

1 The Photon

$$\begin{aligned}
 c &= 2.998 \cdot 10^8 \left[\frac{\text{m}}{\text{s}} \right] \quad \mathbf{C} & \epsilon_0 &= 8.854 \cdot 10^{-12} \left[\frac{\text{F}}{\text{m}} \right] \\
 h &= 6.626 \cdot 10^{-34} \left[\frac{\text{m}^2 \text{kg}}{\text{s}} \right] \quad \mathbf{A} & \hbar &= \frac{h}{2\pi} = 1.055 \cdot 10^{-34} \left[\frac{\text{m}^2 \text{kg}}{\text{s}} \right] \quad \mathbf{B} \\
 e &= 1.602 \cdot 10^{-19} [\text{C}] \quad \mathbf{E} & m_e &= 9.109 \cdot 10^{-31} [\text{kg}] \\
 k_B &= 1.381 \cdot 10^{-23} \left[\frac{\text{m}^2 \text{kg}}{\text{s}^2 \text{K}} \right] \quad \mathbf{D} & 1 [\text{eV}] &= 1.602 \cdot 10^{-19} \left[\frac{\text{kg m}^2}{\text{s}^2} \right] [\text{J}]
 \end{aligned}$$

1.1 Photon & Electron

$$\begin{aligned}
 \lambda [\text{m}], \nu \left[\frac{1}{\text{s}} \right] & \quad \text{Wavelength, Freq.} & \lambda &= \frac{c}{\nu} & \nu &= \frac{c}{\lambda} & \omega &= 2\pi\nu & k &= \frac{2\pi\nu}{c} \\
 k & \quad \text{Wavenumber} \\
 E [\text{J}] & \quad \text{Energy} & E &= h \cdot \nu = \hbar \cdot \omega \\
 \vec{F}_c [\text{N}] & \quad \text{Coulomb Force} & |\vec{F}_c| &= \frac{Q_1 \cdot Q_2}{4\pi\epsilon_0 r^2}
 \end{aligned}$$

1.2 Photoelectric effect

$$\begin{aligned}
 \phi_0 [\text{eV}] & \quad \text{Work function} \\
 I [\text{A}] & \quad \text{Photo-current} & h\nu - \phi_0 &= \frac{1}{2} m_e v^2 = eV \\
 n [\text{m}^{-3}] & \quad \text{Volume density of electrons} & V(\nu) &= \frac{h}{e} \nu - \frac{\phi_0}{e} \\
 N \left[\frac{1}{\text{s}} \right] & \quad \text{Number of photons per second} & I &= nAve, \quad n = \frac{Ndt}{A v dt} \rightarrow I = N \cdot e \\
 A [\text{m}^2] & \quad \text{Area} \\
 v \left[\frac{\text{m}}{\text{s}} \right] & \quad \text{velocity of electrons}
 \end{aligned}$$

1.3 Blackbody Radiation

$$\begin{array}{ll|ll}
 L [\text{m}] & \text{length of blackbody cube} & E_x & \text{Electric field in x-direction} \\
 N & \text{Number of states} & D & \text{Density of states} \\
 u \left[\frac{\text{m kg}^2}{\text{s}^2} \right] & \text{Blackbody energy density} & I \left[\frac{\text{W}}{\text{m}^2} \right] & \text{Power density}
 \end{array}$$

$$\begin{aligned}
 E_x(x, y, z) &= E_{0x} \cos(k_x x) \sin(k_y y) \sin(k_z z) \\
 k_x &= n \frac{\pi}{L} \quad k_y = m \frac{\pi}{L} \quad k_z = l \frac{\pi}{L} \quad k = \sqrt{k_x^2 + k_y^2 + k_z^2} \\
 N(k) &= \text{Num Polarizations} \cdot \frac{1}{2\text{Dim}} \cdot \frac{\text{Volume or Area of sphere or circle with radius } k}{\text{Volume of the elementary cell}} \\
 \text{In 3 Dimensions: } N(k) &= 2 \cdot \frac{1}{8} \cdot \frac{4\pi k^3}{\left(\frac{\pi}{L}\right)^3} = \frac{1}{3\pi^2} k^3 L^3 \quad D(k) = \left(\frac{dN(k)}{dk} \right) \frac{1}{L^3} = \frac{k^2}{\pi^2} \\
 u(\omega) d\omega &= \frac{\omega^2}{\pi^2 c^3} \cdot \frac{\hbar \omega}{\exp\left(\frac{-\hbar \omega}{kT}\right) - 1} d\omega & u(\nu) d\nu &= \frac{8\pi h \nu^3}{c^3 \left(\exp\left(\frac{h\nu}{kT}\right) - 1 \right)} d\nu
 \end{aligned}$$

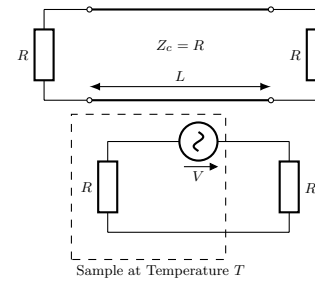
$$I(\omega) d\omega = c \cdot u(\omega) d\omega$$

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

1.4 Johnson-Noise

For Johnson-Noise, we use the model of Blackbody radiation in the 1 dimensional case. We can express $N(k) = \frac{k}{L}$ and $D(k)dk = \frac{1}{\pi} dk$ or $D(\omega) = \frac{1}{\pi c} d\omega$, where c' is the velocity along the transmission line. We have one allowed polarization. The energy density in the line per unit length is: $u(\nu)d\nu = kT \frac{2}{c} d\nu$ and the power radiated at one end of the line is then: $P = \frac{1}{2} c' u(\nu) d\nu = kT d\nu$.

This is the noise created in a one-dimensional circuit (like a coax-cable). If the impedance of the transmission line (TL) is equal to the resistors at the ends, the transmission line can be ignored ($P_R = P_{in}$). $\langle V^2 \rangle$: Noise Voltage and $\delta\nu$: bandwidth



$$D(k) = \frac{1}{L} \frac{dN(k)}{dk} = \frac{1}{\pi} \quad (\text{number of modes in TL})$$

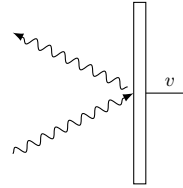
$$E = E_0 \cdot \sin(k_x \cdot x)$$

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

$$\text{if } \frac{\hbar \omega}{kT} > 1 : \langle V^2 \rangle = 3R \cdot k_B T \cdot \delta\nu \cdot \frac{h\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

$$\text{if } Z \neq R \rightarrow P_R = \frac{4RZ}{(R+Z)^2} P_{in}$$

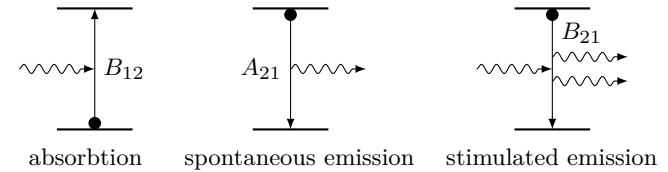
1.5 Momentum of a photon



This process must conserve both total momentum and energy.

$$\begin{aligned}
 p \left[\frac{\text{kg m}}{\text{s}} \right] & \quad \text{momentum} \\
 p_{\text{absorbing}} &= \frac{h\nu}{c} = m \cdot v & p_{\text{reflecting}} &= 2 \cdot \frac{h\nu}{c} \\
 p &= \sqrt{2m_e e \Delta V}
 \end{aligned}$$

1.6 Absorption, spontaneous and stimulated emission

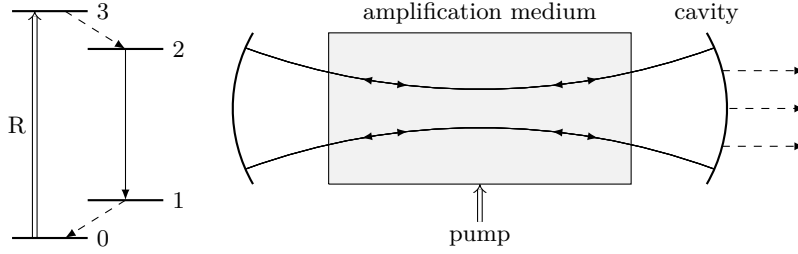


$$\begin{aligned}
 n_1 & \quad \text{Number of electrons in the lower energy state} \\
 n_2 & \quad \text{Number of electrons in the higher energy state}
 \end{aligned}$$

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

$$\begin{aligned}
 \frac{n_2}{n_1} &= e^{-\frac{h\nu}{k_B T}} = \frac{u(\nu) B_{12}}{u(\nu) B_{21} + A_{21}} \\
 B_{21} &= B_{12} = B & A_{21} &= \frac{8\pi h \nu^3}{c^3}
 \end{aligned}$$

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:

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

1.8 Fermi Energy of a metal

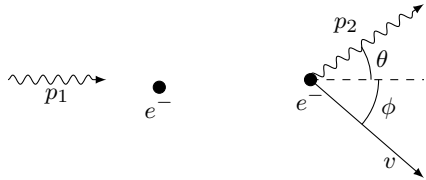
$$E_F = \frac{\hbar^2}{2m_e} (3n\pi^2)^{2/3} \quad n = \frac{\rho}{m} = \frac{\rho \cdot N_A}{m_{mol}}$$

Where m_e [kg] is the mass of the electron, m [kg] is the mass of an single atom of the metal, m_{mol} $\left[\frac{\text{kg}}{\text{mol}}\right]$ is the atomic weight, n $\left[\frac{1}{\text{m}^3}\right]$ is the number of atoms per unit of volume and ρ $\left[\frac{\text{kg}}{\text{m}^3}\right]$ is the density of the metal.

2 Wave mechanics

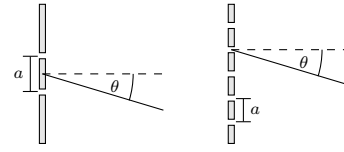
	frequency	wavelength	momentum	energy
Particle	$\nu_b = \frac{E}{h}$	$\lambda_b = \frac{h}{p} = \frac{h}{mv}$	$p = mv$	$E = \frac{1}{2}mv^2$
Wave	ω, ν	$\lambda = \frac{2\pi c}{\omega} = \frac{c}{\nu}$	$p = \hbar k = \frac{\hbar\omega}{c} = \frac{h\nu}{c}$	$E = h\nu = \hbar\omega$

2.1 Compton Scattering



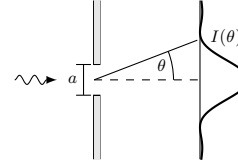
$$\begin{aligned} p_1 &= p_2 + p_e \\ p_1 &= \frac{h\nu_1}{c} \quad p_2 = \frac{h\nu_2}{c} \\ \nu_2 &= \nu_1 - \frac{p_e^2}{2m_e h} \\ \lambda_2 - \lambda_1 &= \frac{h}{m_e c} (1 - \cos \theta); \end{aligned}$$

2.2 Double Slit and Bragg Diffraction



$$\begin{aligned} \text{Constructive} \quad \sin \theta &= \frac{n\lambda}{a} \\ \text{Destructive} \quad \sin \theta &= \frac{(n + \frac{1}{2})\lambda}{a} \\ n &\in \mathbb{Z} \end{aligned}$$

2.3 Single slit and uncertainty relation



$$\begin{aligned} I(\theta) &= I_0 \frac{\sin^2 \theta}{\theta^2} & \sin \theta &= \frac{\lambda}{a} \\ \Delta x \Delta p &\geq \hbar & \Delta t \Delta E &\geq \hbar \quad (E = \hbar\omega) \end{aligned}$$

2.4 Bohr-Sommerfeld quantisation

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

$$\begin{aligned} \int_{length} p \cdot ds &= n \cdot h & n &\in \mathbb{N} \\ p &\text{Momentum of particle} \\ E_n &\text{Energy of the nth state} \\ E_{ry} &\text{Rydberg Energy} \\ a_0 &\text{Bohr-radius} \\ Z &\text{Number of protons} \end{aligned}$$

$$\begin{aligned} E_n &= -\frac{Z^2}{n^2} \cdot \frac{m_e e^4}{8\epsilon_0^2 h^2} = -\frac{Z^2}{n^2} \cdot E_{ry} \\ r_n &= \frac{n^2}{Z} \cdot \frac{2\epsilon_0 h}{m_e e^2} = \frac{n^2}{Z} \cdot a_0 \\ E_{ry} &= 13.6 \text{ [eV]} \end{aligned}$$

$$a_0 = 5.292 \cdot 10^{-11} \text{ [m]}$$

3 Quantum Mechanics

3.1 Wave function

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

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

$$P(x)dx = |\psi(x)|^2 dx \quad P_{ab} = \int_a^b |\psi(x)|^2 dx \quad \langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx$$

3.2 The Schrödinger equation

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

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

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

The wave function and it's derivative must be continuous where the potential $V(x, t)$ is finite.

3.2.1 Phase and Group Velocity

phase velocity v_φ (phase movement), group velocity v_g (movement of wave packet)

$$v_\varphi = \frac{\omega}{k} \quad v_g = \frac{\partial \omega}{\partial k} \quad \text{Particle wave: } v_\varphi \cdot 2 = v_g$$

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.

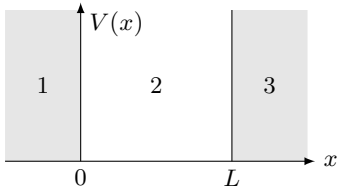
$$\Psi_n(\mathbf{x}, t) = \psi_n(\mathbf{x}) \cdot \chi_n(t) = \psi_n(\mathbf{x}) \cdot e^{-i \frac{E_n}{\hbar} t}$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_n(\mathbf{x}) + V(\mathbf{x}) \psi_n(\mathbf{x}) = \psi_n(\mathbf{x}) \cdot E_n$$

$$\iiint |\Psi|^2 d^3 \mathbf{x} = \iiint |\psi|^2 d^3 \mathbf{x} = 1$$

$$\Psi(\mathbf{x}, t) = \sum a_n \psi_n(\mathbf{x}) \cdot e^{-i \frac{E_n}{\hbar} t} \quad \sum |a_n|^2 = 1$$

3.2.3 Example: 1D infinite potential well



$$\Psi_1 = \Psi_3 = 0$$

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

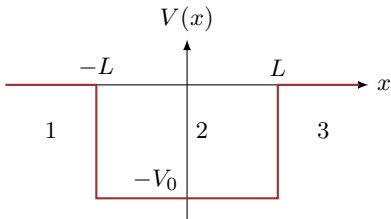
$$\psi_2 = A \sin(kx) + B \cos(kx)$$

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

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

$$E_n = n^2 \cdot \frac{\hbar^2 \pi^2}{2mL} = n^2 \cdot E_0, \quad k_n = \frac{n\pi}{L} \left[\frac{1}{\text{m}} \right]$$

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:

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

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_1(x) = E \psi_1(x) \quad \psi_1 = A_1 e^{ikx} + A'_1 e^{-ikx} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

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**

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

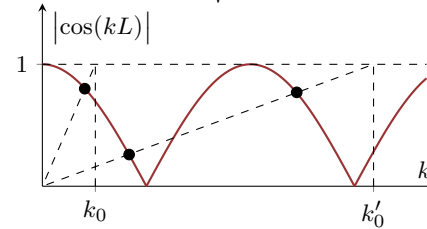
We see that as $x \rightarrow -\infty$, the Term B'_1 , as well as B_3 approaches ∞ . Since the wave function cannot approach ∞ , $B'_1 = B_3 = 0$ is a condition.

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

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

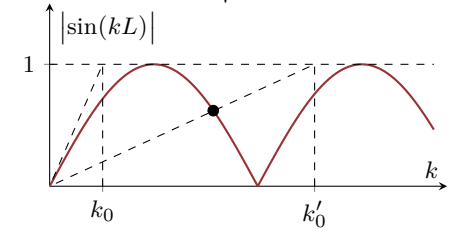
Even solutions: only even (cosine) components

$$\begin{aligned} |\cos(kL)| &= \frac{k}{k_0}, \quad \tan(kL) > 0 \\ k_0 &= \sqrt{\frac{2mV_0}{\hbar^2}} \end{aligned}$$

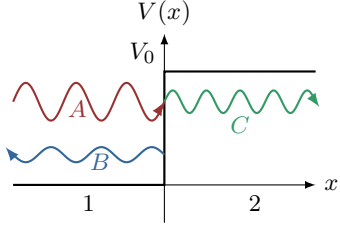


Odd solutions: only odd (sine) components

$$\begin{aligned} |\sin(kL)| &= \frac{k}{k_0}, \quad \tan(kL) > 0 \\ k_0 &= \sqrt{\frac{2mV_0}{\hbar^2}} \end{aligned}$$



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:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_1(x) = E \psi_1(x), \quad \psi_1(x) = A e^{ik_1 x} + B e^{-ik_1 x}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

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

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

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_2 = (E - V_0) \psi_2(x) \quad \psi_2 = C e^{ik_2 x}, \quad k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

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

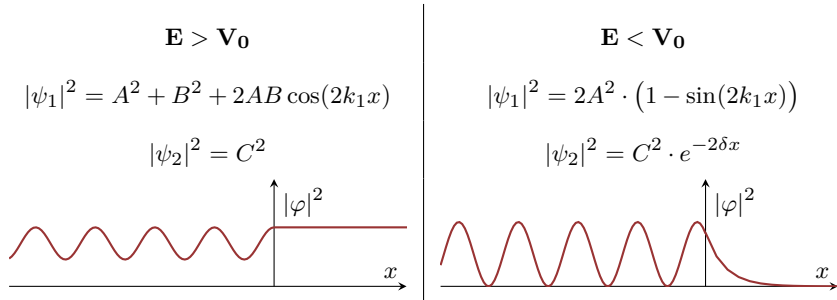
$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_2 = (E - V_0) \psi_2(x) \quad \psi_2 = C e^{\delta_2 x}, \quad \delta_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

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 :

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

$E > V_0$	$E < V_0$
$A + B = C$	$A + B = C$
$k_1(A - B) = k_2 C$	$A = B$

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

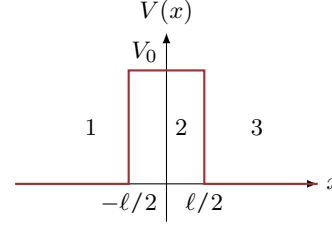


To find the **transmission coefficient** T and the **reflection coefficient** R , we normalize $A = 1$. Then, we can define $B = \sqrt{R}$ and $C = \sqrt{T}$. Then, we can solve for R and T :

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

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:

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

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

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

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

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

$E < V_0$	$E > V_0$
$T = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2(\delta_2 \ell)}$	$T = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sin^2(k_2 \ell)}$

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: $k_2 \ell = \pi/2 + n\pi$.

If $\delta_2 \ell \gg 1$, the transmission coefficient is proportional to: $T \propto e^{-2\delta_2 \ell}$

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 $\langle \psi_1 | \psi_2 \rangle = 0$, ψ_1, ψ_2 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:

$$\langle \mathbf{x} \rangle_\Psi = \iiint \Psi^*(\mathbf{x}, t) \cdot \mathbf{x} \cdot \Psi(\mathbf{x}, t) d^3\mathbf{x} = \iiint \mathbf{x} \cdot |\Psi(\mathbf{x}, t)|^2 d^3\mathbf{x} \quad \langle \psi_m | \psi_n \rangle = \delta_{mn} \quad |\psi_n\rangle \langle \psi_n| = 1$$

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 Canonical commutation relation

The commutators is a way of describing the effect of the order, in which multiple operators are applied.

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}, \quad [\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}], \quad [\hat{A}, \hat{A}] = 0$$

$$[\hat{A}, (\hat{B} + \hat{C})] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

$$[\hat{p}_x, \hat{p}_y] = 0, \quad [\hat{x}, \hat{p}_x] = i\hbar, \quad [\hat{z}, \hat{p}_x] = [\hat{z}, \hat{p}_y] = 0$$

5.2 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.

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

5.3 Harmonic Oscillator

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

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

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

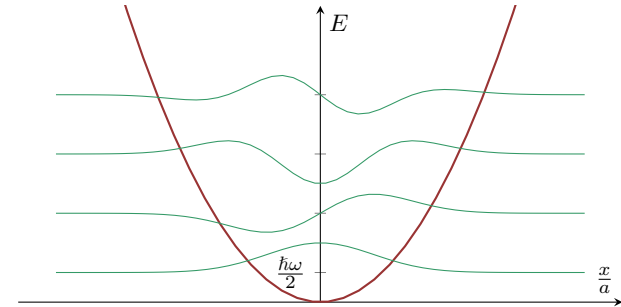
$$a = \sqrt{\frac{\hbar}{m\omega}}, \quad \tilde{x} = \frac{x}{a}, \quad \tilde{E} = \frac{E}{\hbar\omega} \Rightarrow \frac{1}{2} \left[-\frac{\partial^2}{\partial \tilde{x}^2} + \tilde{x}^2 \right] \varphi(\tilde{x}) = \tilde{E} \varphi(\tilde{x})$$

Then, the solutions to the equation is:

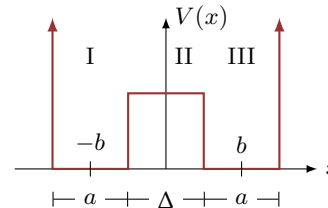
$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega, \quad \psi(\tilde{x}) = c_n H_n(\tilde{x}) e^{-\tilde{x}^2/2}, \quad H_n(\tilde{x}) = (-1)^n e^{\tilde{x}^2} \cdot \frac{\partial^n}{\partial \tilde{x}^n} e^{-\tilde{x}^2}$$

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

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

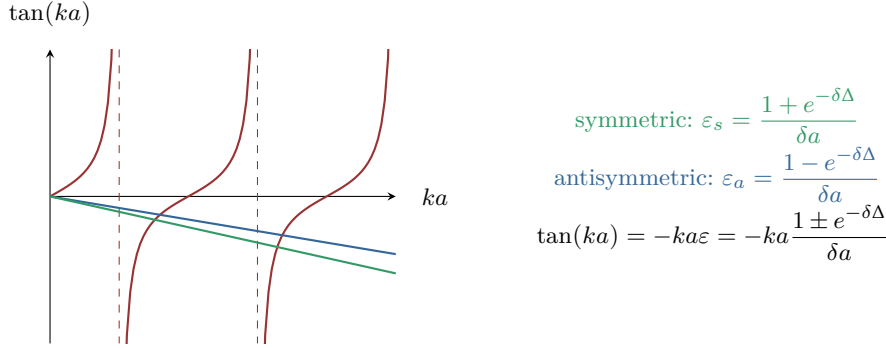


5.4 The coupled quantum well



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: $E < V_0$

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



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

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

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

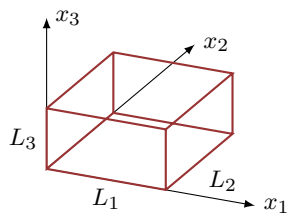
$$\Psi_L = \frac{1}{\sqrt{2}}(\Psi_s - \Psi_a), \quad \Psi_R = \frac{1}{\sqrt{2}}(\Psi_s + \Psi_a)$$

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

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

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

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

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

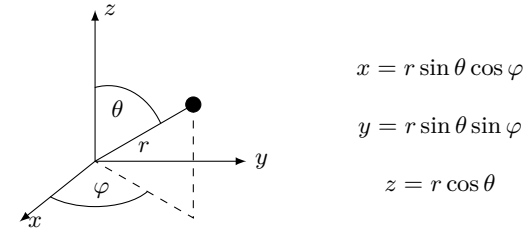
$$E_i^{(n_i)} = n_i^2 \frac{\hbar^2 \pi^2}{2mL_i^2}, \quad \psi_i^{(n_i)} = A \cdot \sin\left(\frac{\pi n_i x}{L_i}\right)$$

After normalizing, the wave function can be written as:

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

When $L_1 = L_2 = L_3$, there sometimes exists multiple states (**degeneracies**) for the same energy $E = E_1 + E_2 + E_3$. Now, we can generate new solutions to the wave function via superposition of those states. In general, degeneracies arise from symmetries (obvious or hidden).

6.1 Schrödinger Equation in spherical coordinates



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

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

Now, we insert this into the Schrödinger equation and try to separate the radial part $R(r)$ from the angular part $Y(\theta, \varphi)$. By introducing a separation constant $\ell(\ell + 1)$, we get:

$$\psi(r, \theta, \varphi) = R(r) \cdot Y(\theta, \varphi)$$

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) - \frac{2mr^2}{\hbar^2} (V - E) = - \left(\frac{1}{Y \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \varphi^2} \right) = \ell(\ell + 1)$$

The angular equation can be rewritten, in order to separate $Y(\theta, \varphi)$ into $\Theta(\theta)\Phi(\varphi)$. With this separation, we get for the angular part:

$$\Phi(2\pi) = \Phi(0) \rightarrow m \in \mathbb{Z}, \quad |m| \leq \ell$$

$$\psi_{n\ell m}(r, \theta, \varphi) = R_{n\ell}(r) \cdot Y_{\ell}^m(\theta, \varphi) = R_{n\ell}(r) \cdot P_{\ell}^m(\cos \theta) e^{im\varphi}$$

The angular part $Y_{\ell}^m(\theta, \varphi)$ can be written as:

$$P_{\ell}^m(x) = (i - x^2)^{\frac{|m|}{2}} \frac{d^{|m|}}{dx^{|m|}} P_{\ell}(x) \quad P_{\ell}(x) = \frac{1}{2^{\ell} \cdot \ell!} \frac{\partial^{\ell}}{\partial x^{\ell}} (x^2 - 1)^{\ell}$$

The solution to Y will be a **spherical harmonic**. Finally, we must apply the normalization

$$\int_0^\infty |R(r)|^2 r^2 dr = 1, \quad \int_{\theta=0}^\pi \int_{\varphi=-\pi}^\pi |Y_\ell^m(\theta, \varphi)|^2 \sin \theta d\varphi d\theta = 1$$

These solutions are the same as **spherical harmonics**. They form an **orthogonal basis**, meaning that every well-behaved function $f(\theta, \varphi)$ can be expressed as a superposition of those harmonics.

6.1.1 Hydrogen Atom

The radial part $R_{n\ell}$ of the hydrogen atom with potential $V(r) = \frac{-e^2}{4\pi\epsilon_0 r}$ can be written as:

$$R_{n\ell}(r) = \frac{1}{r} \rho^{\ell+1} e^{-\rho} v(\rho), \quad \rho = \frac{r}{na_0}, \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \approx 5.29 \cdot 10^{-11} \text{ [m]}$$

$$\psi_{n\ell m}(r, \theta, \varphi) = R_{n\ell}(r) Y_\ell^m(\theta, \varphi) \quad j_{max} = (n - \ell - 1) \geq 0 \quad |m| \leq \ell$$

$$E = -\frac{E_{Ry}}{n^2} \approx -\frac{13.6}{n^2} \text{ [eV]}$$

$v(\rho)$ is a polynomial of degree j_{max} with coefficients: $C_{g+1} = \frac{2(g+l+1-n)}{(g+1)(g+2l+2)} C_g$. For state n , there are $d(n) = n^2$ different solutions (**degeneracies**). The **effective radius** is na_0 . The **probability** of finding an electron between r and $r + dr$ is:

$$p(r)dr = r^2 |R_{n\ell}(r)|^2 dr$$

6.1.2 Quantum Numbers

n is the main quantum number, ℓ is the orbital quantum number and m is the magnetic quantum number (projection of angular momentum). Chemists give the different ℓ 's different names.

- $\ell = 0$: the orbital is called an s-state ($\max p(r)dr$ is at $r = 0$).
- $\ell = 1$: the orbital is called an p-state ($p(r = 0)dr = 0$).
- $\ell = 2$: the orbital is called an d-state.

7 Angular Momentum and Spin

$$\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y & \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z & \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \\ \begin{bmatrix} \hat{L}_x \\ \hat{L}_y \end{bmatrix} &= i\hbar \hat{L}_z & \begin{bmatrix} \hat{L}_y \\ \hat{L}_z \end{bmatrix} &= i\hbar \hat{L}_x & \begin{bmatrix} \hat{L}_z \\ \hat{L}_x \end{bmatrix} &= i\hbar \hat{L}_y \end{aligned} \quad \hat{\mathbf{L}} = \det \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ \hat{x} & \hat{y} & \hat{z} \\ \hat{p}_x & \hat{p}_y & \hat{p}_z \end{vmatrix}$$

$$\hat{L}_x = i\hbar \left(\sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \theta \cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right), \quad \hat{L}_y = -i\hbar \left(\cos \varphi \frac{\partial}{\partial \theta} - \frac{\cos \theta \sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}, \quad \hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]$$

Angular momentum operators do not commute. In order to get commutable operators, we introduce $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

$$\begin{aligned} [\hat{L}^2, \hat{L}_x] &= 0, & [\hat{L}^2, \hat{L}_y] &= 0, & [\hat{L}^2, \hat{L}_z] &= 0 \\ \hat{L}^2 Y_\ell^m(\theta, \varphi) &= \hbar^2 \ell(\ell+1) Y_\ell^m(\theta, \varphi), & \hat{L}_z Y_\ell^m(\theta, \varphi) &= \hbar m Y_\ell^m(\theta, \varphi) \end{aligned}$$

7.1 Ladder Operator

If a ladder operators $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ are used in the following way: Suppose, we have a wave function ψ , which is simultaneously an eigenfunction of \hat{L}^2 and \hat{L}_z . Then, $\hat{L}_\pm \psi$ is also an eigenfunction of \hat{L}^2 and \hat{L}_z with the following eigenvalues:

$$\begin{aligned} \hat{L}^2 \psi &= \lambda \psi, & \hat{L}_z \psi &= \mu \psi & \hat{L}^2 (\hat{L}_\pm \psi) &= \lambda (\hat{L}_\pm \psi), & \hat{L}_z (\hat{L}_\pm \psi) &= (\mu \pm \hbar) (\hat{L}_\pm \psi) \\ \hat{L}_+ Y_\ell^m &= \hbar \sqrt{\ell(\ell+1) - m(m+1)} Y_\ell^{m+1} & \hat{L}_- Y_\ell^m &= \hbar \sqrt{\ell(\ell+1) - m(m-1)} Y_\ell^{m-1} \end{aligned}$$

7.2 Spin

Idea: $\ell = \frac{1}{2} \rightarrow m = \pm \frac{1}{2}$. Instead of using ℓ , we use s to describe the spin. The operators \hat{L}_i are now called \hat{S}_i . We define the spin as $|s, m_s\rangle$:

$$\chi_+ = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad \chi_- = \begin{bmatrix} 1 \\ -2 \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}, \quad \chi = a\chi_+ + b\chi_- = \begin{bmatrix} a \\ b \end{bmatrix}, \quad |a|^2 + |b|^2 = 1$$

Since we have now only two eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$, we can write:

$$\begin{aligned} \hat{S}^2 &= \frac{3}{4} \hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \hat{S}_x &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \hat{S}_y &= \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} & \hat{S}_z &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ |\uparrow_x\rangle &= \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + |\downarrow_z\rangle), & |\downarrow_x\rangle &= \frac{1}{\sqrt{2}} (|\uparrow_z\rangle - |\downarrow_z\rangle) \end{aligned}$$

Now, we define the ladder operators in the same way as for the angular momentum:

$$\hat{S}_+ = \begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix} \quad \hat{S}_- = \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix} \quad \hat{S}_+ |\uparrow\rangle = \hat{S}_- |\downarrow\rangle = 0, \quad \hat{S}_+ |\downarrow\rangle = \hbar |\uparrow\rangle, \quad \hat{S}_- |\uparrow\rangle = \hbar |\downarrow\rangle$$

We can write states in dirac notation as: $|\ell, m\rangle$. For spins, we get:

$$|1, 1\rangle = |\uparrow\uparrow\rangle, \quad |1, -1\rangle = |\downarrow\downarrow\rangle, \quad |1, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad |0, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\text{Clebsch Gordan: } |s, m\rangle = \sum_{m_1+m_2=m} C_{m_1 m_2 m}^{s_1 s_2 s} |s_1, m_1\rangle |s_2, m_2\rangle$$

7.3 Identical Particles

When we have two particles with wave function $\varphi_a(\vec{x}_1)$ and $\varphi_b(\vec{x}_2)$, we can combine them in two different ways:

- **Boson:** $\psi_- = \frac{1}{\sqrt{2}} (\varphi_a(\vec{x}_1)\varphi_b(\vec{x}_2) - \varphi_b(\vec{x}_1)\varphi_a(\vec{x}_2))$: symmetric (electron)
- **Fermion:** $\psi_+ = \frac{1}{\sqrt{2}} (\varphi_a(\vec{x}_1)\varphi_b(\vec{x}_2) + \varphi_b(\vec{x}_1)\varphi_a(\vec{x}_2))$: antisymmetric (photon)

Pauli exclusion principle: **Two fermions cannot occupy the same identical state**

7.3.1 Exchange Interactions

We have two particles, which have normalized and orthogonal wave functions. We have three different interactions:

1. The particles are **distinguishable**: $\psi = \psi_a(x_1)\psi_b(x_2)$

$$\langle (x_1 - x_2)^2 \rangle_\psi = \langle x^2 \rangle_{\psi_a} + \langle x^2 \rangle_{\psi_b} - 2 \langle x \rangle_{\psi_a} \langle x \rangle_{\psi_b}$$

2. **Symmetric** wave function: $\psi_+ = \frac{1}{\sqrt{2}} (|\psi_a\rangle |\psi_b\rangle + |\psi_b\rangle |\psi_a\rangle)$

$$\langle (x_1 - x_2)^2 \rangle_\psi = \langle x^2 \rangle_{\psi_a} + \langle x^2 \rangle_{\psi_b} - 2 \langle x \rangle_{\psi_a} \langle x \rangle_{\psi_b} - 2 |\langle \psi_a | x | \psi_b \rangle|^2$$

3. **Antisymmetric** wave function: $\psi_- = \frac{1}{\sqrt{2}}(|\psi_a\rangle|\psi_b\rangle - |\psi_b\rangle|\psi_a\rangle)$

$$\langle (x_1 - x_2)^2 \rangle_\psi = \langle x^2 \rangle_{\psi_a} + \langle x^2 \rangle_{\psi_b} - 2 \langle x \rangle_{\psi_a} \langle x \rangle_{\psi_b} + 2 \left| \langle \psi_a | x | \psi_b \rangle \right|^2$$

7.4 Many Electrons: Atomic Shells

To write the wave function of an electron, we use the notation indexed by: $|n, \ell, m\rangle$.

shell n	subshell ℓ	max e^- in subshell	max e^- in shell
K	1s	2	2
L	2s 2p	2 6	2 + 6 = 8
M	3s 3p 3d	2 6 10	2 + 6 + 10 = 10

Here, the number of degeneracies per shell is displayed. Remember, we have $n \geq 1$, $0 \leq \ell < n$, $-\ell \leq m \leq \ell$, and for every different state, the electron can have either spin up or spin down. So, the number of electrons in a sub shell is the number of degeneracies.

7.5 Term Symbol

$$^{2S+1}L_J$$

S is the total spin quantum number. $2S + 1$ is the number of possible states of J (total angular momentum quantum number) for a given L and $S \leq L$. $J_{max} = L + S$, $J_{min} = |L - S|$. L is the orbital quantum number in spectroscopic notation: $L = 0 \rightarrow S$, $L = 1 \rightarrow P$, $L = 2 \rightarrow D$, $L = 3 \rightarrow F$...

8 Quantum Statistics and Solid States

8.1 Chemical Potential

For the chemical potential μ , the flux of particles (instead of energy) is important.

$$\mu = \frac{\partial F}{\partial N}, \quad F = U - TS$$

where F is the free energy, U is the total energy, T is the temperature, S is the entropy and N is the number of particles. In other words: **Chemical Potential is the energy exchanged when a particle is added or removed.**

8.2 Fermi-Dirac & Einstein Statistics

What is the probability of a given state to be occupied? And if we have multiple particles, how many electrons are in a state?

$$\text{Fermions: } f_F(E, \mu, T) = \frac{1}{\exp\left(\frac{E-\mu}{kT}\right) + 1}, \quad \text{Bosons: } f_B(E, \mu, T) = \frac{1}{\exp\left(\frac{E-\mu}{kT}\right) - 1}$$

As the energy $E \gg \mu$, both distributions are the same: the classical Boltzmann distribution. If the electrons are far away, we do not need to consider the interaction between single particles.

8.3 Fermi-Dirac statistics of a free electron gas

The number of particles N given an energy E with temperature $T = 0$ is:

$$N(E) = \frac{L^3}{3\pi^2} \frac{(2mE)^{\frac{3}{2}}}{\hbar^2} = \frac{4}{3}\pi k^3 \cdot \frac{1}{8} \cdot \left(\frac{L}{\pi}\right)^3 \cdot 2$$

This equation is derived by multiplying the Volume of a sphere (in the positive k sector) with radius k with the volume of a single state and the number of possible spins (2).

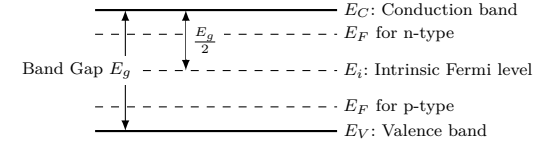
The Density of states $D(E)$ is given by:

$$D(E) = \frac{\partial N(E)}{\partial E} \cdot \frac{1}{V} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar}\right)^{\frac{3}{2}} \sqrt{E}$$

8.4 Semiconductors and Doping

n_c is the electron concentration in the conduction band, and n_i is the intrinsic carrier concentration (depending on the temperature).

$$n_c \left[\frac{1}{\text{m}^3} \right] = n_i \cdot f_{F/B}(E_F, E_i, T) \approx n_i \exp\left(\frac{E_F - E_i}{k_B T}\right) \text{ if } \frac{E_F - E_i}{k_B T} \gg 1$$



8.5 Bloch's Theorem

In a periodic potential, the wave equation can be written as a periodic function $u_{nk}(x)$ multiplied by a complex exponential:

$$\psi_{nk}(x) = e^{ikx} u_{nk}(x)$$

We can apply this theorem the band formation to conclude the following. As soon as we have a crystal, the electrons can be in a continuous band of energies:

$$E = E_0 - 2A \cos(ka) = E(k)$$

where A is the inter-atomic coupling. We can see that the band width is directly proportional to A .

9 Classical Mechanics

Quantity	Symbol	Definition	unit
Momentum	\mathbf{p}	$\mathbf{p} = m\mathbf{v}$	$\left[\frac{\text{kg m}}{\text{s}} \right]$
Force	\mathbf{F}	$\mathbf{F} = \frac{d\mathbf{p}}{dt} = m\mathbf{a}$	$[\text{N}] = \left[\frac{\text{kg m}}{\text{s}^2} \right]$
Angular momentum	\mathbf{L}	$\mathbf{L} = \mathbf{r} \times \mathbf{p}$	$\left[\frac{\text{kg m}^2}{\text{s}} \right]$
Impulse	$\Delta \mathbf{p}$	$\Delta \mathbf{p} = \int \mathbf{F} dt$	$\left[\frac{\text{kg m}}{\text{s}} \right]$
Mechanical Work (Energy)	W	$W = \int_s \mathbf{F} d\mathbf{r} = \frac{1}{2} m v^2$	$[\text{J}] = [\text{N m}] = \left[\frac{\text{kg m}^2}{\text{s}^2} \right]$
Mechanical Power	P	$P = \frac{dE}{dt}$	$[\text{W}] = \left[\frac{\text{J}}{\text{s}} \right] = \left[\frac{\text{kg m}^2}{\text{s}^3} \right]$
Velocity	\mathbf{v}	$\mathbf{v} = \frac{d\mathbf{r}}{dt}$	$\left[\frac{\text{m}}{\text{s}} \right]$
Acceleration	\mathbf{a}	$\mathbf{a} = \frac{d\mathbf{v}}{dt} = \frac{d^2 \mathbf{r}}{dt^2}$	$\left[\frac{\text{m}}{\text{s}^2} \right]$

10 Useful formulas

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

$$\int x^n e^{cx} = e^{cx} \sum_{i=0}^n (-1)^{n-i} \frac{n!}{i! c^{n-i+1}} x^i \quad \int_0^{\infty} x^n e^{-cx} = \frac{n!}{c^{n+1}}$$

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

10.1 Trigonometry

$$\begin{aligned} \sin(2\alpha) &= 2 \sin \alpha \cos \alpha & \cos(2\alpha) &= \cos^2 \alpha - \sin^2 \alpha \\ \sin(\alpha \pm \beta) &= \sin(\alpha) \cos(\beta) \pm \cos(\alpha) \sin(\beta) & \cos(\alpha \pm \beta) &= \cos(\alpha) \cos(\beta) \mp \sin(\alpha) \sin(\beta) \\ \sin(\alpha) \pm \sin(\beta) &= 2 \sin \frac{\alpha \pm \beta}{2} \cos \frac{\alpha \mp \beta}{2} & \cos(\alpha) + \cos(\beta) &= 2 \cos \frac{\alpha + \beta}{2} \cos \frac{\alpha - \beta}{2} \\ \cos(\alpha) - \cos(\beta) &= -2 \sin \frac{\alpha + \beta}{2} \sin \frac{\alpha - \beta}{2} & \sin(\alpha) \sin(\beta) &= \frac{1}{2} (\cos(\alpha - \beta) - \cos(\alpha + \beta)) \\ \cos(\alpha) \cos(\beta) &= \frac{1}{2} (\cos(\alpha - \beta) + \cos(\alpha + \beta)) & \sin(\alpha) \cos(\beta) &= \frac{1}{2} (\sin(\alpha - \beta) + \sin(\alpha + \beta)) \\ \sin^2 \alpha &= \frac{1}{2} (1 - \cos 2\alpha) & \cos^2 \alpha &= \frac{1}{2} (1 + \cos 2\alpha) \\ \sin^3 \alpha &= \frac{1}{4} (3 \sin \alpha - \sin 3\alpha) & \cos^3 \alpha &= \frac{1}{4} (3 \cos \alpha + \cos 3\alpha) \\ \frac{\sin 2\alpha}{\sin \alpha} &= 2 \cos \alpha & \sin \alpha \cos \alpha &= \frac{1}{2} \sin 2\alpha \\ \frac{\sin \alpha}{c^2} &= a^2 + b^2 - 2ab \cos \gamma & \frac{a}{\sin \alpha} &= \frac{b}{\sin \beta} = \frac{c}{\sin \gamma} = 2r = \frac{u}{\pi} \end{aligned}$$

10.2 Differentiation

$$\begin{aligned} \text{Product rule} & \quad (fg)' = f'g + fg' \\ \text{Quotient rule} & \quad \left(\frac{f}{g}\right)' = \frac{f'g - fg'}{g^2} \\ \text{Chain rule} & \quad \frac{d}{dx} (f(g(x))) = f'(g(x)) g'(x) \\ \text{Power rule} & \quad \frac{d}{dx} (x^n) = nx^{n-1} \\ \text{Inverse power rule} & \quad \frac{d}{dx} \left(\frac{1}{x^n}\right) = \frac{-n}{x^{n+1}} \\ \text{Exponential rule} & \quad \frac{d}{dx} (e^{g(x)}) = g'(x) e^{g(x)} \\ \text{Logarithm rule} & \quad \frac{d}{dx} (\ln g(x)) = \frac{g'(x)}{g(x)} \end{aligned}$$

10.3 Integration

$$\begin{aligned} \text{Partial integration} & \quad \int_a^b u(x)v'(x)dx = u(x)v(x)\Big|_a^b - \int_a^b u'(x)v(x)dx \\ \text{Power rule} & \quad \int x^n dx = \frac{1}{n+1} \cdot x^{n+1} + c, \quad n \neq -1 \\ \text{Inverse power rule} & \quad \int \frac{1}{x^n} dx = \frac{1}{-n+1} \cdot \frac{1}{x^{n-1}} + c, \quad n \neq 1 \\ x^{-1} \text{ rule} & \quad \int \frac{1}{x} dx = \ln |x| + c, \quad \int \frac{1}{ax+b} dx = \frac{1}{a} \ln |ax+b| + c \\ \text{Exponential rule} & \quad \int e^x dx = e^x + c \quad \int a^x dx = \frac{a^x}{\ln a} + c \\ \text{Logarithm rule} & \quad \int \ln x dx = x(\ln x - 1) + c \end{aligned}$$

11 Ground State Electron Configuration

This table shows the ground state electron configuration for the four rows of the periodic table:

Z	Element	Configuration
1	H	(1s)
2	He	(1s) ²
3	Li	(He)(2s)
4	Be	(He)(2s) ²
5	B	(He)(2s) ² (2p)
6	C	(He)(2s) ² (2p) ²
7	N	(He)(2s) ² (2p) ³
8	O	(He)(2s) ² (2p) ⁴
9	F	(He)(2s) ² (2p) ⁵
10	Ne	(He)(2s) ² (2p) ⁶
11	Na	(Ne)(3s)
12	Mg	(Ne)(3s) ²
13	Al	(Ne)(3s) ² (3p)
14	Si	(Ne)(3s) ² (3p) ²
15	P	(Ne)(3s) ² (3p) ³
16	S	(Ne)(3s) ² (3p) ⁴
17	Cl	(Ne)(3s) ² (3p) ⁵
18	Ar	(Ne)(3s) ² (3p) ⁶
19	K	(Ar)(4s)
20	Ca	(Ar)(4s) ²
21	Sc	(Ar)(4s) ² (3d)
22	Ti	(Ar)(4s) ² (3d) ²
23	V	(Ar)(4s) ² (3d) ³
24	Cr	(Ar)(4s)(3d) ⁵
25	Mn	(Ar)(4s) ² (3d) ⁵
26	Fe	(Ar)(4s) ² (3d) ⁶
27	Co	(Ar)(4s) ² (3d) ⁷
28	Ni	(Ar)(4s) ² (3d) ⁸
29	Cu	(Ar)(4s)(3d) ¹⁰
30	Zn	(Ar)(4s) ² (3d) ¹⁰
31	Ga	(Ar)(4s) ² (3d) ¹⁰ (4p)
32	Ge	(Ar)(4s) ² (3d) ¹⁰ (4p) ²
33	As	(Ar)(4s) ² (3d) ¹⁰ (4p) ³
34	Se	(Ar)(4s) ² (3d) ¹⁰ (4p) ⁴
35	Br	(Ar)(4s) ² (3d) ¹⁰ (4p) ⁵
36	Kr	(Ar)(4s) ² (3d) ¹⁰ (4p) ⁶

12 Periodic Table of the Elements

<div>2.201s</div> <div>H</div> <div>Hydrogen</div> <div>1.00784–1.00811</div>																		<div>21s</div> <div>He</div> <div>Helium</div> <div>4.002602(2)</div>																	
<div>30.982s</div> <div>Li</div> <div>Lithium</div> <div>6.938–6.997</div>		<div>41.572s</div> <div>Be</div> <div>Beryllium</div> <div>9.0121831(5)</div>																		<div>52.042p</div> <div>B</div> <div>Boron</div> <div>10.806–10.821</div>		<div>62.552p</div> <div>C</div> <div>Carbon</div> <div>12.0096–12.0116</div>		<div>73.042p</div> <div>N</div> <div>Nitrogen</div> <div>14.00643–14.00728</div>		<div>83.442p</div> <div>O</div> <div>Oxygen</div> <div>15.99903–15.99977</div>		<div>93.982p</div> <div>F</div> <div>Fluorine</div> <div>18.998403163(6)</div>		<div>102p</div> <div>Ne</div> <div>Neon</div> <div>20.1797(6)</div>					
<div>110.933s</div> <div>Na</div> <div>Sodium</div> <div>22.98976928(2)</div>		<div>121.313s</div> <div>Mg</div> <div>Magnesium</div> <div>24.304–24.307</div>																		<div>131.613p</div> <div>Al</div> <div>Aluminium</div> <div>26.9815385(7)</div>		<div>141.903p</div> <div>Si</div> <div>Silicon</div> <div>28.084–28.086</div>		<div>152.193p</div> <div>P</div> <div>Phosphorus</div> <div>30.973761998(5)</div>		<div>162.583p</div> <div>S</div> <div>Sulphur</div> <div>32.059–32.076</div>		<div>173.163p</div> <div>Cl</div> <div>Chlorine</div> <div>35.446–35.457</div>		<div>183p</div> <div>Ar</div> <div>Argon</div> <div>39.948(1)</div>					
<div>190.824s</div> <div>K</div> <div>Potassium</div> <div>39.0983(1)</div>		<div>201.004s</div> <div>Ca</div> <div>Calcium</div> <div>40.078(4)</div>		<div>211.363d</div> <div>Sc</div> <div>Scandium</div> <div>44.955908(5)</div>		<div>221.543d</div> <div>Ti</div> <div>Titanium</div> <div>47.867(1)</div>		<div>231.633d</div> <div>V</div> <div>Vanadium</div> <div>50.9415(1)</div>		<div>241.663d*</div> <div>Cr</div> <div>Chromium</div> <div>51.9961(6)</div>		<div>251.553d</div> <div>Mn</div> <div>Manganese</div> <div>54.938044(3)</div>		<div>261.833d</div> <div>Fe</div> <div>Iron</div> <div>55.845(2)</div>		<div>271.883d</div> <div>Co</div> <div>Cobalt</div> <div>58.933194(4)</div>		<div>281.913d</div> <div>Ni</div> <div>Nickel</div> <div>58.6934(4)</div>		<div>291.903d*</div> <div>Cu</div> <div>Copper</div> <div>63.546(3)</div>		<div>301.653d</div> <div>Zn</div> <div>Zinc</div> <div>65.38(2)</div>		<div>311.814p</div> <div>Ga</div> <div>Gallium</div> <div>69.723(1)</div>		<div>322.014p</div> <div>Ge</div> <div>Germanium</div> <div>72.630(8)</div>		<div>332.184p</div> <div>As</div> <div>Arsenic</div> <div>74.921595(6)</div>		<div>342.554p</div> <div>Se</div> <div>Selenium</div> <div>78.971(8)</div>		<div>352.964p</div> <div>Br</div> <div>Bromine</div> <div>79.901–79.907</div>		<div>363.004p</div> <div>Kr</div> <div>Krypton</div> <div>83.798(2)</div>	
<div>370.825s</div> <div>Rb</div> <div>Rubidium</div> <div>85.4678(3)</div>		<div>380.955s</div> <div>Sr</div> <div>Strontium</div> <div>87.62(1)</div>		<div>391.224d</div> <div>Y</div> <div>Yttrium</div> <div>88.90584(2)</div>		<div>401.334d</div> <div>Zr</div> <div>Zirconium</div> <div>91.224(2)</div>		<div>411.64d*</div> <div>Nb</div> <div>Niobium</div> <div>92.90637(2)</div>		<div>422.164d*</div> <div>Mo</div> <div>Molybdenum</div> <div>95.95(1)</div>		<div>431.94d</div> <div>Tc</div> <div>Technetium</div> <div>(98)</div>		<div>442.224d*</div> <div>Ru</div> <div>Ruthenium</div> <div>101.07(2)</div>		<div>452.284d*</div> <div>Rh</div> <div>Rhodium</div> <div>102.90550(2)</div>		<div>462.204d*</div> <div>Pd</div> <div>Palladium</div> <div>106.42(1)</div>		<div>471.934d*</div> <div>Ag</div> <div>Silver</div> <div>107.8682(2)</div>		<div>481.694d</div> <div>Cd</div> <div>Cadmium</div> <div>112.414(4)</div>		<div>491.785p</div> <div>In</div> <div>Indium</div> <div>114.818(1)</div>		<div>501.965p</div> <div>Sn</div> <div>Tin</div> <div>118.710(7)</div>		<div>512.055p</div> <div>Sb</div> <div>Antimony</div> <div>121.760(1)</div>		<div>522.15p</div> <div>Te</div> <div>Tellurium</div> <div>127.60(3)</div>		<div>532.665p</div> <div>I</div> <div>Iodine</div> <div>126.90447(3)</div>		<div>542.605p</div> <div>Xe</div> <div>Xenon</div> <div>131.293(6)</div>	
<div>550.796s</div> <div>Cs</div> <div>Cesium</div> <div>132.90545196(6)</div>		<div>560.896s</div> <div>Ba</div> <div>Barium</div> <div>137.327(7)</div>		<div>57-71</div> <div>*</div> <div>Lanthanides</div>		<div>721.35d</div> <div>Hf</div> <div>Hafnium</div> <div>178.49(2)</div>		<div>731.55d</div> <div>Ta</div> <div>Tantalum</div> <div>180.94788(2)</div>		<div>742.365d</div> <div>W</div> <div>Tungsten</div> <div>183.84(1)</div>		<div>751.95d</div> <div>Re</div> <div>Rhenium</div> <div>186.207(1)</div>		<div>762.25d</div> <div>Os</div> <div>Osmium</div> <div>190.23(3)</div>		<div>772.205d</div> <div>Ir</div> <div>Iridium</div> <div>192.217(3)</div>		<div>782.285d*</div> <div>Pt</div> <div>Platinum</div> <div>195.084(9)</div>		<div>792.545d*</div> <div>Au</div> <div>Gold</div> <div>196.966569(5)</div>		<div>802.005d</div> <div>Hg</div> <div>Mercury</div> <div>200.592(3)</div>		<div>811.626p</div> <div>Tl</div> <div>Thallium</div> <div>204.382–204.385</div>		<div>821.876p</div> <div>Pb</div> <div>Lead</div> <div>207.2(1)</div>		<div>832.026p</div> <div>Bi</div> <div>Bismuth</div> <div>208.98040(1)</div>		<div>842.06p</div> <div>Po</div> <div>Polonium</div> <div>(209)</div>		<div>852.26p</div> <div>At</div> <div>Astatine</div> <div>(210)</div>		<div>862.26p</div> <div>Rn</div> <div>Radon</div> <div>(222)</div>	
<div>870.77s</div> <div>Fr</div> <div>Francium</div> <div>(223)</div>		<div>880.97s</div> <div>Ra</div> <div>Radium</div> <div>(226)</div>		<div>89-103</div> <div>**</div> <div>Actinides</div>		<div>1046d</div> <div>Rf</div> <div>Rutherfordium</div> <div>(261)</div>		<div>1056d</div> <div>Db</div> <div>Dubnium</div> <div>(268)</div>		<div>1066d</div> <div>Sg</div> <div>Seaborgium</div> <div>(269)</div>		<div>1076d</div> <div>Bh</div> <div>Bohrium</div> <div>(270)</div>		<div>1086d</div> <div>Hs</div> <div>Hassium</div> <div>(269)</div>		<div>1096d</div> <div>Mt</div> <div>Meitnerium</div> <div>(278)</div>		<div>1106d</div> <div>Ds</div> <div>Darmstadtium</div> <div>(281)</div>		<div>1116d</div> <div>Rg</div> <div>Roentgenium</div> <div>(282)</div>		<div>1126d</div> <div>Cn</div> <div>Copernicium</div> <div>(285)</div>		<div>1137p</div> <div>Nh</div> <div>Nihonium</div> <div>(286)</div>		<div>1147p</div> <div>Fl</div> <div>Flerovium</div> <div>(289)</div>		<div>1157p</div> <div>Mc</div> <div>Moscovium</div> <div>(289)</div>		<div>1167p</div> <div>Lv</div> <div>Livermorium</div> <div>(293)</div>		<div>1177p</div> <div>Ts</div> <div>Tennessine</div> <div>(294)</div>		<div>1187p</div> <div>Og</div> <div>Oganesson</div> <div>(294)</div>	
<div>*</div> <div>**</div>		<div>571.15d*</div> <div>La</div> <div>Lanthanum</div> <div>138.90547(7)</div>		<div>581.124f*</div> <div>Ce</div> <div>Cerium</div> <div>140.116(1)</div>		<div>591.134f</div> <div>Pr</div> <div>Praseodymium</div> <div>140.90766(2)</div>		<div>601.144f</div> <div>Nd</div> <div>Neodymium</div> <div>144.242(3)</div>		<div>611.134f</div> <div>Pm</div> <div>Promethium</div> <div>(145)</div>		<div>621.174f</div> <div>Sm</div> <div>Samarium</div> <div>150.36(2)</div>		<div>631.24f</div> <div>Eu</div> <div>Europium</div> <div>151.964(1)</div>		<div>641.24f*</div> <div>Gd</div> <div>Gadolinium</div> <div>157.25(3)</div>		<div>651.14f</div> <div>Tb</div> <div>Terbium</div> <div>158.92535(2)</div>		<div>661.224f</div> <div>Dy</div> <div>Dysprosium</div> <div>162.500(1)</div>		<div>671.234f</div> <div>Ho</div> <div>Holmium</div> <div>164.93033(2)</div>		<div>681.244f</div> <div>Er</div> <div>Erbium</div> <div>167.259(3)</div>		<div>691.254f</div> <div>Tm</div> <div>Thulium</div> <div>168.93422(2)</div>		<div>701.14f</div> <div>Yb</div> <div>Ytterbium</div> <div>173.045(10)</div>		<div>711.274f</div> <div>Lu</div> <div>Lutetium</div> <div>174.9668(1)</div>					
		<div>891.16d*</div> <div>Ac</div> <div>Actinium</div> <div>(227)</div>		<div>901.35f*</div> <div>Th</div> <div>Thorium</div> <div>232.0377(4)</div>		<div>911.55f*</div> <div>Pa</div> <div>Protactinium</div> <div>231.03588(2)</div>		<div>921.385f*</div> <div>U</div> <div>Uranium</div> <div>238.02891(3)</div>		<div>931.365f*</div> <div>Np</div> <div>Neptunium</div> <div>(237)</div>		<div>941.285f</div> <div>Pu</div> <div>Plutonium</div> <div>(244)</div>		<div>951.135f</div> <div>Am</div> <div>Americium</div> <div>(243)</div>		<div>961.285f*</div> <div>Cm</div> <div>Curium</div> <div>(247)</div>		<div>971.35f</div> <div>Bk</div> <div>Berkelium</div> <div>(247)</div>		<div>981.35f</div> <div>Cf</div> <div>Californium</div> <div>(251)</div>		<div>991.35f</div> <div>Es</div> <div>Einsteinium</div> <div>(252)</div>		<div>1001.35f</div> <div>Fm</div> <div>Fermium</div> <div>(257)</div>		<div>1011.35f</div> <div>Md</div> <div>Mendelevium</div> <div>(258)</div>		<div>1021.35f</div> <div>No</div> <div>Nobelium</div> <div>(259)</div>		<div>1031.35f</div> <div>Lr</div> <div>Lawrencium</div> <div>(266)</div>					

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.