PHYS 250

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Light Year: years $\times c$
1 eV = 1.6 $\times 10^{-19}$ J
Planck's Constant: $h = 6.626 \times 10^{-34}$ J·s, $hc = 1240$ eV·nm
Electron Rest Mass: 9.11×10^{-31} kg, 0.511×10^{6} MeV/c^2

$$1\,\text{MeV/c}^2 = \frac{1.6 \times 10^{-19} \times 10^{6}}{(3 \times 10^{8})^2}\ \text{kg}$$

$$(a+k)^n = \sum_{k=0}^{n} \frac{n!}{(n-k)!k!} a^{n-k} x^k \qquad \textbf{Binomial Expansion}$$

Vector Calculus

Given $f(x, y, z)$, df is

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz \qquad \textbf{Total Differential}$$

Spherical gradient

$$\boldsymbol{\nabla} = \left\langle \frac{\partial}{\partial r}, \frac{1}{r}\frac{\partial}{\partial \theta}, \frac{1}{\sin(\theta)}\frac{\partial}{\partial \phi} \right\rangle$$

Spherical Laplacian

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

Orthogonality

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right) dx = \begin{cases} 0 & n \neq m \\ \frac{L}{2} & n = m \end{cases} \qquad (1)$$

$$\int_0^L \cos\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right) dx = \begin{cases} 0 & n \neq m \\ \frac{L}{2} & n = m \neq 0 \\ L & n = m = 0 \end{cases} \qquad (2)$$

Fourier Analysis

$$\psi(x) = \int_{-\infty}^{\infty} a(k) e^{ikx}\, dk$$

$$a(k') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \psi(x) e^{-ik'x}\, dx$$

Electromagnetism

Wave Equation

$$u_{xx} = \frac{\mu}{T} u_{tt} \qquad \frac{\mu}{T} = \frac{1}{V^2}$$

μ is mass per unit length, T is tension, V is built in velocity

Coulomb's Law

$$\mathbf{E} = \frac{1}{4\pi\epsilon_0}\frac{Q}{r^2}\hat{\mathbf{r}}$$

Lorentz Force

$$\mathbf{F} = q\mathbf{v} \times \mathbf{B}$$

Maxwell's Equations

Gauss's Law

$$\iint_S \mathbf{E} \cdot d\mathbf{A} = \frac{Q_{encl}}{\epsilon_0} \qquad \nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

Gauss's Law for Magnetic Fields

$$\iint_S \mathbf{B} \cdot d\mathbf{A} = 0 \qquad \nabla \cdot \mathbf{B} = 0$$

ρ is charge volume density

Faraday's Law

$$\oint \mathbf{E} \cdot d\mathbf{l} = -\frac{d\Phi_B}{dt} \qquad \nabla \times \mathbf{E} = -\mathbf{B}_t$$

Ampere's Law

$$\oint \mathbf{B} \cdot d\mathbf{l} = \mu_0 \left(i_C + \epsilon_0 \frac{d\Phi_E}{dt}\right) \qquad \nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \epsilon_0 \mu_0 \mathbf{E}_t$$

$\mathbf{J}$ is current per area

EM Waves

Poynting Vector

$$\mathbf{S} = \frac{1}{\mu_0}\mathbf{E} \times \mathbf{B} \qquad [\text{W/m}^2]$$

gives the rate of energy flow, in the direction of the wave

Energy Densities

$$U_E = \frac{1}{2}\epsilon_0 E^2 = U_M = \frac{1}{2\mu_0}B^2$$

$$U_{tot} = \epsilon_0 E^2 = \frac{B^2}{\mu_0}$$

$$E = \frac{1}{\sqrt{\mu_0 \epsilon_0}} B = cB$$

Momentum Density

$$\mathbf{P} = \epsilon_0 \mathbf{E} \times \mathbf{B} = \epsilon_0 \mu_0 \mathbf{S} = \frac{\mathbf{S}}{c^2} \qquad [\text{N·s/m}^3]$$

Radiation Pressure

$$\mathbf{P}c = \frac{\mathbf{S}}{c} \qquad \text{N/m}^2$$

Interference

Two slit Maxima

$$d \sin\theta = m\lambda$$

d is distance between the slits, θ is angle from horizontal, m is an integer, λ is wavelength

Single Slit Minima

$$\frac{w}{2}\sin(\theta) = m\frac{\lambda}{2}$$

w is the width of the slit, θ is the angle of the central beam from the horizontal.

Special Relativity

1. Pick a moving frame, and a rest frame.
2. Solve via events. Use the Lorentz transform to transform from the rest form into the moving frame.
3. Account of direction of moving frame as seen in the stationary frame

Consider relativity when kinetic energy is a large fraction of the rest energy.

$$\beta = \frac{u}{c} \qquad \gamma = \frac{1}{\sqrt{1-\beta^2}}, \gamma \geq 1$$

$\boldsymbol{u}$: speed of moving frame relative to stationary frame; $\boldsymbol{c}$: 3.00 $\times 10^8$ m/s

$$\gamma^2\left(1-\beta^2\right) = 1$$

Approximations

$$\gamma \approx 1 + \frac{\beta^2}{2} \qquad \text{for low } \beta$$

$$\beta \approx 1 - \frac{1}{2\gamma^2} \qquad \text{for high } \gamma$$

To the rest frame, time periods are longer in moving frame, moving objects are shorter.

$$t' = t\gamma \qquad \text{Time dilation}$$

$$l' = l/\gamma \qquad \text{Length contraction}$$

Warning: these can only be applied when considering length and time measurements to be a *single event*.

Lorentz Transformation

Assuming u is in the x direction, the space-time coordinates of a moving frame S' is related to a stationary frame S by

$$x' = \gamma(x - \beta ct) \qquad x' = \gamma(x - vt)$$

$$y' = y$$

$$z' = z$$

$$ct' = \gamma(ct - \beta x) \qquad t' = \gamma\left(t - \frac{vx}{c^2}\right)$$

Velocity Addition

The speed v an object in a moving frame relative to the stationary frame is

$$v = \frac{v' + u}{1 + v'u/c^2}$$

v': speed of moving object in moving frame relative to the frame
u: speed of moving frame relative to stationary frame

Relativistic Doppler Effect

Longitudinal

$$f_{\text{obs}} = f_{\text{sce}}\sqrt{\frac{1-\beta}{1+\beta}} \qquad \textbf{Source moving away}$$

$$f_{\text{obs}} = f_{\text{sce}}\sqrt{\frac{1+\beta}{1-\beta}} \qquad \textbf{Source moving closer}$$

Transverse

$$f_{\text{obs}} = f_{\text{sce}}\sqrt{1-\beta^2}$$

Source moving closer to observer *blueshifts* frequency. Source moving away *redshifts* frequency.

Proper time τ

As measured by a clock moving with the moving object. Everyone sees that clock, so τ is same in all frames

$$\gamma\tau = t$$

Proper velocity w

$$w = \frac{dx}{d\tau} = \frac{dx}{dt}\frac{dt}{d\tau} = v\gamma$$

Relativistic Momentum

In a single frame, relativistic momentum is conserved

$$\sum P_i = \sum P_f$$

The conservation of momentum and energy:

$$\mathbf{p} = \gamma_{\mathbf{v}} m_0 \mathbf{v}$$

$$p = \beta\gamma m_0 c = \gamma m_0 v$$

Has units of [eV/c]

Relativistic Energy

Total relativistic energy is conserved in any single frame.

Total energy	$E = \gamma m_0 c^2$
Kinetic energy	$K = \gamma m_0 c^2 - m_0 c^2$

Since γ is $\propto v$, we can compare particle speeds by comparing γ.

Energy-Momentum Relation

$$E^2 = p^2c^2 + (m_0c^2)^2$$

Four-Vector Notation

$$\begin{aligned}\mathbf{A} &= [ct_A, x_A, y_A, z_A] \\ &= [ct_A, \mathbf{x}]\end{aligned}$$

Dot Product:

$$\mathbf{A}\cdot\mathbf{B} = A_1B_1 - [A_2B_2 + A_3B_3 + A_3B_3]$$
$$ct_a ct_b - \mathbf{x}_A \cdot \mathbf{x}_B$$

Distributivity:

$$(\mathbf{A}+\mathbf{B})^2 = \mathbf{A}^2 + 2\mathbf{A}\cdot\mathbf{B} + \mathbf{B}^2$$

Invariance:

$$\mathbf{A}\cdot\mathbf{B} = \mathbf{A}'\cdot\mathbf{B}'$$

Lorentz Transformation:

$$\begin{bmatrix} ct' \\ x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} ct \\ x \\ y \\ z \end{bmatrix}$$

Position Four-Vector:

$$\begin{aligned}\mathbf{X}(t) &= [ct, v_xt, v_yt, v_zt] \\ &= t\,[c, v_x, v_y, v_z] \\ &= \gamma\tau\,[c, \mathbf{v}]\end{aligned}$$

Proper Velocity Four-Vector:

$$\mathbf{V} = \frac{d\mathbf{X}}{d\tau} = \gamma\,[c, \mathbf{V}]$$

Momentum Four-Vector:

$$\mathbf{P} = m_0\mathbf{V} = [m_0c\gamma, m_0\gamma\mathbf{v}] = \left[\frac{E}{c}, \mathbf{p}\right]$$

$$\mathbf{P}^2 = (mc)^2$$

Energy-Momentum Invariance:

$$\mathbf{P}\cdot\mathbf{P} = \mathbf{P}'\cdot\mathbf{P}'$$

$$\frac{E^2}{c^2} - \mathbf{p}^2 = \frac{E'^2}{c^2} - \mathbf{p}'^2$$

1. Establish energy momentum 4-vectors
2. Use distributive property to expand squared 4-vector sums
3. Use $\mathbf{P}^2 = m^2$ $(c=1)$ to rewrite expanded terms

Quantization

Photon energy

$$E = pc = hf = \frac{hc}{\lambda}$$

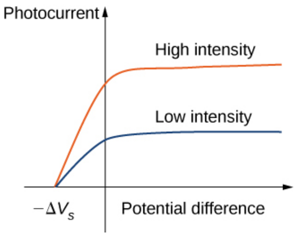
Photoelectric Effect

Maximum photoelectron kinetic energy

$$qV_{\text{stop}} = hf - q\phi_{\text{work}} \Rightarrow hf_{\text{cutoff}} = q\phi_{\text{work}}$$

where q is the electron charge, $q\phi_{\text{work}}$ is the work function. V_{stop} is the magnitude of the potential for which there is no current

- V_{stop} is independent of photon intensity
- Doubling photon energy more than doubles photoelectron energy
- For a single electron atom, only photons with energy equal to energy difference between $n=1$ and $n=m$ will be absorbed



Minimum X-ray Wavelength

$$qV = hf_{\text{max}} = \frac{hc}{\lambda_{\text{min}}}$$

Compton Scattering

A photon of wavelength λ collides with a stationary electron results in a Compton electron and scattered photon of λ'

$$\lambda' = \lambda + \frac{h}{mc}(1-\cos(\theta))$$

Relative frequency change

$$\frac{\Delta f}{f'} = \frac{f'-f}{f'} = \frac{hf}{mc^2}(\cos(\theta)-1)$$

- $\theta = 0$ is no interaction
- Momentum must be conserved

Quantum Mechanics

Rydberg Formula

Predicts spectrum for single electron atoms or ions

$$\frac{hc}{\lambda} = hcRZ^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

where $R = 1/91.13$ nm, and $n_2 > n_1$

Bohr Model

Bohr atoms are planar. Bohr quantized angular momentum:

$$L = rmv = n\hbar$$

Bohr orbital energy	$E = -13.6\,\text{eV}\frac{Z^2}{n^2}$
Bohr radius	$r = 52.97\,\text{pm}\frac{n^2}{Z}$

$n=1$ is ground state, $n=2$ is first excited state. Particles in circular orbits are always accelerated and release radiation, so the orbits cannot be stable.

Moseley's Law

For $2 \to 1$ transitions ($K\alpha$ lines)

$$E = 13.6\,\text{eV}(Z-1)^2\left(\frac{1}{1} - \frac{1}{2^2}\right) = 10.2\,\text{eV}(Z-1)^2$$

De Broglie Waves

$$\lambda = \frac{h}{p} \to p = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k$$

Bragg's Law

For a lattice plane spacing of d, and a incident angle of θ the reflections will be in phase if the extra path length is integer multiple of half wavelength

$$2d\sin(\theta) = n\lambda$$

If λ and d is unknown, but we can measure θ, we can use two x-ray tubes (with peak at λ_1 and λ_2), and two crystals (of spacing d_1 and d_2), then we can find the wavelengths and spacing by

$$\begin{bmatrix} 1 & 0 & -2\sin(\theta_{11}) & 0 \\ 1 & 0 & 0 & -2\sin(\theta_{12}) \\ 0 & 1 & -2\sin(\theta_{21}) & 0 \\ 0 & 1 & 0 & -2\sin(\theta_{22}) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ d_1 \\ d_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- Applies to any radiation (photons, electrons, ...)

Classical Kinetic Energy

$$E = \frac{1}{2}mv^2 = \frac{1}{2}\frac{(mv)^2}{m} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

A free particle only has kinetic energy

Free Particle Schrodinger Equation

$$i\hbar\psi_t = \frac{-\hbar^2}{2m}\psi_{xx}$$

has a plane wave solution

$$\begin{aligned} \psi(x,t) &= A\exp\left(ik\left[x - \frac{\hbar k}{2m}t\right]\right) \\ &= A\exp\left(i\left[\pm kx - \omega t\right]\right) \\ &= A\left(\cos(\pm kx - \omega t) + i\sin(\pm kx - \omega t)\right) \end{aligned}$$

where $k = p/\hbar$, $\omega = 2\pi f = E/\hbar$.

- Plane wave: infinite σ_x; small σ_p
- Wave packet: small σ_x; larger σ_p than plane wave

Phase velocity is the speed of the peaks in the wave packet.
Group velocity is the speed of the wave packet.
Since $E = \hbar\omega$, we have

$$v_{\text{group}} = \frac{d\omega}{dk} = \frac{d}{dk}\left[\frac{\hbar k^2}{2m}\right]$$

Wave Packets

Orthogonality of complex exponentials

$$\int_{-L}^{L} e^{imx}e^{-inx}\,dx = 2\pi\delta_{nm}$$

The wave packet solution is linear combination of a continuous number of functions with different k.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{kx - \frac{\hbar k^2}{2m}t}\,dk$$

where $\phi(k)$ are given by

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)e^{-ikx}\,dx$$

A gaussian wave packet has minimum uncertainty. At $t = 0$.

$$\psi(x, t=0) = \exp\left(\frac{-x^2}{2\sigma_x^2}\right)\exp(ik_0 x)$$

has fourier transform

$$a(k) = \frac{1}{\sqrt{2\pi}\sigma_k}\exp\left(\frac{-(k_0 - k)^2}{2\sigma_k^2}\right),$$

where $\sigma_k = \frac{1}{\sigma_x}$. Since $p = \hbar k$, $\sigma_p = \hbar/\sigma_x$

Conjugate Squared Solution

Is the probability density function of finding the particle at some region.

$$P = \int_{x_1}^{x_2}\psi\psi*\,dx$$

The velocity of $\psi\psi*$ is the group velocity. To normalize $\psi\psi*$, divide it by $\sqrt{V}$, where

$$V = \int_{-\infty}^{\infty}\psi\psi*\,dx$$

Gaussian Function

$G(x)$ has the normalization factor $1/(\sigma\sqrt{2\pi})$

$$G(x) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(\frac{-x^2}{2\sigma^2}\right)$$

has unit area, zero first moments, and second moment equal to σ^2. $G^2(x)$ has standard deviation equal to original $\sigma/\sqrt{2}$.

HW at HM $\quad x = 1.177\sigma = x = \sigma\sqrt{2\ln(2)}$

Uncertainty Principle

Applying to probability density functions

$$\begin{aligned} \Delta x\Delta p &\geq \hbar/2 \\ \Delta E\Delta t &\geq \hbar/2 \end{aligned}$$

When applying to wave functions,

$$\sigma_x\sigma_k = 1 \Rightarrow \sigma_x\sigma_p = \hbar$$

Constant Potential Schrodinger Equation

$$i\hbar\psi_t = \frac{-\hbar^2}{2m}\psi_{xx} + V\psi$$

where V is a constant. It has a plane wave solution

$$\begin{aligned} \psi(x,t) &= A\exp\left(i\left[\pm kx - \omega t\right]\right) \\ &= A\exp\left(i\left[\pm\frac{p}{\hbar}x - \frac{E_k + V}{\hbar}t\right]\right) \end{aligned}$$

Solution by separation of variables

Let $\psi = X(x)T(t)$, and we have

$$T(t) = \exp\left(-i\frac{E}{\hbar}t\right) = \exp\left(-i\omega t\right)$$

and

$$E = \frac{-\hbar^2}{2m}\frac{X''}{X} + V$$

where E is a constant.

- $E > V_{min}$ for every normalizable solution

Step Potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V & x \geq 0 \end{cases}$$

For the eigenvalue problem in X ($X = \psi^x$), the boundary conditions are

$$\begin{aligned} \left[\psi_I^x + \psi_R^x\right](0) &= \left[\psi_T^x\right](0) \\ \left[\frac{d}{dx}\psi_I^x + \frac{d}{dx}\psi_R^x\right](0) &= \left[\frac{d}{dx}\psi_T^x\right](0) \end{aligned}$$

where I is initial, R is reflected, T is transmitted.

At the step, some portion of the wave bounces back with $k_R = -k_I$, some portion is transmitted

$$\begin{aligned} \psi_I^x(x) &= A\exp\left(ik_I x\right) \\ \psi_R^x(x) &= B\exp\left(ik_R x\right) = B\exp\left(-ik_I x\right) \\ \psi_T^x(x) &= C\exp\left[ik_T x\right] \end{aligned}$$

If $V > 0$, then $k_T < k_I$. If $V < 0$ then $k_T > k_I$.

$$k_I = \frac{\sqrt{2mE}}{\hbar} \qquad k_T = \frac{\sqrt{2m(E - V)}}{\hbar}$$

$$A = 1 \qquad B = \frac{k_I - k_T}{k_I + k_T} \qquad C = \frac{2k_I}{k_I + k_T}$$

Reflection probability:

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_I - k_T}{k_I + k_T}\right|^2$$

Transmission Probability:

$$T = 1 - R$$

Potential Barrier

$$V(x) = \begin{cases} 0 & x < 0 \\ V & 0 \le x \le w \\ 0 & x > w \end{cases}$$

$x < 0$, some wave is going to $+\infty$, some is reflected.

$$\psi_I^x = A\exp(ik_I x)$$
$$\psi_R^x = B\exp(-ik_I x)$$

$0 \le x \le w$, opposite travelling waves

$$\psi_{B+}^x = D\exp(ik_B x)$$
$$\psi_{B-}^x = F\exp(-ik_B x)$$

$x > w$, some wave transmitted

$$\psi_T^x = C\exp(ik_I x)$$

With boundary conditions

$$[\psi_I^x + \psi_R^x](0) = [\psi_{B-}^x + \psi_{B+}^x](0)$$
$$\left[\frac{d}{dx}\psi_I^x + \frac{d}{dx}\psi_R^x\right](0) = \left[\frac{d}{dx}\psi_{B-}^x + \frac{d}{dx}\psi_{B+}^x\right](0)$$

$$[\psi_I^x + \psi_R^x](w) = [\psi_{B-}^x + \psi_{B+}^x](w)$$
$$\left[\frac{d}{dx}\psi_I^x + \frac{d}{dx}\psi_R^x\right](w) = \left[\frac{d}{dx}\psi_{B-}^x + \frac{d}{dx}\psi_{B+}^x\right](w)$$

so

$$A + B = D + F$$
$$ik_I(A - B) = ik_B(D - F)$$
$$D\exp(ik_B w) + F\exp(-ik_B w) = C\exp(ik_I w)$$
$$ik_B\left[D\exp(ik_B w) - F\exp(-ik_B w)\right] = ik_I C\exp(ik_I w)$$

Approximate Tunnelling

For $V > E$, let $-a$ be $V(-a) = E$ and $V \le E$ for $x < -a$, the wave function evaluated at some $x > -a$ within the potential barrier is

$$\psi(x) = \exp\left(-\int_{-a}^{x}\sqrt{\frac{2m}{\hbar^2}\left[V(x) - E\right]}\,dx\right)$$

The transmitted wave through the barrier $-a < x < a$ has coefficient $\psi(a)$.

Infinite Square Well

Consider the Potential

$$V(x) = \begin{cases} 0 & 0 \le x \le w \\ \infty & \text{otherwise} \end{cases}$$

$$\psi(x) = \sqrt{\frac{2}{w}}\sin(k_n x) \qquad E_n = \frac{\hbar^2 k_n^2}{2m} \qquad k_n = \frac{n\pi}{w}$$

The most general solution is

$$\Psi = \sum_{n=1}^{\infty} c_n\psi_n(x)\exp(-iEt/\hbar)$$

where

$$c_n = \sqrt{\frac{2}{w}}\int_0^w \sin(k_n x)\,\Psi(x,0)\,dx$$

When we switch to

$$V(x) = \begin{cases} \infty & x = -w/2 \\ 0 & -w/2 < x < w/2 \\ \infty & x = w/2 \end{cases}$$

The solutions are

$$\psi = \begin{cases} A_n\cos(\frac{n\pi x}{w}) & \text{odd}(n) \\ B_n\sin(\frac{n\pi x}{w}) & \text{even}(n) \end{cases}$$

Finite Square Well

When $E < V$, there are a finite number bound states.

$$V(x) = \begin{cases} -V_0 & -a \le x \le a \\ 0 & |x| > a \end{cases}$$

We define

$$\kappa = \frac{\sqrt{-2mE}}{\hbar} \qquad l = \frac{\sqrt{2m(E + V_0)}}{\hbar}$$

For $x < -a$, we have

$$\psi(x) = B\exp(\kappa x)$$

For $|x| > a$, the solutions are either even or odd.

$$\psi(x) = D\cos(lx) \quad \text{or} \quad \psi(x) = F\sin(lx)$$

For $x > a$,

$$\psi(x) = G\exp(-\kappa x)$$

ψ and $\psi_{,x}$ must be continuous at a and $-a$.
Define $z = la$ and $z_0 = a\sqrt{2mV_0}/\hbar$, the bound state energies are indirectly given by the intersections of

$$\sqrt{(z_0/z)^2 - 1} \qquad \tan(z) \qquad -\cot(z)$$

Let E_0 be the ground state energy of a infinite well with width a. The approximate number of bound states for a finite well of depth $-V_0$ is given by

$$n = \sqrt{\frac{V_0}{E_0}}$$

Drawing Wave Functions in Square Wells

- Sinusoidal when $E > V$, decaying exponential when $V > E$
- Greater $|E - V|$ means faster exponential decays, smaller wave function amplitude and wavelength.
- The number of maxima and minima equals the principle quantum number

Harmonic Oscillator Potential

$$E = -\frac{\hbar^2}{2m}\psi_{xx}^x + \frac{1}{2}kx^2$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad \omega = \sqrt{\frac{k}{m}}$$

Has equally space energy levels, non zero ground state energy. The non-normalized stationary states

$$\psi_n(x) = \exp\left(\frac{-x^2}{2b^2}\right)H_n(x)$$

where $1/b^2 = \sqrt{km}/\hbar$.

3D Schrodinger

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

3D Free Particle Solution

$$\psi(\mathbf{x},t) = \exp\left(i\left[\mathbf{k}\cdot\mathbf{x} - \omega t\right]\right)$$

where $E = \mathbf{p}^2/2m = (\hbar\mathbf{k})^2/2m = \hbar\omega$. The k-vector points in the direction the particle is moving.

3D Separation of Variables

Let $\psi = X(\mathbf{x})T(t)$, and we have

$$T(t) = \exp\left(-i\frac{E}{\hbar}t\right) = \exp(-i\omega t)$$

and

$$EX(\mathbf{x}) = \frac{-\hbar^2}{2m}\nabla^2 X(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x})$$

where E is a constant.

3D Infinite Square Well

$$V(\mathbf{x}) = \begin{cases} 0 & \mathbf{x} \in \Omega \\ \infty & \mathbf{x} \notin \Omega \end{cases} \qquad \Omega = \begin{cases} 0 < x < a \\ 0 < y < b \\ 0 < z < c \end{cases}$$

The boundary condition: wave function is zero everywhere on the surface of the box. The solution is

$$\psi(\mathbf{x}) = \sin(k_x x)\sin(k_y y)\sin(k_z z)$$

where

$$\mathbf{k} = \left\langle\frac{n_x\pi}{a}, \frac{n_y\pi}{b}, \frac{n_z\pi}{c}\right\rangle$$

The energy eigenvalues are

$$E = \frac{(\hbar\mathbf{k})^2}{2m}$$

$n > 0$.

3D Harmonic Oscillator

$$V(x) = \frac{1}{2}\left(k_x x^2 + k_y y^2 + k_z z^2\right)$$

Separates into 3 independent oscillator equations

$$\frac{-\hbar^2}{2m}\frac{\partial^2 X}{\partial x^2} + \frac{1}{2}k_x x^2 X(x) = E_x X(x)$$
$$\frac{-\hbar^2}{2m}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{2}k_y y^2 Y(y) = E_y Y(y)$$
$$\frac{-\hbar^2}{2m}\frac{\partial^2 Z}{\partial z^2} + \frac{1}{2}k_z z^2 Z(z) = E_z Z(z)$$

where $E = E_x + E_y + E_z$. The non-normalized stationary states are Gaussian times hermite polynomials

$$\psi_n(x) = \exp\left(\frac{-x^2}{2b^2}\right) H_n(x)$$

where $1/b^2 = \sqrt{km}/\hbar$. When spring constants differ

$$E = \frac{\hbar}{\sqrt{m}}\left[\left(n_x + \frac{1}{2}\right)\sqrt{k_x} + \left(n_y + \frac{1}{2}\right)\sqrt{k_y} + \left(n_z + \frac{1}{2}\right)\sqrt{k_z}\right]$$

when spring constants are all the same

$$E = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\sqrt{\frac{k}{m}}$$

Legendre Polynomials

The degree ℓ of the polynomials determine parity of the function

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell \left(x^2 - 1\right)^\ell$$

Associated Legendre functions

$$P_\ell^m = (-1)^m \left(1 - x^2\right)^{m/2}\left(\frac{d}{dx}\right)^m P_\ell(x)$$

If $m > \ell$ then the Legendre functions is zero. So there is $2\ell + 1$ values of m for some ℓ if we want P_ℓ^m to be nonzero.

Spherical Harmonics

With normalization factor

$$Y_\ell^m(\theta, \phi) = \sqrt{\frac{2\ell + 1}{4\pi}\frac{(\ell - m)!}{(\ell + m)!}} e^{im\phi} P_\ell^m(\cos(\theta))$$

The spherical harmonics are potential independent.

Spherical Schrodinger

Separation of variables of $\psi = R(r)Y(\theta, \phi)$ gives

$$\left[r^2 R_r\right]_r - \frac{2mr^2}{\hbar^2}[V(r) - E]R = R\ell(\ell + 1)$$
$$\frac{-1}{\sin(\theta)}\left[\sin(\theta) Y_\theta\right]_\theta - \frac{1}{\sin^2(\theta)} Y_{\phi\phi} = Y\ell(\ell + 1)$$

where

$$Y = Ae^{im\phi} P_\ell^m(\cos(\theta))$$

such that $m = 0, \pm 1, \pm 2, \ldots$, and $\ell \geq 0$. Using spherical harmonics can be written as

$$Y = AY_\ell^m$$

The R equation can be rewritten using change of variables $R = u/r$. We get the radial equation

$$\frac{-\hbar^2}{2m} u_{rr} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell + 1)}{r^2}\right] u = Eu$$

The effective potential is

$$V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell + 1)}{r^2}$$

The additional term to the potential represents kinetic energy due to angular momentum.

$$\frac{p^2}{2m} = \frac{(rp)^2}{2mr^2} = \frac{L^2}{2mr^2}$$

The full solution is

$$\psi(r, \theta, \phi) = A\frac{u(r)}{r} Y_m^\ell(\theta, \phi)$$

For the function to be normalizable

$$\lim_{r \to \infty} u(r) = 0 \qquad \lim_{r \to 0+} u(r) = 0$$

$\ell = 0, 1, 2, 3, 4$ correspond to s,p,d,f,g waves or states. The normalization condition is

$$\int |\psi|^2 r^2 \sin(\theta)\, dr\, d\theta\, d\phi = 1$$

3D Infinite Spherical Well

$$V(r) = \begin{cases} 0, & r \leq a \\ \infty & r > a \end{cases}$$

Has boundary condition $u(a) = 0$. For $\ell = 0$, the radial equation has solution

$$u_{N0} = \sqrt{\frac{2}{a}} \sin\left(\frac{N\pi r}{a}\right)$$

for $N = 1, 2, 3, \ldots$. The full wave function is

$$\psi_{N00} = A\frac{u_{N0}}{r} Y_0^0(\theta, \phi)$$

since there can only be a single m value for $\ell = 0$. The energy eigenvalues for $\ell = 0$ are are

$$E_{N0} = \frac{N^2(\hbar\pi)^2}{2ma^2}$$

Spherical Finite Well

No bound states when

$$V_0 a^2 < \frac{\pi^2\hbar^2}{8m}$$

Spherical Harmonic Oscillator

$\ell = 0$ and identical spring constants, the radial equation has solution the same as the stationary state of the 1D harmonic oscillator.

$n = 0, 2, 4, \ldots$ cannot be used since the solution is non zero at $r = 0$. (The even ordered Hermite polynomials are non zero at $r = 0$.)

Non-normalized stationary state is

$$\psi(r, \theta, \phi)_{n00} = AH_n \exp\left(\frac{-r^2}{2b^2}\right) Y_0^0(\theta, \phi)$$

For $\ell > 0$,

$$u(r) = F(r)\exp\left(\frac{-r^2}{2b^2}\right)$$

and

$$E = \hbar\sqrt{\frac{k}{m}}\left(p + \frac{1}{2}\right)$$

if

$$p = \begin{cases} \ell + 1 & F(r) = r^p \\ > \ell + 1 & F(r) = r^p + \text{lower powers of r} \end{cases}$$

The Hydrogen Atom

$$\psi_{nlm}(r, \theta, \phi) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n - \ell - 1)!}{2n(n + \ell)!}} \exp\left(\frac{-r}{na}\right) \cdot \left(\frac{2r}{na}\right)^\ell L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na}\right) Y_\ell^m(\theta, \phi)$$

where L_q^p are the associated the Laguerre polynomials

$$L_q^p(x) = (-1)^p\left(\frac{d}{dx}\right)^p L_{q+p}(x)$$

and L_q are the q^{th} Laguerre polynomials

$$L_q = \frac{e^x}{q!}\left(\frac{d}{dx}\right)^q \left(e^{-x} x^q\right)$$

and a is the Bohr radius (52.97 pm).

For any n (principal quantum number) there are $0, 1, 2, \ldots n - 1$ possible values of ℓ. For any ℓ there are $2\ell + 1$ values of m. The hydrogen atom energy levels are n^2 degenerate.

- The number of radial nodes are given by $n - \ell - 1$
- Number of θ nodes (cones centred about the z-axis) are given by $\ell - m$
- m counts the number of nodes in the ϕ direction