Introduction

May 10, 2021 8:21 AM

When is Quantum Mechanics relevant

- When wave energy $E = hf$ (h is the Planck's constant $6.626 \times 10^{-34} Js$).
- When light is dim (individual photons)
- When position uncertainty Δx and momentum uncertainty Δp satisfy Heisenberg's Uncertainty Principle ($\Delta x \times \Delta p \sim h$)
- Low mass particles (low momentum), atoms are completely quantum-mechanical
- Low temperatures
- Superconductivity
- Semiconductor
- Lasers

Mechanical waves and mediums

- Waves travel in a medium
- The wave equation ($\frac{d^2y}{dx^2} = \frac{1}{v^2}\frac{d^2y}{dt^2}$) is only true in the rest frame of the string
  - If moving next to the string at the speed of the wave, we see a non-moving wave, not a solution

Electromagnetic waves and mediums

- Travel in all medium including vacuum
- Velocity is different, because ϵ and μ are different
- Velocity is lower in any medium, the refractive index is $n = \frac{V_{medium}}{c}$
  - $n_{air} = 1.0003$, $n_{water} = 1.333$, $n_{glass} \sim 1.5 - 1.7$, $n_{diamond} = 2.42$.
- Maxwell's equations are only valid in the rest frame

Observer moving through a medium

- Wave has velocity $\vec{v}$, observer has velocity $\vec{u}$, the apparent velocity is $\vec{v} - \vec{u}$

Water-filled telescope

- Deflection angle $n\frac{v}{c}$ (n is the refraction index).

Fresnel drag coefficient

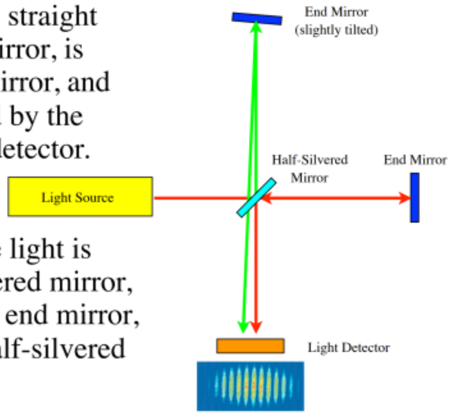
- Aether was dragged with a fraction $D = 1 - \frac{1}{n^2}$ of the velocity of the Earth through the aether (partial aether drag)
  - This D is the Fresnel drag coefficient
- This explain Arago's null result
- No shift in light velocity for air, and half as much for water
- Aether doesn't drag matter, matter drags aether

If moving at a big fraction of the speed of light, this makes half the sky blue-shifted, half red-shifted
If we are moving faster than light, objects behind us are invisible

Michelson-Morley experiment

- The speed of light would be different in different directions if we are moving in the aether
- Compare the speed of light in directions 90° apart using an interferometer

About half of the light goes straight through the half-silvered mirror, is reflected back by the end mirror, and half of that light is reflected by the half-silvered mirror to the detector.



- The other half of the source light is reflected from the half-silvered mirror, then from the slightly tilted end mirror, goes straight through the half-silvered mirror and to the detector.

  The beams interfere at the detector, producing "fringes."
- Let aether wind velocity be v, horizontal (parallel) arm length be L, the round trip time is $T = \frac{2L}{c}\frac{1}{1-\frac{v^2}{c^2}}$.
  - Times in cycles, $cycles = fT = \frac{c}{\lambda}\frac{2L}{c}\frac{1}{1-\frac{v^2}{c^2}} = \frac{2L}{\lambda}\left(1+\frac{v^2}{c^2}\right)$.
- For the other (perpendicular) arm, we have $T = \frac{2L}{c}\frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$.
  - $cycles = \frac{2L}{\lambda}\left(1+\frac{1}{2}\frac{v^2}{c^2}\right)$.
- Perpendicular arm extra delay has the same sign and is half as much as in the parallel arm, so the net effect is cut in half
  - Fringe shift$= \frac{L}{\lambda}\frac{v^2}{c^2}$.

Interpretation
- Earth dragged the aether completely
- Inconsistent with stellar aberration, which requires motion through the aether

FitzGerald-Lorentz contraction
- Motion through the aether caused matter to become compressed by a factor of $\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}} = 1 + \frac{v^2}{2c^2}$.
- This cancels the difference in Michelson-Morley arm transit times without requiring 100% aether drag
- Still needs to be n-dependent partial aether drag to explain the water-filled telescope and Fizeau's result

Einstein's Postulate
- Maxwell's equations (and any correct law of physics) should be valid for all observers, whether stationary or moving

Einstein's explanation
- Since speed of light is the same in all frames, the Michelson and Morley null result is completely expected
- In the Fizeau water-flow interferometer, must use the relativistic velocity addition formula, which gives the Fresnel drag coefficient
- Light propagation direction is frame-dependent

Cherenkov radiation
- Particles can go faster than speed of light in a medium
- The E field lines pile up into a cone
- Moving charges also makes B field lines in the cone
- If the light cone hits a flat surface, it forms a ring

Relativity

May 10, 2021 7:36 PM

Simultaneity

- It is frame dependent
- The time-order of physically separated events can depend on the reference frame

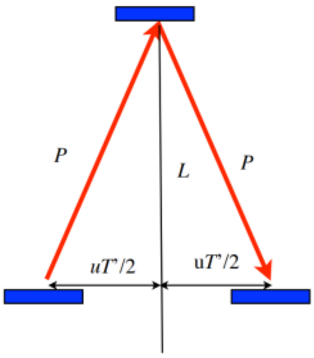
Notations

- S is a frame with origin O for coordinate x and time t
- S' is a frame with origin O' for coordinate x' and time t'
    - It is moving with velocity u in the x-direction of S
- Assume $x = x' = 0$ at $t = t' = 0$.

Galilean Transformations

- $x' = x - ut$ and $t' = t$ (u is the velocity of S').
- To find velocity in S', $v_{S'} = \frac{dx'}{dt} = \frac{dx}{dt} - u = v_S - u$.
- This makes the speed of light frame-dependent, so not the correct transformation.

Vertical light clock (light moving perpendicular to mirror)

- 

- The moving period $T' = \frac{2P}{c} = \frac{2L}{c}\frac{1}{\sqrt{1-u^2/c^2}}$.(the frame is moving with horizontal velocity u)
- The stationary period is $T = \frac{2L}{c}$.
- The outside observer will see the moving clock tick more slowly.

The correct transform

- Distance in S' is $x' = \frac{x-ut}{\sqrt{1-u^2/c^2}}$ (u is the velocity of the frame).
- Time in S' is $t' = \frac{t-ux/c^2}{\sqrt{1-u^2/c^2}}$.

Horizontal light clock (light is moving in the same direction as the mirrors)

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- First half $T_1 = \frac{L}{c-u}$.
- Second half $T_2 = \frac{L}{c+u}$.
- Total period $T = \frac{2L}{c}\frac{1}{1-u^2/c^2}$.
- Still slower than the rate at rest, but the square root is missing, because the length of moving object is also changing
- Object length $L_{moving} = L_{rest}\sqrt{1 - u^2/c^2} < L_{rest}$.

- Then the time period is still $T' = \frac{2P}{c} = \frac{2L}{c}\frac{1}{\sqrt{1-u^2/c^2}}$.

Inverse transform
- Given the position and time change (x' and t') in the moving frame S'.
- The position and time in stationary frame is $x = \frac{x'+ut'}{\sqrt{1-u^2/c^2}}$, $t = \frac{t'+ux'/c^2}{\sqrt{1-u^2/c^2}}$.

Define $\beta = \frac{u}{c}$ and $\gamma = \frac{1}{\sqrt{1-u^2/c^2}} = \frac{1}{\sqrt{1-\beta^2}}$,
We have $x' = \gamma(x-ut) = \gamma(x-\beta ct)$, $t' = \gamma(t-\beta x/c)$.
- $ct' = \gamma(ct-\beta x)$.
- $\beta = 0$ means rest, increasing β means faster.
- $\beta = 1$ is the speed of light, $|\beta| \leq 1$.
- $\gamma = 1$ means rest, increasing γ means faster.
- $\beta \approx 1 - \frac{1}{2}\frac{1}{\gamma^2}$.

Transverse transform
- If frame S' has velocity u in the x-direction, and no velocity in other directions
- Then $y' = y$, $z' = z$. (i.e. they do not change)

3D Lorentz transform
- Given $\beta = \frac{u}{c}$, $\gamma = \frac{1}{\sqrt{1-u^2/c^2}} = \frac{1}{\sqrt{1-\beta^2}}$, where u is velocity along x −direction.
- $x' = \gamma(x-\beta ct)$.
  - $x = \gamma(x'+ut')$.
- $y' = y$.
- $z' = z$.
- $ct' = \gamma(ct-\beta x)$.
  - Equivalently, $t' = \gamma(t-\beta x/c)$.
  - $t = \gamma\left(t' + \frac{ux'}{c^2}\right)$.
- $p = \gamma p' + \beta\gamma E'$.

Simultaneity:
- If $t'_A = t'_B$, we have $t_B - t_A = \frac{\frac{v}{c^2}(x'_B - x'_A)}{\sqrt{1-\left(\frac{v}{c}\right)^2}}$.

Aberration of starlight
- Light from a star in the $+y$ direction of frame S is described by $\cos(ky+\omega t)$. The light is moving in the $-y$ direction
- Observer in frame S', moving in the $+x$ direction with velocity u, $\beta = \frac{u}{c}$.
- This gives $\cos(ky+\omega t) = \cos\left(k\left(y' + \frac{\gamma u}{c}x'\right) + \gamma\omega t'\right)$.
- The first term $k\left(y' + \frac{\gamma u}{c}x'\right)$ has a different direction
- The wave travels in a different direction in the S' frame

Velocity addition
- An object is moving with velocity v' in S' and S' is moving with velocity u.
- The velocity of the object in S is $v = \frac{v'+u}{1+v'u/c^2}$.
  - E.g. two objects moving in opposite direction, then $v_{rel} = \frac{v_1+v_2}{1+v_1v_2/c^2}$.
  - E.g. two objects moving in the same direction, then $v_{rel} = \frac{v_1-v_2}{1-v_1v_2/c^2}$.
- There is no issue about simultaneity

Classical Doppler effect

- Observer at rest and a source moving away with velocity v.
  - $\Delta T_{obs} = \Delta T_{source}\left(1+\frac{v}{c}\right)$.
  - $f_{obs} = \frac{f_{source}}{1+v/c}$.
  - $\lambda_{obs} = \lambda_{source}\left(1+\frac{v}{c}\right)$.
- Source at rest, observer moving away.
  - $\Delta T_{obs} = \frac{\Delta T_{source}}{1-v/c}$.
  - $f_{obs} = f_{source}\left(1-\frac{v}{c}\right)$.

Relativistic Doppler effect

- Observer at rest and a source moving away with velocity v.
  - $\Delta T_{obs} = \Delta T_{source}\frac{1+v/c}{\sqrt{1-v^2/c^2}} = \Delta T_{source}\frac{\sqrt{1+v/c}}{\sqrt{1-v/c}}$.
  - $f_{obs} = f_{source}\sqrt{\frac{1-v/c}{1+v/c}}$.
- Source at rest, observer moving away.
  - $\Delta T_{obs} = \Delta T_{source}\frac{\sqrt{1-v^2/c^2}}{1-v/c} = \Delta T_{source}\frac{\sqrt{1+v/c}}{\sqrt{1-v/c}}$.
  - $f_{obs} = f_{source}\sqrt{\frac{1-v/c}{1+v/c}}$.
- Source moving towards the observer with speed u.
  - $f_{obs} = f_{source}\sqrt{\frac{1+v/c}{1-v/c}}$.
- We have the same result whether the source or the observer is moving
- v is positive if the source and observer are moving away
- If using radar to track, the wave is reflected and shifted twice, we need to use $f_{obs} = f_{source}\left(\frac{1-\frac{v}{c}}{1+\frac{v}{c}}\right)$.
  - At closest point, there will be still time dilation, but no Doppler effect
- Lower frequency means red shift. Higher frequency means blue shift.
  - Approaching reduces wave length, increases frequency
  - Receding increases wave length, reduces frequency.

Time dilation

- It slows moving clocks down to zero at the speed of light
- Get infinite red shift at finite speed

Lorentz contraction and time dilation

- $\gamma = \dfrac{1}{\sqrt{1-u^2/c^2}} = \dfrac{1}{\sqrt{1-\beta^2}}$
  - For small β, $\gamma = 1+\frac{1}{2}\left(\frac{v}{c}\right)^2$.
- Moving objects look shorter: $L_{moving} = \frac{L_{rest}}{\gamma}$.
- Moving clocks tick slower: $f_{moving} = \frac{f_{rest}}{\gamma}$.
- Time periods are longer: $T_{moving} = \gamma T_{rest}$.

Cosmic rays

- High energy particles from space
- In space: protons, atomic nuclei
- At sea level: electrons, muons
  - High velocity (close to speed of light), make muons live long enough to reach the ground

4-vectors

- Define the space-time coordinate 4-vector to be $\underline{X} = (ct, x, y, z) = (ct, \vec{x})$.

- Dot product: $\underline{X_1} \cdot \underline{X_2} = (ct_1)(ct_2) - \vec{x_1} \cdot \vec{x_2}$.
  - Time part has a plus sign, and the space parts have a minus sign
  - $\underline{X} = (ct)^2 - (x^2 + y^2 + z^2)$.
- In a different frame $\underline{X_1'} = (\gamma ct_1 - \beta\gamma x_1, \gamma x_1 - \beta\gamma ct_1, y, z)$, $\underline{X_2'} = (\gamma ct_2 - \beta\gamma x_2, \gamma x_2 - \beta\gamma ct_2, y, z)$.
  - Then $\underline{X_1'} \cdot \underline{X_2'} = \underline{X_1} \cdot \underline{X_2}$
  - Lorentz invariant: 4-vector dot product is the same in any reference frame

Momentum and classical velocity addition
- $m_1 v_{1before} + m_2 v_{2before} = m_1 v_{1after} + m_2 v_{2after}$.
- The relativistic velocity addition causes $p = mv$ to not be conserved.

Clock, proper time, proper velocity and relativistic momentum, mass
- Many clocks in each frame
- Proper time τ: a clock that moves along with the object whose momentum we are defining
  - It is the same in all frames.
- Proper velocity: $w = \frac{v}{\sqrt{1-v^2/c^2}}$.
- Relativistic momentum: $P = m\frac{d}{d\tau}x = mw = \frac{mv}{\sqrt{1-v^2/c^2}}$.
  - The conservation law still holds
- Relativistic mass: $M = \gamma m = \frac{m}{\sqrt{1-v^2/c^2}}$.
  - Moving objects are heavier, acceleration is smaller and this makes it impossible to accelerate any mass beyond the speed of light

Energy
- Define $Q = m\frac{d}{d\tau}ct = \gamma mc = \frac{mc}{\sqrt{1-v^2/c^2}}$.
- Taylor expansion gives $Q = mc\left(1 + \frac{1}{2}\frac{v^2}{c^2}\right)$.
- Relativistic energy $E = Qc = mc^2 + \frac{1}{2}mv^2$.
  - At rest $E = mc^2$
  - $E = Mc^2 = \gamma mc^2 = \sqrt{p^2 + m^2}$ is always true.
  - Kinetic energy: $E = (\gamma - 1)mc^2$.
- For relative momentum to be conserved, relative energy must be conserved
- For relative energy to be conserved, relative momentum must be conserved
- Both momentum and energy are conserved

Proper 4-vector and proper velocity
- $\underline{X} = (ct, v_x t, v_y t, v_z t) = (c, \vec{v})t = (c, \vec{v})\gamma\tau$.
- Proper velocity 4-vector: $\frac{d\underline{X}}{d\tau} = \gamma(c, \vec{v}) = \underline{V}$.
- For low v, $\gamma = 1$, x, y, z part is the frame velocity.

Proper momentum 4-vector (4-momentum):
- $m\frac{d\underline{X}}{d\tau} = m\gamma(c, \vec{v}) = \left(\frac{\gamma mc^2}{c}, \gamma m\vec{v}\right) = \underline{P}$.
- $\gamma m\vec{v}$ is the relativistic momentum and γmc^2 is the relativistic energy, so $\underline{P} = \left(\frac{E_{rel}}{c}, \overrightarrow{p_{rel}}\right)$.
- In center of mass frame $p = 0$, only energy is considered

Electron-volt
- The energy scale of chemistry and atomic physics
- It means the energy change of an electron moving through a potential difference of one Volt.
- $1\ eV = 1.6 \times 10^{-19} J$.
- Ground state of hydrogen is $-13.6eV$.
  - Oxygen: $0.87keV$, uranium: $0.115MeV$.

- Note: $MeV = 10^6 eV, GeV = 10^9 eV, TeV = 10^{12} eV$.
- In $c = 1$ units, momentum is eV/c, masses are eV/c^2.
  - We can use $E = mc^2$ to calculate the mass of a particle.
  - If we use eV unit, we always have $c = 1$
- Nuclear and particle energy scale are usually MeV.
- In relativity, If energy is much greater than its mass, momentum is nearly equal to energy.
- In non-relativity, momentum is much less than mass, energy and momentum are not related

Square of 4-momentum

- $\underline{P}^2 = \frac{E^2}{c^2} - p^2 = E^2 - p^2 = \gamma^2(1-\beta^2)(mc)^2 = (mc)^2 = m^2$ when $c = 1$.
- $E^2 = p^2 + m^2$.
- This is Lorentz invariant and is the same in all frames

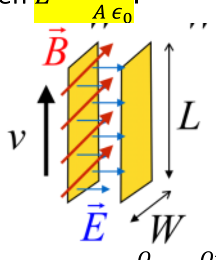
Massless particles

- Since $E^2 = (pc)^2 + (mc^2)^2$, we have $E = pc$.

Lorentz transform for energy, momentum

- $\frac{E'}{c} = \gamma\left(\frac{E}{c} - \beta p_x\right)$.
- $p_x' = \gamma(p_x - \beta\frac{E}{c})$.
- $p_y' = p_y, p_z' = p_z$.
- When energy is in eV, i.e. $c = 1$, we always have $E' = \gamma(E - \beta P)$ and $P' = \gamma(P - \beta E)$.
- E.g. a proton ($M = 938.3 MeV/c^2$) with kinetic energy $K = 6000 MeV$ hits a stationary electron ($m = 0.511 MeV/c^2$), find the momentum of the proton and electron in the CM (center of mass) frame and total kinetic energy
  - $\underline{P} \cdot \underline{e} = \left(K + M, \vec{P}\right) \cdot \left(m, \vec{0}\right) = (K + M)m$.
  - Also $E_{CM}^2 = \left(\underline{P} + \underline{e}\right)^2 = \underline{P}^2 + 2\underline{P} \cdot \underline{e} + e^2 = m_p^2 + 2(K + M)m_e + m_e^2$.
  - $E_{proton\ lab} = K_p + M_p$.

Relativistic capacitor

- By Gauss law, $E = \frac{Q}{A\epsilon_0}$
- If the capacitor moves perpendicular to the plates, the plates appear to be closer together, but the electric field does not change
  - And there is no magnetic field
- If the capacitor moves parallel to the plates, the plates contract along the direction of motion by γ, then $E = \frac{\gamma Q}{A\,\epsilon_0}$.
  - 

  - Current $I = \frac{Q}{LW} = \frac{Qv}{L}$.
  - Magnetic field $B = \frac{\mu_0 I}{W} = \mu_0 \frac{Q}{LW} v$.
    - It is not affected by γ, since E increases by γ, while v decreases by γ.
  - Actually $B = \epsilon_0 \mu_0 E v$, so $B = \frac{Ev}{c^2}$, since $\epsilon_0\mu_0 = 1/c^2$.
- $E_\parallel' = E_\parallel$, $E_\perp' = \gamma(E_\perp + v \times B)$, $B_\parallel' = B_\parallel, B_\perp' = \gamma\left(B_\perp - \frac{1}{c^2} v \times E\right)$.
  - Electric field doesn't transform like other vectors, because it does not have a 4th component

Nuclear reactions

- Given n mole of reactants, there are nN_A reactions.

- $N_A = 6.02 \times 10^{23} mol^{-1}$.
- If $A\ MeV$ energy is produced in the reaction formula, the total energy produced is $A\, n\, N_A$.

Photons

May 10, 2021 7:36 PM

Kinetic theory of gases

- A gas is a collection of small molecules with mass m and average velocity u, bouncing off each other/wall elastically, then collision transfers momentum to the wall $\Delta P = 2mu_x$.
- Force $F = ma = \frac{d}{dt}(mv) = \frac{dP}{dt}$.
- If the container has N molecules of gas in volume V, the number of molecule impacts on area A in time dt is $n = \frac{N}{V}AL$ where $L = |u_x|dt$
- Pressure: $p = \frac{F}{A} = \frac{dP/dt}{A} = \frac{2mu_x \cdot n/dt}{A} = \frac{N}{V}2mu_x^2$.

Statistical mechanics

- Total energy is conserved when atoms collide
- Assume all possible ways to distribute the energy are equally likely, so all molecules have the same average energy $E = \frac{3}{2}kT$, where k is the Boltzmann's constant.
- A small subset of the whole system has energy E, and is in thermal contact with the whole system at temperature T,
    - When E increases, it has more possible states, but the energy of the rest of the system goes down by the same amount, it has fewer possible states.
    - Probability for the subsystem energy, $Prob(E)$ is proportional to $e^{-\frac{E}{kT}}$, Boltzmann factor.

Blackbody radiation

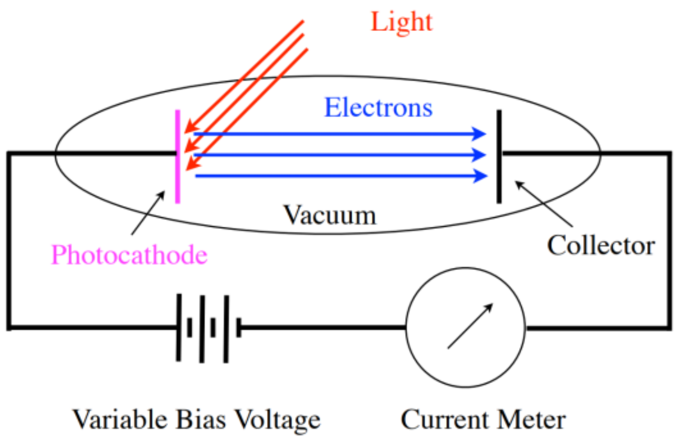
- Hot objects glow red, hotter get yellow, very hot objects get blue, or even ultraviolet
- Shape of black body radiation spectrum should be universal and depend only on f/T (frequency / temperature)
- Rayleigh-Jeans spectrum $dI_{RJ}(f) = \frac{2\pi f^2}{c^2}k_B T df$.
    - Allowed frequencies: $f = \frac{c}{2}\sqrt{\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}}$.
    - k_B is the Boltzmann's constant.
    - Using $f = \frac{c}{\lambda}$, we have $dI_{RJ}(\lambda) = \frac{2\pi c}{\lambda^4}k_B T d\lambda$.
    - Ultraviolet Catastrophe: This predicts that radiated power per unit frequency increases with frequency without limit, so total amount of EM energy inside a metal box should be infinite.
- Wein spectrum $dI_W(f) = Af^3 e^{-\frac{Bf}{T}}df$.
    - Using wavelength, $dI_W(f) = A\frac{c^4}{\lambda^5}e^{-\frac{Bc}{\lambda T}}d\lambda$.
    - Has problem with lower frequency
- Planck spectrum $dI_P(f) = \frac{Af^3}{\exp\left(\frac{Bf}{T}\right)-1}df = \frac{Af^3}{\exp\left(\frac{hf}{k_B T}\right)-1}df$.
    - Satisfies both high and low frequencies

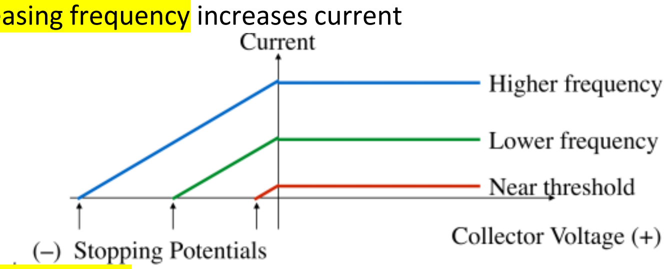
Quantization of EM energy

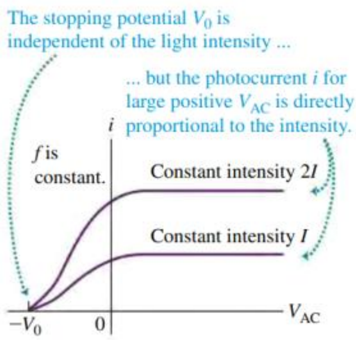
- The energy of frequency f can only be integer multiples of $E = hf = \frac{hc}{\lambda}$
- Planck's Constant: $h = 6.626 \times 10^{-34} Js$.
    - $hc = 1240 eV \cdot nm$.

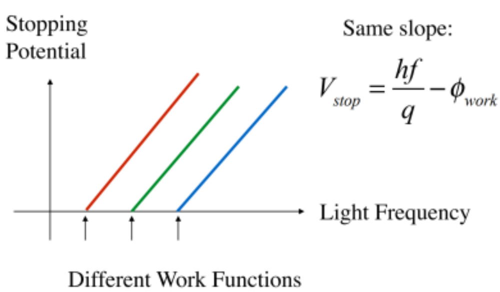
Photoelectric effect

- Shining light on a metal surface (photocathode) ejects electrons

- 

- Light frequency, intensity and current
    - Increasing frequency increases current
        - 

    - Higher intensity increases current, but does not change stopping potential
        - 

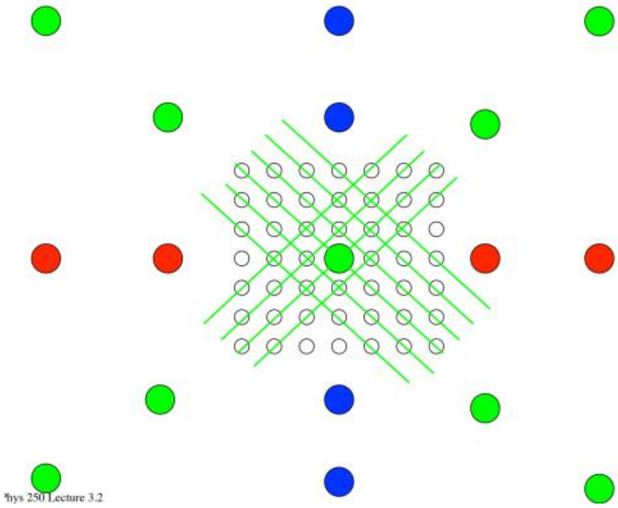
- Stopping potential
    - The maximum ejected electron kinetic (photoelectron) energy is $E = qV_{stop} = hf - q\phi_{work}$.
        - Work function: $q\phi_{work}$ is the energy required to remove an electron from the metal surface
    - Threshold frequency: $q\phi_{work}$.
    - 

- $E = hf$ is intrinsic to the electromagnetic field, independent of atoms.
- Electromagnetic radiation are particles.

Note: we cannot measure the frequency of light directly, but we can use $f = \frac{c}{\lambda}$.

Diffraction
- If light goes through small slits, it emerges in circular waves
- In the forward direction, they are all in phase
- If the wavelength is λ, the waves will be in phase if $d \sin\theta = n\lambda$.

- Diffraction angle θ depends on wavelength
    - d can be the distance between two slits for double slit interference.
- Facts
    - If d is significantly greater than λ then θ will be small and diffraction is invisible.
    - $n = 0$ light goes straight through.
- 2D diffraction



Gas discharge tubes

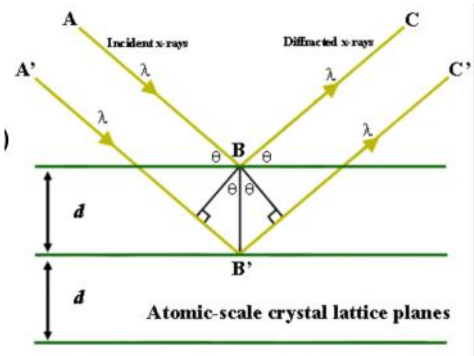
- If pump out all the air inside a glass tube and apply high voltage to electrodes at the end, we get a glowing discharge
- Residual gas gets ionized and can conduct electricity
- Light is produced by electrons recombining with ionized atoms
- Crookes tube
    - Cathode rays come from the negative electrode
    - Horizontal magnetic field deflects cathode rays down. They are charged particles
    - Ionized residual gas shorted out the electric field and does not deflect the cathode rays
- Thomson experiment
    - Velocity $v = \frac{E}{B}$.
    - Charge mass ratio $\frac{q}{m} = \frac{1}{2V}\left(\frac{E}{B}\right)^2$.
- X-ray tube
    - Replace the photocathode by a hot thermionic cathode
    - Apply several thousand volts to attract the electrons to the anode made of tungsten
    - X-rays are scattered as they pass through the crystal, forming an interference pattern on the film
        - Most of the X-rays pass straight through the crystal

X-ray diffraction

- X-ray scatter in all directions from each atom
- Scattered X-rays tend to be out of phase with each other
- In a crystal, atoms are regularly spaced
    - The scattered X-rays are in phase

Diffraction from stacked planes

- If many weakly-reflecting planes are stacked together, we get reflections from all of them
- Reflections will interfere with each other
- Bragg's law: If the plane spacing is d, and the incidence angle from the surface is θ, reflections from all the planes will be in phase if $2d\sin\theta = n\lambda$.

- 

- Bragg X-ray spectrometer
  - Rotate the stack of planes by θ, and move the X-ray detector by 2θ. The detector will see X-ray only with $\lambda = 2\,d\sin\theta$.

X-ray spectrum

- There is a smooth continuous spectrum from electrons hitting the metal anode, where they decelerate rapidly and radiate high-frequency photons
- Deceleration is sudden and the spectrum is broad.
- Sharp peaks at longer wavelengths, the peaks depend on the anode material
- For a given voltage, there is a maximum X-ray frequency which corresponds to a minimum X-ray wavelength $qV = hf_{max} = \frac{hc}{\lambda_{min}}$.

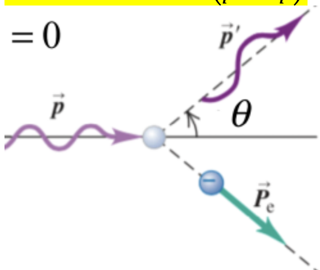
Scattering of light

- When light shines on a material, some of it bounces off
- EM field of light causes charged particles to oscillate at the same frequency as the light
- Particles radiate EM energy at the same frequency
- Reflected/scattered light has the same frequency as the incident light

Scattering of X-rays

- When X-rays scatter through a large angle, the wavelength changes

Quantum scattering of EM radiation

- Incident wave is photons
- An electron absorbs a photon, then immediately emits another photon traveling in another direction
- Energy and momentum of the absorbed and incident photons are conserved
- The absorbed and emitted photon has different momentum (different directions)
  - Electron gains kinetic energy
  - Emitted photon has lower energy than the absorbed photon
- Compton kinematics, let p be the momentum of incident photon, m be the mass of electron, p' be the momentum of emitted photon, θ be the emission angle.
  - $1 - \cos\theta = mc\left(\frac{1}{p'} - \frac{1}{p}\right)$.
  - 

Photons and momentum

- EM waves have a momentum density p as well as and energy density E, $E = pc$.
- Momentum of a photon is $p = \frac{E}{c} = \frac{h}{\lambda}$.
- Then we have $\lambda' - \lambda = \frac{h}{mc}(1 - \cos\theta)$.

- Compton wavelength: $\frac{h}{mc} = 2.426 \times 10^{-12} m$.
- The effect is insignificant unless the light wavelength is in the nanometer range (X-rays or γ-rays)

Photons are particles and waves

The amplitude of electromagnetic waves is quantized such that the energy obeys $E = nhf$.

- It is not continuous.

Photon kinematics

- Velocity $= c$.
- Mass $= 0$.
- $E = pc$.
- Momentum $\gamma mv = p = \frac{E}{c} = \frac{h}{\lambda}$.
- 4-vector momentum $p = (|p|, \vec{p})$.

Photons and intensity

- The energy of a photon is fixed at $E = hf$.
- The intensity of light must be described by photons per second
- More photons per second in the intense part of the light beam.
- If detect light by the photoelectric effect, the photoelectrons will come out one at a time, with the same intensity pattern as the light

Photon flux and density

- An EM wave has flux in $J/m^2/s$, $\vec{S} = \vec{E} \times \frac{\vec{B}}{\mu_0}$.
- Divide by $1.6 \times 10^{-19} J/eV$ to get $\frac{eV}{m^2 s}$.
- Divide by $eV = hf = \frac{hc}{\lambda}$ to get flux of photons/m^2/second.
- Density is $\frac{flux}{c}$.
- E.g. flux from the Sun to Earth is $1.4kW/m^2$, with energy of a solar photon$= 1.4eV$.
  - Solar photon flux is $\frac{1.4\times10^3\ J/(m^2 s)}{1.6\times10^{-19}\ J/eV \times 1.4eV/photon} = 6.24 \times 10^{21} \frac{photons}{m^2 s}$.
  - Photon density is $\frac{6.24\times10^{21}}{3\times10^8} = 2.03 \times 10^{13}\ photons/m^2$.

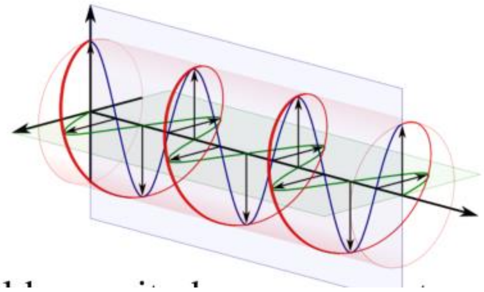
Photons and interference

- Using dim light, there are only a few photons, we see particles
- With more photons, we see the standard interference pattern
- Interference works even when the light is so dim that only one photon at a time is in the apparatus
- Photon must go through both slits and interfere with itself.
- But when absorbing a photon with a detector, the photon collapses to a point
  - A single photoelectron from a single atom, or a single spot on a photographic plate

Size and shape of a photon

- If not absorbed, its size and shape is determined by the classical field pattern
- In a box with conducting sides, the size and shape of a photon is the size and shape of the box
  - Not uniform across the box
  - The energy oscillates between E and B with different shapes
- Transverse size of a laser photon must be the transverse size of the laser beam
  - Any part of the beam can interfere with any other part of the beam
  - If the laser beam diverges, the photons get bigger
  - If focus the laser beam down, the photons get smaller
  - Hard to focus a diameter smaller than the wavelength (not a limit)

Circular & linear polarization

- Superpose vertical polarization with horizontal polarization, that is 90° out of phase.
- The electric field rotates.
- 
- Depending on the relative phase of the two linear polarizations, the rotation can be either right-handed or left-handed
- If we superpose left and right handed circular polarization, we can get either horizontal or vertical polarization
- Linear polarization has regions where the energy density is zero

Coherence length
- Distance over which the phase of the light is stable enough for interference
- For ordinary light, the coherence length is a few millimeters
- It is a better way to define the length of a photon

Shape of a D-line photon
- When an atom emits a photon, we observe the light to go equally in all directions
  - Classical EM field is isotropic.
  - The EM field is a spherical shell with thickness equal to the coherence length
  - The photon is then a spherical shell with this thickness and expanding at the speed of light
- With a hollow spherical detector, the probability that we detect the photon at a given point is proportional to the power per square meter at that point.
  - Power is uniform across the sphere
- Since we only emit one photon, we will detect the photon at just one point, the wave function will collapse from the spherical shell down to the single point that we detect the photon
  - Parts of the photon shell know immediately where to collapse.
- Photon knows where it will be detected, even if we don't detect
- Photon must have all the wave properties that are required for interference, so it can't have a definite direction at the time that it is emitted.

Probability
- The probability that we will detect the photon in a given region is the integral of the photon flux over the region of the detector
- Or the integral over the whole detector of the photon flux times a window function that is 1 for the given region and 0 outside of it
  - The probability for a different region would be the same integral but a different window function
- To find the probability of 2 events, add the individual probabilities of them (add the window function)
- To find the probability of event 1 and 2, multiply the probability and we get 0.

Wave functions and operators and integrals
- Wavefunction $\psi(x)$ represents what we know about a system.
- For any measurement there is an operator W,
  - Window function or manipulation to the wave function
- Prediction for a measurement $\int \psi^*(x) W \psi(x) dx$.
  - $\psi^*(x)$ is the complex conjugate
  - It is over the whole wavefunction
  - The wave function is squared

EPR paradox

- Thought experiment: a pair of particles are put into a state where their properties are correlated, then widely separated, then measured
- The result of measuring one particle instantly influences the result of measuring the other

Bell inequalities

- Standard quantum mechanics frequently predicts stronger correlation than the actual one
- Quantum mechanics is either not local or not realistic

Early Quantum

May 10, 2021 7:37 PM

Balmer formula

- A formula that fits the spectrum of hydrogen.
- $\lambda = B\frac{n^2}{n^2-4}$, $B = 364.5\ nm$.
- Improved version for infrared and ultraviolet
  - $\lambda = B\frac{n^2}{n^2-m^2}$, $B = 364.5\ nm, n > m$.
  - When $m = 1$, ultraviolet (Lyman)
  - When $m = 2$, visible (Balmer).
  - When $m = 3$, infrared (Paschen).

Rydberg formula

- Spectrum of alkali atoms
- $\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$, $n_2 > n_1$, $R = \frac{4}{B} = 1.097 \times 10^7/m$.
- Predicts some alkali atom spectral lines pretty well.
- Inner electrons screen the nuclear, so it looks like the same charge as a proton
- Improved version
  - Remove all but one electron from an atom.
  - $\frac{1}{\lambda} = RZ^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$, Z is the atomic number.
    - Lyman: $n_1 = 1$.
    - Balmer $n_1 = 2$.
    - Paschen: $n_1 = 3$.
  - It predicts the spectrum exactly for hydrogen
- Using Planck's formula in the improved version, we have energy $E = 13.6eV\ Z^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$.

Rutherford orbit energy

- Coulomb's law: $F = \frac{q^2}{4\pi\epsilon_0}\frac{1}{r^2}$, radial acceleration $a = \frac{v^2}{r}$.
- Energy $E_{total} = \frac{1}{2}mv^2 - \frac{q^2}{4\pi\epsilon_0}\frac{1}{r} = -\frac{1}{2}\frac{q^2}{4\pi\epsilon_0}\frac{1}{r}$, $E_k = -E_{total} = -\frac{1}{2}E_{potential}$.
- Problems
  - Orbits can be any size, so atoms of a given element should have a range of sizes
  - Period of the orbit depends on the size of the orbit, so there is no explanation of spectral line frequencies

Rutherford orbit decay

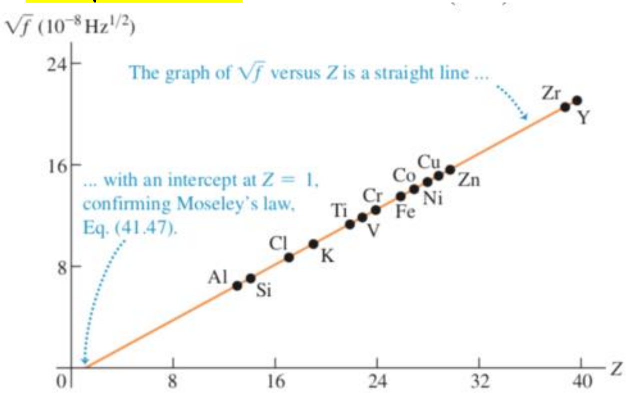
- Larmor radiation: $\frac{dE}{dt} = \frac{q^2}{6\pi\epsilon_0 c^3}a^2$, $a = \frac{v^2}{2} = \frac{2|E_{total}|}{mr}$ is acceleration.
  - t is the decay time.
  - $\frac{dE}{dt} = \frac{256}{6}\frac{\pi\epsilon_0}{m^2q^2c^3}E^4$, let the constant be A.
  - $E = -\left(|E_0|^{-3} - 3At\right)^{-1/3}$.
  - So when $E = 0$ (orbit radius goes to 0), $t = \frac{|E_0|^{-3}}{3A}$, $A = \frac{256}{6}\frac{\pi\epsilon_0}{m^2q^2c^3}$.
    - Can be rewritten as $t = 3.92 \times 10^{-8}|E_0|^{-3}$, E_0 in eV.
    - If $E_0 = -1eV$, decay time is 40ns.
    - If $E_0 = -13.6eV$, decay time is 16ps.

Bohr model

- Angular momentum can only be integer multiples of Planck's constant but divided by 2π.

- $L = n\frac{h}{2\pi} = n\hbar, n \in \mathbb{N}$.
  - Reduced Planck's constant $\hbar = 1.055 \times 10^{-34} J/s$.
  - $\hbar c = \frac{1240 eV \cdot nm}{2\pi} = 197.4 eV \cdot nm$.
- Orbit energy: $E = -\frac{m}{2}\left(\frac{qQ}{4\pi\epsilon_0}\right)^2 \frac{1}{L^2}$.
  - Quantization by $L = n\hbar$, $E = -13.6eV\frac{Z^2}{n^2}$.
- Radius $r = 52.97pm\frac{n^2}{Z}$.
- The predicted energies come out exactly right for hydrogen
- The lowest energy orbit has a definite size, so all hydrogen atoms are the same size
- Problems
  - Hydrogen atoms are spherical, but Bohr hydrogen is planar
  - Charge moving in a circular orbit generates a magnetic moment. Ground state hydrogen atoms do have a magnetic moment, but it's not the value predicted by the Bohr model
  - There is no magnetic moment from orbital motion, because there is no orbital motion

De Broglie waves
- Particles have wave properties
- For both matter and photons, $\lambda = \frac{h}{p}$.
  - For a particle in an orbit with radius r and angular momentum $L = rp$ would have a wavelength of $\lambda = \frac{hr}{L}$.
  - If we require an integer n wavelengths, $L = n\hbar$.
- This avoids the problem of the electron radiating away its energy
- A uniform and constant current following a circular path makes a static magnetic field, but it doesn't radiate
- For photons, $p = \frac{E}{c}$, $\lambda = \frac{hc}{E}$.
- For non-relativistic matter, $E = \frac{p^2}{2m}$, $\lambda = \frac{h}{\sqrt{2mE_k}} = \frac{hc}{\sqrt{2mc^2E_k}}$.

X-ray spectral lines
- As the atomic number Z goes up, the Rydberg wavelengths go into X-ray range. It gets increasingly hard to get rid of all but one electron
- Moseley's law: The energy of the most prominent X-ray line ($K\alpha$) is $E_{k\alpha} = 10.2eV(Z-1)^2$.
  - $E_{k\alpha} = 13.6eV \cdot \frac{3}{4} \cdot (Z-1)^2$.
  - So $Z = \sqrt{\frac{91.13}{\lambda} \cdot \frac{4}{3}} + 1$.
  - 

- Note: $E_{Rydberg} = 13.6eV\ Z^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$, if $n_1 = 1$, and $n_2 = 2$, it is the Mosley's law.
  - $K\alpha$ line comes from an electron in the second Bohr orbit dropping into the first Bohr orbit.
- $(Z-1)^2$ implies that there was still one electron in the first Bohr orbit, which partially screens the nuclear charge.
- Can be used to determine the elemental composition of a sample
- K-β: transition from $n = 3$ to $n = 1$.

- $L-\alpha$: transition from $n=3$ to $n=2$, $E=13.6eV\ (Z-7.4)^2\left(\frac{1}{2^2}-\frac{1}{3^2}\right)$.

Franck-Hertz experiment
- Mercury vapor has a spectral line at $250nm$, $E=4.96eV$.
- Increase the voltage until the electron energy reaches $5eV$, we can repeat to excite all mercury atoms
- If use neon gas, the emitted photon is visible
- The same discrete atomic energy levels, correlated with photon wavelengths via Planck's constant, also showed up in the interactions of electrons with atoms

Davisson-Germer experiment
- Electrons diffract like waves
- $\lambda=\frac{h}{\sqrt{2mE_k}}=\frac{hc}{\sqrt{2mc^2qV}}=\frac{1240}{\sqrt{2\cdot 511keV\cdot 54eV}}=167pm$.
- $d=91pm$ from X-ray diffraction, follows the Bragg formula $\lambda=2d\sin\theta=2\cdot 91\cdot\sin 65=165pm$.

Quantum: Schrodinger

June 7, 2021 8:28 AM

Schrodinger equation gives a much better explanation of atomic physics than the Bohr Model
But it's more complicated to find solutions to it

Wave equation: $y_{xx} = \frac{1}{v^2} y_{tt}$.

- Solution: $y(x,t) = g(x \pm vt)$ for any g.
  - Any linear combination is also a solution
  - Doesn't have to be a sinusoid
- If it is a sinusoid with wavelength λ and period T, we have $y = A \sin\left(2\pi\left(\pm\frac{x}{\lambda} - \frac{t}{T}\right) + \phi\right)$.
  - $v = \frac{\lambda}{T}$.
  - Can be written as $y = A\sin(\pm kx - \omega t + \phi)$.
    - $k = \frac{2\pi}{\lambda}$, $\omega = \frac{2\pi}{T} = 2\pi f$.
    - $v = \frac{\omega}{k}$.
- Complex exponential: $y(x,t) = e^{i(kx - \omega t)}$.

Quantum relations + classical energy

- Plank-Einstein: $E = hf = \hbar\omega$.
- De Broglie: $p = \frac{h}{\lambda} = \hbar k$.
- $E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$.
- With $v = \frac{\omega}{k}$ defined as above.

Free-particle Schrodinger equation

- Complex wave: $y(x,t) = e^{2\pi i\left(\frac{x}{\lambda} - \frac{t}{T}\right)}$.
  - Definitions: $k = \frac{2\pi}{\lambda}$, $\omega = \frac{2\pi}{T} = 2\pi f$.
  - Simplified: $y(x,t) = e^{i(kx - \omega t)}$.
- Define: $\hbar = \frac{h}{2\pi}$.
- De Broglie: $\lambda = \frac{h}{p}$, $p = \hbar k$.
- Energy: $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$.
- Planck: $E = hf = \hbar\omega$.
- Equation: $i\hbar y_t = -\frac{\hbar^2}{2m} y_{xx}$.

Time-stepping the equation

- $\Delta y = i\frac{\hbar}{2m}\frac{\Delta^2 y}{\Delta x^2}\Delta t$.
- Define $y(x)$ at discrete points at $t = 0$.
- Do numerical solutions to $\frac{\Delta^2 y}{\Delta x^2}$ at each point.
- Take a finite time step, and repeat

E.g.

- Wave solution with $E = 1eV$, real and imaginary out of phase, everywhere
- Wave solution with $E = 0.25eV$, same, but moves slower
- Gaussian with $E = 0$, starts real, gets imaginary part, magnitude stays Gaussian
- Narrower Gaussian, spreads into wider, area looks constant
- Gaussian with $E \neq 0$, Gaussian can move

Area and normalization

- Define complex conjugate $(x+iy)^* = (x-iy)$.
- $\frac{\partial}{\partial t}\int_{-\infty}^{\infty} y^*(x,t)y(x,t)dx = -\frac{i\hbar}{2m}\frac{\partial}{\partial x}(y'^*y - y^*y') = 0$.
- Define $A = \int_{-\infty}^{\infty} y^*(x,t)y(x,t)dx$.
  - Only need to consider x part here.
- Redefine $y = \frac{y}{A}$, then $\int_{-\infty}^{\infty} y^*(x,t)y(x,t)dx = 1$.
  - Then $\int_{-\infty}^{\infty} y^*(x,t)y(x,t)dx$ can be interpreted as the probability of finding the particle at position x at time t.

Moving particles

- Guess $y(x,t) = F(x-vt)e^{i(kx-\omega t)}$ with $v = \frac{p}{m} = \frac{\hbar k}{m}$, $k = \frac{mv}{\hbar}$.
- Plug into $i\hbar y_t = -\frac{\hbar^2}{2m}y_{xx}$, and $E = \frac{\hbar^2 k^2}{2m}$.
  - $EF = EF - E\frac{F''}{k^2}$.
  - So the guess is not exact, but close if $\frac{F''}{k^2} < F$, i.e. curvature of F is much less than curvature of the wave $e^{i(kx-\omega t)}$.

Fourier analysis

- For N discrete data samples x_j, the transform X_k is $X_k = \sum_{j=0}^{N-1} x_j e^{-2\pi i\frac{jk}{N}}$.
  - Note when x_j are real, the transform X_k is complex.
- Inverse transform $x_j = \sum_{k=0}^{N-1} X_k e^{2\pi i\frac{jk}{N}}$.
- For continuous case: $S(f) = \int_{-\infty}^{\infty} s(t)e^{-2\pi i f t}dt$.
  - Inverse: $s(t) = \int_{-\infty}^{\infty} S(f)e^{2\pi i f t}df$.
- In quantum mechanics convention:
  - $y(x) = \int_{-\infty}^{\infty} a(k)e^{ikx}dk$.
  - $a(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} y(x)e^{-ikx}dx$.
    - It is the amplitude function

Gaussian Fourier transform

- Take a Gaussian with width σ_x at $t=0$, $y(x,t=0) = \exp\left(-\frac{x^2}{2\sigma_x^2}\right)$.
  - Decompose into spatial frequencies $a(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left(-\frac{x^2 - 2ik\sigma_x^2 x}{2\sigma_x^2}\right)dx = A\exp\left(-\frac{k^2\sigma_x^2}{2}\right)$
  - Define $\sigma_k = \frac{1}{\sigma_x}$, $a(k) = \exp\left(-\frac{k^2}{2\sigma_k^2}\right)$.
- So Gaussian in x of width σ_x Fourier transforms into a Gaussian in k of width $\sigma_k = \frac{1}{\sigma_x}$.
  - This is how we find minimum length of wave packet by $a(k)$, σ_x is the minimum wavelength.
- Shorter width spreads faster, longer width travels faster

Heisenberg uncertainty principle

- $a(k) = \frac{1}{\sqrt{2\pi}\sigma_k}\exp\left(-\frac{k^2}{2\sigma_k^2}\right)$.
- Gaussian in k, centered on $k=0$, width $\sigma_k = \frac{1}{\sigma_x}$.
- Width in momentum space is $\sigma_p = \hbar\sigma_k$, $\sigma_x\sigma_p = \hbar$
- Heisenberg principle: $\sigma_x\sigma_p \geq \frac{\hbar}{2}$.
  - The 2 comes from squaring a Gaussian (width goes down by $\sqrt{2}$).
  - Gaussian wave functions are minimum uncertainty, and give the lower limit
- Wave packet spreads in x, but stays the same width in k
  - Get the minimum product at $t=0$.

- Position uncertainty of wave function: σ, then position uncertainty of probability is $\frac{\sigma}{\sqrt{2}}$.
  - Then momentum uncertainty of wave function $\frac{\hbar}{\sigma}$, momentum uncertainty of probability is $\frac{\hbar}{\sqrt{2}\sigma}$.
  - Velocity uncertainty: $\sigma_v = \frac{\sigma_p}{m} = \frac{\hbar}{m\sigma}$.

Adding forces to Schrodinger

- Free particle means it doesn't include any forces, but it has dimensions of energy
- Include forces by adding a potential energy function: $i\hbar y_t = -\frac{\hbar^2}{2m} y_{xx} + V(x)y$.
- Potential: minus the integral of force over distance
  - Constant force F: $V(x) = -Fx$ (linear potential).
  - Restoring force $F = -kx$: $V = \frac{1}{2}kx^2$ (harmonic oscillator).
  - Step potential:
    - if a particle comes in from the left with energy E and $V > E$, particle bounce back.
    - If $V < E$, the particle moves forward at a reduced velocity.
    - E.g. with $E = 0.8V$
      - $V = 0.6eV$, wave is transmitted, also reflected to a standing wave.
      - $V = 1.0eV$, wave is completely reflected as a standing wave.
      - $V = 1.0eV$, then back to $V = 0$, some of the wave crosses the step, the rest reflected.
    - Analysis for $V < E$
      - Incident wave: $y_I(x,t) = e^{i(kx-\omega t)}$, $\omega = \frac{E}{\hbar}$, $E = \frac{\hbar^2 k^2}{2m}$, $k = \frac{\sqrt{2mE}}{\hbar}$.
      - Both reflected and transmitted, and boundary conditions at the step
        - All three waves must have the same frequency ω.
      - Let R be the amplitude of reflected wave, $y_R = Re^{-ikx}e^{-i\omega t}$.
      - Let T be the transmitted wave, $y_T = Te^{ik'x}e^{-i\omega t}$.
        - $k' = \frac{\sqrt{2m(E-V)}}{\hbar}$.
      - $R = \frac{k-k'}{k+k'}$.
      - $T = \frac{2k}{k+k'}$.
      - Density will be $R^2 A$ and $T^2 A$
      - $V = 0, k' = k, R = 0, T = 1$.
      - V small, $k' < k$, R small, $T < 1$.
      - $V \sim E, R = 1, T = 2$.
    - Analysis for $V > E$.
      - $k' = \frac{\sqrt{2m(E-V)}}{\hbar} \in \mathbb{C}$.
      - $y_T = Te^{-k''x}e^{-i\omega t}$, $k'' = \frac{k'}{i} \in \mathbb{R}$.
      - $R = \frac{k-ik''}{k+ik''}$.
      - $T = \frac{2k'}{k+ik''}$.
      - $V = E, k'' = 0, R = 1, T = 2$.
      - $V > E, k''$ big, $|R| = 1$, T small.
      - V infinite, k'' infinite, $|R| = 1, T = 0$.

Potential barrier ($V < E$)

- Similar to the potential step, have an incident wave, a reflected wave and a transmitted wave
- Two waves inside the potential barrier, one going right and one going left.
  - Require the wave function and its derivative to be continuous at both sides of the barrier
  - $A = 1$, 4 wave amplitudes, 4 boundary conditions.
- Components:
  - $y_I = Ae^{ik_I x}$, $k_I = \frac{\sqrt{2mE}}{\hbar}$.

- $y_R = Be^{-ik_R x}$.
- $y_T = Ce^{ik_I x}$.
- $y_{B^+} = De^{ik_B x}$, $y_{B^-} = Fe^{-ik_B x}$, $k_B = \frac{\sqrt{2m(E-V)}}{\hbar}$.

- Requirements
  - $A + B = D + F$.
  - $ik_I(A - B) = ik_B(D - F)$.
  - $De^{ik_B x} + Fe^{-ik_B x} = Ce^{ik_I x}$.
  - $ik_B\left(De^{ik_B x} - Fe^{-ik_B x}\right) = ik_I Ce^{ik_I x}$.
- Amplitudes example ($k_I = 1, k_B = 0.5, x = 2\pi$)
  - $B = 0$ means zero reflection.
  - $C = -1$ means 100% transmission with a phase flip.
    - Zero reflection means 100% transmission.
  - $D = 1.5$ means forward wave inside barrier is big, $F = -0.5$ means the backward wave is significant but smaller.

Tunnelling ($V > E$)

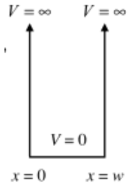
- $k_B = \frac{\sqrt{2m(E-V)}}{\hbar}$ is imaginary
- Wave components are the same, $k_I = \frac{\sqrt{2mE}}{\hbar}$.
- $y_{B^+} = De^{ik_B x}$, $y_{B^-} = Fe^{-ik_B x}$ becomes real exponentials
- example ($k_I = 1, k_B = 0.5i, x = 2\pi$)
  - $B = 0.5971 - 0.7992i$.
  - $C = 0.0554 + 0.0414i$.
  - $D = 1.5977 - 0.8024i$.
  - $F = -0.0006 + 0.0033i$.
  - $|B|^2 = 0.9952$, $|C|^2 = 0.0047$, 99.5% reflection, 0.5% transmission.
  - D and F gives decaying exponential.

Approximate tunnelling

- Potential barrier is not flat
- Often the decay-distance is short compared to the shape of the potential barrier
- Assume wave in the barrier $\psi(x) = e^{-f(x)}$.
  - $E\psi = -\frac{\hbar^2}{2m}\psi_{xx} + V(x)\psi$.
  - Need: $\psi_x = -f_x e^{-f(x)}$, $\psi_{xx} = \left(f_x^2 - f_{xx}\right)e^{-f(x)}$.
  - So $E = -\frac{\hbar^2}{2m}\left(f_x^2 - f_{xx}\right) + V(x)$.
  - If $\psi = e^{f(x)}$ is a simple deaying exponential, then f is linear, $E = -\frac{\hbar^2}{2m}f_x^2 + V$.
  - Then $f_x = \frac{\sqrt{2m(V(x)-E)}}{\hbar}$, $\psi = \exp\left(-\frac{\sqrt{2m}}{\hbar}\int_{x_1}^{x}\sqrt{V(x) - E}\,dx\right)$.
    - x_1 is the point where the potential first becomes equal to the particle energy.
    - Only take the part where $V(x) > E$.
    - The value squared is the probability that it got transmitted
- Incident wave $x = x_1$ $\psi\left(x_1\right) = 1$.
- Transmitted wave $\psi(x_2)$.
  - x_2 is where the potential becomes equal to the particle energy again.
- Another probability of tunneling:
  - $T = Ge^{-2kL}$.
  - $G = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)$, $k = \frac{\sqrt{2m(U_0-E)}}{\hbar}$.

Infinite potential barrier

- $k_T = \frac{\sqrt{2m|V-E|}}{\hbar}$ infinite positive, $\psi_T = e^{-k_T x}$, transmitted wave is zero.
- Incident + reflected must be continuous with transmitted, so the total wave function at the barrier must be zero

- Infinite square well
  - 

  - $E\psi = -\frac{\hbar^2}{2m}\psi_{xx} + 0\psi$.
  - BC: $\psi(0) = \psi(w) = 0$.
  - Wave: $\psi(x) = \sin(k_n x)$, $k_n = \frac{n\pi}{w}$.
    - Normalization: $\psi_n(x) = \sqrt{\frac{2}{w}}\sin(k_n x)$.
  - Energy: $E_n = n^2 \frac{\hbar^2\pi^2}{2mw^2}$.

Uncertainty principle and energy
- Take $p = \Delta p = \frac{\hbar}{2w}$ $(\Delta x = w, \Delta x \Delta p \geq \frac{\hbar}{2})$.
- $E = \frac{p^2}{2m} = \left(\frac{\hbar}{2w}\right)^2 \frac{1}{2m} = \frac{1}{8}\frac{\hbar^2}{mw^2}$.
- Ground state energy: $E_1 = 4.935\frac{\hbar^2}{mw^2}$.
- Flat distribution, $\sigma_x = \frac{w}{\sqrt{12}}$, $E = 1.5\frac{\hbar^2}{mw^2}$
- Flipped parabola, $\sigma_x = \frac{w}{\sqrt{20}}$, $E = 2.5\frac{\hbar^2}{mw^2}$.

Finite square well
- $E > V$, plane wave with reflections
- $E < V$, bound states.
  - Look like infinite potential step, wave functions will not be zero at boundaries, but with some decaying-exponential
  - Finite number of bound states
- Center at $x = 0$, wave: $\sin(kx)$ or $\cos(kx)$, with $k = \frac{\sqrt{2mE}}{\hbar}$.
- Decaying exponential outside $Ae^{\pm k'x}$, $k' = \frac{\sqrt{2m(V-E)}}{\hbar}$.
- $\frac{\sqrt{E}}{\sqrt{V-E}} = -\tan\left(\sqrt{E}\frac{\sqrt{2mw^2}}{2\hbar} + \frac{\pi}{2}\right)$ if wave is $\sin(kx)$.
  - Use $\hbar = \frac{1240}{2\pi}$ here, m in eV/c^2, V, E in eV, w in nm.
- $\frac{\sqrt{E}}{\sqrt{V-E}} = -\tan\left(\sqrt{E}\frac{\sqrt{2mw^2}}{2\hbar}\right)$ if wave is $\cos(kx)$.
- When V is infinite, we have $\frac{\sqrt{E/E_1}}{\sqrt{\frac{V}{E_1}-\frac{E}{E_1}}} = -\left[\tan\left(\frac{\pi}{2}\sqrt{\frac{E}{E_1}}+\frac{\pi}{2}\right), \tan\left(\frac{\pi}{2}\sqrt{\frac{E}{E_1}}\right)\right]$.
  - ith energy level in the infinite square well is $i^2 E_1$.
- Shift the potential, 0 at the top, $-V$ at the bottom.
  - Energy levels become: $E_i = E_i - V < 0$ if $E < V$.
  - When $E > 0$, travelling plane waves instead of bound states.

For an infinite long wave, wavelength and frequency are well-defined
For a wave packet, they can vary.

Electrons per second is conserved, but electrons per length is not conserved

Separating time dependence
- $\psi(x,t) = F(x)G(t)$.
- So $i\hbar\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + V\psi$ becomes $i\hbar F G_t = -\frac{\hbar^2}{2m}GF_{xx} + VFG$.
- Then we have $i\hbar\frac{1}{G}G_t = -\frac{\hbar^2}{2m}\frac{1}{F}F_{xx} + V(x) = E$, where E is a constant.

- Multiply F on the right side, $-\frac{\hbar^2}{2m}F_{xx}+V(x)F=EF$ is time independent, and it is real.
  - For different E, there is a different F
- Left equation can be integrated to $G=e^{-i\frac{E}{\hbar}t}$.

Infinite square well

- Wave function must satisfy: $E\psi=-\frac{\hbar^2}{2m}\psi_{xx}$, boundary at $x=0$ and $x=L$.
- Then $\psi_n(x)=\sin\left(\frac{n\pi x}{L}\right)$, $E_n=\frac{\hbar^2k_n^2}{2m}=n^2\frac{\hbar^2\pi^2}{2mL^2}$.
- If steps at $-\frac{L}{2},\frac{L}{2}$, we have $\psi(x)=\cos\left(\frac{(2n+1)\pi x}{L}\right),\sin\left(\frac{2n\pi x}{L}\right)$.
  - Energy solutions are $E_n=n^2\frac{\hbar^2\pi^2}{2mw^2}$, $w=\frac{L}{2}$ (the boundary).

Operators

- Turns a function into another
- Momentum operator
  - Since $p=\hbar k$, $\frac{1}{i}\frac{\partial}{\partial x}\exp(ikx-\omega t)=k\exp(ikx-\omega t)$.
  - Define $p_{op}=\frac{\hbar}{i}\frac{\partial}{\partial x}$.
- Hamiltonian operator
  - $H_{op}=\frac{p_{op}^2}{2m}+V(x)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)$.
  - $E\psi(x)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi(x)=H_{op}\psi(x)$.
- Parity operator
  - P_{op} swaps x to $-x$, $P_{op}V(x)=V(-x)$.
  - $P_{op}\frac{\partial}{\partial x}=-\frac{\partial}{\partial x}$.
  - $P_{op}\frac{\partial^2}{\partial x^2}=\frac{\partial^2}{\partial x^2}$.
  - P_{op} does not change the Hamiltonian operator if the potential is symmetric.
    - $P_{op}(H_{op}\psi)=P_{op}(E\psi)$, so $H_{op}(P_{op}\psi)=E(P_{op}\psi)$.
    - P_{op} can only do nothing to ψ or change ψ to $-\psi$.
    - The solution must be symmetric $\psi(-x)=\psi(x)$ or anti-symmetric $\psi(-x)=-\psi(x)$.

3D Laplacian:

- cartesian: $\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$
- spherical: $\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$
- cylindrical: $\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+\frac{\partial^2}{\partial z^2}$.
  - 2D circular: $\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}$.

3D Schrodinger

- $-\frac{\hbar^2}{2m}\psi_{xx}$ comes from kinetic energy $\frac{p_x^2}{2m}$, 3D equivalent: $\frac{p_x^2+p_y^2+p_z^2}{2m}$.
  - So we have $-\frac{\hbar^2}{2m}\left(\psi_{xx}+\psi_{yy}+\psi_{zz}\right)=-\frac{\hbar^2}{2m}\nabla^2\psi$.
- 3D Schrodinger equation: $i\hbar\psi_t=-\frac{\hbar^2}{2m}\nabla^2\psi+V\cdot\psi$.
- Probability:
  - $\int\int\int|\psi|^2dx\,dydz$.
  - $\int\int\int|\psi|^2r^2\sin\phi\,dr\,d\phi\,d\theta$.

3D free particle ($V=0$)

- $\psi(x,t)=\exp(i(k\cdot x-\omega t))=\exp\left(i\left(k_xx+k_yy+k_zz-\omega t\right)\right)$, $E=\frac{p^2}{2m}=\frac{(\hbar k)^2}{2m}=\hbar\omega$.
- k vector points in the direction the particle is moving.

3D time independent Schrodinger

- $g(t) = \exp\left(-i\frac{Et}{\hbar}\right) = \exp(-i\omega t)$.
- Space equation: $E\psi(x) = -\frac{\hbar^2}{2m}\nabla^2\psi + V\cdot\psi$.

Particle in 3D box

- Assume $V(x) = 0$, for $0 < x < a$, $0 < y < b$, $0 < z < c$, and $V(x) = \infty$ otherwise.
- $E\psi = -\frac{\hbar^2}{2m}\nabla^2\psi$, boundary condition: $\psi = 0$ at $x = 0, a$, $y = 0, b$, $z = 0, c$.
- Solution: $\psi = A\sin(k_x x)\sin(k_y y)\sin(k_z z)$.
  - $k_x = \frac{n_x\pi}{a}$, $k_y = \frac{n_y\pi}{b}$, $k_z = \frac{n_z\pi}{c}$.
  - $A^2\left(\frac{a}{2}\right)\left(\frac{b}{2}\right)\left(\frac{c}{2}\right) = 1$.
- $E = \frac{\hbar^2}{2m}\left(\left(\frac{n_x\pi}{a}\right)^2 + \left(\frac{n_y\pi}{b}\right)^2 + \left(\frac{n_z\pi}{c}\right)^2\right) = \frac{(\hbar k)^2}{2m}$.
  - Rewrite as $E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$.
  - Lowest energy state: $n_x = n_y = n_z = 1$.
  - If all 3 dimensions are the same value w: $E = E = \frac{\hbar^2\pi^2}{2mw^2}\left(n_x^2 + n_y^2 + n_z^2\right)$.
    - Some states will have the same energy, these states are called degeneracy.

Spherical symmetry

- Coulomb potential: $V(r) = \frac{qQ}{4\pi\epsilon_0}\frac{1}{r}$.
- 3D harmonic oscillator potential with all spring constant the same: $V = \frac{1}{2}(kx^2 + ky^2 + kz^2) = \frac{1}{2}kr^2$.
  - Kinetic energy doesn't depend on direction
- Spherical gradient
  - $\nabla F = rF_r + \theta\frac{1}{r}F_\theta + \phi\frac{1}{r\sin\theta}F_\phi$.
- Divergence (net flux of a vector function out of a cube, divided by the volume)
  - Vector function: $G = rG_r + \theta G_\theta + \phi G_\phi$.
  - Flux of the r-component: $\Phi_r = G_r\cdot\Delta_\theta\cdot\Delta_\phi = G_r\cdot r\Delta\theta\cdot r\sin\theta\,\Delta\phi$.
  - Volume: $V = \Delta r\Delta\theta\Delta\phi\, r^2\sin\theta$.
  - Partial divergence: $\frac{\Delta\Phi_r}{V} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2G_r)$, $\frac{\Delta\Phi_\theta}{V} = \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\, G_\theta)$, $\frac{\Delta\Phi_\phi}{V} = \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(G_\phi)$.
  - Total divergence: $\nabla\cdot G = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2G_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\, G_\theta) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(G_\phi)$.
- Spherical Laplacian: $\nabla^2F = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2F_r) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\, F_\theta) + \frac{1}{r^2\sin^2\theta}F_{\phi\phi}$.
- So the spherical Schrodinger: $E\psi = -\frac{\hbar^2}{2M}\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\psi_r) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\,\psi_\theta) + \frac{1}{r^2\sin^2\theta}\psi_{\phi\phi}\right) + V(r)\psi$.
- Separation:
  - $\psi(r,\theta,\phi) = F(r)G(\theta)H(\phi)$.
  - $EF(r) = -\frac{\hbar^2}{2Mr}\frac{\partial}{\partial r}(r^2F_r) + \left(V(r) + \frac{\hbar^2\lambda}{2Mr^2}\right)F(r)$.
  - $\sin\theta\frac{\partial}{\partial\theta}(\sin\theta\ G_\theta) = (-\lambda\sin^2\theta + \mu)G(\theta)$.
    - $G(\theta) = \sin^{\mathrm{M}}\theta$, $\lambda = M(M+1)$.
    - $G(\theta) = \sin^{\mathrm{M}}\theta\cos\theta$, $\lambda = (M+1)(M+2)$.
    - General case: $G(\theta) = \sin^{\mathrm{M}}\theta\, Q_{N,M}(\cos\theta)$.
      - $Q_{N,M}(\cos\theta)$ is a polynomial of order N, with only even or only odd powers of $\cos\theta$.
      - M, N need to be positive integers.
      - $\lambda = (M+N)(M+N+1) = l(l+1)$.

- $G(\theta)$ are called associated Legendre functions $P_l^m(\cos\theta)$, $l = M + N$, $m = M$.
  - When $m = 0$, they are called Legendre polynomials $P_n(x)$.
  - $P_l^m = (-1)^m (\sin\theta)^m \frac{d^m}{d(\cos\theta)^m}\big(P_l(\cos\theta)\big)$.
- $H_{\phi\phi} = -\mu H(\phi)$.
  - $H(\phi) = \exp(im\phi)$.
  - It must be continuous as ϕ crosses from 2π to 0.
  - m must be an integer.
- E, λ, μ are constants.

Spherical Harmonics

- Combine the Legendre function with ϕ dependence.
- $Y_l^m(\theta,\phi) = P_l^m(\theta)\exp(im\phi)$.
- They are also normalized

Radial Schrodinger equation

- $\frac{2Mr^2}{\hbar^2}\big(E - V(r)\big) + \frac{\partial}{\partial r}\left(r^2 \frac{\partial F}{\partial r}\right)\frac{1}{F} = \lambda$.
- Then $EF(r) = -\frac{\hbar^2}{2Mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial F}{\partial r}\right) + \left(V(r) + \frac{\hbar^2\lambda}{2Mr^2}\right)F(r)$.
- Kinetic energy due to angular momentum $\frac{\hbar^2\lambda}{2Mr^2} = \frac{\hbar^2 l(l+1)}{2Mr^2}$.
  - Classically, $\frac{L^2}{2Mr^2}$.
- For each given potential and l, we have many radial solutions, each with its own energy, and radial quantum number k. If $l > 0$, there will be several different m values with same E
- Each different l gives a new set of radial functions, with own energies and radial quantum numbers.
- Substitute $F(r) = \frac{U(r)}{r}$, $F_r = \frac{rU_r - U}{r^2}$, we get $-\frac{\hbar^2}{2M}U_{rr} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2Mr^2}\right)U = EU$ (radial Schrodinger, 1D Schrodinger with modified potential).
  - Full wave function: $\psi_{klm}(r,\theta,\phi) = \frac{1}{r}U_{kl}(r)Y_l^m(\theta,\phi)$.
  - Three quantum numbers k, l, m.
  - Effective potential: $V(r) + \frac{\hbar^2 l(l+1)}{2Mr^2}$.
- Boundary conditions
  - $U(r) = 0$ at $r = 0$, otherwise $\frac{1}{r}U(r)$ will be infinite.
  - $U(r) \to 0$ as $r \to \infty$, otherwise, it cannot be normalized.

Infinite spherical square well

- If $l = 0$, $u_{n0}(r) = \sin\left(\frac{n\pi r}{R}\right)$, $E_{n0} = n^2\frac{(\hbar\pi)^2}{2MR^2}$, $\psi_{n00} = \frac{1}{r}\sin\left(\frac{n\pi r}{R}\right)Y_0^0(\theta,\phi)$.
- For $l > 0$, energy of the lowest state for a given l increases with l, but the states don't line up horizontally.

Energy levels

- Centrifugal potential: $\frac{\hbar^2 l(l+1)}{2Mr^2}$ always increases the energy.
  - Lowest state $l = 0$, labelled with $k = 0$, we must have $m = 0$.
  - Energies of $l = 0$ states increase with k.
  - $l = 1$ states will have higher energy than the lowest state, but not necessarily higher than $l = 0$ states with higher k.
  - $l = 1$ states can have $m = 0, \pm 1$, there are 3 states with the same energy for each one.
- $l = 0$ solutions are independent of angle or spherically symmetric, s-waves, s-states.
- $l = 1$, p-waves, p-states.
- $l = 2$, d-waves, d-states.
- $l = 3$, f-waves, f-states.
- $l = 4$, g-waves, g-states.

Radial equation for hydrogen

- Define $X = \frac{2m}{\hbar^2}$, $Y = \frac{Mq^2}{2\pi\hbar^2\epsilon_0}$.
- $U_{rr} = \left(-XE - Y\frac{1}{r} + l(l+1)\frac{1}{r^2}\right)U(r)$.
- Guess $U(r) = r^n \exp(-br)$.
  - $n = l + 1, b = \frac{Y}{2}\frac{1}{n} = \frac{1}{n\,a_0}, E = -\frac{Y^2}{4X}\frac{1}{n^2}$.
- It agrees the Bohr model, where radius $a_0 = \frac{4\pi\hbar^2\epsilon_0}{q^2 M}$, so $b = \frac{1}{na_0}$.
- Guess $U(r) = \left(r^n + Ar^{n-1}\right)\exp(-br)$, $n = l + 2, b = \frac{1}{n\,a_0}$.
  - $E = -\frac{Y^2}{4X}\frac{1}{n^2}, A = -n(n-1)a_0$.
- Guess $U(r) = \left(r^n + Ar^{n-1} + Br^{n-2}\right)\exp(-br), n = l + 3$.
  - E and b are fixed, we can solve for A and B.

Hydrogen states

- $l = 0$ has a single state $m = 0$.
  - $n = 1$, single 1s state (for $l = 0$).
- $l = 1$ has 3 states, $m = 0, \pm 1$.
  - $n = 2$, one 2s state, three 2p states (for $l = 1$).
- $l = 2$ has 5 states, $m = 0, \pm 1, \pm 2$.
  - $n = 3$, One 3s state, three 3p states, five 3d states (for $l = 2$)
- $l = 3$ has 7 states, $m = 0, \pm 1, \pm 2, \pm 3$.

Pauli exclusion principle

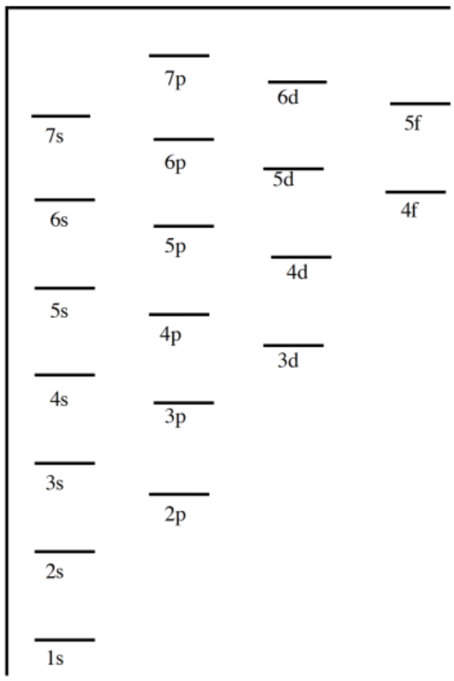
- Only 2 electrons per state
- Due to electrons having intrinsic spin of $\frac{1}{2}$ (spin-up or spin-down).
- Real rule: there can be only one electron per state, but the state includes the intrinsic spin of the electron
- Particles with zero spins (pions) or spin 1 (photons) don't care, can put as many per state as we want

Bigger atoms

- Helium has a charge of 2, for the first electron, that cuts the radius in half, and quadruples the binding energy
  - 2 electrons, both of them go into the lowest energy state, the energies are different due to screening
- Lithium has a charge of 3
  - First electron is the same.
  - Second electron does what it does in helium
  - Third electron goes to the 2s state.
- Can put 2 electrons into the 1s state, 2 more into the 2s state for a total of 4.
- 2p state has 3 different m states, all with the same energy as the 2p states, so we can put in 6 more electrons, for a total of 10

Multiple electron atoms

- Lowest states fill up first
- Each state can hold 2 electrons
- When there are multiple electrons, the inner electrons shield the outer electrons from some of the nuclear charge
  - 2p level shifts up relative to the 2s level.
  - 3d is higher than 3p than 3d

- 

Spectroscopic notation

- Superscript means how many electrons are in the state
- Hydrogen: $1s^1$.
- Helium: $1s^2$.
- Lithium: $1s^2 2s^1$.
- Oxygen with 8 electrons: $1s^2 2s^2 2p^4$.
- Iron: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$.
    - 4s orbit fills up before the 3d starts.

Applications

June 9, 2021 9:34 AM

Contradiction (interaction of photons):

- Black-body radiation spectrum: smooth function of frequency
- Structure of atoms: discrete frequency

Plasma:

- Electrons and protons or helium nuclei too hot to form atoms
- Charged particles are free, not bound into quantum states
- Interact into a Maxwellian thermal equilibrium
- When charged particles scatter from each other, the acceleration creates EM radiation: photons
- Photons Rayleigh-scatter from the charged particles, making the blackbody radiation spectrum

Solid matter

- Solids are atoms packed together
- Behave differently from isolated atoms
- X-ray frequency range (Moseley): quantum properties of energy levels of individual atoms
- Infrared frequency rage (thermal): collective motions of many atoms
- Visible lights (in between): complicated

Non-conducting solids

- Electrons shared between atoms, but not free to move between molecules
- Pure material is transparent (crystal, glass)
- Impurities give the material color
  - Pure aluminum oxide (corundum) is transparent
  - Chromium impurity absorbs blue and green, making ruby
- Speed of light in the material is different than vacuum
  - Refraction at interfaces
  - Powdered crystals become white and opaque

Conducting solid

- Some electrons can move fairly freely between atoms, with a continuous energy distribution
- In UV and above, photons can knock electrons out of the atoms (photoelectric effect)
  - EM radiation is absorbed
- Below UV, EM field causes the free electrons to move, generating other EM fields
  - Waves reflect from the material

Atomic gases

- Isolated single atoms emit or absorb discrete wavelengths
- Atoms that are hot, or are excited by higher energy photons, emit spectral lines
- Against bright background, like thermal radiation from a star, cold gases will absorb light at their spectral lines
- Ring nebula
  - Hot blue star in the middle makes thermal UV photons
  - Absorbed by the gas cloud, radiates the visible spectral lines of the elements in the gas cloud
- Solar absorption lines
  - The sun has an atmosphere above the hot plasma that emits blackbody radiation
  - Atoms in the atmosphere absorb discrete frequencies, which gives narrow dark lines in the spectrum

Molecular gases

- Atoms in molecules can vibrate relative to each other
- Frequency and energy of atom vibration is lower than electrons
- Have absorption bands in the infrared, causing greenhouse effect

Photon absorption rate

- Transitions between states
- Absorb a photon of energy E_γ, causing an atom to go from E_1 to E_2
  - Final state: $\psi_F = \psi_2(x)e^{-i\frac{E_2}{\hbar}t}$.
  - Initial state $\psi_I = \psi_1(x)e^{-i\frac{E_1}{\hbar}t} \times \Gamma(x)e^{-i\frac{E_\gamma}{\hbar}t}$.
- Interaction rate:
  - $\int \psi_F^* \cdot \psi_I dxdt = \int \left(e^{i\frac{E_2-E_1-E_\gamma}{\hbar}t}\right) dt\left(\psi_2^*\psi_1\Gamma\right)dx$.
  - If $E_2 = E_1 + E_\gamma$, the integral grows with time.
  - Otherwise, it just oscillates around zero
  - The photon is absorbed only if energy is conserved
  - Space integral depends on the wavefunctions, but not on time, so some transitions that are allowed could be faster or slower than others, and some may not happen
- EM field of photon with frequency $\frac{E_\gamma}{\hbar}$ shakes the atom with resonant frequency $\frac{E_2-E_1}{\hbar}$.
  - If the resonant frequency is the same as the photon frequency, the atom gets excited into E_2 by absorbing the photon.

Photon emission rate

- Final state: $\psi_F = \psi_1(x)e^{-i\frac{E_1}{\hbar}t} \times \Gamma(x)e^{-i\frac{E_\gamma}{\hbar}t}$.
- Initial state: $\psi_I = \psi_2(x)e^{-i\frac{E_2}{\hbar}t}$.
- Integral becomes $\int \psi_F^* \cdot \psi_I dxdt = \int \left(e^{i\frac{E_1+E_\gamma-E_2}{\hbar}t}\right) dt\left(\psi_1^*\Gamma^*\psi_2\right)dx$.
- No initial EM field, we can think that the EM field is quantized and has zero point energy at all possible frequencies
  - It shakes the atom at its resonant frequency and cause the photon to be emitted
- Simulated emission:
  - If an atom is in E_2, a photon comes along with energy E_γ.
  - Shake the atom at $\frac{E_2-E_1}{\hbar}$, which cause it to emit a photon energy E_γ, but the initial photon would still exist
  - Energy conservation: $E_2 + E_\gamma = E_1 + E_\gamma + E_\gamma$.
  - Best to think of the process not as emitting an extra photon, but as doubling the intensity of the original photon, from $n = 1$ to $n = 2$.

Absorption, emission, and temperature

- If a gas is cold, only the ground state is populated, only absorption, no emission
- If a gas is hot, some atoms will be in excited states, but many more will be in the ground state
- Spontaneous emission, and some stimulated emission, but the photons tend to be absorbed by the more numerous atoms in the ground state
  - Re-emitted in random directions, resulting in a diffuse glow

Stimulated emission chain reaction

- One photon could cause an atom to emit a second photon, which could generate more and more photons
- Problem: absorption integral is the same as the stimulated emission integral
- Since there are more ground-state atoms than excited atoms, the absorption would be larger than the stimulated emission, and the chain reaction would die out
- Population inversion:
  - More atoms in the excited state than in the ground state to make the chain reaction work
  - Population is proportional to $e^{-\frac{\Delta E}{kT}}$, so lower energy states are always more populated

        - Normal thermal ways cannot achieve the effect.
    - Microwave Amplification by Stimulated Emission of Radiation (MASER) can be used to achieve this
        - Low-power microwaves went into the resonator, caused stimulated emission from excited atoms, and microwaves came out at higher power
        - Does not work for visible light

Optical pumping
- Pumping is self-limiting, because it causes random stimulated emission back down to the ground state
- 3-level optical pumping
    - Can work if there is another state between the upper state we are pumping to and the ground state
    - Populate state E_3 by optical pumping.
    - Spontaneous emission from state E_3 populates state E_2
    - If spontaneous emission from E_2 is low, we can have more atoms in E_2 than E_1 and get population inversion.
- 4-Level pumping
    - If there is another state with a very short lifetime between the long-lived intermediate state and the ground state, optical pumping works even better
    - The laser uses the transitions between the two middle states
    - The lower state population cleans itself out quickly

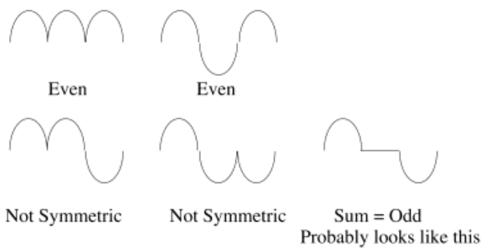
Gas-discharging laser
- Excite gas atoms with an electrical discharge
- One gas is excited, and transfers its excitation to another, which does the actual lasing
- He-Ne lasers excite He, which transfers to Ne, which has the desired long and short lived states

CO2 laser transitions
- Discharge excited N_2, transfers to CO_2, molecular vibrations make photons

Semiconductors
- They are at the borderline between insulators and metallic conductors

Double square well
- Two identical square wells separated by some distance
- Wavefunction extends beyond the well, and the particle tunnels into the other well
- The tunnelling doesn't stop when the particle is half in one well and half in the other. It goes completely into the other well. Then tunnels back into the first well and process repeats
- Wavefunction inside each well is a sinusoid
    - Can be the same sign or opposite sign in the two wells
    - If add together, they add in one well and cancel in the other, so we get a particle in one well
- Wavefunction between the wells is real exponential
- Wavefunctions are either even or odd
- All the energy levels split

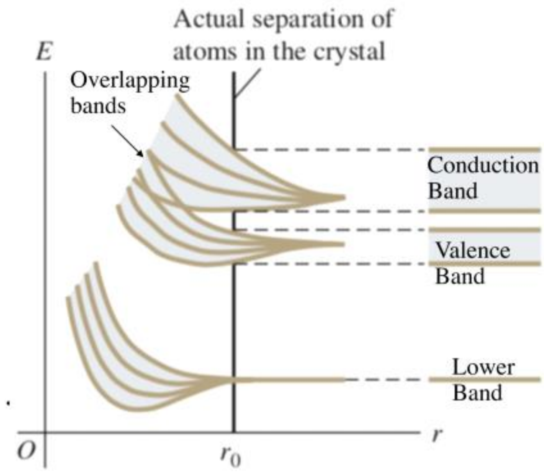
Three potential wells
- Let the first well always have a positive bump
- The second and third well could have either sign of bump
- If the potential is symmetric, there is also requirement that the wavefunction be either even or odd, and not all the shapes satisfy that

- 

N potential wells

- If there are N potential wells, each energy level splits into N closely-spaced energy level
- The amount of splitting depends on how close together the wells are, and the height of the barriers between them
- Allowing particles to flow between wells increases the wavelength, which reduces the kinetic energy contribution
- If the wavefunction is large in the barriers, that increases the potential energy

Level splitting in crystals

- If the atoms are far apart, they will have the usual Schrodinger equation levels, the same for each atom
- When atoms are closer, the energy levels split more and more
- At the actual separation of atoms, there are N closely spaced levels split from the original levels
- Energy bands
    - The possible electron energies form effectively continuous energy bands
    - Can be energy gaps between different bands
    - Bands can overlap
    - 

Pauli principle and bands

- If we have N atoms, each level splits into N levels
- The first 2N electrons go into the lowest band
- The next 2N electrons go into the next band
- This contines until we have assigned all the electrons
- There are still possible wavefunctions corresponding to higher electron energies. They are just not occupied

Conductivity

- Even though electrons can tunnel from atom to atom, that may not result in electrical conductivity
- If a band is fully occupied, there are no empty states for electrons to move into, so full bands don't conduct
- If a band is completely empty, there are no electrons to move, so that doesn't conduct
- If a band is not full, there are un-occupied states that electrons can use to move, that gives conductivity

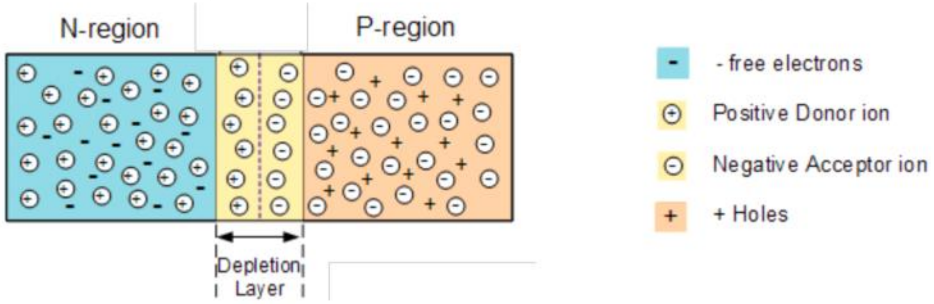
Insulator, conductor, semiconductor

- Insulator: at absolute zero, there are no electrons in the conduction band with large energy gap
- Conductor: partially filled conduction band with large energy gap
- Semi-conductor: empty conduction band, but a smaller gap between the valence and conduction bands

Semiconductors and doping

- Doping: putting impurities into the semiconductors
- Pure germanium (or silicon) has a full valence band and empty conduction band, with a small gap between them
- Arsenic has 5 outer electrons. Normal thermal excitation can detach the extra electron from its atom, and it can wander around the conduction band
- Gallium has 3 outer electrons. This leaves a hole in the valence band. The hole can be detached from the atom and move around, contributing to conductivity

PN junction

- Start with a pure silicon wafer
- Diffuse some P-type impurity into the whole thickness
- Then diffuse enough N-type impurity to reverse the polarity, but just of the surface
- 

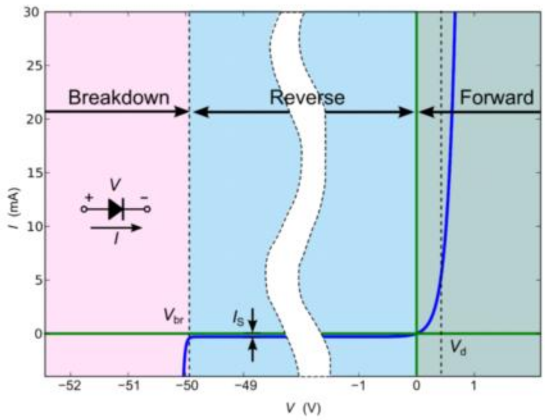
- The electrons and holes neutralize each other in a thin depletion layer that has the low conductivity of pure silicon
- The N-region and P-region conduct
- The charge flow to form the depletion layer results in a built-in potential difference across the junction

Solar cell

- Photons that enter the silicon can detach an electron from an atom, leaving a hole behind
- The built-in electric field separates the electron from the hole, causing an electric current to flow

Rectifier diode

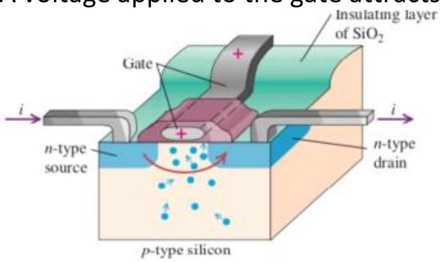
- Thickness of the depletion layer can be changed by applying an external voltage to the PN junction
- Standard rectifier: If a large enough positive voltage is applied to the P-side (0.6V for silicon), the depletion layer gets o thin that significant conduction occurs.
- Zener mode: for negative voltage, there is a tiny reverse current, until a sudden breakdown at a large voltage

- 

Light-emitting diode

- When a diode is conducting, there are lots of electrons and holes in the depletion region
- They can re-combine, annihilating each other
- The energy of recombination can turn into a photon

Field-effect transistor

- 2 N-type islands in P-type silicon.
- Grow an insulating layer of oxide on tope
- Etch holes above the N-type islands and deposit metal connecting wires
- Deposit another metal wire over the region between the N-type islands without a hole
- One of the PN junctions is always reverse-biased
    - No current flow between the source and the drain
- A voltage applied to the gate attracts holes to the region, allowing current to flow
- 

Harmonic Oscillator

July 12, 2021 8:37 AM

Classical

- Force: $F = -kx$.
- $F = ma$ gives $-kx = m\frac{d^2x}{dt^2}$.
- Solution is $x = A\cos\omega t$, $\omega = \sqrt{\frac{k}{m}}$.
- Potential: $V(x) = \frac{1}{2}kx^2$.
- Energy: $E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$ constant.
- Maximum displacement for a given energy is at $v = 0$, $x = A$
  - $E = \frac{1}{2}kA^2$.
  - $\frac{E}{\omega} = \frac{A^2}{2}\sqrt{km}$.

1D harmonic oscillator

- Potential: $V = \frac{1}{2}kx^2$.
- Schrodinger equation: $\frac{\hbar^2}{2m}\psi_{xx} = \left(\frac{1}{2}kx^2 - E\right)\psi$.
- With large x, E is negligible, $\frac{\hbar^2}{2m}\psi_{xx} = \frac{1}{2}kx^2\psi$.
- Solutions:
  - $\psi = \exp\left(-\frac{x^2}{2b^2}\right)$, $b^2 = \frac{\hbar}{\sqrt{km}}$, $E = \frac{1}{2}\hbar\sqrt{\frac{k}{m}} = \frac{1}{2}\hbar\omega_{classical}$.
  - $\psi = x\exp\left(-\frac{x^2}{2b^2}\right)$, $b^2 = \frac{\hbar}{\sqrt{km}}$, $E = \frac{3}{2}\hbar\sqrt{\frac{k}{m}} = \frac{3}{2}\hbar\omega_{classical}$.
- If we rewrite $E = \eta\hbar\omega$, $x = by = y\sqrt{\frac{\hbar}{\sqrt{km}}}$ and plug into Schrodiner equation.
  - $\psi = fg = f(x)\exp(-\frac{x^2}{2b^2})$.
  - $\frac{1}{2}f'' - yf' + \left(\eta - \frac{1}{2}\right)f = 0$.
  - When $f = 1, \eta = \frac{1}{2}, \psi_0 = e^{-\frac{y^2}{2}}, E = \frac{1}{2}\hbar\omega$.
  - When $f = y, \eta = \frac{3}{2}, \psi_1 = ye^{-\frac{y^2}{2}}, E = \left(1 + \frac{1}{2}\right)\hbar\omega$.
  - When $f = y^2 - \frac{1}{2}, \eta = \frac{5}{2}, \psi_2 = \left(y^2 - \frac{1}{2}\right)e^{-\frac{y^2}{2}}, E = \left(2 + \frac{1}{2}\right)\hbar\omega$.
  - When $f = y^3 - \frac{3}{2}y, \eta = \frac{7}{2}, \psi_3 = \left(y^3 - \frac{3}{2}y\right)e^{-\frac{y^2}{2}}, E = \left(3 + \frac{1}{2}\right)\hbar\omega$.
  - When $f = y^4 - 3y^2 + \frac{3}{4}, \eta = \frac{9}{2}, \psi_4 = \left(y^4 - 3y^2 + \frac{3}{4}\right)e^{-\frac{y^2}{2}}, E = \left(4 + \frac{1}{2}\right)\hbar\omega$.
  - $y = \frac{x}{b}$, $b^2 = \frac{\hbar}{\sqrt{km}}$, $\omega = \sqrt{\frac{k}{m}}$.
  - Width of the wave function is $2b$.

Summary of solutions

- Wave functions: $\psi_n = H_n(y)\exp\left(-\frac{y^2}{2}\right)$, $n \geq 0$.
  - Gaussian with a polynomial H_n of order n.
- Solutions alternate between even and odd, the polynomials have either all even powers or all odd powers
- H_n are called Hermite polynomials, with first factor 2^n as normalization.
  - $H_0 = 1$.
  - $H_1 = 2x$.
  - $H_2 = 4x^2 - 2$.

- $H_3 = 8x^3 - 12x$.
- $H_4 = 16x^4 - 48x^2 + 12$.

Comparing solutions

- Infinite square well
  - $\psi_n = \sin\left(\frac{nx}{w/\pi}\right), n \geq 1, E_n = n^2 E_1$.
- Harmonic oscillator
  - $\psi_n = H_n\left(\frac{x}{b}\right)\exp(-\frac{x^2}{2b^2}), n \geq 0, E_n = \left(n + \frac{1}{2}\right)\hbar\omega$.
- Coulomb potential ($l = 0$)
  - $\psi_n = \frac{1}{r}L_n\left(\frac{r}{a_0}\right)\exp\left(-\frac{r}{na_0}\right), n \geq 1, E_n = -\frac{1}{n^2}E_1$.

XYZ harmonic oscillator

- 3D potential: $V = \frac{1}{2}\left(k_x x^2 + k_y y^2 + k_z z^2\right)$.
  - If spring constants are the same: $V = \frac{1}{2}k\left(x^2 + y^2 + z^2\right)$.
- Can get three independent harmonic oscillator equations
- $E = \left(n_x + \frac{1}{2}\right)\hbar\omega + \left(n_y + \frac{1}{2}\right)\hbar\omega + \left(n_z + \frac{1}{2}\right)\hbar\omega = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega$.
- The total wave function is the product of one wave function for each of x, y, z each with its own quantum number.
  - $\psi_{n_X n_Y n_Z} = H_{n_X}\left(\frac{x}{b}\right)e^{-\frac{x^2}{2b^2}}H_{n_Y}\left(\frac{y}{b}\right)e^{-\frac{y^2}{2b^2}}H_{n_Z}\left(\frac{z}{b}\right)e^{-\frac{z^2}{2b^2}}$.

States

- Lowest state: $n_x = n_y = n_z = 0, E = \frac{3}{2}\hbar\omega$.
- One dimension excited: $E_{100} = E_{010} = E_{001} = \left(1 + \frac{3}{2}\right)\hbar\omega$.
- 6 ways to get $E = \left(2 + \frac{3}{2}\right)\hbar\omega$.
- 10 ways to get $E = \left(3 + \frac{3}{2}\right)\hbar\omega$.
- 15 ways to get $E = \left(4 + \frac{3}{2}\right)\hbar\omega$.
- 21 ways to get $E = \left(5 + \frac{3}{2}\right)\hbar\omega$.

Probability density

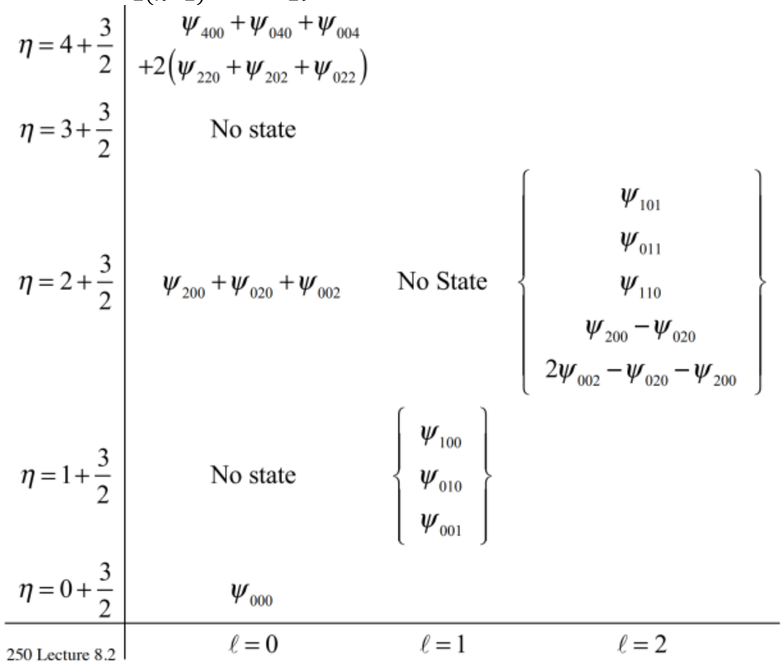
- One unit vibration in x: $\psi_{100} = xe^{-\frac{x^2+y^2+z^2}{2b^2}} = xe^{-\frac{r^2}{2b^2}}$.
  - Probability density $\psi_{100}^*\psi_{100} = x^2 e^{-\frac{r^2}{b^2}}$.
- One unit vibration in x and y: $\psi_{100} + \psi_{010} = (x + y)e^{-\frac{r^2}{2b^2}}$.
  - Probability density: $\left(\psi_{100}^* + \psi_{010}^*\right)\left(\psi_{100} + \psi_{010}\right) = (x + y)^2 e^{-\frac{r^2}{b^2}}$.

Spherical harmonic oscillator

- Reduced radial equation: $-\frac{\hbar^2}{2M}u_{rr} + \frac{1}{2}kr^2 u + \frac{\hbar^2 l(l+1)}{2Mr^2}u = Eu$.
- $l = 0$, it is 1D oscillator equation $u_n(x) = H_n(x)e^{-\frac{x^2}{2b^2}}, \frac{1}{b^2} = \frac{\sqrt{kM}}{\hbar}, E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \omega = \sqrt{\frac{k}{m}}$.
  - But extra boundary condition: $u = 0$ at $r = 0$, so $n = 0,2,4, \ldots$ cannot be used.
  - Lowest usable state: $n = 1, E = \left(1 + \frac{1}{2}\right)\hbar\omega$ (same to XYZ).
    - Full wave function $\psi = e^{-\frac{r^2}{2b^2}}$.
  - $n = 3, E = \left(3 + \frac{1}{2}\right)\hbar\omega$.
    - $\psi = \left(\frac{r^2}{b^2} - \frac{3}{2}\right)e^{-\frac{r^2}{2b^2}}$.
  - $n = 5, E = \left(5 + \frac{1}{2}\right)\hbar\omega$.

        - $\psi = \left(\frac{r^4}{b^4} - \frac{5r^2}{b^2} + \frac{15}{4}\right) e^{-\frac{r^2}{2b^2}}$.
    - Spherical harmonic is $Y_0^0 = 1$, so no angle dependence.

Dimensionless variables

- Let $E = \eta\hbar\omega, r = b\rho, \omega = \sqrt{\frac{k}{m}}, b^2 = \frac{\hbar}{\sqrt{km}}$.
- Then $-\frac{1}{2}u_{\rho\rho} + \frac{1}{2}\rho^2 u + \frac{1}{2}\frac{l(l+1)}{\rho^2}u = \eta u$.
- Rearrange: $u_{\rho\rho} = \left(\rho^2 + \frac{l(l+1)}{\rho^2} - 2\eta\right)u$.
- Product wave function: $u_{\rho\rho} = \left(f'' - 2\rho f' + (\rho^2 - 1)f\right)g$ (with $u = fg, g = e^{-\frac{\rho^2}{2}}$).
- So $f'' - 2\rho f' + \left(2\eta - 1 - \frac{l(l+1)}{\rho^2}\right)f = 0$.
- Guess $f = \rho^n$.
    - $n = l + 1$.
    - $\eta = l + \frac{3}{2}, E = \left(l + \frac{3}{2}\right)\hbar\omega$.
    - $\psi = \frac{b}{r}u_{0l} = \frac{r^l}{b^l}e^{-\frac{r^2}{2b^2}}$.
- Guess $f = \rho^n + A\rho^{n-2}$.
    - $n = l + 2$.
    - $\eta = l + \frac{5}{2}, E = \left(l + \frac{5}{2}\right)\hbar\omega$.
    - $A = \frac{n(n-1)}{2(n-2)} = \frac{(l+2)(l+1)}{2l}$.
- 

Complex spherical harmonics

- $Y_{l=1}^{\pm 1} = Y_{l=1}^X \pm iY_{l=1}^Y$.
    - $Y_{l=1}^X = \frac{Y_{l=1}^1 + Y_{l=1}^{-1}}{2} = \sin\theta\cos\phi, Y_{l=1}^Y = \frac{Y_{l=1}^1 - Y_{l=1}^{-1}}{2} = \sin\theta\sin\phi$.
    - Using $z = r\cos\theta, x = r\sin\theta\cos\phi, y = r\sin\theta\sin\phi$, we get.
        - $Y_{l=1}^X = \frac{x}{r}, Y_{l=1}^Y = \frac{y}{r}, Y_{l=1}^Z = \frac{z}{r}$
- $l = 1, m = \pm 1$ wave function is $\psi_{100} + i\psi_{010} = \frac{x}{b}e^{-\frac{r^2}{2b^2}} \pm i\frac{y}{b}e^{-\frac{r^2}{2b^2}}$.
    - $\left(\psi_{100} \pm i\psi_{010}\right)^* = \left(\psi_{100}^* \mp i\psi_{010}^*\right)$.
    - Probability density: $\frac{x^2+y^2}{r^2}e^{-\frac{r^2}{b^2}}$.