1 The Photon

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

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

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

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

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

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

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

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

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

1.1 Photon & Electron

λ [m] , ν $\left[\frac{1}{\mathrm{s}}\right]$	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 $\left[\mathrm{m}^{-3}\right]$	Volume density of electrons
A $\left[\mathrm{m}^2\right]$	Area
v $\left[\frac{\mathrm{m}}{\mathrm{s}}\right]$	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	$< E >$	Average Energy
N	Number of states	D	Density of states
u	Blackbody radiation	I	Power radiated

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

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

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

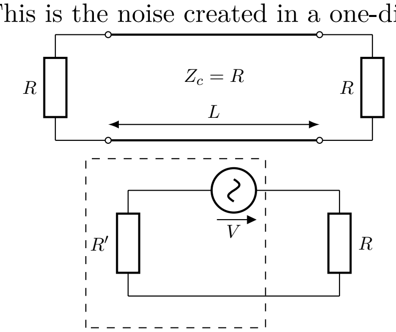
$$u(\omega) = \frac{\omega^2}{\pi^2 c^3} \cdot \frac{\hbar\omega}{\exp\left(\frac{-\hbar\omega}{kT}\right) - 1}d\omega \qquad u(\nu) = \frac{8\pi h\nu^3}{c^3\left(\exp\left(\frac{h\nu}{kT}\right) - 1\right)}d\nu$$

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

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).

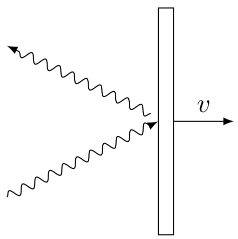


$\langle V^2 \rangle$	Noise Voltage
$\Delta\nu$	Bandwidth

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

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

1.5 Momentum of a photon



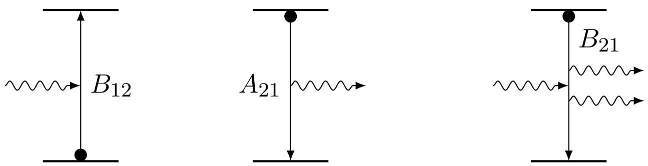
$p \left[\frac{\mathrm{kg\,m}}{\mathrm{s}}\right]$ momentum

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

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

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

1.6 Absorption, spontaneous and stimulated emission



absorbtion spontaneous emission stimulated emission

n_1 Number of electrons in the lower energy state

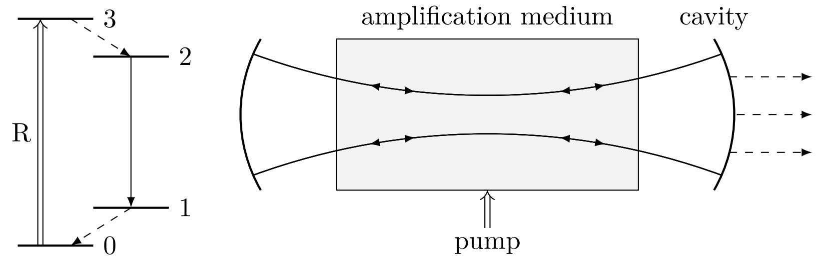
n_2 Number of electrons in the higher energy state

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

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

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

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:

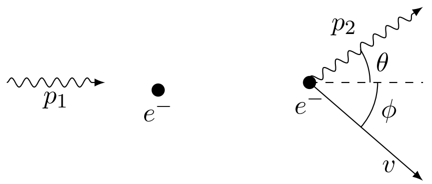
$$n_2 = \frac{R}{A_{21}} \quad \text{whereas} \quad n_1 \approx 0 \quad \text{because} \quad A_{21} < \frac{1}{\tau_1}$$

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

2 Wave mechanics

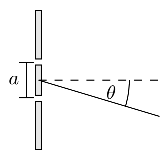
	frequency	wavelength	momentum	energy
Particle		$\lambda_b = \frac{h}{p}$	$p = mv$	$E = \frac{1}{2} m v^2$
Wave	ω	$\lambda = \frac{2\pi c}{\omega}$	$p = \frac{\hbar \omega}{c}$	$E = \hbar \omega$

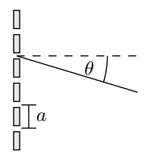
2.1 Compton Scattering



$$p_1 = \frac{h\nu_1}{c} \qquad p' = \frac{h\nu_2}{c}$$
$$\nu_2 = \nu_1 - \frac{P_e^2}{2m_e h}$$
$$\lambda_2 - \lambda_1 = \frac{h}{m_e c}(1 - \cos\theta);$$

2.2 Double Slit and Bragg Diffraction



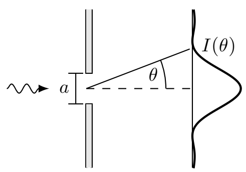


Constructive $\quad \sin\theta = \frac{n\lambda}{a}$

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

$$n \in \mathbb{Z}$$

2.3 Single slit and uncertainty relation



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

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
E_n	Energy of the nth state
E_{ry}	Rydberg Energy
a_0	Bohr-radius
Z	Number of protons

$$\int_{length} p \cdot ds = n \cdot h \qquad n \in \mathbb{N}$$
$$E_n = -\frac{Z^2}{n^2} \cdot \frac{m_e e^4}{8\epsilon_0^2 h^2} = -\frac{Z^2}{n^2} \cdot E_{ry}$$
$$r_n = \frac{n^2}{Z} \cdot \frac{2\epsilon_0 h}{m_e e^2} = \frac{n^2}{Z} \cdot a_0$$
$$E_{ry} = 13.6 \ \text{[eV]}$$
$$a_0 = 5.292 \cdot 10^{-11} \ \text{[m]}$$

3 Quantum Mechanics

3.1 Wave function

$$\psi(\boldsymbol{x}, t) : \mathbb{R}^4 \to \mathbb{C} \qquad \iiint \left|\psi(\boldsymbol{x}, t)\right|^2 d^3r = 1$$
$$\psi(\boldsymbol{x}, t) = a\psi_1(\boldsymbol{x}, t) + b\psi_2(\boldsymbol{x}, t), \qquad |a|^2 + |b|^2 = 1$$
$$P(x)dx = \left|\psi(x)\right|^2 dx \qquad P_{ab} = \int_a^b \left|\psi(x)\right|^2 dx \qquad \langle x \rangle = \int_{-\infty}^{\infty} x \left|\psi(x)\right|^2 dx$$

3.2 The Schrödinger equation

$V(x,t)$ potential | m mass

$$i\hbar \cdot \frac{\partial \Psi}{\partial t}(\boldsymbol{x}, t) = -\frac{\hbar^2}{2m} \cdot \nabla^2 \Psi(\boldsymbol{x}, t) + V(\boldsymbol{x}, t)\Psi(\boldsymbol{x}, t)$$
$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$
$$\Psi = A \cdot e^{i(\boldsymbol{kx} - \omega t)} \qquad \boldsymbol{k} = \begin{bmatrix} k_x & k_y & k_z \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$
$$E = \omega\hbar = \frac{\hbar^2 k^2}{2m}, \qquad k^2 = |k|^2$$
$$V(r) = -\frac{e^2}{4\pi\epsilon_0 |r|}$$

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.

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

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 $\varphi(\boldsymbol{x})$ independent of time and a function $\chi(t)$ independent of space.

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

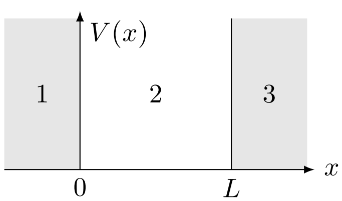
$$-\frac{\hbar^2}{2m}\nabla^2\psi_n(\boldsymbol{x}) + V(\boldsymbol{x})\psi_n(\boldsymbol{x}) = \psi_n(\boldsymbol{x}) \cdot E_n$$

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

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

Requirements: The wave function must be continous, as well as it's derivative

3.2.3 Example: 1D infinite potential well



$$\Psi_1 = \Psi_3 = 0$$

$$-\frac{\hbar^3}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x,t) = E\psi_2(x,t)$$

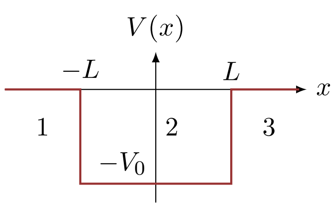
$$\psi_2 = A\sin(kx) + B\cos(kx)$$

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

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

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

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:

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

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

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

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

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

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

   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**

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

   We see that as $x \to -\infty$, 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 it's spacial derivative. Therefore, we have:

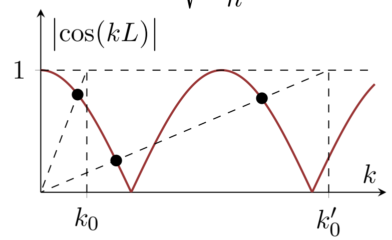
$$\psi_1(-L) = \psi_2(-L) \qquad \psi_2(L) = \psi_3(L)$$

$$\frac{\partial}{\partial x}\psi_1(-L) = \frac{\partial}{\partial x}\psi_2(-L) \qquad \frac{\partial}{\partial x}\psi_2(L) = \frac{\partial}{\partial x}\psi_3(L)$$

Even solutions: only even (cosine) components

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

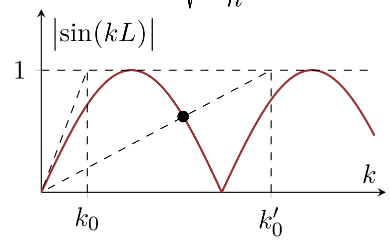
$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$$



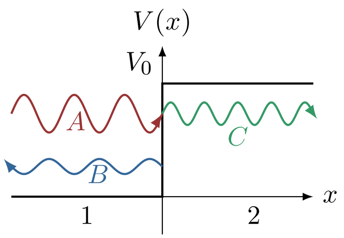
Odd solutions: only odd (sine) components

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

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



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. $\mathbf{E > V_0}$: **Transmission**

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

2. $\mathbf{E < V_0}$: **Complete reflection**

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

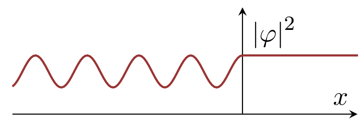
Applying the **initial conditions**, which require the wave function and it's derivative to be continuous at $x = 0$, we get the following expression for A, B, C:

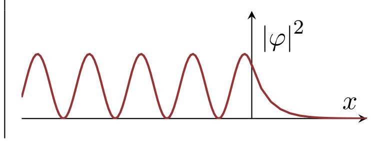
$$\psi_1(x = 0) = \psi_2(x = 0) \qquad \frac{\partial}{\partial x}\psi_1(x = 0) = \frac{\partial}{\partial x}\psi_2(x = 0)$$

$\mathbf{E > V_0}$	$\mathbf{E < V_0}$
$A + B = C$	$A + B = C$
$k_1(A - B) = k_2C$	$A = B$

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

$\mathbf{E > V_0}$	$\mathbf{E < V_0}$
$\lvert\psi_1\rvert^2 = A^2 + B^2 + 2AB\cos(2k_1x)$	$\lvert\psi_1\rvert^2 = 2A^2 \cdot \big(1 - \sin(2k_1x)\big)$
$\lvert\psi_2\rvert^2 = C^2$	$\lvert\psi_2\rvert^2 = C^2 \cdot e^{-2\delta x}$



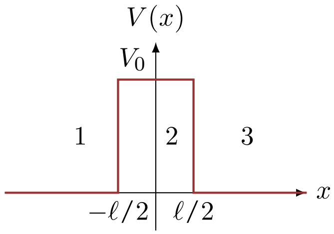


To find the **transmission coefficient** T and the **reflection coefficient** R, we normalize $A = 1$. Then, we can define $B = \sqrt{R}$ and $C = \sqrt{T}$. Then, we can solve for R and T:

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

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:

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

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

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

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

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:

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

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

If $\mathbf{E > V_0}$, the transmission coefficient has a maximum. If $k_2\ell = n\pi \Rightarrow T = 1$ (**resonance**). The minimum of Tu 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**.

$$\langle\psi_1|\psi_2\rangle = \int_{-\infty}^{\infty} \psi_1^*(\boldsymbol{x}, t)\psi_2(\boldsymbol{x}, t) d^3\boldsymbol{x}$$
$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(\boldsymbol{x}, t)\psi(\boldsymbol{x}, t) d^3\boldsymbol{x} = \int_{-\infty}^{\infty} \left|\psi(\boldsymbol{x}, t)\right|^2 d^3\boldsymbol{x} = 1$$

4.2 Fourier Transform

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

5 Observable Measurements, Time-dependence

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

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

Name	Operator	
Position	$\widehat{\boldsymbol{x}} = [\boldsymbol{x}]$	
Momentum	$\widehat{\boldsymbol{p}} = [-i\hbar\boldsymbol{\nabla}]$	$\boldsymbol{\nabla} = \left[\frac{\partial}{\partial x} \quad \frac{\partial}{\partial y} \quad \frac{\partial}{\partial z}\right]^T$
Hamiltonian	$\widehat{H} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x})\right]$	$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Canonical commutation relation: $[\widehat{A}, \widehat{B}] = \widehat{A}\widehat{B} - \widehat{B}\widehat{A}$

5.1 Eigenstates and Eigenvalues

An Observable has an Operator $\widehat{A}$. 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.

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

5.2 Harmonic Oscillator

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

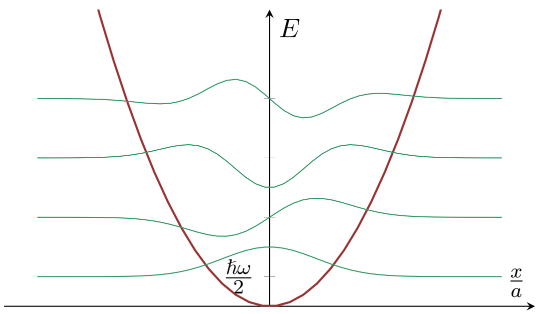
$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x), \quad V(x) = \frac{1}{2}kx^2 = \frac{m\omega^2}{2}x^2$$

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

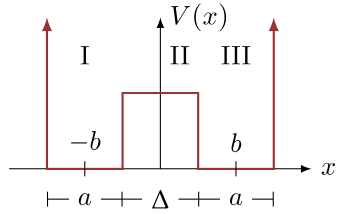
$$a = \sqrt{\frac{\hbar}{m\omega}}, \quad \tilde{x} = \frac{x}{a}, \quad \tilde{E} = \frac{E}{\hbar\omega} \Rightarrow \frac{1}{2}\left[-\frac{\partial^2}{\partial\tilde{x}^2} + \tilde{x}^2\right]\varphi(\tilde{x}) = \tilde{E}\varphi(\tilde{x})$$

Then, the solutions to the equation is:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad \psi(\tilde{x}) = c_n H_n(\tilde{x})e^{-\tilde{x}/2}, \quad H_n(\tilde{x}) = (-1)^n e^{\tilde{x}^2}\cdot\frac{\partial^n}{\partial\tilde{x}^n}e^{-\tilde{x}^2}$$
$$H_0(\tilde{x}) = 1, \quad H_1(\tilde{x}) = 2\tilde{x}, \quad H_2(\tilde{x}) = 4\tilde{x}^2 - 2, \quad H_3(\tilde{x}) = 8\tilde{x}^3 - 12\tilde{x}$$
$$\Psi_n(x) = \frac{1}{\sqrt[4]{\pi}\sqrt{2^n n! a}}\cdot H_n\left(\frac{x}{a}\right)e^{-\frac{x^2}{2a^2}}$$

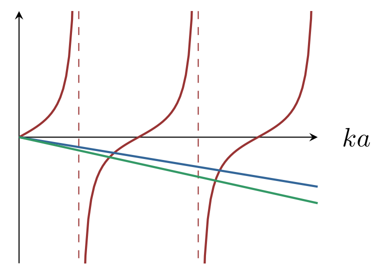


5.3 The coupled quantum well



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: $\boldsymbol{E < V_0}$

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



$$\text{symmetric: } \varepsilon_s = \frac{1 + e^{-\delta\Delta}}{\delta a}$$
$$\text{antisymmetric: } \varepsilon_a = \frac{1 - e^{-\delta\Delta}}{\delta a}$$
$$\tan(ka) = -ka\varepsilon = -ka\frac{1 \pm e^{-\delta\Delta}}{\delta a}$$

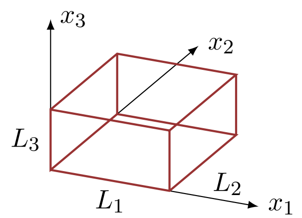
Now, we can create a superposition of both the symmetric and the antisymmetric case:

$$\psi_{s_{\text{I}}} = +\lambda\sin\left(k\left(b - \frac{a}{2} + x\right)\right), \quad \psi_{s_{\text{III}}} = +\lambda\sin\left(k\left(b - \frac{a}{2} + x\right)\right)$$
$$\psi_{a_{\text{I}}} = -\lambda\sin\left(k\left(b - \frac{a}{2} + x\right)\right), \quad \psi_{a_{\text{III}}} = +\lambda\sin\left(k\left(b - \frac{a}{2} + x\right)\right)$$
$$\Psi_L = \frac{1}{\sqrt{2}}(\Psi_s - \Psi_a), \qquad \Psi_R = \frac{1}{\sqrt{2}}(\Psi_s + \Psi_a)$$
$$\Psi_L(x,t) = \frac{1}{\sqrt{2}}e^{-i\omega_s t}\left(\psi_s(x) - e^{-i(\omega_a - \omega_s)t}\psi_a(x)\right)$$
$$\omega_a = \frac{E_a}{\hbar}, \quad \omega_s = \frac{E_a}{\hbar}, \quad E_a - E_s = \frac{\hbar^2\pi^2}{2m\delta a^2}\cdot 8e^{-\delta\Delta}$$

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

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

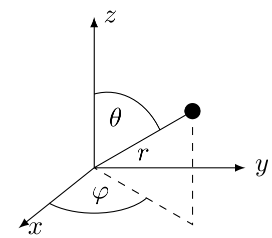
$$E_i^{(n_i)} = n_i^2 \frac{\hbar^2\pi^2}{2mL_i^2}, \qquad \psi_i^{(n_1)} = A \cdot \sin\left(\frac{\pi n_i x}{L_i}\right)$$

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



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

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

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

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

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

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

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:

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

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

$v(\rho)$ 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 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 Useful formulas

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \qquad \int_{0}^{\infty} x e^{-ax^2} dc = \frac{1}{2a} \qquad \int_{-\infty}^{\infty} x^2 e^{-ax^2} = \frac{\sqrt{\pi}}{2a^{3/2}}$$

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

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

7.1 Trigonometry

$$\sin\beta = \frac{b}{a} = \frac{\text{Gegenkathete}}{\text{Hypotenuse}} \qquad \tan\beta = \frac{c}{b} = \frac{\text{Gegenkathete}}{\text{Ankathete}}$$

$$\cos\beta = \frac{c}{a} = \frac{\text{Ankathete}}{\text{Hypotenuse}} \qquad \cot\beta = \frac{c}{b} = \frac{\text{Ankathete}}{\text{Gegenkathete}}$$

$\cos(a + k\cdot 2\pi) = \cos(a) \qquad \sin(a + k\cdot 2\pi) = \sin(a) \qquad (k \in \mathbb{Z})$
$\sin(a \pm b) = \sin(a)\cdot\cos(b) \pm \cos(a)\cdot\sin(b)$
$\cos(a \pm b) = \cos(a)\cdot\cos(b) \mp \sin(a)\cdot\sin(b)$
$\tan(a \pm b) = \dfrac{\tan(a) \pm \tan(b)}{1 \mp \tan(a)\cdot\tan(b)}$
$\sin(2a) = 2\sin(a)\cos(a)$
$\cos(2a) = \cos^2(a) - \sin^2(a) = 2\cos^2(a) - 1 = 1 - 2\sin^2(a)$

$c^2 = a^2 + b^2 - 2\cdot a\cdot b\cdot\cos\gamma$
$\frac{a}{\sin\alpha} = \frac{b}{\sin\beta} = \frac{c}{\sin\gamma} = 2r = \frac{u}{\pi}$
$\sin(a)\sin(b) = \frac{1}{2}(\cos(a-b) - \cos(a+b))$
$\cos(a)\cos(b) = \frac{1}{2}(\cos(a-b) + \cos(a+b))$
$\sin(a)\cos(b) = \frac{1}{2}(\sin(a-b) + \sin(a+b))$

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

$\sin(a) + \sin(b) = 2\cdot\sin\left(\frac{a+b}{2}\right)\cdot\cos\left(\frac{a-b}{2}\right)$
$\sin(a) - \sin(b) = 2\cdot\sin\left(\frac{a-b}{2}\right)\cdot\cos\left(\frac{a+b}{2}\right)$
$\cos(a) + \cos(b) = 2\cdot\cos\left(\frac{a+b}{2}\right)\cdot\cos\left(\frac{a-b}{2}\right)$
$\cos(a) - \cos(b) = -2\cdot\sin\left(\frac{a+b}{2}\right)\cdot\sin\left(\frac{a-b}{2}\right)$
$\tan(a) \pm \tan(b) = \dfrac{\sin(a \pm b)}{\cos(a)\cos(b)}$
$\sin(x) = \frac{1}{2j}\left(e^{jx} - e^{-jx}\right) \qquad \cos(x) = \frac{1}{2}\left(e^{jx} + e^{-jx}\right)$
$e^{x+jy} = e^x \cdot e^{jy} = e^x \cdot \left(\cos(y) + j\sin(y)\right)$
$e^{j\pi} = e^{-j\pi} = -1$

8 Periodic Table of the Elements

Z eneg ss
Sy
Name
saw

Z = atomic number; eneg = electronegativity; ss = subshell; Sy = Symbol, Name = element name, saw = standard atomic weight

1 2.20 1s **H** Hydrogen 1.00784–1.00811																	2 1s **He** Helium 4.002602(2)
3 0.98 2s **Li** Lithium 6.938–6.997	4 1.57 2s **Be** Beryllium 9.0121831(5)											5 2.04 2p **B** Boron 10.806–10.821	6 2.55 2p **C** Carbon 12.0096–12.0116	7 3.04 2p **N** Nitrogen 14.00643–14.00728	8 3.44 2p **O** Oxygen 15.99903–15.99977	9 3.98 2p **F** Fluorine 18.998403163(6)	10 2p **Ne** Neon 20.1797(6)
11 0.93 3s **Na** Sodium 22.98976928(2)	12 1.31 3s **Mg** Magnesium 24.304–24.307											13 1.61 3p **Al** Aluminium 26.9815385(7)	14 1.90 3p **Si** Silicon 28.084–28.086	15 2.19 3p **P** Phosphorus 30.973761998(5)	16 2.58 3p **S** Sulphur 32.059–32.076	17 3.16 3p **Cl** Chlorine 35.446–35.457	18 3p **Ar** Argon 39.948(1)
19 0.82 4s **K** Potassium 39.0983(1)	20 1.00 4s **Ca** Calcium 40.078(4)	21 1.36 3d **Sc** Scandium 44.955908(5)	22 1.54 3d **Ti** Titanium 47.867(1)	23 1.63 3d **V** Vanadium 50.9415(1)	24 1.66 3d* **Cr** Chromium 51.9961(6)	25 1.55 3d **Mn** Manganese 54.938044(3)	26 1.83 3d **Fe** Iron 55.845(2)	27 1.88 3d **Co** Cobalt 58.933194(4)	28 1.91 3d **Ni** Nickel 58.6934(4)	29 1.90 3d* **Cu** Copper 63.546(3)	30 1.65 3d **Zn** Zinc 65.38(2)	31 1.81 4p **Ga** Gallium 69.723(1)	32 2.01 4p **Ge** Germanium 72.630(8)	33 2.18 4p **As** Arsenic 74.921595(6)	34 2.55 4p **Se** Selenium 78.971(8)	35 2.96 4p **Br** Bromine 79.901–79.907	36 3.00 4p **Kr** Krypton 83.798(2)
37 0.82 5s **Rb** Rubidium 85.4678(3)	38 0.95 5s **Sr** Strontium 87.62(1)	39 1.22 4d **Y** Yttrium 88.90584(2)	40 1.33 4d **Zr** Zirconium 91.224(2)	41 1.6 4d* **Nb** Niobium 92.90637(2)	42 2.16 4d* **Mo** Molybdenum 95.95(1)	43 1.9 4d **Tc** Technetium (98)	44 2.2 4d* **Ru** Ruthenium 101.07(2)	45 2.28 4d* **Rh** Rhodium 102.90550(2)	46 2.20 4d* **Pd** Palladium 106.42(1)	47 1.93 4d* **Ag** Silver 107.8682(2)	48 1.69 4d **Cd** Cadmium 112.414(4)	49 1.78 5p **In** Indium 114.818(1)	50 1.96 5p **Sn** Tin 118.710(7)	51 2.05 5p **Sb** Antimony 121.760(1)	52 2.1 5p **Te** Tellurium 127.60(3)	53 2.66 5p **I** Iodine 126.90447(3)	54 2.60 5p **Xe** Xenon 131.293(6)
55 0.79 6s **Cs** Cesium 132.90545196(6)	56 0.89 6s **Ba** Barium 137.327(7)	57-71 ***** Lanthanides	72 1.3 5d **Hf** Halfnium 178.49(2)	73 1.5 5d **Ta** Tantalum 180.94788(2)	74 2.36 5d **W** Tungsten 183.84(1)	75 1.9 5d **Re** Rhenium 186.207(1)	76 2.2 5d **Os** Osmium 190.23(3)	77 2.20 5d **Ir** Iridium 192.217(3)	78 2.28 5d* **Pt** Platinum 195.084(9)	79 2.54 5d* **Au** Gold 196.966569(5)	80 2.00 5d **Hg** Mercury 200.592(3)	81 1.62 6p **Tl** Thallium 204.382–204.385	82 1.87 6p **Pb** Lead 207.2(1)	83 2.02 6p **Bi** Bismuth 208.98040(1)	84 2.0 6p **Po** Polonium (209)	85 2.2 6p **At** Astatine (210)	86 2.2 6p **Rn** Radon (222)
87 0.7 7s **Fr** Francium (223)	88 0.9 7s **Ra** Radium (226)	89-103 ****** Actinides	104 6d **Rf** Rutherfordium (261)	105 6d **Db** Dubnium (268)	106 6d **Sg** Seaborgium (269)	107 6d **Bh** Bohrium (270)	108 6d **Hs** Hassium (269)	109 6d **Mt** Meitnerium (278)	110 6d **Ds** Darmstadtium (281)	111 6d **Rg** Roentgenium (282)	112 6d **Cn** Copernicium (285)	113 7p **Nh** Nihonium (286)	114 7p **Fl** Flerovium (289)	115 7p **Mc** Moscovium (289)	116 7p **Lv** Livermorium (293)	117 7p **Ts** Tennessine (294)	118 7p **Og** Oganesson (294)

*	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 LaTeX Periodic Table. © 2017 Paul Danese

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