

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

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

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

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

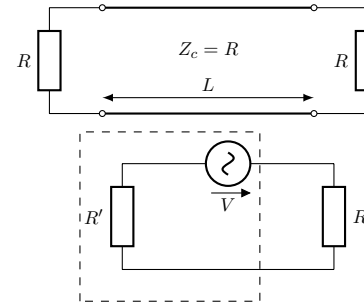
$$u(\omega) = \frac{\omega^2}{\pi^2 c^3} \cdot \frac{\hbar \omega}{\exp\left(\frac{\hbar \omega}{kT}\right) - 1} d\omega \quad u(\nu) = \frac{8\pi h \nu^3}{c^3 \left(\exp\left(\frac{h\nu}{kT}\right) - 1\right)} d\nu$$

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

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).

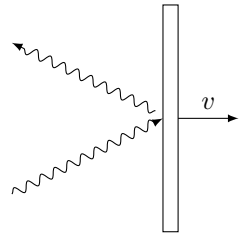


$\langle V^2 \rangle$	Noise Voltage
$\Delta\nu$	Bandwidth

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

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

1.5 Momentum of a photon



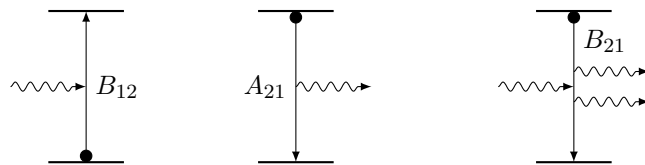
$$p \left[\frac{\text{kg m}}{\text{s}} \right] \quad \text{momentum}$$

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

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

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

1.6 Absorption, spontaneous and stimulated emission



absorption spontaneous emission stimulated emission

n_1 Number of electrons in the lower energy state

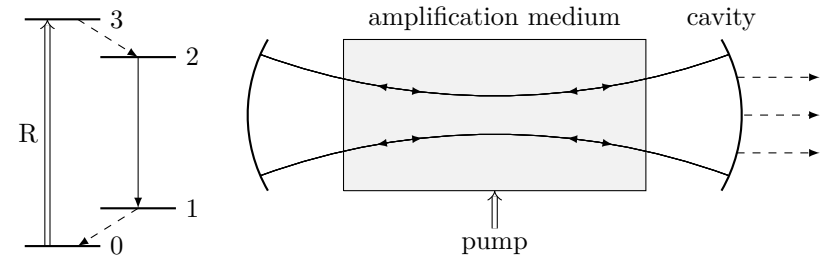
n_2 Number of electrons in the higher energy state

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

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

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

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:

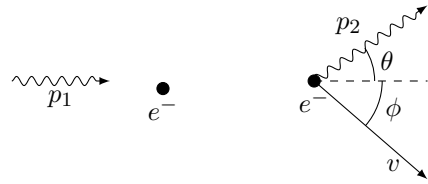
$$n_2 = \frac{R}{A_{21}} \quad \text{whereas} \quad n_1 \approx 0 \quad \text{because} \quad A_{21} < \frac{1}{\tau_1}$$

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

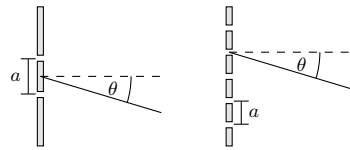


$$p_1 = \frac{h\nu_1}{c} \quad p' = \frac{h\nu_2}{c}$$

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

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

2.2 Double Slit and Bragg Diffraction

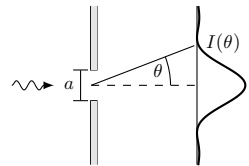


Constructive $\sin \theta = \frac{n\lambda}{a}$

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	$\int_{\text{length}} p \cdot ds = n \cdot h \quad n \in \mathbb{N}$
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

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

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

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

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

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

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

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

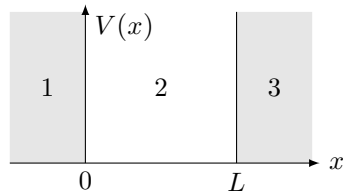
3.2.2 Stationary (Time independent) States

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

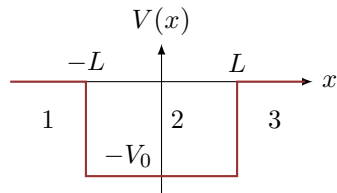


$$\begin{aligned}\Psi_1 = \Psi_3 &= 0 \\ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_2(x, t) &= E \psi_2(x, t) \\ \psi_2 &= A \sin(kx) + B \cos(kx)\end{aligned}$$

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

$$\begin{aligned}\psi_{2n} &= A \cdot \sin(k_n x) \quad \Psi_{2n} = A \cdot \sin(k_n x) \cdot e^{-i \frac{E_n}{\hbar} t}, \quad \text{Normalize: } A = \sqrt{\frac{2}{L}} \\ E_n &= n^2 \cdot \frac{\hbar^2 \pi^2}{2mL} = n^2 \cdot E_0, \quad k_n = \frac{n\pi}{L}\end{aligned}$$

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:

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

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.

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

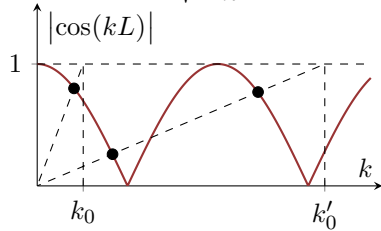
Boundary conditions: We require, that the wave function is continuous, as well as its spacial derivative. Therefore, we have:

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

Even solutions: only even (cosine) components

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

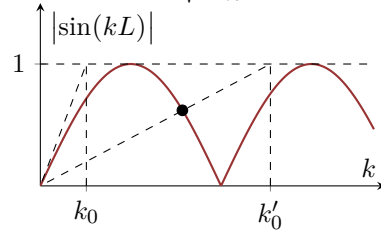
$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$$



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 :

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

$E > V_0$

$$A + B = C$$

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

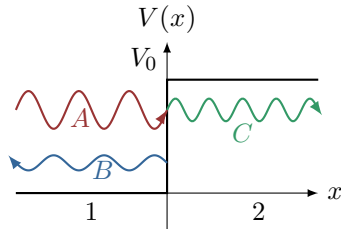
$E < V_0$

$$A + B = C$$

$$A = B$$

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**

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

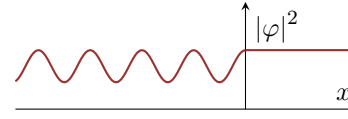
2. **$E < V_0$: Complete reflection**

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

$E > V_0$

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

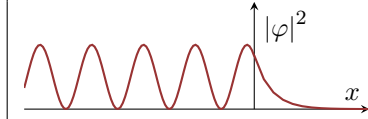
$$|\psi_2|^2 = C^2$$



$E < V_0$

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

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

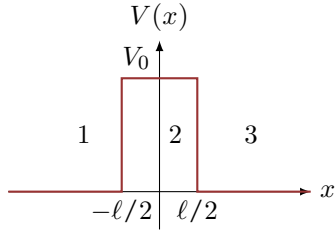


To find the **transmission coefficient** T and the **reflection coefficient** R , we normalize $A = 1$. Then, we can define $B = \sqrt{R}$ and $C = \sqrt{T}$. Then, we can solve for R and T :

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

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:

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

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 $A'_3 = 0$.

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

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

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

$$T = \frac{\mathbf{E} < \mathbf{V_0}}{4E(V_0 - E) + V_0^2 \sinh^2(\delta_2 \ell)} \quad \left| \quad T = \frac{\mathbf{E} > \mathbf{V_0}}{4E(V_0 - E) + V_0^2 \sin^2(k_2 \ell)} \right.$$

If $\mathbf{E} > \mathbf{V_0}$, 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

$$\begin{aligned} \psi(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \varphi(p) dp, \quad \varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \psi(x) dx \\ \psi(\vec{x}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} e^{\frac{i\vec{p}\vec{x}}{\hbar}} \varphi(\vec{p}) d\vec{p}, \quad \varphi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} e^{\frac{i\vec{p}\vec{x}}{\hbar}} \psi(\vec{x}) d\vec{x} \\ \int_{-\infty}^{\infty} \psi_1^*(x) \cdot \psi_2(x) \cdot dx &= \int_{-\infty}^{\infty} \varphi_1^*(p) \cdot \varphi_2(p) \cdot dp \end{aligned}$$

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:

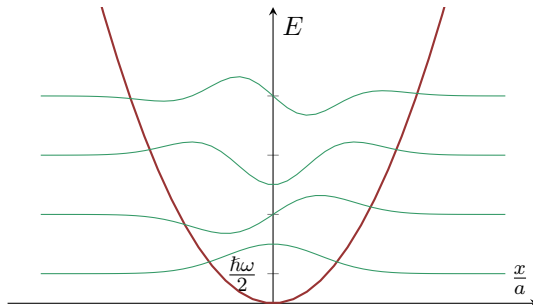
$$a = \sqrt{\frac{\hbar}{m\omega}}, \quad \tilde{x} = \frac{x}{a}, \quad \tilde{E} = \frac{E}{\hbar\omega} \Rightarrow \frac{1}{2} \left[-\frac{\partial^2}{\partial \tilde{x}^2} + \tilde{x}^2 \right] \varphi(\tilde{x}) = \tilde{E} \varphi(\tilde{x})$$

Then, the solutions to the equation is:

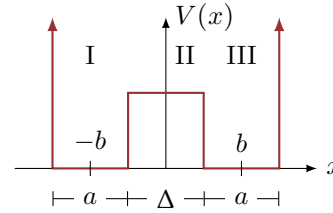
$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega, \quad \psi(\tilde{x}) = c_n H_n(\tilde{x}) e^{-\tilde{x}^2/2}, \quad H_n(\tilde{x}) = (-1)^n e^{\tilde{x}^2} \cdot \frac{\partial^n}{\partial \tilde{x}^n} e^{-\tilde{x}^2}$$

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

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



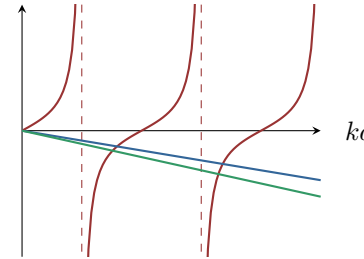
5.3 The coupled quantum well



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:

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

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

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

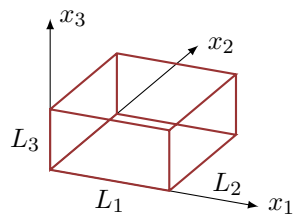
$$\Psi_L(x, t) = \frac{1}{\sqrt{2}} e^{-i\omega_s t} \left(\psi_s(x) - e^{-i(\omega_a - \omega_s)t} \psi_a(x) \right)$$

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

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 spacial dimension x_i

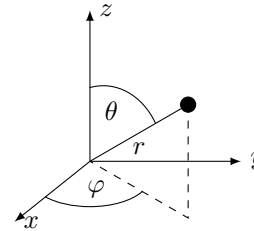
$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} \psi_i(x_i) + V(x_i) \psi_i(x_i) = E_i \psi_i(x_i)$$

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

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

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

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

1 <div>2.20</div> <div>H</div> <div>Hydrogen</div> <div>1.00784–1.00811</div>	2 <div>4.00</div> <div>He</div> <div>Helium</div> <div>4.002602(2)</div>																
3 <div>0.98</div> <div>Li</div> <div>Lithium</div> <div>6.938–6.997</div>	4 <div>1.57</div> <div>Be</div> <div>Beryllium</div> <div>9.0121831(5)</div>	<div> <div>Z</div> <div>eneg</div> <div>ss</div> </div> <div> <div>Sy</div> <div>Name</div> <div>saw</div> </div> <div> <div>Z = atomic number; eneg = electronegativity; ss = subshell;</div> <div>Sy = Symbol, Name = element name, saw = standard atomic weight</div> </div>	5 <div>2.04</div> <div>B</div> <div>Boron</div> <div>10.806–10.821</div>	6 <div>2.55</div> <div>C</div> <div>Carbon</div> <div>12.0096–12.0116</div>	7 <div>3.04</div> <div>N</div> <div>Nitrogen</div> <div>14.00643–14.00728</div>	8 <div>3.44</div> <div>O</div> <div>Oxygen</div> <div>15.99903–15.99977</div>	9 <div>3.98</div> <div>F</div> <div>Fluorine</div> <div>18.998403163(6)</div>	10 <div>19.99</div> <div>Ne</div> <div>Neon</div> <div>20.1797(6)</div>									
11 <div>0.93</div> <div>Na</div> <div>Sodium</div> <div>22.98976928(2)</div>	12 <div>1.31</div> <div>Mg</div> <div>Magnesium</div> <div>24.304–24.307</div>		13 <div>1.61</div> <div>Al</div> <div>Aluminium</div> <div>26.9815385(7)</div>	14 <div>1.90</div> <div>Si</div> <div>Silicon</div> <div>28.084–28.086</div>	15 <div>2.19</div> <div>P</div> <div>Phosphorus</div> <div>30.973761998(5)</div>	16 <div>2.58</div> <div>S</div> <div>Sulphur</div> <div>32.059–32.076</div>	17 <div>3.16</div> <div>Cl</div> <div>Chlorine</div> <div>35.446–35.457</div>	18 <div>39.96</div> <div>Ar</div> <div>Argon</div> <div>39.948(1)</div>									
19 <div>0.82</div> <div>K</div> <div>Potassium</div> <div>39.0983(1)</div>	20 <div>1.00</div> <div>Ca</div> <div>Calcium</div> <div>40.078(4)</div>	21 <div>1.36</div> <div>Sc</div> <div>Scandium</div> <div>44.955908(5)</div>	22 <div>1.54</div> <div>Ti</div> <div>Titanium</div> <div>47.867(1)</div>	23 <div>1.63</div> <div>V</div> <div>Vanadium</div> <div>50.9415(1)</div>	24 <div>1.66</div> <div>Cr</div> <div>Chromium</div> <div>51.9961(6)</div>	25 <div>1.55</div> <div>Mn</div> <div>Manganese</div> <div>54.938044(3)</div>	26 <div>1.83</div> <div>Fe</div> <div>Iron</div> <div>55.845(2)</div>	27 <div>1.88</div> <div>Co</div> <div>Cobalt</div> <div>58.933194(4)</div>	28 <div>1.91</div> <div>Ni</div> <div>Nickel</div> <div>58.6934(4)</div>	29 <div>1.90</div> <div>Cu</div> <div>Copper</div> <div>63.546(3)</div>	30 <div>1.65</div> <div>Zn</div> <div>Zinc</div> <div>65.38(2)</div>	31 <div>1.81</div> <div>Ga</div> <div>Gallium</div> <div>69.723(1)</div>	32 <div>2.01</div> <div>Ge</div> <div>Germanium</div> <div>72.630(8)</div>	33 <div>2.18</div> <div>As</div> <div>Arsenic</div> <div>74.921595(6)</div>	34 <div>2.55</div> <div>Se</div> <div>Selenium</div> <div>78.971(8)</div>	35 <div>2.96</div> <div>Br</div> <div>Bromine</div> <div>79.901–79.907</div>	36 <div>3.00</div> <div>Kr</div> <div>Krypton</div> <div>83.798(2)</div>
37 <div>0.82</div> <div>Rb</div> <div>Rubidium</div> <div>85.4678(3)</div>	38 <div>0.95</div> <div>Sr</div> <div>Strontium</div> <div>87.62(1)</div>	39 <div>1.22</div> <div>Y</div> <div>Yttrium</div> <div>88.90584(2)</div>	40 <div>1.33</div> <div>Zr</div> <div>Zirconium</div> <div>91.224(2)</div>	41 <div>1.6</div> <div>Nb</div> <div>Niobium</div> <div>92.90637(2)</div>	42 <div>2.16</div> <div>Mo</div> <div>Molybdenum</div> <div>95.95(1)</div>	43 <div>1.9</div> <div>Tc</div> <div>Technetium</div> <div>(98)</div>	44 <div>2.2</div> <div>Ru</div> <div>Ruthenium</div> <div>101.07(2)</div>	45 <div>2.28</div> <div>Rh</div> <div>Rhodium</div> <div>102.90550(2)</div>	46 <div>2.20</div> <div>Pd</div> <div>Palladium</div> <div>106.42(1)</div>	47 <div>1.93</div> <div>Ag</div> <div>Silver</div> <div>107.8682(2)</div>	48 <div>1.69</div> <div>Cd</div> <div>Cadmium</div> <div>112.414(4)</div>	49 <div>1.78</div> <div>In</div> <div>Indium</div> <div>114.818(1)</div>	50 <div>1.96</div> <div>Sn</div> <div>Tin</div> <div>118.710(7)</div>	51 <div>2.05</div> <div>Sb</div> <div>Antimony</div> <div>121.760(1)</div>	52 <div>2.1</div> <div>Te</div> <div>Tellurium</div> <div>127.60(3)</div>	53 <div>2.66</div> <div>I</div> <div>Iodine</div> <div>126.90447(3)</div>	54 <div>2.60</div> <div>Xe</div> <div>Xenon</div> <div>131.293(6)</div>
55 <div>0.79</div> <div>Cs</div> <div>Cesium</div> <div>132.90545196(6)</div>	56 <div>0.89</div> <div>Ba</div> <div>Barium</div> <div>137.327(7)</div>	57–71 <div>1.05</div> <div>*</div> <div>Lanthanides</div>	72 <div>1.3</div> <div>Hf</div> <div>Hafnium</div> <div>178.49(2)</div>	73 <div>1.5</div> <div>Ta</div> <div>Tantalum</div> <div>180.94788(2)</div>	74 <div>2.36</div> <div>W</div> <div>Tungsten</div> <div>183.84(1)</div>	75 <div>1.9</div> <div>Re</div> <div>Rhenium</div> <div>186.207(1)</div>	76 <div>2.2</div> <div>Os</div> <div>Osmium</div> <div>190.23(3)</div>	77 <div>2.20</div> <div>Ir</div> <div>Iridium</div> <div>192.217(3)</div>	78 <div>2.28</div> <div>Pt</div> <div>Platinum</div> <div>195.084(9)</div>	79 <div>2.54</div> <div>Au</div> <div>Gold</div> <div>196.966569(5)</div>	80 <div>2.00</div> <div>Hg</div> <div>Mercury</div> <div>200.592(3)</div>	81 <div>1.62</div> <div>Tl</div> <div>Thallium</div> <div>204.382–204.385</div>	82 <div>1.87</div> <div>Pb</div> <div>Lead</div> <div>207.2(1)</div>	83 <div>2.02</div> <div>Bi</div> <div>Bismuth</div> <div>208.98040(1)</div>	84 <div>2.0</div> <div>Po</div> <div>Polonium</div> <div>(209)</div>	85 <div>2.2</div> <div>At</div> <div>Astatine</div> <div>(210)</div>	86 <div>2.2</div> <div>Rn</div> <div>Radon</div> <div>(222)</div>
87 <div>0.7</div> <div>Fr</div> <div>Francium</div> <div>(223)</div>	88 <div>0.9</div> <div>Ra</div> <div>Radium</div> <div>(226)</div>	89–103 <div>1.0</div> <div>**</div> <div>Actinides</div>	104 <div>1.3</div> <div>Rf</div> <div>Rutherfordium</div> <div>(261)</div>	105 <div>1.6</div> <div>Db</div> <div>Dubnium</div> <div>(268)</div>	106 <div>2.3</div> <div>Sg</div> <div>Seaborgium</div> <div>(269)</div>	107 <div>2.6</div> <div>Bh</div> <div>Bohrium</div> <div>(270)</div>	108 <div>2.7</div> <div>Hs</div> <div>Hassium</div> <div>(269)</div>	109 <div>2.7</div> <div>Mt</div> <div>Meitnerium</div> <div>(278)</div>	110 <div>2.7</div> <div>Ds</div> <div>Darmstadtium</div> <div>(281)</div>	111 <div>2.7</div> <div>Rg</div> <div>Roentgenium</div> <div>(282)</div>	112 <div>2.7</div> <div>Cn</div> <div>Copernicium</div> <div>(285)</div>	113 <div>1.7</div> <div>Nh</div> <div>Nihonium</div> <div>(286)</div>	114 <div>1.7</div> <div>Fl</div> <div>Flerovium</div> <div>(289)</div>	115 <div>1.7</div> <div>Mc</</div>			

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