## PHY293: Modern Physics

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## 1 Introduction to Modern Physics

• Classical Physics (1400-1900): heliocentric model, force laws, electromagntism, classical mechanics etc.

- Modern Physics (1900-today): special & general relativity, quantum mechanics, big bang, particle physics etc.
- Classical Physics faced several crises
  - Galilean relativity didnt define a preferred reference frame
  - Photoelectric effect
  - Nature of electromagnetism
  - Ultraviolet catastrophe
  - Speed of light constant?
- Hints of modern physics
  - emergence on "quanta" explained Photoelectric effect
- Special relativity motivated by constant c

#### 2 Introduction to Special Relativity

- Galilean principle of relativity
  - Cant tell whether you are in uniform motion or at rest wrt another observer
  - The laws of nature are the same in a laboratory moving relative to an observer or a laboratory at rest
- Inertial reference frame
  - a reference frame where Newton's law of inertia holds
- Concept of Simultaniety
  - Observers in different inertial frames agree on simultaneous "events"
- Nature insists that light has the same speed regardless of reference frame (this is a well established fact)
- Consider a train (3 cars) that has a flash bulb in the centre of the train and two photo cells and clocks at each end
  - Clocks will record light pulse at  $\Delta t_{train} = \frac{d}{2c}$  where d is the length of the train
- Now consider the train in motion so that its length is now d'
  - Flashes going forward and backward travel at c in the observer's reference frame
  - Since the train is moving forward, light will reach the back of the train first i.e. not simultaneous
  - Clocks don't appear synchronized

- What happens to the length?
  - Conclude that distances perpendicular to relative motion don't change between inertial frames.
- Clocks at rest & in motion
  - Light clock using light bouncing from end of metre stick to another
  - In rest frame of metre stick, a tick is  $\frac{2m}{c}$ .
  - In our frame, light travels further so that  $\Delta t' = \Delta t \gamma$  where  $\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$
  - Called time dilation
  - Conclusion: Any clock relative to us is keeping time at a different rate
- What happens with distances parallel to velocity?
  - After some algebra and using t', we get  $l' = l \cdot \sqrt{1 \frac{v^2}{c^2}} = \frac{l}{\gamma}$
  - Phenomena known as Lorentz contraction!
- GPS: Example of time dilation
  - Time slip per day relative to the transmitter on the ground is around 5  $\mu$  s
  - Synchronization of time is important since the precision is of order > 100ns.

## 3 Lorentz Transformations

- In rest frame of ruler, bulb flashes at t=0 and ruler has length l so  $\Delta t=\frac{l}{C}$ .
- In the observer's frame, metre stick is travelling to the left with velocity v. First, metre stick is Lorentz contracted with  $l' = l\sqrt{1 \frac{v^2}{c^2}}$ .
  - When flash detected, clock reads  $\frac{l}{c}$ .
  - But time to go from bulb to detector in observer frame is  $\Delta t' = \frac{l\sqrt{1-\frac{v}{c}}}{c\sqrt{1+\frac{v}{c}}}$
  - Clocks run slowly when moving so observed elapsed time is  $\Delta t' \sqrt{1 \frac{v^2}{c^2}} = \frac{l}{c} \frac{lv}{c^2}$

#### • Summary

- Time in a frame moving wrt rest frame is shifted proportional to time and distance
- Distances in a frames moving wrt rest frame shifted proportional to time and distance
- Leads to Lorentz transformation equations:

$$* ct' = \gamma(ct - \beta x)$$

- $* x' = \gamma(x \beta ct)$
- \* Note:  $\beta = \frac{v}{a}$
- General approach to 4 vector transformations
  - Define a 4-vector x = (ct, x, y, z)
  - Define "boost matrix" from frame S to S' moving along x-axis with speed v:

$$B = \begin{bmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Use matrix algebra to transform x
- Space time 4 vector defines "event"
- typically use inertial frames with relative velocity in x direction
- $-\gamma \ge 1$  at all times
- set of all Lorentz matrices form a group
- Minkowski diagrams are a graphical approach
  - One dimension is the x axis (scaled by c units of light-s)
  - Use time in seconds
  - Define axes in boosted frame by lines of constant  $\frac{x'}{c}$  and t'.
  - Angle to axes in rest frame of observer given by velocity of boosted frame
  - Specifically, the angle formed between events is  $\theta = \tan^{-1}(\frac{v}{c})$
  - More details and graphs in the lecture notes

## 4 Apparent Paradoxes in Special Relativity

- Simultaniety now depends on the inertial frame
  - Simultaniety is relative i.e. simulataneous events in a rest frame are not simulataneous in an inertial frame in motion
  - But when 2 events coincide in space and time, observers have to agree
- Pole in the barn problem
  - In rest frame, barn has a length  $L_b'$  and a pole with length  $L_p$  where  $L_b' < L_p$
  - Runner with the pole running at a velocity v
  - From the runner's perspective, the length of the barn is too short even shorter when Lorentz contracted

- Let t = t' = 0 be when pole enters barn
- In runners frame, barn is Lorentz contracted so time when pole hits other end of barm  $t_{front} = \frac{L_b}{v} = \frac{L_b'}{v} \cdot \frac{1}{\gamma}$
- At that point, back of pole sticks out of barn with length  $L_p L_b' \cdot \frac{1}{\gamma}$
- Time when back of pole enters barn in runners frame is  $t_{back} = \frac{L_p}{v}$
- In the barn frame, pole is Lorentz contracted so time when pole hits other end of the barn is  $t'_{front} = t_{front} \cdot \gamma$
- Observer sees time dilation in pole's rest frame
- Back of pole doesnt stick out of the barn
- Time back of pole enters barn in barn frame is  $t'_{back} = \frac{L_p}{v} \cdot \frac{1}{\gamma}$
- All of pole is in barn at the same time
- In runner's frame, there is time dilation so  $t_{back} = \frac{L_p}{v}$

#### • Twin Paradox

- Two twins one that is earth bound (Alice) and other (Berta) which takes a rocket trip returning to earth
- Who is older? Alice knows time dilation occurs on the rocket so will she be older? Berta knows time dilation occurs on Earth so is she older?
- Minkowski diagram provides the answer
- Earth time is dilated according to Berta
- But turning around at the planet, puts Berta in a non-inertial accelerating frame.
- Time on Earth runs faster as rocket ship turns around
- So Alice is older

#### • Relativistic Doppler Shift

- Special Relativity affects light frequencies
- Consider waves with frequency  $f_s$  in source frame with receiver moving away
- Period and wavelength of waves emitted by source in rest frame  $\Delta t_s = \frac{1}{f_s}$ ,  $\lambda_s = \frac{c}{f_s}$
- But receiver moves so time interval at receiver  $\Delta t_r$  satisfies:  $\lambda_s + v\Delta t_r = c\Delta t_r$  so  $\Delta t_r = \frac{1}{f_s(1-\beta)}$  where  $\beta = \frac{v}{c}$
- But there is time dilation in receiver frame so that  $\Delta t'_r = \Delta t_r \sqrt{1-\beta^2} = \frac{1}{f_s} \sqrt{\frac{1+\beta}{1-\beta}}$
- Can use relativistic doppler shifts to measure the expansion of universe
  - \* Use doppler shift of distant supernovae to measure speed of recession
  - \* Define redshift as  $z=\frac{\lambda_r-\lambda_s}{\lambda_s}=\frac{\lambda_r}{\lambda_s}-1=\frac{f_s}{f_r}-1$

# 5 Four-vectors, Lorentz invariants, Relativistic Energy and Momentum

- General approach to 4-vector transformations
  - Start with spacetime 4-vector x = (ct, x, y, z)
  - Define boost matrix B
  - Use matrix algebra to transform x' = Bx
  - Assumes inertial frames have relative velocity in x direction
  - Lorentz factor  $\gamma$  is always  $\geq 1$
  - The inverse of B is Lorentz transformation in the opposite direction
  - Many kinds of 4-vectors e.g. energy-Momentum, charge and current density, electric and magnetic potential
- Lorentz transformations classify observables
  - Lorentz scalars
  - Lorentz vectors
  - Tensors (e.g. Faraday Tensor)
  - Useful to introduce metric tensor
  - GO OVER THE NOTES AGAIN AND UPDATE
- Using relativistic energies and momenta
  - 4-vector momentum is  $p = (\frac{E}{c}, p_x, p_y, p_z)$
  - Quantity m is the "rest mass" i.e. mass of object in its rest frame
  - Specific to each particle
  - For massless particles  $\frac{E}{c} = p$ .
  - Lorentz invariant of 4-momentum is  $p^T \eta p = (\frac{E}{c})^2 p_x^2 p_y^2 p_z^2 = (m\gamma)^2 (c^2 v_x^2 v_y^2 v_z^2) = (mc\gamma)^2 \left(1 \frac{v_x^2 + v_y^2 + v_z^2}{c^2}\right) = m^2 c^2$
  - This can also be seen by looking at this in the rest frame  $p^T \eta p = (\frac{E}{c})^2 = m^2 c^2 \Rightarrow E = mc^2$

#### 6 Light Cones in Minkowski Diagrams

- ADD IMAGE FROM THE LEC SLIDES
- When considering 4-momentum, we can generalize Minkowski diagram to momentum space
- Defined as 4-D space with axes  $\frac{E}{c}$ ,  $p_x$ ,  $p_y$ ,  $p_z$

- The "mass shell" defines the physical region for a massive particle. Hyperboloid defines possible energy-momentum values of a particle
- Gives a heuristic way of looking at energy and momentum correlations

#### 7 Introduction to Quantum Mechanics

- Look at how light interacts with matter
- Black-body radiation became the stumbling block
  - Walls emit radiation but also have to absorb radiation
  - If walls black, then equal at all wavelengths
  - However spectrum of radiation in box depends on temperature
- Planck first noted quantization as the solution
- Particle nature of light was a second challenge

#### 8 Photoelectric Effect and Compton Scattering

- Photoelectric effect was discovered in 1887 and was the first evidence for light acting as a particle
  - Observed that metals appeared to release free charges when exposed to UV light
  - Observed sparking happened at lower voltage across two metal plates
  - Other features include negative particles being emitted from metal, requirement of a minimum frequency of light and the energy of charged particles being dependent on the metal
- Measure proerties of photoelectrons
  - Can measure energy of electrons given off as a function of frequency
  - Minimum energy needed to free electron ins called the "work energy"
- Einstein applied quanta to problem
  - Hypothesised that light consists of particles
    - \* Each had quanta of energy  $h\nu$
    - \* Work function was energy binding electrons to metal
    - \* Photoelectron created when  $h\nu > W$
- Compton scattering was a 2nd early application of QM
  - X-rays can produce electrons

- There was a shift in the frequency of the incident atom and the recoiled atom
- Assume an elastic collision of photon with electron at rest with photon 4-momentum  $(\frac{\omega}{c}, k)$
- $-E = \bar{h}\omega, p = (p_x, p_y, p_z) = hk = h(k_x, k_y, k_z)$
- Note:  $\bar{h} = \frac{h}{2\pi}$
- Assume the binding energy of an electron is negligible
- Use conservation of energy-momentum to find "Compton shift":  $\bar{h}\omega' = \frac{\bar{h}\omega}{1+\frac{h}{m_0c^2}(1-\cos\theta)}$
- This formula works when we don't take the binding energy of electron into account
- Maximum energy order of magnitude is 2keV
- Compton scattering calculation employs 4-vectors
  - $-p_{\gamma}=(\frac{hw}{c},hk), p_e=(cm,0)$  for incoming particles and  $p'_{\gamma}=(\frac{hw'}{c},hk'), p'_e=(\frac{E'}{c},p'_e)$  for the outgoing particles
  - Use conservation of momentum
  - Ends up leading to Compton shift equation which we had before
  - $-\frac{2\pi h}{m_e c}$  is the Compton wavelength of an electron

#### 9 Atomic Spectra

- Light interacts strongly with matter
  - Light absorption in a material
  - Light reflection & diffraction
  - Absorption except for specific wavelengths
  - Emission when matter is emitting energy
  - Absorption spectrum and emission spectrum when combined form the complete spectrum
  - The light coming through has not been affected by the gas while the black region is because of light interacting and being emitted everywhere
- Empirical Relationship between emission
  - Hydrogen discharge lamp: send current through a lap and light at specific wavelengths is generated
  - Wavelengths measured in visible spectrum are 656, 486, 434 and 410 nm
  - Relates to the Rydberg constant
- This led to several different models for atoms

- Rutherford-Bohr model with electrons surrounding nucleus in orbit was basis for modern theory of atomic structure
- Bohr model started with four postulates
  - The Coulomb force on an electron provides the force needed to keep it into orbit
  - The angular momentum is quantized:  $L = \bar{h}n$
  - An electron in a stationary orbit doesn't radiate
  - Emission or absorption of radiation causes an electron to move from one orbital to the next
  - The radius of the electron orbit can be predicted using the first two postulates.
  - The Bohr radius is the size of the lowest energy electron orbit
- "Stationary states" explained spectra nicely
  - Rutherford-Bohr model with stationary states explained atomic spectra
  - the problem was that classical physis could not describe these states
  - This set for the introduction of quantum wave mechanics

#### 10 de Broglie Waves

- The problem of making a particle a wave
  - Photons demonstrated both wave and particle properties
  - The frequency of light wave is proportional to its momentum
  - Has clear diffraction properties
  - Has clear particle properties: Photoelectric effect and compton Scattering
  - But actual particles (like electrons) behave like particles. They can be localized and have particle like trajectories - predictable and exact
  - The Sommerfeld-Bohr model of the atoms was seen as the place to start
  - Uses the kinematics of electrons in orbits:  $\frac{mv^2}{r} = \frac{Ze^2}{r^2}$  and  $mvr = n\bar{h}$
  - Using  $n\lambda = 2\pi r_n$ , we got  $n\lambda = \frac{2\pi n\bar{h}}{mv}$  so that  $\lambda = \frac{h}{p}$  where p is the momentum of the electron
- Matter waves appear to be very small
  - The challenge with a matter wave is the scale set by Planck's constant
  - When calculating the momentum, there is an additional unit of c
  - The de Broglie wavelength is  $1.23 \times 10^{-9} m$
- Davison and Germer demonstrate matter waves

- For an electron, de Broglie wavelength is comparable to atomic spacings
- Davisson & Germer used nickel crystal to see if electrons behave like waves
- Bragg scattering predicts diffracted beams constructively interfere and require a path difference of  $n\lambda$
- Neutron scattering is another clear example
  - Experiment with ultra cold neutron beam showed that wavelengths of neutrons varied from 1.5 to 3 nm

#### 11 Wave Particle Duality

- Case for wave particle duality
  - Wave Nature: Light is a wave of the EM field, De Broglie matter waves exist
  - Particle Nature: Photoelectric effect, compton scattering, Rutherford scattering
- Particles can be modelled as wave packets
  - We can create a wave packet through the superposition of several frequencies using functions of the form  $\sum_{n=-\infty}^{\infty} a_n \cos(k_n x \omega_n t) + b_n \sin(k_n x \omega_n t)$
  - The coefficients and wave vectors are given by boundary conditions and this describes a wave packet moving with velocity  $v_n = \frac{\omega_n}{k_n}$
  - The resulting wave packet will spread as it travels as a result of it being made up of numerous frequencies
- Single-slit makes neutron look like a wave
  - Suppose we have a one-slit neutron scattering experiment
  - We see a diffraction pattern with a wave diffracting through a slit
  - The angles of the diffraction peaks depend on the slit width
  - Can calculate the angles of minima and maxima
  - $-a\sin T = \lambda_n \implies T = \sin^{-1}(\frac{\lambda_n}{a}) = 2 \times 10^{-5} rad$
- The double-slit experiment shows wave infterference
  - The experiment has cold neutrons go through two slits
  - An interference pattern is formed
  - This is the same phenomena as waves of light, sound and surface and the classical description of interference of waves works
  - If the neutron flux is low enough that no more than one electron passes through the slits, what happens? We still get an interference pattern and there is no definitive answer for why this is the case

$$-\lambda_n = d_{slit}\theta_{peak} = (1.2 \times 10^{-4})(1.5 \times 10^{-5}) = 1.8 \times 10^{-9}$$

- Example of diffraction: "Bucky Balls"
  - Buckministerfullerene is a molecule consisting of 60 C atoms, 1 nm in diameter
  - Diffraction is seen in a two slit experiment with 200 m/s molecule bucky balls
  - The de Broglie wavelength is  $\frac{h}{mV} = 2.77 \times 10^{-12}$
  - To see diffraction, need a large enough angle  $(\frac{\lambda}{d})$
  - If the detector can resolve angles  $\frac{\delta}{D}=10^{-5}$ , the slit satisfies  $\frac{\lambda}{d}>\frac{\delta}{D}\Longrightarrow d<\frac{\lambda D}{\delta}=\frac{(2.77\times 10^{-12})(1)}{1\times 10^{-5}}=277nm$
  - $-\delta$  is the resolution
- Behaviour of particle changes if we get involved
  - If we put a detector on one slit, we know which slit the particle went through
  - Doing this with an electron beam, we can detect the electron without "disturing" it too much
  - We no longer see an inference pattern
  - This does not depend on how we detect the electon. Double slit interference disappears when we can determine which slit the particle goes through

## 12 Heisenberg Uncertainty Principle

- Wave-particle duality has other implications
  - Single particles behave like waves
  - Detecting particle trajectories changes wave like behaviour
  - Consider a localized wave packet
  - Lets attempt to measure a particles position and momentum
- Wave packet calculation illustrates uncertainty
  - Wave packet is a superposition of plane waves given by  $A \exp(i(kx \omega t))$
  - Take this over all waves numbers of some function f(k) reflecting the distribution of wave numbers as  $\Psi(x,t) = \int_{k=-\infty}^{\infty} f(k) \exp(i(kx-\omega x)) dk$
  - Need to have f(k) large around  $k \sim k_0$
  - $-v = \frac{\omega}{k}, \, \bar{h}k = p, \, k = \frac{\omega}{v} = \frac{2\pi}{\lambda}, \, v = \nu\lambda = \frac{\omega\lambda}{2\pi}$
  - We can write  $\Delta k = \left| \frac{dk}{d\lambda} \right| \Delta \lambda = \frac{2\pi}{\lambda^2} \Delta \lambda$  since  $k = \frac{2\pi}{\lambda}$
  - $-\Delta x = N\lambda$  so  $\Delta x \simeq \frac{\lambda^2}{4\Delta\lambda} = \frac{1}{4}\frac{2\pi}{\Delta k} \implies \Delta x\Delta k \simeq \frac{\pi}{2}$  and  $\Delta x\Delta k \geq \frac{1}{2}$
  - Multiplying both sides by  $\bar{h}$ , we get  $\Delta x \Delta p \geq \frac{\bar{h}}{2}$  which is known as the Heisenberg Uncertainty Relationship

- Practical measurement illustrates principle
  - Lets think of a practical experiment
  - Use photons to measure the position of electron
  - Photons interact with electron and bounce into microscope
  - Given a finite aperture of microscope subtending  $\alpha$  from electron,  $\Delta x \simeq \frac{\lambda_{\gamma}}{\sin \alpha}$
  - The uncertainty in momentum  $\Delta p_x \simeq p \sin \alpha = 2\pi \bar{h} \frac{\sin \alpha}{\lambda_{\gamma}} \implies \Delta x \Delta p_x \simeq 2\pi \bar{h}$
- Heisenberg Uncertainty Principle is fundamental
  - Position and momentum:  $\Delta x \Delta p_x \geq \frac{1}{2}\bar{h}$
  - Time and energy:  $\Delta t \Delta E \geq \frac{1}{2}\bar{h}$
  - Angular momentum and angle:  $\Delta L \Delta \varphi \geq \frac{1}{2}\bar{h}$
  - This does not relate to the precision of the apparatus or the technique used for the measurements
  - Can be an infinite number of complementary variables

### 13 The Schrödinger Equation and Wave Functions

- Schrödinger found an equation that predicted waves
  - Light can be modelled with plane waves  $A \exp(i(kx \omega t))$
  - This is a solution to the wave equation  $\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2}$  where  $k^2 = \frac{\omega^2}{c^2}$
  - Schrödinger noted that if  $\frac{\partial^2 \Psi}{\partial x^2}=\alpha \frac{\partial \Psi}{\partial t}$  then  $-k^2=-i\alpha\omega$
  - If  $\alpha = -\frac{2mi}{\bar{h}}$  then  $-hk^2 = -2m\omega$  so that  $\frac{\bar{h}^2k^2}{2m} = \bar{h}\omega$  and using Plancks relationship,  $\frac{p^2}{2m} = E$ , this implies that it is a particle
  - Rearranging gives  $i\bar{h}\frac{\partial\Psi}{\partial t}=-\frac{\bar{h}^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$  which is the Schrödinger equation for a free particle
  - This can be generalized with a potential V(x) as  $E\Psi = \left(\frac{p^2}{2m} + V(x)\right)\Psi$
- The wave function  $\Psi$  has some physical meaning
  - It is a complex function and so gives interference
  - Max Born suggested that it could be a probability density:  $|\Psi(x,t)|^2 \delta x$
  - Needs to be normalized so its a probability:  $\int_{all space} |\Psi(x,t)|^2 dx = 1$
  - Physically, consider a free particle with momentum  $\Psi(x,t) = C \exp(i(kx \omega t))$

  - Equal probability to be anywhere
- Gives interference but what about quanta?

- This theory had to explain wave phenomena, explain matter waves and photons, be consistent with classical physics and predict quantization of systems
- By construction, the first two points have been take care of but the third needs to be checked
- Schrödinger equation is a differential equation so we need boundary conditions to solve
- From the free particle "solution"  $\Psi(x,t) = C \exp(i(kx \omega t))$
- Momentum is constant and given by  $p = \bar{h}k$
- Wave function is constant in all of space since equal probability of being anywhere
- Need to confine it within some region
- Particle confined to circle gives some insight
  - Consider a toy system
  - Particle with mass m free to move in a circular track with radius R (x is an angular coordinate  $(0, 2\pi R)$ )
  - Solutions to Schrödinger Equation are still plane waves:  $\Psi(x,t) = C \exp(i(kx \omega t))$
  - Boundary conditions are periodic:  $\Psi(x,t) = \Psi(x+2\pi nR,t)$
  - $-\exp(i(kx \omega t)) = \exp(i(k(x + 2\pi R) \omega t))$
  - $-\implies 2\pi kR = n2\pi \implies k_n = \frac{n}{R}$
  - $-p_n = \bar{h}k_n$  so that it is quantized

### 14 Time-Independent Schrödinger Equation

- Wave equation in 1-D can have stationary solutions
  - Closed systems conserve energy (not a totally unrealistic assumption)
  - Examples of real closed systems: frictionless pendulum, isolated or non interacting atomic or molecular systems and stable, non-interacting nuclei
  - Many systems are good approximations to being closed
  - In such systems, the potential energy must be time-independent: V(x,t) = V(x)
  - Going back to the Schrödinger equation  $i\bar{h}\frac{\partial\Psi}{\partial t}=-\frac{\bar{h}^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x)\Psi$
  - Assume that one can find a solution through separation of variables. Let  $\Psi(x,t) = u(x)T(t)$
  - Then  $i\bar{h}u(x)\frac{dT}{dt} = -\frac{\bar{h}^2T(t)}{2m}\frac{d^2u}{dx^2} + V(x)u(x)T(t)$
  - $-\frac{i\bar{h}}{T(t)}\frac{dT}{dt} = -\frac{\bar{h}^2}{2mu(x)}\frac{d^2u}{dx^2} + V(x) = E$
  - This gives us the "seperation of variables" where the LHS only depends on time and the RHS only depends on x

- The equation must hold  $\forall x, t$  and therefore must equal a constant
- Means that time-dependence is simple
  - Solve first for T(t):  $\frac{dT}{dt} = \frac{E}{i\hbar}T(t) \implies T(t) = \exp(\frac{Et}{i\hbar})$
  - So the time dependence is just a phase that is linear in time
  - Apart from interference effects, this doesnt affect the modulus:  $|\Psi(x,t)|^2 = |u(x) \exp(\frac{Et}{i\hbar})|^2 = |u(x)|^2$  since the exponential has modulus 1
  - This leads to the time-independent Schrödinger equation:  $Eu(x) = -\frac{\bar{h}^2}{2m}\frac{d^2u}{dx^2} + V(x)u(x)$
  - The first RHS term can be interpreted as the kinetic energy and the second RHS term is the potential energy
  - The RHS is the "energy operator" for the system
  - Need to have V(x) and specified boundary conditions
  - In principle, we can then solve for the spatial dependence. For V(x) = 0, we have the wave equation: a free particle is described by plane waves
  - We can then use  $u(x) \to \Psi(x)$  since time dependence does not matter
- Conditions on  $\Psi(x)$  can be more formally stated
  - We need solutions to be continuous and single-valued, otherwise  $\Psi(x)$  to describe a physical system
  - The integral of the wave function over any interval must be finite otherwise it cannot be interpreted as a probability
  - The first derivative of  $\Psi(x)$  must be continuous everywhere. This ensures that the second derivative is well behaved
  - The boundary conditions must also be satisfied
- Solve problem of particle in infinite square well
  - Consider a closed 1D system
  - Particle with mass m freely moving in region x < |a| V(x) = 0
  - Potential for x > |a| is infinite i.e.  $V(x) = \infty$ : a particle cannot go beyond |x| = a
  - Classically, we expect that the particle will move freely in x < |a| and bounce back at each boundary with an equal probability of finding the particle anywhere
  - Boundary conditions for a quantum particle:  $\Psi(x)=0$  for  $|x|>a \implies \Psi(x)=0$  for |x|=a
  - This should be integrable and normalizable:  $\int_{-a}^{a} |\Psi(x)|^2 dx = C$
  - Continuous and Single valued
- Can now solve Schrödinger equation

- Inside region |x| < a,  $\Psi(x)$  satisfies  $E\Psi(x) = -\frac{\bar{h}^2}{2m}\frac{d^2\Psi}{dx^2}$
- Assume  $\Psi(x) = A\cos(kx) + B\sin(kx)$
- This gives  $E = \frac{\bar{h}^2 k^2}{2m}$  so that energy depends on k
- Applying the boundary conditions  $\Psi(-a) = \Psi(a) = 0$  gives  $A\cos(ka) + B\sin(ka) = 0$ ,  $A\cos(-ka) + B\sin(-ka) = 0$ ,  $A\cos(ka) B\sin(ka) = 0$
- Two possible solutions:  $B=0 \implies ka=\frac{n\pi}{2}$  for n=1,3,5,...,  $A=0 \implies ka=\frac{n\pi}{2}$  for n=2,4,6,...
- Defines possible values of k:  $k_n = 1, 2, 3, ...$
- Energy is quantized:  $E = \frac{h^2 \pi^2 n^2}{8ma^2}$

#### • Let's normalize the wave function

- Normalization requires  $\int_{allspace} |\Psi(x)|^2 dx = 1 \implies \int_{-a}^a A^2 \cos^2(k_n x) dx = 1$
- Integrating and simplifying  $\frac{A^2}{k_n}(\frac{k_n x}{2} + \frac{1}{4}\sin(2k_n x))|_{-k_n a}^{k_n a} = 1$
- Thus  $A^2a=1$  or  $A=\frac{1}{\sqrt{a}}$
- $-\Psi_n(x) = \frac{1}{\sqrt{a}}\cos(k_n x)$  or  $\Psi_n(x) = \frac{1}{\sqrt{a}}\sin(k_n x)$
- The resulting wave functions are  $B=0 \implies ka=\frac{n\pi}{2}$  for  $n=1,3,5,\cdots \implies \Psi_n(x)=\frac{1}{\sqrt{a}}\cos((\frac{n\pi x}{2a}))$ . Similarly  $\Psi_n(x)=\frac{1}{\sqrt{a}}\sin((\frac{n\pi x}{2a}))$  for  $n=2,4,6,\ldots$

#### • These solutions have non-trivial behaviour

- -N=1, particle found near the centre
- -N=2, particle avoids the centre
- -N=3, particle prefers centre and edges
- -N = 8, almost uniform
- This agrees with the quantum prediction but not from classical physics
- $-E_n$  is  $n^2$  times  $E_1$

#### • Classical Limit and Correspondence Principle

- The energy spacing provides a way of seeing what limit we are in  $:E_n = \frac{\bar{h}^2 \pi^2 n^2}{8ma^2}$
- In a quantum scale, we can look at the atomic length scale for an electron
- Several ways of going to the classical limit: e.g. make size of well macroscopic:  $a\sim 10^{-6}$  which makes energy spacings  $<10^{-7}eV$
- The wave function is uniform for any macroscopic energy state. Need a very high energy level,  $n \sim 10^4$

#### 15 Particle in Finite Square Well

- The finite square well is a more complex problem
  - Consider a particle in a potential well. Depth of the well is  $V_0$ , width is 2a and we look at "confined states" i.e. states where total energy  $E < V_0$
  - This system is an approximation for many physical systems
  - More complex boundary conditions
  - Classically, it has a simple solution (particle trapped in well, moving back and forth)
- Solve Schrodinger equation as before
  - Have to consider two regions:  $|x| > a \implies V(x) = V_0$  and  $|x| < a \implies V(x) = 0$
  - Find solutions in each region and match boundary conditions at transition between one region and the next
  - In region 1:  $E\Psi(x) = -\frac{\bar{h}^2}{2m} \frac{d^2\Psi}{dx^2} + V_0\Psi(x)$  for  $|x| > a \implies \frac{d^2\Psi}{dx^2} = \frac{2m(V_0 E)}{\bar{h}^2}\Psi(x)$
  - Solutions of the form  $\Psi(x) = C \exp(\pm \kappa x)$  where  $\kappa = \frac{\sqrt{2m(V_0 E)}}{\bar{h}}$
  - But expoentially growing solutions would not be normalizable so we reject the solutions  $\exp(\kappa x)$  for x > a and  $\exp(-\kappa x)$  for x < -a
  - We are then left with  $\Psi(x) = C \exp(\kappa x)$  for x < -a and  $\Psi(x) = D \exp(-\kappa x)$  for x > a
- Region 2: Solve Schrodinger for |x| < a
  - Solutions are of the form  $\Psi(x) = A\cos(kx)$  or  $\Psi(x) = B\sin(kx)$
  - However boundary conditions are different: doesn't have to go to zero at  $x = \pm a$  but we still require continuity
  - A lot of algebra