

# Introduction to Quantum Phenomenon

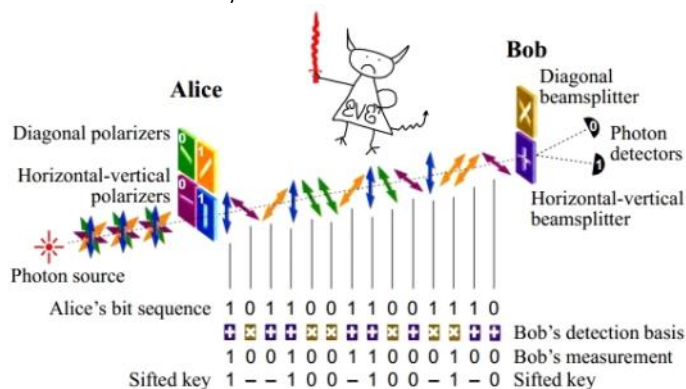
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## Introduction

- Quantum mechanics is generally considered to be separate to classical mechanics, however the correct approach is that quantum is the superset of classical mechanics
- Quantum mechanics is difficult to perceive because it is often contrary to the classical mechanics we do perceive.
- Quantum gives us a certainty if something is possible or impossible.
- We place classical information into a quantum system and can only receive a classical output.
- The wavefunction is a complete description of all understanding we could derive from a system

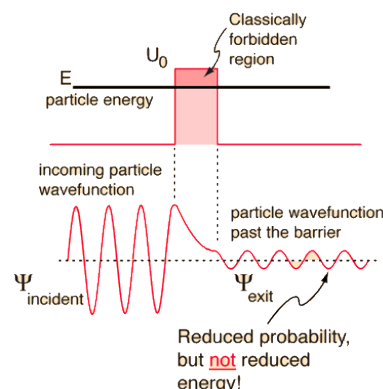
## Quantum Encryption

- Consider a case where Alice is sending Bob a series of bits. She sends them either in the up-down basis or in the diagonal basis. Bob randomly will choose to read in either basis. If the basis match, the bit will be 100% correct, if it doesn't it has a 50% chance of being correct.
  - If Eve intercepts these messages, she will read the basis, but she changes the fragile state of the bits. She does not know if the bit she reads is correct and cannot send the same bit she read to Bob, as there is only a 75% chance she made the correct reading. At best she can only send the same bit 25% of the time.
  - Bob must call Alice (it is okay if this communication is intercepted). Alice and Bob tell each other the base, in which they sent or read the message. If the basis match, then Bob and Alice know that part of the message was sent correctly.
    - Even if Eve can listen to this call, she is only able to discern which bits are correct.
  - Alice and Bob can detect if there is an eavesdropper by sharing the state of the matching basis. If the observation always matches the bit sent, then they are confident their information is safe. However if some of them are wrong, they know the bits have been tampered with on the way.



## The Fundamental rules of Quantum Mechanics

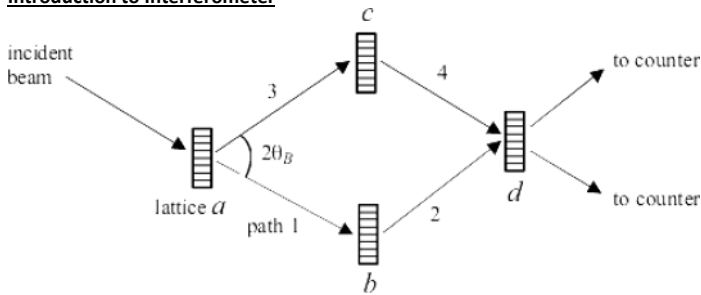
- Everything is quantized (mass, energy, force etc.)
  - We can use this to provide reliable outputs, such as CdSe quantum dots which output a specific wavelength of light depending on their size.
- Superposition: The combination of any solutions to a quantum problem is also a solution
- Quantum Mechanics is linear: this means if we go through a system, each input must give us a unique output. There must be a 1 to 1 mapping that can be reversed.
- Measurements influence the system. Every time a system is measured, we must update the wave function with the information we know
  - If we measure the position of a particle, we must update our wave function to that specific position.
    - An electron can be spin up or spin down, but once we measure it, we know it to be one of the two
- Quantum states are fragile. This means that quantum state (such as superposition)
- Quantum mechanics is non-local.
  - If we set one coin to heads and one to tails and without looking at them separate them across the universe, when we reveal one, the superposition of the other collapses instantly
    - This does not violate special relativity
- Quantum Tunneling
  - There is a finite probability that something can teleport over an energy barrier based on the thickness of the barrier.



# Neutron Interferometer

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## Introduction to Interferometer



- In the neutron interferometer, a neutron beam impacts a thin Silicon wafer. This silicon wafer splits the incoming beam equally with a momentum up and down.
- These beams then impact a second wafer, which redirects them towards the center, before they are finally split again by the third wafer, which is of the same operator as the first.
- The splitting is due to Bragg diffraction of the neutron wave.
- A detector for this system is made of  $\text{He}^3$ . This is an incredibly good absorber of neutrons and will emit a quantized energy of light when absorbing one. Thus it is easy to tell when a neutron has reached the detector.

## Normalization

- All wave functions must have a probability of 1. We can check the probability of a wave function by taking the probability amplitude of each component, finding the magnitude of the probability amplitude (because amplitudes are complex numbers) and summing the results together. If it is greater than 1, it is not normalized.
  - To normalize a vector, we must divide each component by the magnitude of the vector.

## Polarizer

- A polarizer can be added to the system to change the phase of the light. This imparts a phase angle  $\phi$  to one of the beams
- This operator can be expressed as, if it is being imparted on the momentum up beam.
 
$$\begin{pmatrix} 1 & 0 \\ 0 & \exp(i\phi) \end{pmatrix}$$
- We can check that this matrix does not violate linearity or normalization by passing our wave function through it. We see that the momentum down component is not effected, but the momentum up component becomes exponential.
  - This will change our final result and the resulting probabilities. The probability of finding it in momentum up or down is different depending on the phase angle imparted.
  - The resulting probability from applying a phase angle to the momentum up beam is
 
$$\frac{1}{2}(1 - \cos \phi) \text{ for momentum up and } \frac{1}{2}(1 + \cos \phi)$$
- A phase angle is essentially a delay wave function by a phase. A phase is a proportion of the wave.  $a/\lambda = \phi/2\pi$
- The expectation value of the system is the average result of the measurements. When we measure the system, the neutron is NEVER in 2 places at the same time.

## Solving the Interferometer problem

- The first key to solving a quantum situation is to defining a unique basis. These basis are components to build all other things. You should not be able to define a basis with another basis
- Let's define two basis, one with a component of momentum up and one with momentum down. We'll define them as column vectors respectively. The labelling is arbitrary and we can choose any axis.
 
$$\text{Up: } \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{Down: } \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
- Contrary to the diagram shown, we'll consider a beam with a momentum going upwards at first. We will try and derive an operator for each Silicon blade.
- Let's map out the second blade first since it is the easiest. We must understand what the wafer is doing to each of the components of the problem
  - The middle wafer take a beam with momentum up and switches it to down. It takes a beam with momentum down and switches it to up.
  - Therefore we need to solve for an operator that takes  $(x \ y)$  and maps out  $(y \ x)$ .
  - The solution is:
 
$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
- Now let's consider what happens at the first wafer. We are taking a component in and mapping it to an equal probability of going up and down.
  - Let take a second to define some limitations to our solutions.
    - Based on the principle of linearity, the total probability must be equal to the probability going in. Since the probability going in is 1. The total probability of the output must be 1
    - The wave function defines probability amplitude which is the square root of probability.
      - Since there is an equal probability of both solutions is  $1/2$ , the probability amplitude can be  $\pm 1/\sqrt{2}$
  - We know the wafer takes both a wave with momentum and maps it to a wave function with equal probability of being both momentums. Therefore, we need to solve for an operator that will give us a unique solution to the input.
  - We find that the operator is equal to:
 
$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$
    - Why can't it be a matrix of all 1s. Because that would violate the normalization/linearity of the problem
  - We see that passing a wavefunction of momentum up yields the solution. We need to break down this solution for us to truly understand its meaning
 
$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
    - We see in this solution that if we square the front term, we see that both basis have a probability of  $1/2$ . The sum of these probabilities is equal to 1, Therefore it does not violate normalization.
- Since the third blade is the same as the first, it has the same operator as the first blade.
- If we pass a beam with momentum up, we will see that the outgoing wave is fully momentum down!
  - The splitting seems to have a cancellation effect when a wave up and wave down are passed in
    - If we block one of the beams from hitting the last wafer, we collapse one of the components. This means all the probability is in the last component. We are required to redefine our wave function as we have measured the system.
    - When passed through the last wafer, the single component cannot have a destructive interference pattern with the other component and thus produces a light splitting similar to the first wafer.
- We can multiple the operators together to have a single operator which represents the entire system.

# Particle in a Box

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## Schrodinger's Equation

- Schrodinger's Equation states that  $H\phi = E\phi$ , where  $H$  is the Hamiltonian,  $E$  is the energy of the system and  $\phi$  is the wave function.
  - This is an eigenvalue problem.
  - The Hamiltonian represents the total energy of the system, which is obvious why this equation works. The Hamiltonian finds the total energy of the system.
- Let's try to define the Hamiltonian: We know the total energy of the system is the sum of the Kinetic and Potential Energy. The kinetic energy can be described with respect to the momentum of the system in question.

$$H = KE + PE = \frac{p^2}{2m} + P(x) = -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)$$

## The Wave Function

- We define the wave function as a combination of Eigenstates.

$$\psi = \sum c_n \phi_n$$

- As  $n$  approaches infinity, we can describe any normalized function in this boundary.
- If we know the wavefunction, how can we solve for the coefficients?

$$c_n = \int \phi_n^* \psi dx$$

- We can substitute in the wave function to prove the equality of this relationship
- We can calculate the expected value of an operator by solving.

$$\langle \Omega \rangle = \int \psi^*(x) \Omega \psi(x)$$

Expected Value	Operator to Substitute In
Total Energy	Hamiltonian
Potential	$V(x)$
Momentum	$-i\hbar \frac{d}{dx}$
Position	$x$

- The wave function is complete as it contains information about position, energy, momentum etc.
- Gibb's ringing are interference patterns towards the edge of the wave function. This is caused by the wave interacting with the walls of the well.
- If we had a wavefunction composed of a single eigenfunction, then we suddenly moved the edges of the walls, we would have to redefine the wavefunction with respect to the eigenfunctions of the new parameters.

## Time Dependence

- The probability of the location of the wave will change with respect to time based on the energy of the wave.
- Higher energy waves tend to propagate faster over time. We can add a time dependence to each of our eigenfunctions

$$a. \Phi_n = \phi_n \exp\left(-\frac{iE_n t}{\hbar}\right)$$

- We composed our wavefunction of a series of time dependent eigenstates.
  - The expected values of the wavefunction will change with time, however the eigenstates are time independent functions.
- The complete Schrodinger Equation is equal to:

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

- We can solve this wave equation by a separation of variables method. We find that our wave equation is of the form.

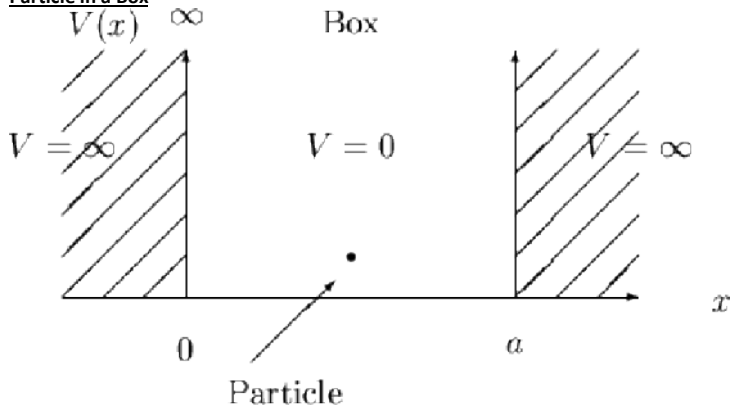
$$\Psi = \exp\left(-\frac{iEt}{\hbar}\right) \sum c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

- We can see from our expected values that eigenstates are time independent, which is consistent with our solution from earlier. We also see that our evolution of our wavefunction is dependent on the energy difference between the individual eigenstates.

## Neutron Interferometer

- We can model a neutron interferometer with a circular boundary to a box.
  - We can split a Gaussian wave packet (normal distribution) in to two opposite directions
  - We can model a way to switch the momentums of the wave packets.
  - However we haven't learned yet, the model for recombining the wave packet.

## Particle in a Box



- Consider an electron on a finite piece of wire. We can define the voltage of the wire to be 0 and since the electron cannot leave the wire, the potential elsewhere to be infinite.
- If we substitute this relationship into the Schrodinger Equation, we see that on the wire we have the Hamiltonian.

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = H$$

- With this we can solve the Schrodinger Equation for the particle in the box.
- First let us define a set of eigenstates which satisfy the Schrodinger Equation. We can construct our wave function of these eigenstates.

- This is a differential equation and we can easily solve, where the second derivative is related to the function. Solving for the differential equation we get that the solution is

$$\phi = A_n \sin\left(\frac{n\pi x}{a}\right) \text{ where } n = 1, 2, 3 \dots$$

- As we increase in wavenumber, we add one node for every number we go up. This increases the energy of the eigenstate

- We can solve for the energy eigenvalue solution. We see that
 
$$E = \frac{\hbar^2 n^2}{8ma^2}$$

- We need to solve for  $A_n$ . We should let this coefficient equal 1 because when we construct a wave function of eigenstates, we will be assigning the probability of each eigenstate to a different coefficient. Thus these should be normalized to make our lives easier ahead.
- A normalized eigenstate obeys the following relationship

$$\int \phi^* \phi = 1. \rightarrow A_n = \sqrt{\frac{2}{a}}$$

- We can test the eigenstates are both normalized and orthogonal by integrating.

$$\int \phi_n^* \phi_m = \delta_{nm}$$

- Where the dirac delta function is equal to 1, when  $n=m$  and 0 otherwise.

## Heisenberg Uncertainty Principle

- We can plot wavefunctions, but instead of showing the probability of position, we can show the probability of momentum.
  - Classically, a discrete energy would provide us with a positive and negative momentum.
  - However due to Heisenberg Uncertainty principle, we see an uncertainty in our momentum at discrete energy levels. We see a positive and negative peak.
    - These probability distributions are centered around the expected or classical solution to the problem.
- We can quantify the Heisenberg Uncertainty Principle, such that:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

## Numerical Methods of Approximation.

- We can subdivide our region of interest into many small intervals,  $w$ . We treat each of these intervals as a basis  $b_n = [0, 0, 0, 1, 0, \dots]$ .
  - We multiply each basis by the probability amplitude that the particle is in that interval. These amplitudes should have a combined magnitude of 1 to obey normalization.
- Now we can represent the wave function as a vector  $[a, b, c, \dots]$  which is normalized.
- We can now write an operator, which acts on the vector and maps it to a new vector one small time step later. This matrix operator is the Hamiltonian.
- For a vector  $a_t$ , when we multiply it by the Hamiltonian Operator  $U$ , we get  $a_{t+1}$ . Such that  $H a_t = a_{t+1}$
- How do we write our Hamiltonian

opposite directions

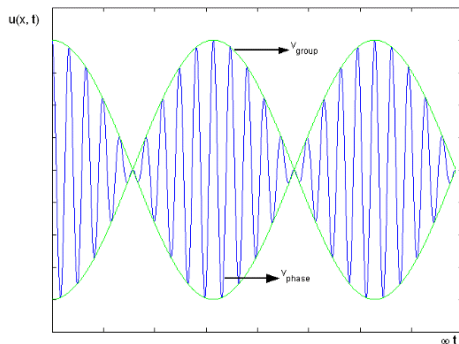
- We can model a way to switch the momentums of the wave packets.
- However we haven't learned yet, the model for recombining the wave packet.
  - This is related to the fact that our current model cannot track the phase of particle.

### Step Potential

- Consider a free electron, the potential on this electron is 0 everywhere.
- We can apply Schrodinger Equation the a free electron and we see that the eigenstates are.

$$k = \frac{\sqrt{2mE_k}}{\hbar} \quad E_k = \frac{\hbar^2 k^2}{2m} \quad \phi_k = \exp(ikx)$$

- We see that we cannot normalize the eigenstate, as it has infinite possibility. This represents that the electron is spread over all space.
  - This is non-physical and is not allowed. However we can use the eigenstates to create a wave function, since it is a combination of these. The eigenstates alone are not allowed.
- $$\psi = \sum f(k) \phi_k(x)$$
- We can add a time dependence to this relationship so that we get  $\exp(i(kx - \omega t))$
- In this free electron moving through space, we see 2 velocities, The phase velocity, which is  $\omega/k$ . This is the internal movement of the peaks
- The group velocity is the movement of the Gaussian wave packet over time. This is the classical velocity and is equal to double the phase velocity.



- Consider this free electron moving through space impacts a potential wall, that steps up.
  - Some of the wave will continue moving at a higher potential and some will bounce back.
    - We know that the wavefunction and its derivative are always continuous.
- Consider the incident, reflect and forward wave packet of electron.

Wave Packet	Incident	Reflected	Forward
Wavefunction	$e^{ikx}$	$Re^{ikx}$	$fe^{ikfx}$
Probability Amplitude at $x=0$	1	R	f
Derivative at $x=0$	ik	$-ikr$	$ikrf$

- We see the same potential between the reflected and incident wave, but an increased potential from  $k$  to  $k_f$  for the forward wave.

$$kf = \sqrt{\frac{2m(E_k - V)}{\hbar}}$$

- Since we have two different equations from left of 0 and right of 0, we know the two equations must be equal at 0 for the function to be continuous.
  - We also know the derivative must be smooth thus they must also be equal for it to be continuous.
- We can solve for  $r$  and  $f$  of the system. The ratio of reflected to forward waves

$$r = \frac{k - k_f}{k + k_f} \quad f = \frac{2k}{k + k_f}$$

- There are some unique situations
  - When the incoming energy is equal to the step potential, we no longer get a wave packet moving forward, but an exponentially decaying probability amplitude.
    - This decaying probability amplitude is the tunnelling effects
    - We also see a phase change in the reflected wave.
  - As  $V(x)$  approaches infinity, our phase change for our reflected wave becomes 90 degrees or  $\pi/2$ .
    - Our tunnelling probability also drops as  $V(x)$  increase. This decreases exponentially.
    - The reflected wave generally has the form of  $2r \cos(kx)$ . This is because the sum of the reflected component ( $re^{-ikx}$ ) and the

We can now write an operator, which acts on the vector and maps it to a new vector one small time step later. This matrix operator is the Hamiltonian.

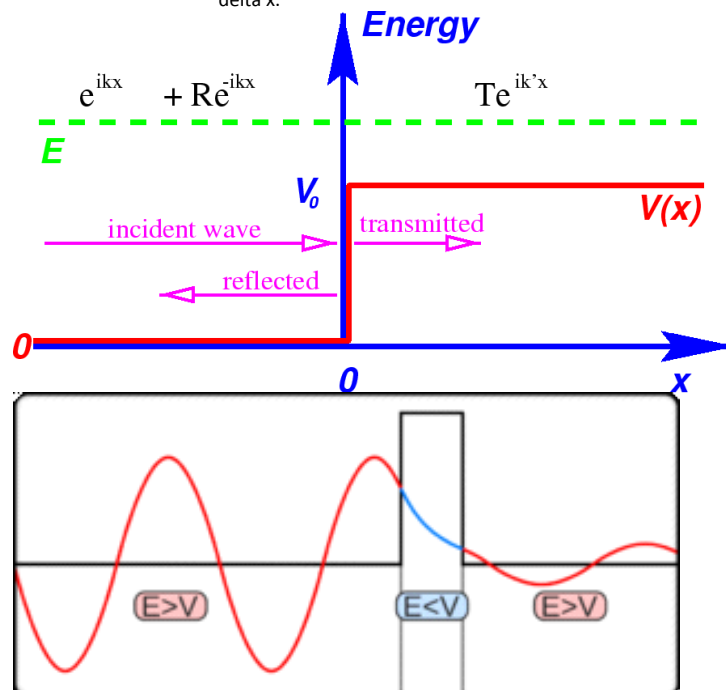
- For a vector  $a_t$ , when we multiply it by the Hamiltonian Operator  $U$ , we get  $a_{t+1}$ . Such that  $Ha_t = a_{t+1}$
- How do we write our Hamiltonian.
  - We know that if we multiply a vector, by the identity matrix, it is as if the vector did not move.
  - If we multiply by the sub diagonal, all terms shift down 1, such that we are moving to the right.
    - The sub diagonal is a diagonal of 1s starting one below the top left corner
  - If we multiply by the super diagonal, we shift all terms up 1, such that we appear to be moving to the left
    - The sub diagonal is a diagonal of 1s starting one to the right of the top left corner.
  - These 3 pieces of information are enough for us to move the wavefunction in any direction
  - $U = c_1 I + c_2 (\text{Subdiagonal}) + c_3 (\text{Superdiagonal})$ 
    - $c_1$  is the probability amplitude the wavefunction will stay still,  $c_2$  the probability amplitude it will move to the right and  $c_3$  the probability amplitude it will move to the left.
  - We have to make one consideration as information is lost on the side of the matrix. We have several options. We can have the probability accumulate on the edges, or we can have a cyclic BC such that it moves back to the start when it reaches the end and vice versa.
    - To do this, we need to add a 1 to first column of the super diagonal in the last row (bottom left term) and a 1 to the top right corner of the sub diagonal
  - We can combine several time steps into a single operator.
- We can have an estimate for the Hamiltonian based on the finite difference method. Knowing that the Hamiltonian is related to the second derivative.

$$f_{xx}(x, y) \approx \frac{f(x+h, y) - 2f(x, y) + f(x-h, y)}{h^2}$$

- We use this method to approximate the size of each time step, such that

$$H = \frac{\hbar^2}{2m\omega^2} (\text{Identity Matrix}) + V(x)(\text{Identity Matrix}) - \frac{\hbar^2}{2m\omega^2} (\text{Super} + \text{Sub Diagonal})$$

- We can solve for eigenvector to this state, which replace our eigenstates. We need to ensure these eigenstates are orthonormal.
- Then we can compose a wavefunction of these eigenstates. We can then add a time dependence to each eigenstate. This allows our wavefunction to have time dependence.
- Using this we can take measurements
  - To approximate the value of something instead of integrating, we take a sum of the series
    - In general, when you see an integral turn it into a sum notation across every interval within the bounds of integration
    - Multiply the result of the sum by the size of the intervals.
      - Replace integral signs with summation notation and  $dx$  with  $\delta x$ .



- Multi step potential wells can also be considered (picture above)

- Our tunnelling probability also drops as  $V(X)$  increase. This decreases exponentially.
- The reflected wave generally has the form of  $2r\cos(kx)$ . This is because the sum of the reflected component ( $re^{-ikx}$ ) and the incident wave  $e^{ikx}$  can be factored out to form  $2r\cos(kx)$
- However as  $k_f$  approaches  $i\infty$ . We see that  $r$  approaches -1. Thus when we factor we see  $e^{ikx} - e^{-ikx} = 2\sin(kx)$ .
  - This is the 90 degree phase shift

- The phase is equal to  $2\pi/k$ .
- The 1D step potential is useful for modelling the transition between two metals in a wire
- The flux is defines as, this is a combination of probability and velocity.  $f = \frac{f \cdot \hbar k_f}{m}$

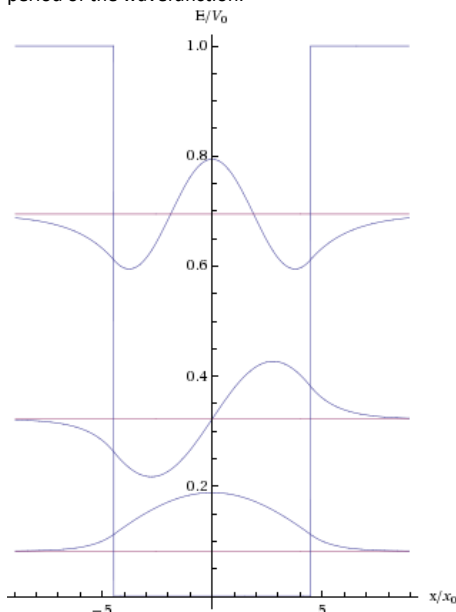
- Current Density is directly related to the flux.

#### Dirac Delta Function

- Dirac delta functions are infinitely high potential barriers that span an infinitely small region. These barriers normalize to 1. The only way through one of these barriers is tunnelling.
- Given a barrier of  $V_0 \delta$ . These equations govern the tunnelling  $\psi_{left} = \psi(0) = \psi_{right}$   $\frac{d\psi_{left}(0)}{dx} = \frac{d\psi_{right}(0)}{dx} = -\frac{2V_0 m}{\hbar^2} \psi(0)$
- We can create a set of bound states by these dirac delta functions. We use a negative function to trap it in an infinitely small well.
- We can also have 2 infinitely high barriers to model a 1D square well
- We see resonant tunneling effects when a plane wave impacts 2 dirac delta functions.

#### Finite Square Well

- These are square wells whos barriers are not infinite. We see tunnelling at the edges of the well. (Picture to the right)
- We see trapped states are of the form  $\cos(kx)$  and the tunnelling at the edges is modelled by a negative exponential  $\exp(-x/K_f)$ 
  - These follow the rules that the wavefunction and its derivative are continuous at all points.
- There are a finite number of eigenstates that sit in the well. There are more the larger and deeper the well. Eventually the eigenstates are free electrons outside of the well.
- Travelling electrons outside of the well can experience resonance tunnelling through the well. The odds of them being trapped in the well are lower if the period in the well is related to the width of the well by an integer factor.
- We can also get reflection as the well approaches an infinitely deep well and resonance effects are perfectly misaligned.
  - The misalignment means that the width is equal to a half value of the period of the wavefunction.

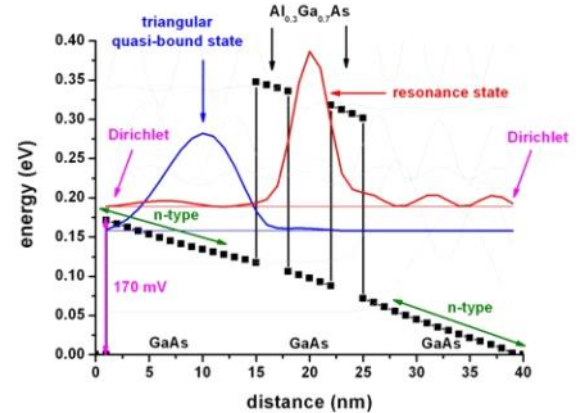


#### Triangular Wavefunction

- We can also have a sloping potential in our well. The solution to these are Airy functions. These are special functions. In order to produce these solutions, we need some clever algebra that is not worth our time to do. The solutions look like:



- Multi step potential wells can also be considered (picture above)
- In order to solve these systems, one must create 2 sets of equations at each interface.
  - At our second interface we will not be able to make our simplification as  $x$  will not be equal to 0.  $x$  will be equal to some value  $a$ , which is the width of the barrier.
  - We see a phenomenon of resonant tunnelling in multi-step potential. If the energy is higher than the potential barrier and the wavefunction spans an integer value multiplied by half the phase of the wavefunction, we see a near 100% probability of tunnelling through the barrier.



#### Perturbation Theory

- Consider the Schrodinger Equation  $H^0 \Phi_n^0 = E_n^0 \Phi_n^0$ . We can add a small modification in the Hamiltonian, either a small potential change or size change. Using perturbation theory, we can estimate the new solutions.
- Let  $H = H^0 + H^1$ , where  $H^1$  is the modification in the Hamiltonian. We can write a series expansion for all other term. For simplicity  $\Phi_n$  will just be represented by  $\Phi$ .
  - The superscripts represent the order of approximation
- $(H^0 + H^1)(\Phi^0 + \Phi^1 + \Phi^2 + \dots) = (E^0 + E^1 + E^2 + \dots)(\Phi^0 + \Phi^1 + \Phi^2 + \dots)$
- We can focus on the terms that produce a total of first order error.  $H^0 \Phi^1 + H^1 \Phi^0 = E^0 \Phi^1 + E^1 \Phi^0$ . We know all the 0th order terms as well as  $H^1$ , since we applied the perturbation to the system.
- We can left multiply all terms by  $\Phi^{0*}$  and integrate both sides.

$$\int \Phi^{0*} H^0 \Phi^1 + \int \Phi^{0*} H^1 \Phi^0 = \int \Phi^{0*} E^0 \Phi^1 + \int \Phi^{0*} E^1 \Phi^0$$

We can left multiply the first integral because it is the conjugate.

$$\int \Phi^{0*} E^0 \Phi^1 + \int \Phi^{0*} H^1 \Phi^0 = \int \Phi^{0*} E^0 \Phi^1 + \int \Phi^{0*} E^1 \Phi^0$$

$$E^0 \int \Phi^{0*} \Phi^0 + \int \Phi^{0*} H^1 \Phi^0 = E^0 \int \Phi^{0*} \Phi^1 + \int \Phi^{0*} E^1 \Phi^0$$

We can cancel the first term on both sides as they are equal

$$\int \Phi^{0*} H^1 \Phi^0 = \int \Phi^{0*} E^1 \Phi^0$$

$$\int \Phi^{0*} H^1 \Phi^0 = E^1 \int \Phi^{0*} \Phi^0$$

$$E^1 = \int \Phi^{0*} H^1 \Phi^0$$

We can sub the result back into our initial equation

$$H^0 \Phi^1 + H^1 \Phi^0 = E^0 \Phi^1 + E^1 \Phi^0 \text{ to solve for the perturbation in the eigenstate.}$$

Since our original eigenstates formed a complete basis we can represent  $\Phi^1$  as a sum of our original basis set

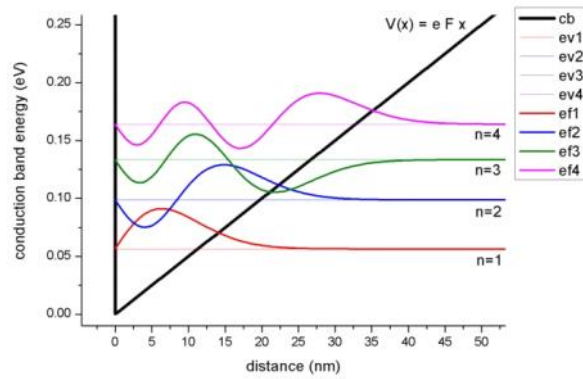
$$\Phi^1 = \sum_{m \neq n} c_{m,n} \Phi_m$$

We can solve for each coefficient by rearranging our original equation.

$$(H^0 - E^0) \Phi^1 = E^1 \Phi^0 - H^0 \Phi^1$$

$$c_{m,n} = - \frac{\int \Phi_m H^1 \Phi_n}{E_n - E_m}$$

Using these 2 equations we can estimate the change in the eigenstates due to small changes in the Hamiltonian



- We see tunnelling into the barriers that are slope. However at higher and higher energies we see the sloping potential affecting our wavefunctions less and less.
  - They look like our 1D well solutions, but shifted to the side of lower potential

# Harmonic Oscillator

July 7, 2015 1:01 PM

## Potential of a Harmonic Oscillator

- The potential of the harmonic oscillator is based on the potential well formed by a spring. The potential well is equal to  $\frac{1}{2}kx^2$ . When we substitute this into our Schrodinger Equation we come up with 
$$\frac{1}{2m}(p^2 + (m\omega x)^2)\phi = E\phi$$
 Where  $p$  and  $x$  are the momentum and position operator respectively.  $M$  is the mass of the particle and  $\omega$  is equal to  $\sqrt{k/m}$ .  $K$  is a constant in Hooke's Law.
- We define two fundamental operators in this case 
$$a_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)$$
- Consider  $a_+a_-$ . We get 
$$\frac{1}{2\hbar m\omega}(p^2 + (m\omega x)^2 - im\omega(px - xp)) = \frac{1}{2\hbar m\omega}(p^2 + (m\omega x)^2 - \hbar m\omega)$$
 Notice the first 2 terms in the bracket are equal to our Hamiltonian! 
$$\frac{1}{\hbar\omega}H - \frac{1}{2}$$
- We can do a similar thing for  $a_-a_+$  and we get 
$$\frac{1}{\hbar\omega}H + \frac{1}{2}$$
  - It is clear the commutator of the two operators is equal to -1 based on the above expression.
- We can rewrite our Hamiltonian as  $\hbar\omega\left(a_+a_- - \frac{1}{2}\right)$
- These two operators are known as the raising and lowering operators. There are 3 rules to these operators
  - $a_+\Phi_n = \sqrt{n+1}\Phi_{n+1}$
  - $a_-\Phi_n = \sqrt{n}\Phi_{n-1}$
  - $a_-\Phi_0 = 0$
- The last rule prevents us from creating an eigenfunction below the ground state. We can also use it to solve for the equation of the groundstate as that is a partial differential equation. 
$$\phi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$
- We can show that the eigenstates are equally spaced in terms of energy by using our new expression of the Hamiltonian we determined. 
$$\hbar\omega\left(a_+a_- - \frac{1}{2}\right)a_+\Phi = \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\Phi$$
 
$$= \hbar\omega a_+\left(a_-a_+ - \frac{1}{2}\right)\Phi = \hbar\omega a_+\left(a_-a_+ - \frac{1}{2} + 1\right)\Phi = \hbar\omega a_+(H + 1)$$
 
$$= a_+(E + \hbar\omega)\phi = (E + \hbar\omega)a_+\phi$$
  - This shows when we go up a single eigenstates by the raising operator, the energy raises by a constant amount.
- At low eigenstates, we have a high probability of being in the middle. This fits a pendulum swinging. The lower energy it has the closer, the more likely it is in the middle. As we get to higher energies there is a higher probability of being on the edges.
- A super position of  $n$  and  $n+1$  eigenstates will have the same frequency as a superposition of the first 2 eigenstates.
  - This oscillation represents an oscillation in the dipole moment of the system.

## Commutator

- In Quantum Mechanics, the order of the applied operators is very important. The difference order makes is known as the commutator.
- The commutator of  $p$  and  $x$  is  $[p, x]$
- This can be calculated by  $px - xp$ . 
$$[px - xp] = -i\hbar \frac{d}{dx}x - \left(-i\hbar \frac{d}{dx}\right)$$
 We apply a dummy wave function to help us solve this. 
$$-i\hbar \frac{d}{dx}x\Phi - \left(-i\hbar \frac{d}{dx}\right)\Phi = -i\hbar\left(\Phi + x\frac{d\Phi}{dx} - \frac{xd\Phi}{dx}\right) = -i\hbar\phi$$
 Therefore the commutator is equal to  $-i\hbar$ . This can be done for any series of operators. If the result is equal to 0, then we know the order of these operators does not matter.

## Applications of the Harmonic Oscillator

- We can use the harmonic oscillator to model a double well potential.
- We can model the potential well formed by a diatomic molecule.
- We can model an oscillating circuit
- An excited electrons transition through the bands
- A beam of light bouncing between two perfect mirrors.

## Summary of Equations

$$a_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)$$

$$H = \hbar\omega\left(a_+a_- - \frac{1}{2}\right) = \hbar\omega\left(a_-a_+ + \frac{1}{2}\right)$$

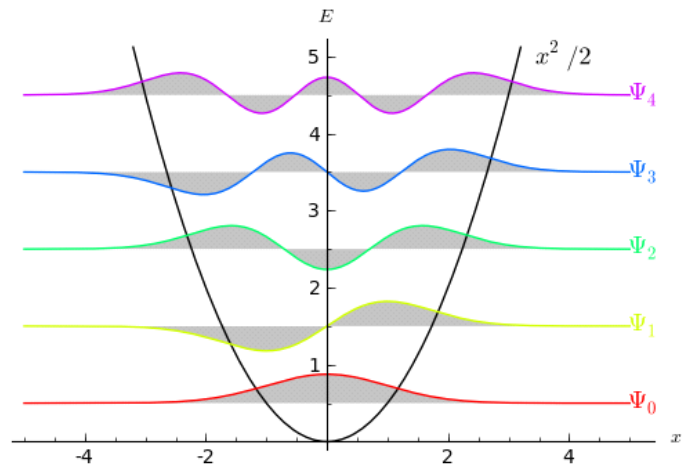
$$x = (a_+ + a_-)\sqrt{\frac{\hbar}{2m\omega}}$$

$$p = (a_+ - a_-)i\sqrt{\frac{2m\omega}{\hbar}}$$

$$\phi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

$$\phi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(y) \exp\left(-\frac{y^2}{2}\right)$$

Where  $H$  is the hermite polynomial and  $y = \sqrt{\frac{m\omega}{\hbar}}x$



# Hydrogen Atom

July 21, 2015 5:10 PM

## Expanding into Multiple Dimensions

- In our general case we define our Hamiltonian to be a Laplacian operator.
 
$$\left( \frac{-\hbar^2}{2m} \nabla^2 + V(x, y, z) \right) \Psi(x, y, z) = E \Psi(x, y, z)$$
- We also will generally use cylindrical and spherical coordinates to define our system.

- The gradient operator has a slightly different definition in each of these. We use  $\alpha$  rather than  $\Phi$  in our angle definitions to avoid confusion

Cylindrical Gradient

$$\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial z^2}$$

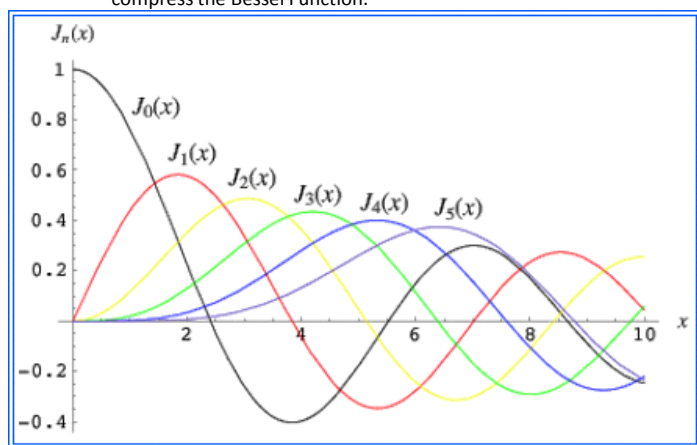
Spherical Gradient

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

- To solve our Hydrogen atom example, we will assume that our equations are always separable.
  - This means we can apply separation of variables to solving our PDE.
  - This allows us to solve each PDE independently of one another.
- This means we generate eigenstates in each direction (x,y,z) for Cartesian and r,  $\alpha$ ,  $\theta$  in spherical coordinates.
  - We will get different quantum numbers in each coordinate as well as a different energy in that direction.
- The energy will be roughly proportional to the sum of the squares of the quantum numbers.

## Particle on a Disk

- This varies from particle on a ring because r is now a variable.
 
$$\left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \alpha^2} \right) \Psi(\alpha, r) = E \Psi(\alpha, r)$$
- We assume our equation is separable and thus we can salvage our equations from our particle on a ring equation.
  - We redefine these eigenstates as defined by the angular momentum quantum number  $n\alpha$
- The solution to our radial part is Bessel Function. A Bessel Function is defined by  $n_r$ . The type of Bessel Function is  $J_n$ 
  - We do not need to know the mathematical representation of the Bessel Function. The important thing to know is that the larger  $n_r$ , the more shifted away from the central axis it is.
  - $N_r$  also determines the number of nodes in the radial direction.
  - However our Bessel function is not directly controlled by  $n_r$ .
  - Our type of Bessel function  $J_n$  is actually dictated by the angular quantum number. Such that  $J_{n\alpha}$ .
  - Our radial dependence comes in becomes our  $n_r$  will stretch or compress the Bessel Function.



- The general solution to the radial direction is
 
$$R(r) = J_{n\alpha} \left( \frac{\rho_{nr, n\alpha} r}{a} \right)$$
 The J is the Bessel function. The  $\rho_{nr, n\alpha}$  component states that we only allow the Bessel function to exist up to the  $n_r$  node. The  $r/a$  part will stretch it to keep our function limited to our disk.
 
$$P_{1,2}$$
 states that we allow up to the 1st node of  $J_2$  that is our function. This would be the yellow line above going to ~5.
- We still see our degeneracy where the two different directions matter. We say that  $n\alpha$  can be  $0, \pm 1, \pm 2 \dots$  and  $n_r = 1, 2, 3, 4$ 

$$\varphi = R(r) A(\alpha) = J_{n\alpha} \left( \frac{\rho_{nr, n\alpha} r}{a} \right) \frac{1}{\sqrt{2\pi}} \exp(in\alpha) E = \frac{\hbar \rho_{nr, n\alpha}^2}{2m a^2}$$
 Where  $a$  is the radius of the disk

## Particle in a Sphere

## Particle on a Ring

- We will use cylindrical coordinates to represent this system. Since the radius is constant. The Laplacian operator is only a function of  $\alpha$ . We can write Schrodinger's Equation as

$$\frac{-\hbar^2}{2m r_0^2} \frac{\partial^2}{\partial \alpha^2} \Psi(\alpha) = E \Psi(\alpha)$$

- We know that since it is a particle on the ring, the wave function must be cyclical and return to the same point.
- We are also setting up a boundary condition that all points in space outside of this well have an infinite potential.
- The eigenstate solution to this problem is:

$$\frac{1}{\sqrt{2\pi}} \exp(in\alpha), \text{ where } n = 0, \pm 1, \pm 2, \pm 3 \dots \text{ and } E_n = \frac{\hbar^2 n^2}{2m r_0^2}$$

- Why do we get +n and -n states existing, where as before we didn't need to worry about negatives.
  - In our previous 1D derivations, the -n state was degenerate and was identical to the positive n case. Thus we could ignore it as it was the same state.
  - To understand why the negative is no longer degenerate. Let's consider the angular momentum of the system. Recall our classical definition of angular momentum is  $r \times p$ . Since it is a ring all of the angular momentum is along the z-direction.

$$L_z = \frac{-i\hbar}{d\alpha} \rightarrow L_z \varphi_n = n\hbar \varphi_n$$

- We see with positive and negative n we know have different angular momentums (different directions of orbit). Therefore our states are no longer degenerate.
  - We see energy splitting for each energy level, we know have 2 states.
- We see that angular momentum is also an eigenfunction problem that is solved by our eigenfunctions. We say that the quantum number for angular momentum along z is equal to  $n\hbar$

- We can also define angular momentum operators in other directions.

- Commutation Rules:

- Momentum commuted with a different direction will always yield 0.  $[z, p_x] = 0$
- Angular momentums commuted IN order will yield the next operator  $[L_x, L_y] = L_z$ , but  $[L_x, L_z]$  will NOT yield  $L_y$

- We can simplify Schrodinger's Equation by substituting in the moment of inertia and using our angular momentum operator.

- The moment of inertia of a system is the distance between all points and the center integrated over the mass. For a ring it is simply  $mr^2$

$$\frac{L_z^2}{2I} \frac{\partial^2}{\partial \alpha^2} \Psi(\alpha) = \frac{\hbar^2 n^2}{I} \Psi(\alpha)$$

- If we substitute 0 in, we see that our ground state energy is 0, but we know that is forbidden in quantum mechanics.

- This is because it is unrealistic of us to say we have infinite potential everywhere.
- If we shift the potential of our state to have negative infinite potential and the rest of the system to have 0 potential. We see a ground state energy falls out. This is added to all energies as there true energy.
- $V_0 \delta$  is the depth of the well

$$E_0 = -\frac{mV_0}{2\hbar^2}$$

## Particle on a Sphere

- We solve this system by using our spherical coordinates system. Thus we have a function of  $\theta$  and  $\alpha$ .

Our Schrodinger Equation is already solved for us! It is expressed as.

$$\frac{-\hbar^2}{2m r_0^2} L^2 Y_{n\text{total}}^{nz}(\theta, \alpha) = E_{n\text{total}} Y_{n\text{total}}^{nz}(\theta, \alpha)$$

- Note that despite our eigenfunction being dependent on 2 quantum numbers, the total energy is only dependent on  $n_{\text{total}}$ . This is because  $n_{\text{total}}$  quantifies the total angular momentum of the system.
- $L^2$  is the total angular momentum operator and is equal to a linear combination of the angular momentum in each direction  $L^2 = (L_x)^2 + (L_y)^2 + (L_z)^2$
- The magnitude  $n_z$  is limited to being less than or equal to the total angular momentum

- The angular momentum in one component cannot be greater than all of the angular momentum

$$E_{n\text{total}} = \frac{n_{\text{total}}(n_{\text{total}} + 1)\hbar^2}{2m r_0^2}$$

- What is the our eigenfunction equal to as it has been represented by this Y term.

$$\phi_{n\text{total}, n_z} = L^2 Y_{n\text{total}}^{nz} = n_{\text{total}}(n_{\text{total}} + 1)\hbar Y_{n\text{total}}^{nz}$$

$$Y_{n\text{total}}^{nz}(\theta, \alpha) = \exp(in_z \alpha) P_{n\text{total}}^{n_z}$$

P is the Legendre Polynomial

$$\varphi = R(r)A(\alpha) = J_{n\alpha} \left( \frac{\rho_{nr,n\alpha} r}{a} \right) \frac{1}{\sqrt{2\pi}} \exp(in\alpha) E = \frac{\hbar \rho_{nr,n\alpha}}{2m a^2}$$

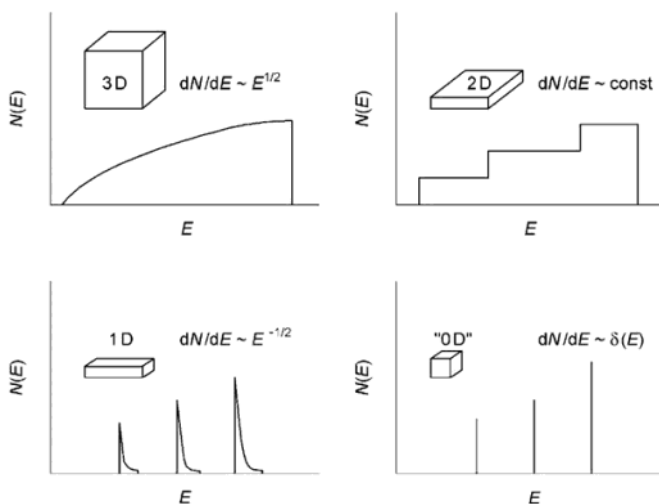
Where  $a$  is the radius of the risk

### Particle in a Sphere

- We simply added in our Bessel function term when we moved from a ring to a disk. We can basically do the same thing to our solution from on a sphere
- We have 3 quantum numbers  $n_r$ , the radial quantum number,  $n_\theta$  describes the total angular momentum and  $n_z$  describes the z-component of our angular momentum.
- $N = 2n_r + n_\theta$ .  $N^2$  is proportional to our energy.
  - We see a high amount of degeneracy. Consider  $N=2$ . We can make that up with a great deal of combinations of  $n_r$  and  $n_\theta$ . Then we can further have varying  $n_z$  terms depending on  $n_\theta$ . Thus we get the degeneracy expected in our terms.
- Our expected atomic orbital diagrams appear when we plot only the real part of our eigenfunctions.
  - We can ignore the imaginary component when we are talking about bonding

### Density of States

- As we increase our energy, we increase  $N$ , thus we get more states when we increase the energy.
  - The density of states is the number of states per energy level.
- This means as we get to higher energies, we have more and more states to place an electron.
  - This is only true for 3D. In each dimension we get a different rate of increasing states compared to the increase energy



term.

$$\phi_{n_{total} n_z} = L^2 Y_{n_{total}}^{n_z} = n_{tot}(n_{tot} + 1) \hbar Y_{n_{total}}^{n_z}$$

$$Y_{n_{total}}^{n_z}(\theta, \alpha) = \exp(in_z \alpha) P_{n_{total}}^{n_z}$$

$P$  is the legendre Polynomial

- Similar to the Legendre Polynomial the most important thing to discern about the Legendre Polynomial is the number of nodes..
  - $N_z$  will indicate the number of nodes in the equatorial direction. If we spin in the direction of  $\alpha$ . We will have that many nodes
  - If we move up and down our sphere (along the "z-direction") we will see our remaining nodes.
  - This caps our number of nodes to  $n_{total}$  nodes
- Another way to think of it.
- Since our equation is separable, our legendre polynomial describes the state of the system in the  $\theta$  direction. It has  $n_{total} - n_z$  nodes
  - Nodes at the poles are not considered nodes as they do not separate 2 regions
- Our alpha direction is still described by our  $e^{in_z \alpha}$  term. The number of nodes is equal to  $n_z$

TABLE 3.7  
Some Spherical Harmonics

Symbol	Polar	Cartesian	Normalization Constant
$Y_{00}$	1	1	$\frac{1}{2}(1/\pi)^{1/2}$
$Y_{10}$	$\cos \theta$	$z/r$	$\frac{1}{2}(3/\pi)^{1/2}$
$Y_{1\pm 1}$	$\mp(\sin \theta)e^{\pm i\phi}$	$\mp(x \pm iy)/r$	$\frac{1}{2}(3/2\pi)^{1/2}$
$Y_{20}$	$(3 \cos^2 \theta - 1)$	$(3z^2 - r^2)/r^2$	$\frac{1}{4}(5/\pi)^{1/2}$
$Y_{2\pm 1}$	$\mp(\sin \theta)(\cos \theta)e^{\pm i\phi}$	$\mp z(x \pm iy)/r^2$	$\frac{1}{2}(15/2\pi)^{1/2}$
$Y_{2\pm 2}$	$(\sin^2 \theta)e^{\pm 2i\phi}$	$(x \pm iy)^2/r^2$	$\frac{1}{4}(15/2\pi)^{1/2}$
$Y_{30}$	$(5 \cos^3 \theta - 3 \cos \theta)$	$z(5z^2 - 3r^2)/r^3$	$\frac{1}{4}(7/\pi)^{1/2}$
$Y_{3\pm 1}$	$\mp \sin \theta (5 \cos^2 \theta - 1)e^{\pm i\phi}$	$\mp (x \pm iy)(5z^2 - r^2)/r^3$	$\frac{1}{8}(21/\pi)^{1/2}$
$Y_{3\pm 2}$	$(\sin^2 \theta)(\cos \theta)e^{\pm 2i\phi}$	$z(x \pm iy)^2/r^3$	$\frac{1}{4}(105/2\pi)^{1/2}$
$Y_{3\pm 3}$	$\mp(\sin^3 \theta)e^{\pm 3i\phi}$	$\mp(x \pm iy)^3/r^3$	$\frac{1}{8}(35/\pi)^{1/2}$

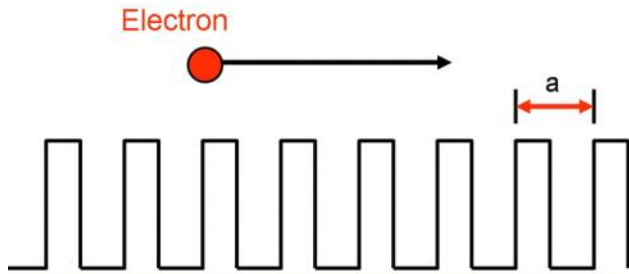
Douglas, Bodie E. and Hollingsworth, Charles A. *Symmetry in Bonding and Spectra - An Introduction* (Orlando, Florida: Academic Press, Inc., 1985) p. 88.

# Periodic Potential Wells

July 23, 2015 7:27 PM

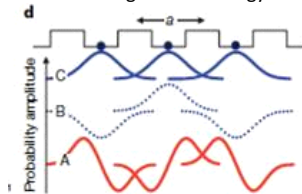
## Periodic Crystals

- Periodic Crystals can be modelled using an infinite square well.
- We can model each bond as a finite square well



## Approximation of the Periodic Potential of the Crystal

- Our eigenstates look roughly like our original eigenstates. For our ground state we can see that we have an overall shape across the crystal of a ground state and each small well has a ground state
  - For our 1st excited state, the overall lattice looks like the 1st excited state, but inside each peak we still see our ground state peaks
    - This means there is one node across the lattice, but no nodes in the well
  - Due to this we see a near degeneracy in the energy. For N wells, N eigenstates have degenerate energy



- When we move up to N+1 eigenstate, we see that each well adopts the configuration of the 1st excited state, but the overall structure returns to the ground state. This cycle repeats itself

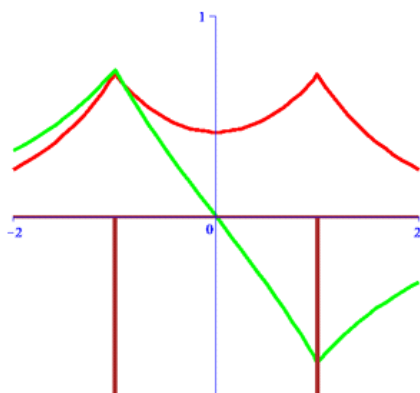
## Simple 2 Well System

- Now that we have solved the energy for one well, we can move on to building the eigenstate for the entire crystal lattice.
- Consider a simple 2 well system. We are going to assume they are the same depth and thus it is reasonable to assume that the probability being in both wells is the same.
- We can say we have an eigenstate for the entire system
 
$$\Phi_k^l = \sum \frac{1}{\sqrt{N}} \exp(inla) \phi_k(x + na)$$
- Confusingly enough l represents the number of periods the eigenstate has over the entire crystal. If it is just half a sine wave over the crystal l=1 (Plot C in the graph to the left), if it is a complete sine wave then l=2 etc. This is related to the wave number
- K is equal to the eigenstate of each well.
- N indicates which well we are summing over and a is the distance between wells.
- It should be obvious that there are only 2 possible states with a ground state well energy.

$$\Phi_1^1 = \frac{1}{\sqrt{2}} \phi_1(x) + \frac{1}{\sqrt{2}} \phi_2(x) \quad \Phi_1^2 = \frac{1}{\sqrt{2}} \phi_1(x) - \frac{1}{\sqrt{2}} \phi_2(x)$$

We see that the energy of the whole crystal is equal to  $E_1^1 = \alpha + \beta$   $E_1^2 = \alpha - \beta$

The red line shows the 1st eigenstate and the green line shows the second eigenstate.



## Solving Schrodinger's Equation for Periodic states

- We can represent the wavefunction as a linear combination of atomic orbitals as the eigenstates of each well represent a complete basis set.
  - We make 2 assumptions. There is no hybridization of atomic orbitals and we have tight binding. This is the assumption that we only consider overlap from the nearest neighbouring wells.
- We can represent the Hamiltonian as a matrix again.
 
$$\begin{matrix} \alpha & \beta & 0 \\ \beta & \alpha & \beta \\ 0 & \beta & \alpha \end{matrix}$$

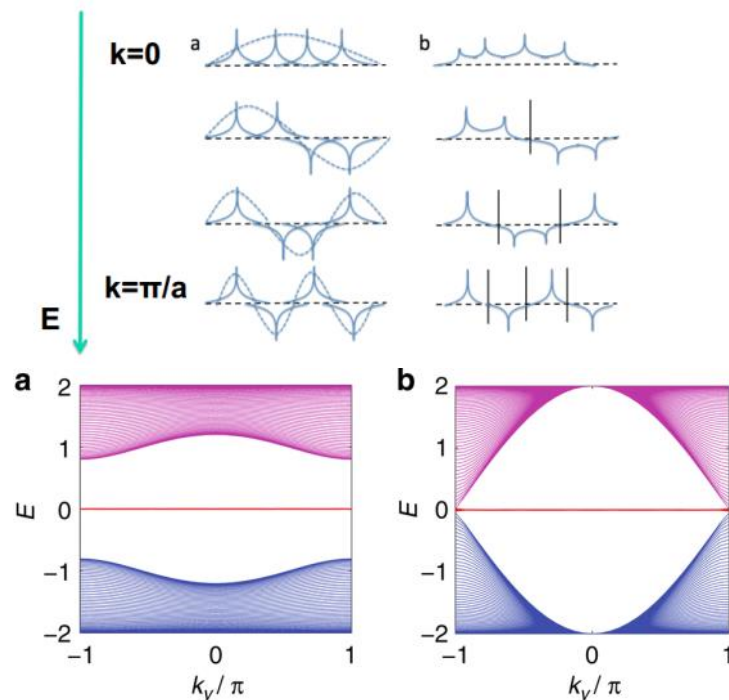
Where alpha is the energy at the well and beta is the hopping probability between the wells.

$$\alpha = \int \varphi_{n,x} * H \varphi_{n,x} dx \quad \beta = \int \varphi_{n,x} \varphi_{n+1,x}$$

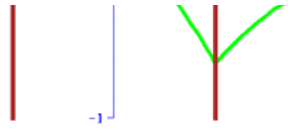
- Where x indicates which well the eigenstate is for and n indicates the quantum number of the state.
- We assume that we have cyclic boundary conditions. There is a very small error associated with this.
- We know the eigenstate of a finite square well is  $Ae^{-inka}$ , where n indicates the state of each well. A is the normalization constant K is the wave number and is equal to  $q2\pi/l$ . "a" is the length of the well
- We can say that the eigenstate in each well is equal to  $\beta \exp(-i(n-1)ka) + \alpha \exp(-inka) + \beta \exp(-i(n+1)ka) = \varphi_{well}$
- We can sub this into Schrodinger's Equation and solve for the energy of the eigenstate in the crystal
 
$$E = 2\beta \cos(ka) + \alpha$$
- We see that the energy in each well depends on the wave number of the overall crystal.
  - The wave number indicates the periodicity of the entire crystal. Recall this is governed by the overall eigenstate of the system.

## Generalized Lattice

- As stated in the previous section the general energy is a function of K is equal to  $E = 2\beta \cos(ka) + \alpha$ 
  - Recall  $k=2\pi q/l$ , where q is the number of periods and l the length of the crystal
  - When the length of the period is equal to the length of the crystal we see that k reaches its minimum and so does the energy. This is when we have 1 period over the well
  - When the length of the period is equal to the length of the well, meaning we have the maximum number of oscillations with N periods.
  - For those that do not form good integers, we see the individual eigenstates rotating into the imaginary plane. Thus creating a smooth curve.
  - With these we form our energy bands



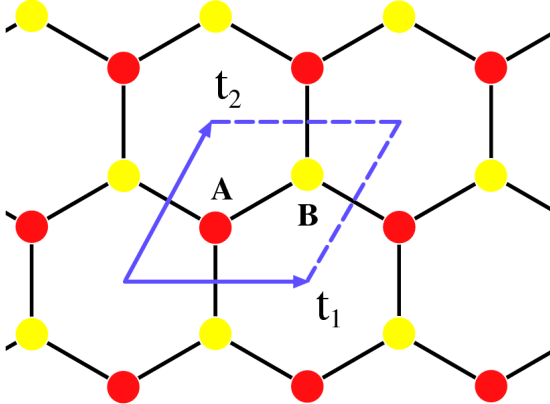
- We have a different energy function depending on the eigenstate in the well. For instance the second eigenstate has the opposite relation, where the most periodic, has the lowest energy.
- This is the formation of energy bands and the bands formed have a gap



- This is the formation of energy bands. These energy bands

### Graphene

- Graphene can be easily broken down into a simple lattice structure



- We can apply the same assumptions, we did to solving our periodic well to graphene as the simplest unit is composed of 2 atoms. (Tight Binding) and we are only interested in the valence electron in the p-orbital.
- We can express our Hamiltonian by using vectors to indicate the voltage at a specific region. Let  $V_{at}$  be operator that gives the atomic potential from an atom on a point

$$H = \frac{p^2}{2m} + \sum V_{at}(\vec{x} - \vec{x}_{c1} - \vec{R}) + V_{at}(\vec{x} - \vec{x}_{c2} - \vec{R})$$

When we substitute in our basic Eigen function we see that

$$H\phi_1 = \phi_1 E_1$$

$$+ \phi_1 \left( \sum V_{at}(\vec{x} - \vec{x}_{c1} - \vec{R}) + V_{at}(\vec{x} - \vec{x}_{c2} - \vec{R}) + V_{at}(\vec{x}_{c1} - \vec{x}_{c2}) \right)$$

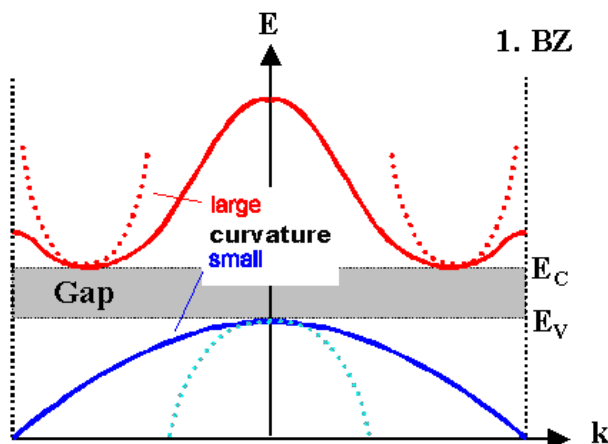
We represent the massive summation term as  $\Delta u_1$

- We will define the energy state of individual carbons to be the 0 energy level.
- Knowing that the carbon atoms are identical, we can rewrite Schrodinger's Equation as  $H\phi_1 = \Delta u_1 \phi_1, H\phi_2 = \Delta u_2 \phi_2$
- Know that we have solved our equation for our individual well, we must solve it for the entire lattice. When we solve the energy of this system we find that

$$E(k_x, k_y) = \pm \sqrt{1 + 4\cos\left(\frac{\sqrt{3}ak_y}{2}\right)\cos\left(\frac{ak_x}{2}\right) + 4\cos^2\left(\frac{ak_x}{2}\right)}$$

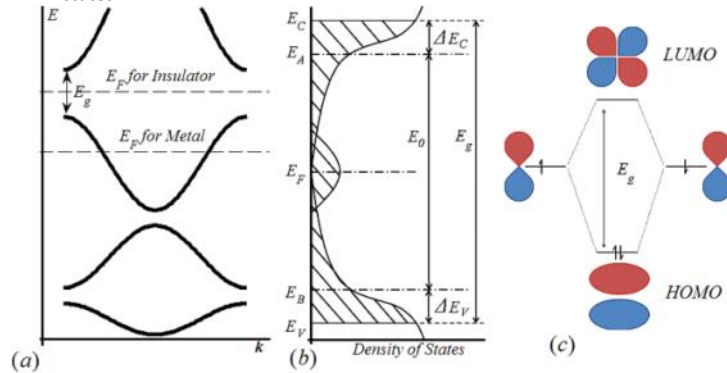
### Effective Mass

- Consider if had holes stuck in the conduction band. They would migrate to the highest point in the CB. This is analogous to air in a bottle of water migrating to the top.
- We can apply an electric field to the semi-conductor and the carriers will begin to move because they are charged.
  - We are applying a force and thus the electrons will move, but how easy is it to move

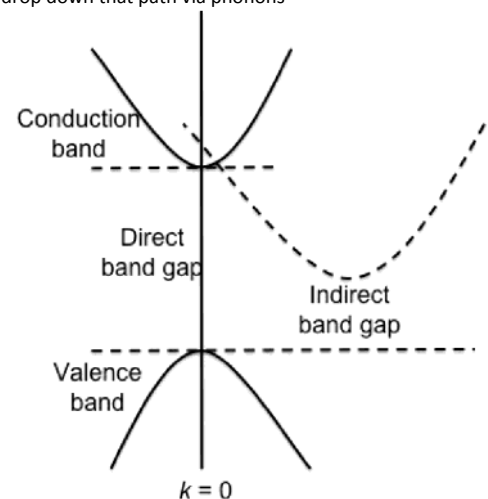


- The amount they are effected by the force applied is based on the effective mass of the particle.  $F_{ext} = m^*a$ , where  $m^*$  is defined as the effective mass.

- We have a different energy function depending on the eigenstate in the well. For instance the second eigenstate has the opposite relation, where the most periodic, has the lowest energy.
- This is the formation of energy bands and the bands formed have a gap inbetween. This gap is known as the band gap.
- The density of states is the integration over all wave numbers at a certain energy slice. The more flat the band is at that energy the larger the density of states.



- Direct Gap Semi-Conductors have the minimum of the conduction band and the maximum of the valence band aligned. These are useful for light emitters. Since they reliably and easily produce this fall for the electron, generating the same energy photon every time. This is reliable light production (LEDs)
- Indirect-Gap Semi conductors have their k values not aligned. Therefore the electron becomes trapped in the conduction band until a phonon (random vibration) changes its momentum to allow its fall. This process will still occur but takes significantly longer. This is good if we want to exploit this energy (Solar panels)
  - In indirect gap semi conductors, electrons will look for alternative pathways. This means if there is a defect that lowers the band, it will drop down that path via phonons



- The Brillouin Zone is only interesting space as it is the smallest repeatable space. We can draw all of our bands by using the energy level over one band.
  - We only need to know the periodicity over the whole well to determine energy, not

### Hybridization

- We can hybridize our orbitals by taking a superposition of the well eigenstates in at different energy levels.
  - Since we can add a phase to each eigenstate, we can create 3 hybridized states with 3 input states.
  - Each of these states has characteristics of their inputs states corresponding to the probability
  - Each of these states has equal energy.
  - Hybridization occurs because the unequal distribution of the atom results in a greater overlap between atoms.

- The force is less effective in a region of high curvature as to accelerate the particle, we require additional energy to move up the edge of the band
  - Think of this as rolling a ball across a hilly road. A flat road makes the ball feel easy to roll, while a steep hill makes it feel hard.

- Effective mass is directly related to the curvature.

$$m = \hbar^2 \left( \frac{d^2 E}{dx^2} \right)^{-1}$$

- Using a 2nd order Taylor expansion we can simplify this to be

$$m^* = \frac{\hbar^2}{|\beta| \alpha}$$

# Spin

July 25, 2015 4:56 PM

## Spin and Dirac Notation

- The spin of an electron is related to the magnetic moment of an electron. The  $1/2$  indicates that it is a magnetic dipole, this means the north pole can point either up or down.
- We represent this in dirac delta notation  $|\frac{1}{2}\rangle$  and  $|\frac{-1}{2}\rangle$ , for spin up and spin down.
- They can also be written as column vectors.
  - This is very similar to our neutron interferometer
- We represent the conjugated states as  $\langle \frac{1}{2}|$  and  $\langle \frac{-1}{2}|$ 
  - These are the equivalent of row vectors
- This gives us a condensed way of taking the inner product of two eigenstates as  $\langle \phi_n | \phi_n \rangle = \delta_{nn}$
- we can represent a wave function by a series of coefficients that indicate the magnitude of each eigenstate.
- The general wave function for our spin is:

$$\Psi = \cos \alpha |\frac{1}{2}\rangle + \exp(i\beta) \sin \alpha |\frac{-1}{2}\rangle$$

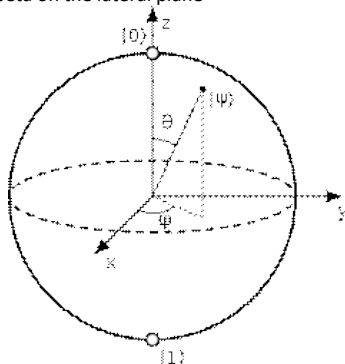
- The alpha term gives magnitudes and the beta term serves as a phase.
- This is a simple 2D system so representing it with matrices will be simple.
- An operator in dirac notation is denoted by  $|\text{out}\rangle = \Omega |\text{input}\rangle$
- In matrix notation, we can write out any operator as a combination of the following.
- Identity =  $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$   $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$   $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$   $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
- The operator can be written as a linear combination of the 4 operators  $\Omega = aI + b\sigma_x + c\sigma_y + d\sigma_z$ , where each coefficient is  $\text{Trace}(\Omega\sigma)$
- The trace (sum of the diagonal) of the sigma (Pauli) operators is equal to 0.
- The poly operators do not commute in general two poly operators  $[\sigma_a, \sigma_b] = 2i \epsilon_{abc} \sigma_c$  (epsilon is the Levi Civitan Symbol. If the commutators are in order like they are a,b, c then it returns 1, if they are out of order b,a,c then it returns -1. If there is any symbol repeating itself then it returns 0. (aba)

$$\Omega^+ = \Omega, \text{ where } \Omega = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \text{ and } \Omega^+ = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}$$

Operators can be written as outer products. For instance the Pauli operator in z rotates a matrix. We can rewrite it as

$$|\frac{1}{2}\rangle\langle\frac{-1}{2}| + |\frac{-1}{2}\rangle\langle\frac{1}{2}|$$

- There is a certain class of operators known as projectors. This is when the square of the operator returns the same operator. The following is a projector operator.
- The probability that the wavefunction is in that eigenstate is still equal to the probability amplitude (coefficient) squared.
- The Bloch Sphere gives us a physical representation. Consider the spin up to be oriented pointing in positive z and spin down pointing in negative z. We can represent any wavefunction by plotting the vector alpha on the x-y plane and beta on the lateral plane

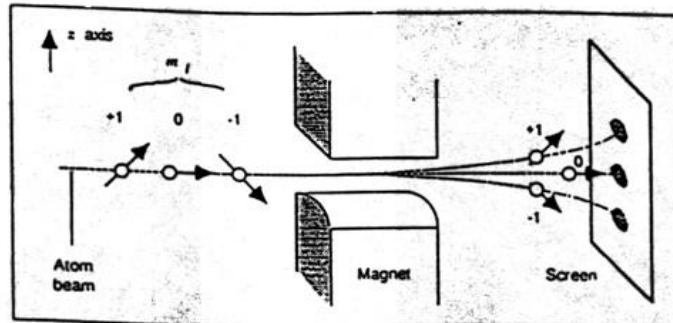


We can then define spins to be in the positive x and y direction.

- Spin up and spin down eigenstates are also eigenstates of the Pauli-Z operator.
- The eigenstates for the Pauli-X operator lie on the x-axis, they can be represented as spin up and down as  $\frac{1}{\sqrt{2}}(|\frac{1}{2}\rangle + |\frac{-1}{2}\rangle)$  and  $\frac{1}{\sqrt{2}}(|\frac{1}{2}\rangle - |\frac{-1}{2}\rangle)$
- We can rotate on the bloch sphere in a certain direction by  $\theta$ . Say we want to rotate around x with an angle  $\theta$ . We apply the following operator to the

## Stern Gerlach Experiment

- In the Stern-Gerlach experiment silver atoms were passed through a magnetic field, due to the spin up and spin down nature. They head to two quantized positions as they either have a spin up or spin down.
  - The probability of where it heads depends on the probability it is in the + or - eigenstate.



- Consider now we pass the bottom beam, with  $-1/2$  spin, into another magnetic field oriented along the z direction.
  - We will not see beam splitting as the wavefunction is updated to contain only atoms with  $-1/2$  spin
- Instead consider, we pass the bottom beam with  $-1/2$  spin, into another magnetic field along the x-axis.
  - We will see beam splitting. If we think of the Bloch sphere, when we take the projection of a z-component on the x-axis, we can make an equal projection in both directions
- If we pass one of our resulting x-direction beams through another magnetic field aligned in z, we will once again see beam splitting, similar to the neutron interferometer.
- If we pass both of our resulting x-direction beams through the magnetic field aligned in z, we will return our  $-1/2$  spin.

## Time Evolution with Pauli Operators

- The time evolution of the system can be added and is equal to.  $|\Psi\rangle = \exp\left(\frac{iHt}{\hbar}\right) |\Psi(0)\rangle$
- The time dependence is a unitary which means, the magnitude is constantly 1, this ensure normalization
- We can apply a Taylor expansion to the exponential time term. We'll take the Hamiltonian to be equal to  $\omega\sigma_z/2$ . The time term is equal to  $\exp\left(\frac{iHt}{\hbar}\right) = I \cos\left(\frac{\theta}{2}\right) - i \sin\left(\frac{\theta}{2}\right) \sigma_z$  Where  $\theta = \omega t$  which describes the frequency of the system and capital I stands for the identity matrix.
- We can convert this to Matrix Form  $\begin{pmatrix} \cos\frac{\theta}{2} - i \sin\frac{\theta}{2} & 0 \\ 0 & \cos\frac{\theta}{2} + i \sin\frac{\theta}{2} \end{pmatrix}$
- We can perform a similar process subbing different Pauli Operators as our Hamiltonian.  $\sigma_x \rightarrow \begin{pmatrix} \cos\frac{\theta}{2} & -i \sin\frac{\theta}{2} \\ -i \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$   $\sigma_y \rightarrow \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$
- On our Bloch Sphere this is equivalent to rotating around the axis over time. " $\sigma_y$ " as our Hamiltonian will have the wavefunction rotating ABOUT the y-axis in the X-Z plane.
  - Spinner Dynamics States that we must rotate around twice to return to our initial state. There is a period of  $4\pi$ , since all of our time factors have the angle divided by two.
- This can be shown by subbing any initial wave function and propagate it through time with our equation.

## MRI

- All protons have a magnetic dipole that are rotating. We can write a Hamiltonian for each hydrogen atom as  $H = \frac{\gamma B \sigma_z}{2}$
- Where gamma describes the frequency of the electro magnetic field, B is the applied magnetic field
- MRI work by placing a person in a strong magnetic field parallel in the Z-direction.
  - The spins will all be sitting along z, since they are in their lowest energy

represented as spin up and down as

$$\frac{1}{\sqrt{2}} \left( \left| \frac{1}{2} \right\rangle + \left| -\frac{1}{2} \right\rangle \right) \text{ and } \frac{1}{\sqrt{2}} \left( \left| \frac{1}{2} \right\rangle - \left| -\frac{1}{2} \right\rangle \right)$$

- We can rotate on the Bloch sphere in a certain direction by  $\theta$ . Say we want to rotate around x with an angle  $\theta$ . We apply the following operator to the wavefunction.

$$\exp\left(\frac{i\theta}{2}\sigma_x\right)|\Psi\rangle$$

applied magnetic field

- MRI works by placing a person in a strong magnetic field parallel in the Z-direction.
  - The spins will all be sitting along z, since they are in their lowest energy eigenstates.
- We apply a rotation to the eigenstate to rotate the state on to the X-Y plane. This will cause it to rapidly spin around the Z-Axis.
  - We have a detector, which is capable of detecting the frequency it passes through one of these axes.
    - If there are no hydrogens there, then we get no resulting spin.
- We apply a gradient magnetic field because it assigns each location with a unique frequency. Thus we can measure the intensity of each frequency to determine the concentration of hydrogen in the area.
  - The direction of our applied magnetic field allows us to choose which slices we are looking at.
  - This allows us to map the hydrogen concentration across the body. We can also apply this to other paramagnetic elements, such as oxygen in the brain.

# Tutorial Information (Useful for Course Material)

June 7, 2015 7:40 PM

## Complex Numbers

- A complex number has a real and imaginary component ( $a+bi$ )
  - Imaginary numbers are equal to the square root of -1.
- We can represent them as a sum of trigonometric terms  $R \cos \theta + Ri \sin \theta$ , where  $R=\sqrt{a^2+b^2}$  and  $\theta$  is  $\arctan(b/a)$
- By Euler's formula, we can represent it as an exponential  $Re^{i\theta}$ 
  - When applying Euler's formula be careful when evaluating the angle, as there are sometimes two possible answers. Think about the angle plotted out from the x-axis to determine which is correct
- Properties of Complex Sets
  - Conjugate: The conjugate to a complex number is equal to  $a-bi$ . The result of multiplying  $A$  by its conjugate  $A^*$  if we find the magnitude  $|A|$ .
  - Normalization involves dividing a complex number by its magnitude
  - For adding two conjugate numbers  $a+bi+c+di$ , we can say that  $(a+c)+i(b+d)$
  - When multiplying two complex numbers, we use our FOIL rules.  $(a+bi)(c+di)=(ac-bd)+i(bc+ad)$
  - When dividing two complex numbers it is easier to convert to Euler's Formula and apply exponential rules to evaluate.
    - Another possibility is to multiply the top and bottom by the conjugate of the denominator and evaluate

## Expectation Value

- The expectation value of a system, is the value you expect to get when you average all the measurements of the system.
- The expectation value of an operator  $\Omega$  from the wavefunction is always equal to

$$\int \varphi^*(x) \Omega \varphi(x) dx$$

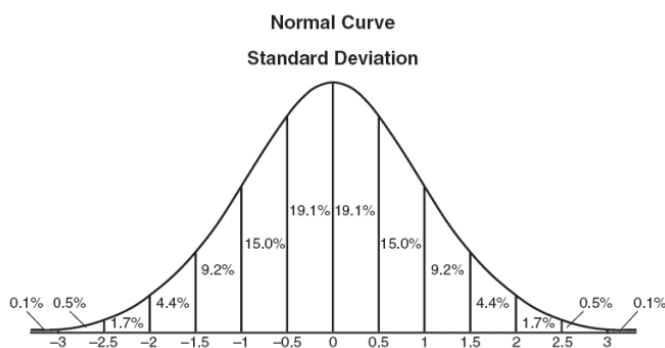
- We can solve for the expected energy, position, momentum etc. of a particle in a box system.

## Standard Deviation

- The standard deviation of a system tell us the spread of the measurements from the average value. It is defined as, where  $\mu$  is the expected value  $\sigma = \sqrt{\langle (x - \mu)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$
- If we consider the eigenstates of a particle in a box, the standard deviation of the eigenstates approaches 0.29. Why is that?
  - The higher the eigenstate, the more it looks like a flat line distributed across the region. Therefore the limit for the standard deviation as  $N$  approaches infinity is the standard deviation of a line over space.

## Gaussian Distribution

- The Gaussian or normal distribution is shown below.



- The wave function for a gaussian distribution is the square root of the gaussian function. This has a positive and negative component to it

## Eigenvectors

- An eigenstate/vector for operator  $A$ , is a state that when operated on by  $A$  only changes by a scalar value.
  - In other words, the magnitude of each component of the state increase by the same proportion.
- The eigenvalue, is the scalar that the state is multiplied by when passing through the operator  $A$ . This is represented by  $\lambda$ .
- We can solve for the eigenvalues of a problem by finding values of  $\lambda$  that satisfy the following relationship  $\det[A-\lambda I]=0$ .
- To solve for the eigenstate/vector, we substitute our solved eigenvalue into the relationship that  $Ax=\lambda x$  and solve for each component of the vector.
- Eigenstates are unique as there is no fundamental shift in their state, when an operator is applied to them.

## The Nature of Light

- Light exists as a wave-particle duality, meaning it shares properties of both waves and particles
  - It behaves wavelike as it is travelling, but still may only impact one position as a particle.
- Light is an electromagnetic vibration that travels through space as a wave.
- Unpolarised light is light that oscillates in every direction.
- A polarizer filters the light to have a oscillate in a single direction.
  - This polarizer cuts the intensity in half.
    - Consider if we define a basis set in the direction of the polarizer and orthogonal to the polarizer. All directions of oscillation can be broken up into those two components.
      - Thus if we fully eliminate the orthogonal component, we only get half the light from unpolarised light.
  - If we have polarized light passing through another polarizer, that is orthogonal to the first filter, we lose all amplitude.
  - If we have 3 polarizers, one 45 degrees to the first and one orthogonal to the first, we don't see total annihilation.
    - This is because the middle filter, converts the light to another direction, that is not orthogonal to the final filter, thus allowing some light to pass through the final filter. There is a loss of intensity of 1/8 however.
  - This final property is used when analyzing materials as they will impart a polarization on passing light.
- The wavenumber of a particle, decreases the wavelength of the particle. This increases the momentum of the particle, the higher the wave numbers.
  - This higher momentum leads to a higher energy, which is represented by  $\frac{h^2 k^2}{2m}$
- A Gaussian distribution in a 1D square well problem will spread out before interacting with the walls and returning to its initial state.
- The momentum of light can be express as  $h/\lambda$ , where  $h$  is Planck's constant. The momentum is also equal to  $mv$ . Therefore  $h/\lambda=mv$ .
  - This is known as DeBroglie's Equation

## Quantum Dots

- Quantum dots are homogenous spheres. They are important because they have very homogenous band gaps. The size of the band gap is controlled by the size
- Therefore we can get colours of high quality and brilliance by exciting electrons in a Quantum dot.
- We can also build quantum dots as sections of a pillar or as a single electron trapped in a well.
  - This well is made by placing an electron on a conductor. The electron is surrounded by a region of negative charge to remove all other electrons.
- Quantum dots are used in industry, but it is challenging to have 3 quantum dots for each primary colour per pixel.
  - Instead the quantum dots are coated. We can apply an electric field to these quantum dots to change the boundaries.
  - The field slopes the potential lines in a 1D well and allows us to control the band gap.