{E_n}{\hbar} t} \quad \sum |a_n|^2 = 1\end{aligned}$$

Requirements: The wave function must be continuous, as well as its derivative

3.2.3 Example: 1D infinite potential well



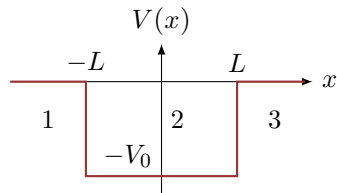
$$\begin{aligned}\Psi_1 = \Psi_3 &= 0 \\ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_2(x, t) &= E \psi_2(x, t) \\ \psi_2 &= A \sin(kx) + B \cos(kx)\end{aligned}$$

$$\text{Boundary cond.: } \psi_2(0) = \psi_2(L) = 0$$

$$\psi_{2n} = A \cdot \sin(k_n x) \quad \Psi_{2n} = A \cdot \sin(k_n x) \cdot e^{-i \frac{E_n}{\hbar} t}, \quad \text{Normalize: } A = \sqrt{\frac{2}{L}}$$

$$E_n = n^2 \cdot \frac{\hbar^2 \pi^2}{2mL} = n^2 \cdot E_0, \quad k_n = \frac{n\pi}{L}$$

3.2.4 Example: 1D finite potential well



The Energy E can be either bigger or smaller than 0. If $E > 0$, the wave function will decay exponentially in region 1 and 3. If $E < 0$, the wave will propagate away from the potential well.

Inside the well: The general solution to the rearranged Schrödinger's is:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_2(x) = (E - V_0) \psi_2(x)$$

$$\psi_2(x) = A_2 e^{ikx} + A'_2 e^{-ikx} \quad E = \frac{k^2 \hbar^2}{2m} \quad k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

Outside the well: There are two cases, which can apply:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_1(x) = E \psi_1(x)$$

1. $E > 0$: **Unbound state**

$$\psi_1 = A_1 e^{ikx} + A'_1 e^{-ikx} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

The unbound state does not make sense to be investigated, because the particle is free to be anywhere. In the following, only the unbound state is considered.

2. $E < 0$: **Bound state**

$$\psi_1 = B_1 e^{\delta x} + B'_1 e^{-\delta x} \quad \delta = \sqrt{-\frac{2mE}{\hbar^2}}$$

We see that as $x \rightarrow -\infty$, the Term B'_1 , as well as B_3 approaches ∞ . Since the wave function cannot approach ∞ , $B'_1 = B_3 = 0$ is a condition.

$$\psi = \begin{cases} \psi_1 = B_1 e^{\delta x} & x < -L \\ \psi_2 = A_2 e^{ikx} + A'_2 e^{-ikx} & -L < x < L \\ \psi_3 = B'_3 e^{-\delta x} & L < x \end{cases}$$

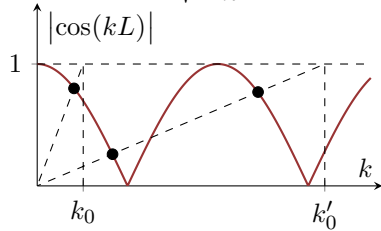
Boundary conditions: We require, that the wave function is continuous, as well as its spacial derivative. Therefore, we have:

$$\begin{aligned}\psi_1(-L) &= \psi_2(-L) & \psi_2(L) &= \psi_3(L) \\ \frac{\partial}{\partial x} \psi_1(-L) &= \frac{\partial}{\partial x} \psi_2(-L) & \frac{\partial}{\partial x} \psi_2(L) &= \frac{\partial}{\partial x} \psi_3(L)\end{aligned}$$

Even solutions: only even (cosine) components

$$|\cos(kL)| = \frac{k}{k_0}, \quad \tan(kL) > 0$$

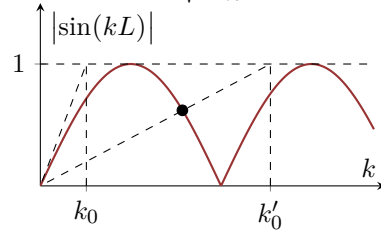
$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$$



Odd solutions: only odd (sine) components

$$|\sin(kL)| = \frac{k}{k_0}, \quad \tan(kL) > 0$$

$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$$



Applying the **initial conditions**, which require the wave function and its derivative to be continuous at $x = 0$, we get the following expression for A , B , C :

$$\psi_1(x=0) = \psi_2(x=0) \quad \frac{\partial}{\partial x} \psi_1(x=0) = \frac{\partial}{\partial x} \psi_2(x=0)$$

$E > V_0$

$$A + B = C$$

$$k_1(A - B) = k_2C$$

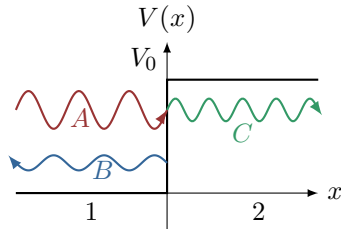
$E < V_0$

$$A + B = C$$

$$A = B$$

The **probability density function** $|\psi(x,t)|^2 = |\varphi(x)|^2 = \varphi \cdot \varphi^*$ can then be computed and sketched:

3.3 Example: 1D potential step function



An incoming plane wave from the left hits a potential step at $x = 0$. In region 1, two waves are added together, one is traveling to the right and one to the left. If $E > V_0$, the wave is transmitted to region 2. If $E < V_0$, the wave decays exponentially in region 2.

In **Region 1**, the general solution to the Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_1(x) = E\psi_1(x), \quad \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

In **Region 2**, there are two cases, which can apply:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_2 = (E - V_0)\psi_2(x)$$

1. **$E > V_0$: Transmission**

$$\psi_2 = Ce^{ik_2x}, \quad k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

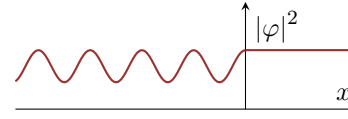
2. **$E < V_0$: Complete reflection**

$$\psi_2 = Ce^{\delta_2x}, \quad \delta_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$E > V_0$

$$|\psi_1|^2 = A^2 + B^2 + 2AB \cos(2k_1x)$$

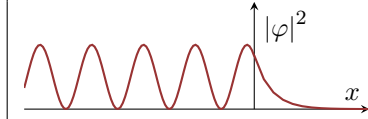
$$|\psi_2|^2 = C^2$$



$E < V_0$

$$|\psi_1|^2 = 2A^2 \cdot (1 - \sin(2k_1x))$$

$$|\psi_2|^2 = C^2 \cdot e^{-2\delta x}$$

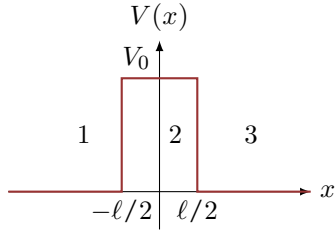


To find the **transmission coefficient** T and the **reflection coefficient** R , we normalize $A = 1$. Then, we can define $B = \sqrt{R}$ and $C = \sqrt{T}$. Then, we can solve for R and T :

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} \quad R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

If $E < V_0$, nothing is transmitted and therefore $T = 0$ and $R = 1$.

3.3.1 Example: 1D finite potential barrier



An incoming plane wave from the left hits a potential barrier with length l . The Transmission coefficient tells, how much of the wave can continue at the other side of the barrier (quantum tunneling).

In **Region 1 and 3**, the general expression for the wave equation is the following:

$$\psi_j(x) = A_j e^{ik_j x} + A'_j e^{-ik_j x}, \quad k_j = \sqrt{\frac{2mE}{\hbar^2}}, \quad j \in \{1, 3\}$$

In **Region 2**, the expression is depending on V_0 . There are two cases:

1. $E < V_0$: $\varphi_2 = B_2 e^{\delta_2 x} + B'_2 e^{-\delta_2 x}$, $\delta_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$
2. $E > V_0$: $\varphi_2 = A_2 e^{ik_2 x} + A'_2 e^{-ik_2 x}$, $k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$

Apply **boundary conditions** at $x = -\ell/2$ and $x = \ell/2$ in order to determine all constants. If the wave is only traveling from left to right, then $A'_3 = 0$.

$$\psi_1(-\ell/2) = \psi_2(-\ell/2), \quad \psi_2(\ell/2) = \psi_3(\ell/2)$$

$$\frac{\partial}{\partial x} \psi_1(-\ell/2) = \frac{\partial}{\partial x} \psi_2(-\ell/2), \quad \frac{\partial}{\partial x} \psi_2(\ell/2) = \frac{\partial}{\partial x} \psi_3(\ell/2)$$

Then, the **transmission coefficient** T and the **reflection coefficient** R can be calculated as following:

$$R = \left(\frac{A_1}{A'_1} \right)^2, \quad T = \left(\frac{A_3}{A_1} \right)^2$$

$$T = \frac{E < V_0}{4E(V_0 - E)} \quad \left| \quad T = \frac{E > V_0}{4E(V_0 - E) + V_0^2 \sin^2(k_2 \ell)} \right.$$

If $E > V_0$, the transmission coefficient has a maximum. If $k_2 \ell = n\pi \Rightarrow T = 1$ (**resonance**). The minimum of T is at: $k_2 \ell = \pi/2 + n\pi$.

4 Wave Function Space (Hilbert Space)

4.1 Inner Product

The inner product $\langle \psi_1 | \psi_2 \rangle$ is defined like the scalar product for vectors. If the inner product of two wave functions is 0, those two wave functions are **orthogonal**.

$$\langle \psi_1 | \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_1^*(\mathbf{x}, t) \psi_2(\mathbf{x}, t) d^3 \mathbf{x}$$

$$\langle \psi | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t) d^3 \mathbf{x} = \int_{-\infty}^{\infty} |\psi(\mathbf{x}, t)|^2 d^3 \mathbf{x} = 1$$

4.2 Fourier Transform

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \varphi(p) dp, \quad \varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \psi(x) dx$$

$$\psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} e^{\frac{i\vec{p}\vec{x}}{\hbar}} \varphi(\vec{p}) d\vec{p}, \quad \varphi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} e^{\frac{i\vec{p}\vec{x}}{\hbar}} \psi(\vec{x}) d\vec{x}$$

$$\int_{-\infty}^{\infty} \psi_1^*(x) \cdot \psi_2(x) \cdot dx = \int_{-\infty}^{\infty} \varphi_1^*(p) \cdot \varphi_2(p) \cdot dp$$

5 Observable Measurements, Time-dependence

Doing a measurement in quantum mechanics (observable) can be interpreted as applying an operator \hat{A} on the wave function $\psi(\mathbf{x}, t)$. For example, to compute the expected position $\langle \mathbf{x} \rangle_\psi$, we apply the operator $\hat{\mathbf{x}} = \mathbf{x}$ to average the wave function:

$$\langle \mathbf{x} \rangle_\Psi = \iiint \Psi^*(\mathbf{x}, t) \cdot \mathbf{x} \cdot \Psi(\mathbf{x}, t) d^3 \mathbf{x} = \iiint \mathbf{x} \cdot |\Psi(\mathbf{x}, t)|^2 d^3 \mathbf{x}$$

Name	Operator
Position	$\hat{\mathbf{x}} = [\mathbf{x}]$
Momentum	$\hat{\mathbf{p}} = [-i\hbar \nabla]$
Hamiltonian	$\hat{H} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right]$

$$\nabla = \left[\frac{\partial}{\partial x} \quad \frac{\partial}{\partial y} \quad \frac{\partial}{\partial z} \right]^T$$

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

5.1 Eigenstates and Eigenvalues

An Observable has an Operator \hat{A} . a state $u_n(x)$ is called an eigenstate the operator applied on the wave function acts like a scalar multiplication to it. Then, the measurement of the general state $\psi(x)$ is a superposition of all the eigenstates.

$$\hat{A}u_n(x) = a_n u_n(x), \quad \int_{-\infty}^{\infty} u_n^*(x) \hat{A}u_n(x) dx = a_n$$

$$\hat{A}\psi(x) = \sum_n c_n u_n(x)$$

5.2 Harmonic Oscillator

A Quantum mechanical harmonic oscillator can be interpreted as the solution to the Schrödinger equation:

$$\left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E \psi(x), \quad V(x) = \frac{1}{2} k x^2 = \frac{m\omega^2}{2} x^2$$

To simplify the equation, we define a new length scale and energy:

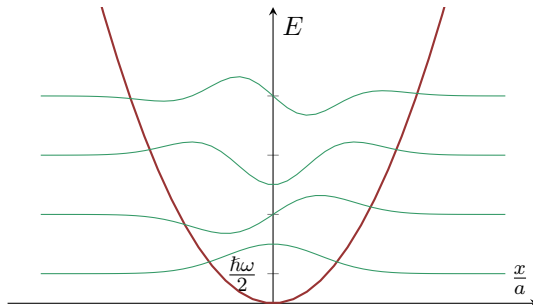
$$a = \sqrt{\frac{\hbar}{m\omega}}, \quad \tilde{x} = \frac{x}{a}, \quad \tilde{E} = \frac{E}{\hbar\omega} \Rightarrow \frac{1}{2} \left[-\frac{\partial^2}{\partial \tilde{x}^2} + \tilde{x}^2 \right] \varphi(\tilde{x}) = \tilde{E} \varphi(\tilde{x})$$

Then, the solutions to the equation is:

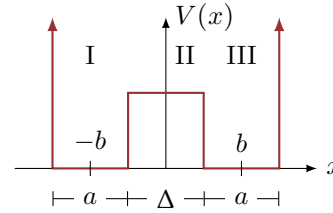
$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega, \quad \psi(\tilde{x}) = c_n H_n(\tilde{x}) e^{-\tilde{x}^2/2}, \quad H_n(\tilde{x}) = (-1)^n e^{\tilde{x}^2} \cdot \frac{\partial^n}{\partial \tilde{x}^n} e^{-\tilde{x}^2}$$

$$H_0(\tilde{x}) = 1, \quad H_1(\tilde{x}) = 2\tilde{x}, \quad H_2(\tilde{x}) = 4\tilde{x}^2 - 2, \quad H_3(\tilde{x}) = 8\tilde{x}^3 - 12\tilde{x}$$

$$\Psi_n(x) = \frac{1}{\sqrt[4]{\pi} \sqrt{2^n n!} a} \cdot H_n\left(\frac{x}{a}\right) e^{-\frac{x^2}{2a^2}}$$



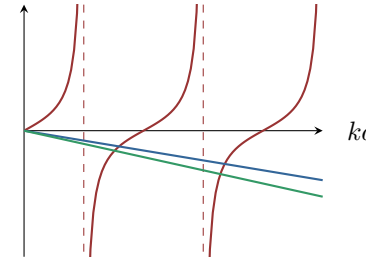
5.3 The coupled quantum well



This is the simplified potential of an ammonia molecule NH_3 . The wave function outside the well ($|x| > b + \frac{a}{2}$) is zero. There exists a symmetric, as well as an antisymmetric solution. We consider the case: $E < V_0$

$$\psi_{\text{II}} = \begin{cases} \mu \cosh(\delta x) & \text{symmetric} \\ \mu \sinh(\delta x) & \text{antisymmetric} \end{cases} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad \delta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$\tan(ka)$



$$\text{symmetric: } \varepsilon_s = \frac{1 + e^{-\delta\Delta}}{\delta a}$$

$$\text{antisymmetric: } \varepsilon_a = \frac{1 - e^{-\delta\Delta}}{\delta a}$$

$$\tan(ka) = -ka\varepsilon = -ka \frac{1 \pm e^{-\delta\Delta}}{\delta a}$$

Now, we can create a superposition of both the symmetric and the antisymmetric case:

$$\psi_{s\text{I}} = +\lambda \sin\left(k\left(b - \frac{a}{2} + x\right)\right), \quad \psi_{s\text{III}} = +\lambda \sin\left(k\left(b - \frac{a}{2} + x\right)\right)$$

$$\psi_{a\text{I}} = -\lambda \sin\left(k\left(b - \frac{a}{2} + x\right)\right), \quad \psi_{a\text{III}} = +\lambda \sin\left(k\left(b - \frac{a}{2} + x\right)\right)$$

$$\Psi_L = \frac{1}{\sqrt{2}}(\Psi_s - \Psi_a), \quad \Psi_R = \frac{1}{\sqrt{2}}(\Psi_s + \Psi_a)$$

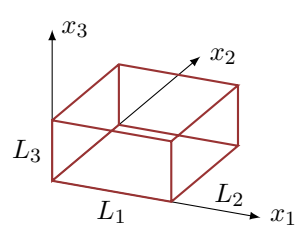
$$\Psi_L(x, t) = \frac{1}{\sqrt{2}} e^{-i\omega_s t} \left(\psi_s(x) - e^{-i(\omega_a - \omega_s)t} \psi_a(x) \right)$$

$$\omega_a = \frac{E_a}{\hbar}, \quad \omega_s = \frac{E_s}{\hbar}, \quad E_a - E_s = \frac{\hbar^2 \pi^2}{2m\delta a^2} \cdot 8e^{-\delta\Delta}$$

From the formula describing the wave equation, we can see that at t_0 , the particle can only be found in region I, and after some time $t_{1/2}$, the particle can only be found in region III. The particle has tunneled from one side to the other. Now, we can define a period T :

$$T = \frac{2\pi\hbar}{E_a - E_s}$$

6 Schrödinger Equation in 3D



$$V(x_i) = \begin{cases} 0 & \text{if } 0 < x_i < L_i \\ \infty & \text{otherwise} \end{cases}$$

$$V(x, y, z) = V(x_1) + V(x_2) + V(x_3)$$

$$\psi(x_1, x_2, x_3) = \psi_1(x_1) \cdot \psi_2(x_2) \cdot \psi_3(x_3)$$

$$-\frac{\hbar^2}{2m} \left[\frac{\psi_1''(x_1)}{\psi_1(x_1)} + \frac{\psi_2''(x_2)}{\psi_2(x_2)} + \frac{\psi_3''(x_3)}{\psi_3(x_3)} \right] + V(x_1) + V(x_2) + V(x_3) = E$$

This equation can be separated into three smaller equations for every spatial dimension x_i

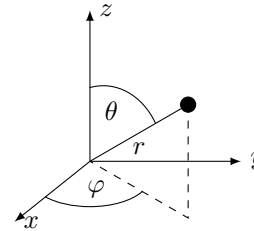
$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} \psi_i(x_i) + V(x_i) \psi_i(x_i) = E_i \psi_i(x_i)$$

$$E_i^{(n_i)} = n_i^2 \frac{\hbar^2 \pi^2}{2m L_i^2}, \quad \psi_i^{(n_i)} = A \cdot \sin\left(\frac{\pi n_i x}{L_i}\right)$$

After normalizing, the wave function can be written as:

$$\psi(x_1, x_2, x_3) = \sqrt{\frac{8}{L_1 L_2 L_3}} \sin\left(\frac{\pi n_1 x_1}{L_1}\right) \sin\left(\frac{\pi n_2 x_2}{L_2}\right) \sin\left(\frac{\pi n_3 x_3}{L_3}\right)$$

6.1 Schrödinger Equation in spherical coordinates



$$x = r \sin \theta \cos \varphi$$

$$y = r \sin \theta \sin \varphi$$

$$z = r \cos \theta$$

To use the Schrödinger equation, we must define the Laplacian operator ∇^2 :

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

7 Useful formulas

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad \int_0^{\infty} x e^{-ax^2} dx = \frac{1}{2a} \quad \int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}}$$

$$\text{Gaussian: } G = A \cdot e^{-\frac{x^2}{2\sigma^2}}$$

7.1 Trigonometry

$$\sin \beta = \frac{b}{a} = \frac{\text{Gegenkathete}}{\text{Hypotenuse}} \quad \cos \beta = \frac{c}{a} = \frac{\text{Ankathete}}{\text{Hypotenuse}}$$

$$\tan \beta = \frac{c}{b} = \frac{\text{Gegenkathete}}{\text{Ankathete}} \quad \cot \beta = \frac{c}{b} = \frac{\text{Ankathete}}{\text{Gegenkathete}}$$

$$\cos(a + k \cdot 2\pi) = \cos(a) \quad \sin(a + k \cdot 2\pi) = \sin(a) \quad (k \in \mathbb{Z})$$

$$\sin(a \pm b) = \sin(a) \cdot \cos(b) \pm \cos(a) \cdot \sin(b)$$

$$\cos(a \pm b) = \cos(a) \cdot \cos(b) \mp \sin(a) \cdot \sin(b)$$

$$\tan(a \pm b) = \frac{\tan(a) \pm \tan(b)}{1 \mp \tan(a) \cdot \tan(b)}$$

$$\sin(2a) = 2 \sin(a) \cos(a)$$

$$\cos(2a) = \cos^2(a) - \sin^2(a) = 2 \cos^2(a) - 1 = 1 - 2 \sin^2(a)$$

$$c^2 = a^2 + b^2 - 2 \cdot a \cdot b \cdot \cos \gamma$$

$$\frac{a}{\sin \alpha} = \frac{b}{\sin \beta} = \frac{c}{\sin \gamma} = 2r = \frac{u}{\pi}$$

$$\sin(a) \sin(b) = \frac{1}{2} (\cos(a-b) - \cos(a+b))$$

$$\cos(a) \cos(b) = \frac{1}{2} (\cos(a-b) + \cos(a+b))$$

$$\sin(a) \cos(b) = \frac{1}{2}(\sin(a-b) + \sin(a+b))$$

$$\cos^2\left(\frac{a}{2}\right) = \frac{1+\cos(a)}{2} \quad \sin^2\left(\frac{a}{2}\right) = \frac{1-\cos(a)}{2}$$

$$\sin(a) + \sin(b) = 2 \cdot \sin\left(\frac{a+b}{2}\right) \cdot \cos\left(\frac{a-b}{2}\right)$$

$$\sin(a) - \sin(b) = 2 \cdot \sin\left(\frac{a-b}{2}\right) \cdot \cos\left(\frac{a+b}{2}\right)$$

$$\cos(a) + \cos(b) = 2 \cdot \cos\left(\frac{a+b}{2}\right) \cdot \cos\left(\frac{a-b}{2}\right)$$

$$\cos(a) - \cos(b) = -2 \cdot \sin\left(\frac{a+b}{2}\right) \cdot \sin\left(\frac{a-b}{2}\right)$$

$$\tan(a) \pm \tan(b) = \frac{\sin(a \pm b)}{\cos(a) \cos(b)}$$

$$\sin(x) = \frac{1}{2j} \left(e^{jx} - e^{-jx} \right) \quad \cos(x) = \frac{1}{2} \left(e^{jx} + e^{-jx} \right)$$

$$e^{x+jy} = e^x \cdot e^{jy} = e^x \cdot (\cos(y) + j \sin(y))$$

$$e^{j\pi} = e^{-j\pi} = -1$$

8 Periodic Table of the Elements

2.20 H Hydrogen 1.00784– 1.00811																		2 He Helium 4.002602(2)	1s																
3 0.98 Li Lithium 6.938–6.997	2s	4 1.57 Be Beryllium 9.0121831(5)	2s	<div><div>Zenegss</div><div>Sy</div><div>Name</div><div>saw</div></div> <div>Z = atomic number; eneg = electronegativity; ss = subshell; Sy = Symbol, Name = element name, saw = standard atomic weight</div>																5 2.04 B Boron 10.806–10.821	2p	6 2.55 C Carbon 12.0096– 12.0116	2p	7 3.04 N Nitrogen 14.00643– 14.00728	2p	8 3.44 O Oxygen 15.99903– 15.99977	2p	9 3.98 F Fluorine 18.998403163(6)	2p	10 Ne Neon 20.1797(6)	2p				
11 0.93 Na Sodium 22.98976928(2)	3s	12 1.31 Mg Magnesium 24.304–24.307	3s																	13 1.61 Al Aluminium 26.9815385(7)	3p	14 1.90 Si Silicon 28.084–28.086	3p	15 2.19 P Phosphorus 30.973761998(5)	3p	16 2.58 S Sulphur 32.059–32.076	3p	17 3.16 Cl Chlorine 35.446–35.457	3p	18 Ar Argon 39.948(1)	3p				
19 0.82 K Potassium 39.0983(1)	4s	20 1.00 Ca Calcium 40.078(4)	4s	21 1.36 Sc Scandium 44.955908(5)	3d	22 1.54 Ti Titanium 47.867(1)	3d	23 1.63 V Vanadium 50.9415(1)	3d	24 1.66 3d* Cr Chromium 51.9961(6)	3d	25 1.55 Mn Manganese 54.938044(3)	3d	26 1.83 Fe Iron 55.845(2)	3d	27 1.88 Co Cobalt 58.933194(4)	3d	28 1.91 Ni Nickel 58.6934(4)	3d	29 1.90 3d* Cu Copper 63.546(3)	3d	30 1.65 Zn Zinc 65.38(2)	3d	31 1.81 Ga Gallium 69.723(1)	4p	32 2.01 Ge Germanium 72.630(8)	4p	33 2.18 As Arsenic 74.921595(6)	4p	34 2.55 Se Selenium 78.971(8)	4p	35 2.96 Br Bromine 79.901–79.907	4p	36 3.00 Kr Krypton 83.798(2)	4p
37 0.82 Rb Rubidium 85.4678(3)	5s	38 0.95 Sr Strontium 87.62(1)	5s	39 1.22 Y Yttrium 88.90584(2)	4d	40 1.33 Zr Zirconium 91.224(2)	4d	41 1.6 4d* Nb Niobium 92.90637(2)	4d	42 2.16 4d* Mo Molybdenum 95.95(1)	4d	43 1.9 4d Tc Technetium (98)	4d	44 2.2 4d* Ru Ruthenium 101.07(2)	4d	45 2.28 4d* Rh Rhodium 102.90550(2)	4d	46 2.20 4d* Pd Palladium 106.42(1)	4d	47 1.93 4d* Ag Silver 107.8682(2)	4d	48 1.69 Cd Cadmium 112.414(4)	4d	49 1.78 In Indium 114.818(1)	5p	50 1.96 Sn Tin 118.710(7)	5p	51 2.05 Sb Antimony 121.760(1)	5p	52 2.1 5p Te Tellurium 127.60(3)	5p	53 2.66 I Iodine 126.90447(3)	5p	54 2.60 Xe Xenon 131.293(6)	5p
55 0.79 Cs Cesium 132.90545196(6)	6s	56 0.89 Ba Barium 137.327(7)	6s	57–71 * Lanthanides	72 1.3 5d Hf Hafnium 178.49(2)	5d	73 1.5 5d Ta Tantalum 180.94788(2)	5d	74 2.36 5d W Tungsten 183.84(1)	5d	75 1.9 5d Re Rhenium 186.207(1)	5d	76 2.2 5d Os Osmium 190.23(3)	5d	77 2.20 5d Ir Iridium 192.227(3)	5d	78 2.28 5d* Pt Platinum 195.084(9)	5d	79 2.54 5d* Au Gold 196.966569(5)	5d	80 2.00 5d Hg Mercury 200.592(3)	5d	81 1.62 6p Tl Thallium 204.382– 204.385	6p	82 1.87 Pb Lead 207.2(1)	6p	83 2.02 6p Bi Bismuth 208.98040(1)	6p	84 2.0 6p Po Polonium (209)	6p	85 2.2 6p At Astatine (210)	6p	86 2.2 6p Rn Radon (222)	6p	
87 0.7 7s Fr Francium (223)	7s	88 0.9 7s Ra Radium (226)	7s	89–103 ** Actinides	104 Rf Rutherfordium (261)	6d	105 Db Dubnium (268)	6d	106 Sg Seaborgium (269)	6d	107 Bh Bohrium (270)	6d	108 Hs Hassium (269)	6d	109 Mt Meitnerium (278)	6d	110 Ds Darmstadtium (281)	6d	111 Rg Roentgenium (282)	6d	112 Cn Copernicium (285)	6d	113 Nh Nihonium (286)	7p	114 Fl Flerovium (289)	7p	115 Mc Moscovium (289)	7p	116 Lv Livermorium (293)	7p	117 Ts Tennessine (294)	7p	118 Og Oganesson (294)	7p	
* **				57 1.1 5d* La Lanthanum 138.90547(7)	58 1.12 4f* Ce Cerium 140.116(1)	59 1.13 4f Pr Praseodymium 140.90766(2)	60 1.14 4f Nd Neodymium 144.242(3)	61 1.13 4f Pm Promethium (145)	62 1.17 4f Sm Samarium 150.36(2)	63 1.2 4f Eu Europium 151.964(1)	64 1.2 4f* Gd Gadolinium 157.25(3)	65 1.1 4f Tb Terbium 158.92535(2)	66 1.22 4f Dy Dysprosium 162.500(1)	67 1.23 4f Ho Holmium 164.93033(2)	68 1.24 4f Er Erbium 167.259(3)	69 1.25 4f Tm Thulium 168.93422(2)	70 1.1 4f Yb Ytterbium 173.045(10)	71 1.27 4f Lu Lutetium 174.9668(1)	89 1.1 6d* Ac Actinium (227)	90 1.3 5f* Th Thorium 232.0377(4)	91 1.5 5f* Pa Protactinium 231.03588(2)	92 1.38 5f* U Uranium 238.02891(3)	93 1.36 5f* Np Neptunium (237)	94 1.28 5f Pu Plutonium (244)	95 1.13 5f Am Americium (243)	96 1.28 5f* Cm Curium (247)	97 1.3 5f Bk Berkelium (247)	98 1.3 5f Cf Californium (251)	99 1.3 5f Es Einsteinium (252)	100 1.3 5f Fm Fermium (257)	101 1.3 5f Md Mendelevium (258)	102 1.3 5f No Nobelium (259)	103 1.3 5f Lr Lawrencium (266)		

Standard atomic weights taken from the Commission on Isotopic Abundances and Atomic Weights (ciaaw.org/atomic-weights.htm). Adapted from Ivan Griffin's L^AT_EX Periodic Table. © 2017 Paul Danese

An asterisk (*) next to a subshell indicates an anomalous (Aufbau rule-breaking) ground state electron configuration.