

# Introduction to Quantum Physics

## PH107 TSC

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# Outline

- 1 Introduction
- 2 Duality
- 3 Mathematical Interlude
- 4 Quantum Mechanics
- 5 Statistical Mechanics

# A Touch of Philosophy

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- So how do we go about studying the rather non-trivial universe around us?
- Experiments! What better way to analyse our surroundings than to be in them. Then, we create theories and models to explain the results of these experiments.

We are both spectators and actors in the great drama of existence  
- Bohr

# Failure of the Classical Theory

And then Newton said<sup>1</sup>,  $F = ma$ . Claps!

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# Failure of the Classical Theory

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- Blackbody Radiation
- Compton effect
- Various other reasons as to why classical theory was inadequate.

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# Blackbody Radiation

Consider a body in thermal equilibrium. It was argued<sup>2</sup> that the emitted power is proportional to the power absorbed.

$$e_f = J(f, T)A_f \quad (1)$$

where  $e_f$  is the power emitted per unit area per unit frequency by a particular heated object,  $A_f$  is the absorption power (fraction of the incident power absorbed per unit area per unit frequency by the heated object), and  $J(f, T)$  is a universal function (the same for all bodies) that depends only on  $f$ , the light frequency, and  $T$ , the absolute temperature of the body.

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<sup>2</sup>Using some thermodynamics, not a part of the course 

# Blackbody Radiation

## Definition (Blackbody)

A blackbody is defined as an object that absorbs all the electromagnetic radiation falling on it

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## Stefan Boltzmann Law

The total radiant heat power emitted from a surface is proportional to the fourth power of its absolute temperature

Mathematically,

$$e_{total} = \int_0^{\infty} e_f df = \sigma T^4 \quad (2)$$

# Blackbody Radiation

## Wien's Displacement Law

The wavelength marking the maximum power emission of a blackbody, is inversely proportional to its absolute temperature

Mathematically,

$$\lambda_{max} T = 2.898 \times 10^{-3} mK \quad (3)$$

# Blackbody Radiation

At this stage, it is more convenient to talk in terms of energy per unit volume per unit frequency of the radiation within the blackbody cavity,  $u(f, T)$  instead of the power radiated per unit area per unit frequency. We can evaluate<sup>3</sup>

$$J(f, T) = u(f, T) \times \frac{c}{4} \quad (4)$$

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So where's the problem? Let us try to evaluate  $u(f, T)$

$$u(f, T)df = \bar{E}N(f)df \quad (5)$$

Where  $N(f)df = \frac{8\pi f^2}{c^3}df$  is the number of modes of vibration <sup>4</sup>

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# Blackbody Radiation

Let us compute the above, particularly  $\bar{E}$  using classical theories. Considering a Maxwell-Boltzmann distribution, we know that the probability of being in a state with energy  $E$  is proportional to  $\exp(-E/k_B T)$ . Thus,<sup>5</sup>

$$\bar{E} = \frac{\sum E P(E)}{\sum P} = \frac{\int_0^\infty E e^{-\frac{E}{k_B T}}}{\int_0^\infty e^{-\frac{E}{k_B T}}} = k_B T \quad (6)$$

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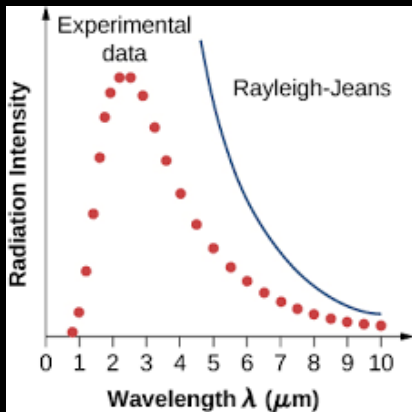
Plugging it back into the equation (5),

$$u(f, T) df = \frac{8\pi f^2}{c^3} k_B T df$$

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# Blackbody Radiation



The disagreement of Rayleigh Jeans at low wavelength is called Ultraviolet catastrophe

# Blackbody Radiation

Wien made another estimate for blackbody radiation. This was made from a purely thermodynamic argument and Planck's constant was not introduced at this stage. However, we express the constants in terms of  $h$  and  $c$  to observe that the estimate only holds good at lower wavelengths. Thus, there was a disconnect between not just between classical theory and experimental data but within classical theories themselves!

$$I(\nu, T) = \frac{2h\nu^3}{c^2} e^{-\frac{h\nu}{k_B T}}$$

# Blackbody Radiation

Now, Plank proposed that energies could only be integral multiples of  $hf$ , for Plank's constant  $h$ <sup>6</sup>. Let us calculate  $u(f,T)$  now

$$\bar{E} = \frac{\sum E P(E)}{\sum P} = \frac{\sum n h f e^{n h f / k_B T}}{\sum e^{n h f / k_B T}} = \frac{h f}{e^{\frac{h f}{k_B T}} - 1} \quad (7)$$

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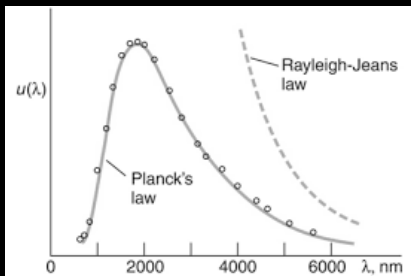
Plugging it back into the equation (5),

$$u(f, T) df = \frac{8 \pi f^2}{c^3} \left( \frac{h f}{e^{\frac{h f}{k_B T}} - 1} \right) df$$

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# Blackbody Radiation



Plank's formula fits the data better! Check on your own for the sake of completeness that in the high wavelength region, Plank's formula becomes equivalent to Rayleigh Jeans' formula (and to Wien's exponential law in the low wavelength region)

# Compton Scattering

Another classic example where classical theory was inadequate was Compton Scattering.



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- incident radiation of frequency  $f_0$  should accelerate an electron in the direction of propagation of the incident radiation
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# Compton Scattering

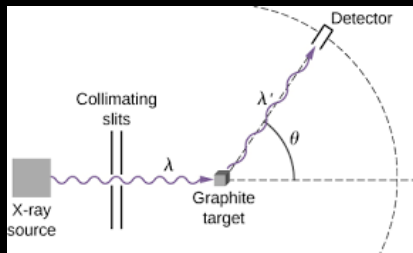
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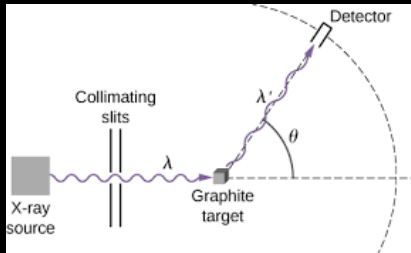
Clearly, experimental data from Compton's experiment tells us otherwise

# Compton Scattering

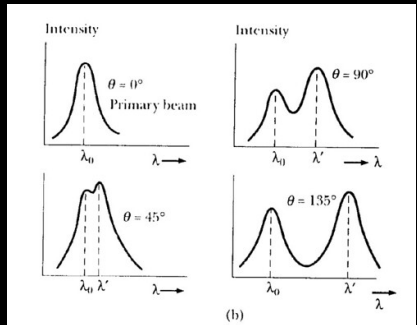


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# Compton Scattering

Let us obtain the above equations from modern physics

$$hf + m_e c^2 = hf' + \sqrt{p_e^2 c^2 + m_e^2 c^4} \quad (\text{Energy conservation})$$

$$\vec{p} = \vec{p}_e + \vec{p}' \quad (\text{Momentum conservation})$$

$$f = \frac{c}{\lambda}$$

Simplifying the above, we obtain equation (8)

# Need for a new Theory

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But where and how to start?

Let us start by challenging a few more ideas of the classical theory  
- particles and waves.

# Wave-Particle Duality

Particle nature and wave nature are entities which have been analysed in rather great detail in classical theories. We refer to light waves and matter particles extensively.

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Particle nature and wave nature are entities which have been analysed in rather great detail in classical theories. We refer to light waves and matter particles extensively.

But as light does show particle nature<sup>7</sup>, it is not a dystopian idea that matter can show wave like behaviour.

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# De-Broglie Equation

Inspired by the inadequacies<sup>8</sup> of the Bohr model of the atom, De Broglie stated,

## De - Broglie Hypothesis

Since photons have wave and particle characteristics, perhaps all forms of matter have wave as well as particle properties.

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He concluded that the wavelength and frequency of a matter wave associated with any moving object were given by

$$\lambda = \frac{h}{p} \quad (9)$$

---

<sup>8</sup>Such as inability to explain quantization amongst many others

## Davisson Germer Experiment

Of course, such radical sounding ideas cannot be accepted without any evidence, and as mentioned before, experiments are evidence. Thus, came the Davisson Germer Experiment.

# Davisson Germer Experiment

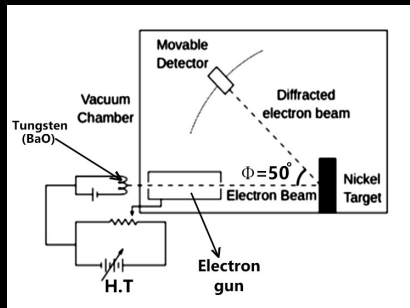
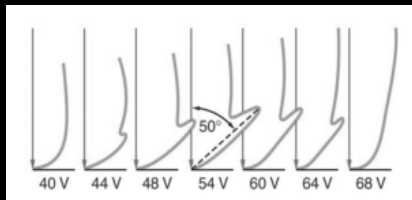
The experiment consisted of firing an electron beam at a nickel crystal, perpendicular to the surface of the crystal, and measuring how the number of reflected electrons varied as the angle between the detector and the nickel surface varied. The electrons were accelerated through an electric potential difference, giving them a certain amount of kinetic energy, towards the nickel crystal.

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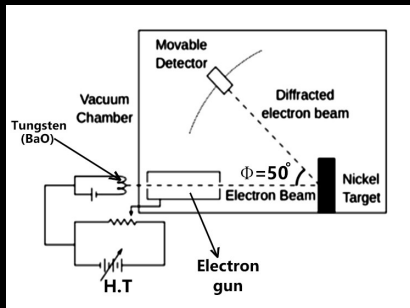
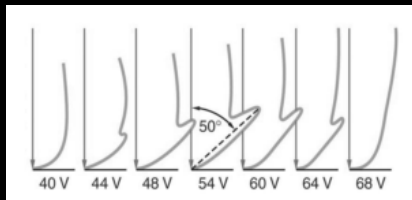


# Davisson Germer Experiment



<sup>9</sup>Note that  $\theta$  here is not the same angle as in the figure above

# Davisson Germer Experiment



Davisson-Germer experiment results in an interference pattern expected from waves with the calculated wavelength according to Bragg's Law

$$^9 n\lambda = 2d\sin\theta \text{ (path difference)} \quad (10)$$

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## Group and Phase Velocity

Something just doesn't add up though. When we think of waves, say on a string, we don't or rather, can't ask questions like where is the wave on the string. It's everywhere! The whole string is vibrating. However, we can talk about the location of an object <sup>10</sup>. Why's that?

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The matter wave representing a moving particle must reflect the fact that the particle has a large probability of being found in a small region of space only at a specific time. This means that a traveling sinusoidal matter wave of infinite extent and constant amplitude cannot properly represent a localized moving particle. What is needed is a pulse, or “wave group,” of limited spatial extent.

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## Group and Phase Velocity

Let us examine this situation mathematically. Consider a one-dimensional wave propagating in the positive  $x$  direction with a phase speed  $v_p$ . Note that  $v_p$  is the speed of a point of constant phase on the wave. This traveling wave with wavelength  $\lambda$ , frequency  $f$ , and amplitude  $A$  may be described by

$$y = A \cos\left(\frac{2\pi x}{\lambda} - 2\pi f t\right) = A \cos(kx - \omega t)$$

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## Group and Phase Velocity

We can visualize the above as a wave of high frequency and low wavelength bound inside an envelope of higher wavelength (the wave packet). The packet moves with a velocity

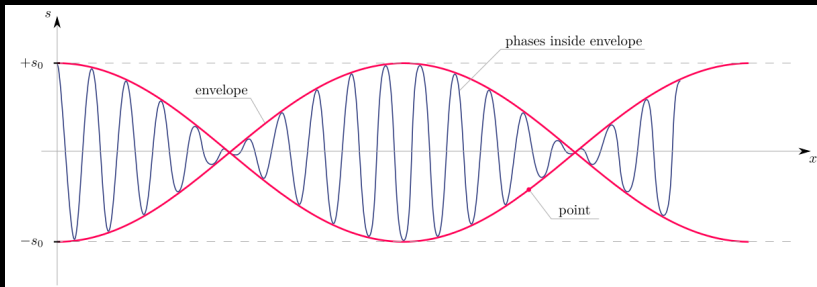
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$$E = \hbar\omega, p = \hbar k$$

$$\implies v_p = \frac{E}{p}, v_g = \frac{\partial E}{\partial p}$$

### Result

Using  $E^2 = p^2 c^2 + m_0^2 c^4$ , we can show that  
 $v_p > c, v_g < c, v_p \times v_g = c^2$

# Dispersion Relation

Dispersion relations describe the effect of dispersion on the properties of waves in a medium. A dispersion relation relates the wavelength or wave-number of a wave to its frequency, say  $w(k)$

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Wait a minute! In Result 1 above, we calculated the phase and group velocities. Did we use any dispersion relation there? Yep!  $E^2 = p^2 c^2 + m_0^2 c^4$  is the relativistic dispersion relation.



# The question of Duality

So finally, are electrons particles or waves?

## Duality

Electrons are very delicate and rather plastic—they behave like either particles or waves, depending on the kind of experiment performed on them. In any case, it is impossible to measure both the wave and particle properties simultaneously

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In a YDSE experiment, in all cases if the detector collects electrons at different positions for a long enough time, a typical wave interference pattern for the counts per minute or probability of arrival of electrons is found.

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In a YDSE experiment, in all cases if the detector collects electrons at different positions for a long enough time, a typical wave interference pattern for the counts per minute or probability of arrival of electrons is found.

However, if we determine which slit the electron passes through, the interference pattern is lost and the accumulated result is simply the sum of the individual results.

# Doubts and Difficulties!

So do we start the cool stuff like Schrodinger's equation now?

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# Fourier Transform

Let's start with some inspiration. Suppose I wanted to analyse the momentum of a particle represented by a matter wave. The current mathematical form is not very simple to analyse for momentum especially when the form of the matter wave becomes arbitrary. This is where Fourier Transforms are a handy tool.

# Fourier Transform

## Theorem (Dirichlet)

*"Any" function  $f(x)$  on the interval  $[-a, +a]$  can be expanded as a Fourier series*

$$f(x) = \sum_{n=0}^{\infty} (a_n \sin(n\pi x/a) + b_n \cos(n\pi x/a)) \quad (11)$$

# Fourier Transform

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$$f(x) = \sum_{n=0}^{\infty} (a_n \sin(n\pi x/a) + b_n \cos(n\pi x/a)) \quad (11)$$

This can be simplified to

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/a} \quad (12)$$

$$c_n = \frac{1}{2a} \int_{-a}^a f(x) e^{-in\pi x/a} dx \quad (13)$$



# Fourier Transform

Let  $k = n\pi/a$  and  $F(k) = \sqrt{2/\pi}ac_n$  and plugging it into above equations

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} F(k)e^{ikx} \Delta k \quad (14)$$

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As we take the limit  $a \rightarrow \infty$ , we obtain the Fourier Transform equations

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)e^{ikx} dk \quad (16)$$

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{-ikx} dx \quad (17)$$

# Fourier Transform

That's a lot of hand wavy math but we're finally done. We have a tool to now analyse the matter wave in  $k$ -space. Also, the same equations are used to transform between  $t$ -space and  $\omega$ -space.

# Statistics

Consider you have an experiment where the result of the experiment is some real number. The probability of obtaining a number between  $x$  and  $dx$  is modelled by a probability distribution function  $P(x)dx$  where  $\int_{-\infty}^{\infty} P(x)dx = 1$

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## Definition (Expectation Value)

The average of all results of an experiment over infinite trials of the experiment is the expectation value

$$\langle x \rangle = \int_{-\infty}^{\infty} xP(x)dx$$

# Statistics

To measure the "spread" of  $P(x)$  we use a quantity known as variance

## Definition (Variance)

The expectation value of the square of the difference between the obtained value and the expectation value is variance

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Square root of the variance is the standard deviation.



# Gaussian

Gaussian is a family of distributions characterised by 2 parameters.

## Exercise

Find mean and variance of the Gaussian function

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

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$\langle x \rangle = \mu$ . Variance =  $\sigma^2$ ,

# Problems

- The phase velocity of ripples on a liquid surface is given by  $v_p = \sqrt{2\pi S / \lambda \rho}$ , where  $S$  is the surface tension,  $\lambda$  is the wavelength and  $\rho$  is the density of the liquid. Find the group velocity ( $v_g$ ) of the ripples. Obtain the relation between  $v_p$  and  $v_g$ .

# Problems

- Consider Sun and Earth as ideal black bodies in empty space. The Sun's temperature is  $T_S = 6000K$  and the heat transfer by oceans and Earth's atmosphere keep the Earth's surface at a uniform temperature. Radius of Earth  $R_E = 6.4 \times 10^6 m$ , radius of Sun  $R_S = 7 \times 10^8 m$ , mass of Sun  $M_S = 2 \times 10^{30} \text{ kg}$  and Earth-Sun distance  $d = 1.5 \times 10^{11} m$ .
  - Find the temperature of the Earth
  - Find the radiation force on the Earth.
  - Find the distance from the Sun at which a substance, having a melting point of  $T_m = 1550K$ , will melt.

# Problems

- Electrons with kinetic energy 54 eV are diffracted by crystal panes with interplanar spacing  $d = 0.107$  nm.
  - 1 Calculate the Bragg angle at which the diffraction maximum occurs for  $n = 1$ .
  - 2 Calculate the de Broglie wavelengths if the electron energy is changed to 100 MeV and 520 KeV. Will there be a diffraction from the the crystal planes at these energies? Justify your answer.

# Quantum Mechanics! - At Last

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Let us, as always, start by reviewing how it's done classically



## More Classical Mechanics

Imagine a particle of mass  $m$ , constrained to move along the  $x$ -axis, subject to some specified force  $F(x, t)$ . The program of classical mechanics is to determine the position of the particle at any given time:  $x(t)$ . Once we know that, we can figure out the velocity ( $v=dx/dt$ ), the momentum ( $p=mv$ ), the kinetic energy ( $T=(1/2)mv^2$ ), or any other dynamical variable of interest. And how do we go about determining  $x(t)$ ? We apply Newton's second law:  $F = ma$ . (For conservative systems-the only kind we shall consider, and, fortunately, the only kind that occur at the microscopic level-the force can be expressed as the derivative of a potential energy function,  $F = -\partial v/\partial x$ , and Newton's law reads  $m d^2x/dt^2 = -\partial v/\partial x$ .) This, together with appropriate initial conditions (typically the position and velocity at  $t = 0$ ), determines  $x(t)$ .

# Schrodinger Equation

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## Schrodinger Wave Equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi$$

# Statistical Interpretation

Though, due to various reasons is a way of describing the evolution of the system, it is absurd physically because we haven't associated the wavefunction with any physical interpretation. How can such an object be said to describe the state of a particle?

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<sup>11</sup>Normalisation condition

# Statistical Interpretation

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The answer is provided by Born's statistical interpretation of the wave function, which says that the square of the magnitude of the wavefunction gives the probability of finding the particle at point  $x$ , at time  $t$  and consequently<sup>11</sup>,

$$\int_{all\ space} |\psi(r, t)|^2 dr = 1$$

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This is where the fun begins.

### <sup>11</sup>Normalisation condition

# Normalisation

A small caveat about normalisation that I did not mention is that since, the normalisation condition holds for all time  $t$ , is it possible to ensure this?

Fortunately, the wavefunction obeys Schrodinger wave equation and because of that, it is possible to show that

$$\frac{d}{dt} \int_{all\ space} |\psi(r, t)|^2 dr = 0$$

And hence, if the wavefunction is normalised at one time instant, it is normalised at all time instants

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And now, from position, we can obtain other quantities, for instance,

$$\langle p \rangle = m \langle v \rangle = m \frac{d \langle x \rangle}{dt} = -i \hbar \int \psi^*(r, t) \frac{\partial \psi}{\partial x} dr$$

Thus, we can view momentum as an operator  $-i\hbar\frac{\partial}{\partial \mathbf{x}}$ .

## Statistical Interpretation

Similarly, we can extend other observables to be represented by operators and for a particular observable  $O$  with corresponding operator  $\hat{O}$ , we have

$$\langle o \rangle = \int \psi^*(r, t) \hat{O} \psi(r, t) dr$$

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The most accepted answer to this comes through the Copenhagen interpretation, which states that the act of measurement forces the particle to 'take a stand'.

## Catching up

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Observables in Quantum Mechanics are associated with a Linear Hermitian operator, which ensures the linearity of expectation and that the values obtained on measurement are real.

# Heisenberg Uncertainty Principle

A major result of the statistical interpretation is the concept of uncertainty.

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where  $\Delta x$  is the standard deviation of the probability distribution of position and  $\Delta p$  is the standard deviation of the probability distribution of momentum

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This can be extended to the idea of any 2 observables  $A, B$  which have a non-zero commutator.

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# Operators and Eigenvalue Equation

Firsly, what is an operator?

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The possible outcomes are the solutions to the eigenvalue equation

$$\hat{A}\psi = a\psi$$

where  $a$  is called the eigenvalue and is a possible result of this measurement and  $\psi$  is an eigenstate/ eigenvector/ eigenfunction which is the state the particle will be in after the measurement.<sup>13</sup>

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# Properties of the Operator

By a postulate of quantum mechanics, Every observable in quantum mechanics is represented by a Linear Hermitian operator which is used to obtain physical information about the observable from the state function

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## Linearity

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## Hermitian

Operators that are their own Hermitian Conjugate are called Hermitian Operators ( $H^\dagger = H$ ). These operators have real eigenvalues and a complete orthogonal set of eigenvectors

## Properties of the Operator

Since an operator has a complete set of eigenvectors, we can write any wavefunction as a linear combination of the eigenvectors of an operator.

$$\psi(r, t) = c_1\phi_1 + c_2\phi_2 + \dots$$



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# Yep! Fourier Transforms!

# Problems

An observable  $A$  is represented by the operator  $\hat{A}$ . Two of its normalized eigenfunctions are given as  $\phi_1(x)$  and  $\phi_2(x)$ , corresponding to distinct eigenvalues  $a_1$  and  $a_2$ , respectively. Another observable  $B$  is represented by an operator  $\hat{B}$ . Two normalized eigenfunctions of this operator are given as  $u_1(x)$  and  $u_2(x)$  with distinct eigenvalues  $b_1$  and  $b_2$ , respectively. The eigenfunctions  $\phi_1(x)$  and  $\phi_2(x)$  are related to  $u_1(x)$  and  $u_2(x)$  as,  $\phi_1 = D(3u_1 + 4u_2)$ ;  $\phi_2 = F(4u_1 - Pu_2)$  At time  $t = 0$ , a particle is in a state given by  $\frac{2}{3}\phi_1 + \frac{1}{3}\phi_2$ .

- 1 Find the values of  $D$ ,  $F$  and  $P$ .
- 2 If a measurement of  $A$  is carried out at  $t = 0$ , what are the possible results and what are their probabilities ?
- 3 Assume that the measurement of  $A$  mentioned above yielded a value  $a_1$ . If a measurement of  $B$  is carried out immediately after this, what would be the possible outcomes and what would be their probabilities ?
- 4 If instead of following the above path, a measurement of  $B$  was carried out initially at  $t = 0$ , what would be the possible outcomes and what would be their probabilities ?
- 5 Assume that after performing the measurements described in (c), the outcome was  $b_2$ . What would be the possible outcomes, if  $A$  were measured immediately after this and what would be the probabilities ?

# Solving the Schrodinger Equation

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Clearly, Schrodinger's equation is a differential equation and like any good natured physicist, our first line of attack is variable separation.

Let us assume the solutions to be of the form

$$\psi(x, t) = \phi(x)f(t)$$

# Solving the Schrodinger Equation

Plugging in the separable solutions into the equation,

$$i\hbar\phi\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2}f + V\phi f$$

Dividing by  $\phi f$

$$i\hbar\frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m\phi}\frac{d^2\phi}{dx^2} + V$$

Equating both sides to a constant (why?), say  $E$ (again why?)

$$i\hbar\frac{1}{f}\frac{df}{dt} = E \implies f(t) = e^{-iEt/\hbar}$$

And the Time Independent Schrodinger Equation

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- They are states of definite total energy. In classical mechanics, the total energy (kinetic plus potential) is called the Hamiltonian. And the time independent Schrodinger equation is the eigenvalue equation for the Hamiltonian

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- And thus, most importantly, the general solution(to TDSE) is a linear combination of separable solutions.(why?)

# Intermission

This ends the discussion of the first half of the quantum mechanics course PH107.

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We have seen what quantum mechanics says. Our new theory must now be put to some use. We look into some common potential fields to analyse what quantum mechanics has to say about it and whether quantum mechanics truly does a better job of explaining what classical theories could not.



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The next major section of the course revolves around solving the Schrodinger equation for some common occurring potentials. For the preliminary discussion, we restrict the analysis to one dimension only. Let us make a note of them here before diving deep into each one

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# Free Particle

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$$H\psi = E\psi$$

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi = E\psi$$

$$\psi = Ae^{i(kx - \omega t)}$$

where  $k = \pm \frac{\sqrt{2mE}}{\hbar}$ ,  $\omega = \frac{\hbar k^2}{2m}$ ,



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- Some linear combinations(wave-packets) of the stationary states are normalisable. - Free particle has possible states
- On measurement of energy, the wavefunction does not collapse to a stationary state - There is no such thing as a free particle with a definite energy

# Free Particle

Sanity check - Is the quantum model consistent with experimental data?

# Free Particle

Sanity check - Is the quantum model consistent with experimental data? Let us consider velocity. The classical picture for a free particle states the velocity as

$$v_{classical} = \sqrt{\frac{2E}{m}}$$

The quantum picture associates a free particle with a wave packet with the individual waves moving with velocity

$$v_{phase} = \frac{v_{classical}}{2}$$

# Free Particle

Is this an inconsistency?



# Free Particle

Is this an inconsistency? Obviously not!

We have seen that it is the group velocity, which talks about the velocity with which the wave-packet moves and represents the velocity of the particle. Using the dispersion relation  $\omega = \frac{\hbar k^2}{2m}$ , we obtain

$$v_{group} = v_{classical}$$

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One of the classic examples to witness the difference between quantum and classical theory is that of the particle in the Box. It is one of the few problems in quantum mechanics which can be solved entirely analytically. We deal with the following potential in one-dimension.

$$V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & \text{elsewhere} \end{cases}$$

## Particle in a Box

We begin our analysis in the same way as always, by identifying the stationary states using the Time-Independent Schrodinger Equation.

$$H\psi = E\psi$$

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi = E\psi$$

$$\psi = A \sin kx + B \cos kx \text{ (Inside the box)}$$

where  $k = \frac{\sqrt{2mE}}{\hbar}$

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 \psi &= A \sin kx + B \cos kx \text{ (Inside the box)}
 \end{aligned}$$

where  $k = \frac{\sqrt{2mE}}{\hbar}$

Applying continuity boundary conditions to  $\psi$  at  $x = 0$  and  $x = a$ , we obtain  $B = 0$  and  $k = \frac{n\pi}{a}$ .

Thus,  $\psi_n = A \sin \frac{n\pi x}{a}$ ,  $E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$

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## Particle in a Box

And we are essentially done. All we need to do is normalise, obtain stationary states and the linear combination of these states will be the general solution. Let's start by normalisation

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\implies |A|^2 = \frac{2}{a}$$

This fixes magnitude<sup>14</sup> of A to be  $\sqrt{\frac{2}{a}}$ . Thus, the general solution can be expressed as

$$\psi = \sum_i c_i \phi_i e^{-jE_i t/\hbar}, \quad \phi_i = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

<sup>14</sup>The absolute phase factor is redundant, only relevant phase factor matters

# Particle in a Box

Some notable observations

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- Orthogonality

$$\int \phi_m^* \phi_n dx = \delta_{mn}$$

- Completeness

$$\psi = \sum_i c_i \phi_i, c_i = \int \phi_i^* \psi d\mathbf{x}$$

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# Particle in a Finite Well

We now handle the potential of the finite well. This is where things start becoming interesting (but also more complicated mathematically) We deal with the following potential in one-dimension.

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ V_0, & \text{elsewhere} \end{cases}$$

Let us analyse the bound states, that is, those with energy less than  $V_0$ . The scattering states will be analysed later.

# Particle in a Finite Well

$$\frac{1}{\psi(x)} \frac{d^2\psi(x)}{dx^2} = \begin{cases} \kappa^2 & x < 0 \\ -k^2 & 0 \leq x \leq L \\ \kappa^2 & x > L \end{cases}$$

$$\psi(x) = \begin{cases} 0 & x \rightarrow -\infty \\ Ae^{\kappa x} + Be^{-\kappa x} & x < 0 \\ C \cos(kx) + D \sin(kx) & 0 \leq x \leq L \\ Fe^{\kappa x} + Ge^{-\kappa x} & x > L \\ 0 & x \rightarrow \infty \end{cases}$$

Where

$$\kappa^2 = \frac{2m(V_0 - E)}{\hbar^2}, \quad k^2 = \frac{2mE}{\hbar^2}$$

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- Continuity and differentiability at  $x = L$

$$\begin{aligned} C \cos(kL) + D \sin(kL) &= Ge^{-\kappa L} \\ -k(C \sin(kL) - D \cos(kL)) &= -\kappa Ge^{-\kappa L} \end{aligned}$$



# Particle in a Finite Well

A very natural simplification follows

$$\begin{aligned}
 \frac{C \cos(kL) + D \sin(kL)}{k(C \sin(kL) - D \cos(kL))} &= \frac{1}{\kappa} \\
 \Rightarrow \frac{\cos(kL) + \frac{\kappa}{k} \sin(kL)}{\sin(kL) - \frac{\kappa}{k} \cos(kL)} &= \frac{k}{\kappa} \\
 \Rightarrow \frac{1 + \frac{\kappa}{k} \tan(kL)}{\tan(kL) - \frac{\kappa}{k}} &= \frac{k}{\kappa} \\
 \Rightarrow \tan(kL) &= \frac{2k\kappa}{k^2 - \kappa^2} \\
 \Rightarrow \tan\left(\frac{kL}{2}\right) = \frac{\kappa}{k} \text{ OR } -\cot\left(\frac{kL}{2}\right) &= \frac{\kappa}{k}
 \end{aligned}$$

## Particle in a Finite Well

We are done. The above is a formula for the allowed energies; the only unknown in the above equation is energy.

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We will analyse 2 special cases

- $V_0 \rightarrow \infty$ : This reduces to the infinite potential well

$$\frac{kL}{2} = (n + \frac{1}{2})\pi \implies E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

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- $V_0 \rightarrow 0$ : We lower the 'walls' of the potential well. There is always one bound state, no matter how "weak" the well becomes.<sup>15</sup>

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## Particle in a Finite Well

We can normalise the above wavefunction to obtain the stationary states. And then, the general solution is a linear combination of the stationary states.

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We can approximate the finite potential well to be an infinite potential well of greater width due to the exponential decay of the wavefunction on either side. We call this the penetration depth( $d$ ) and then use the simple expression<sup>16</sup> for the energy of an infinite potential well

$$d = \frac{\hbar}{\sqrt{2mE}}, \quad E \approx \frac{n^2 \pi^2 \hbar^2}{2m(L + 2d)^2}$$

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# Scattering and Tunnelling

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- Bound State: If  $V(x)$  rises higher than the particle's total energy ( $E$ ) on every 'side', then the particle is "stuck" in the potential well. We call this a bound state.

$$E < \min(V(\infty), V(-\infty))$$

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$$E < \min(V(\infty), V(-\infty))$$

- Scattering State: If, on the other hand,  $E$  exceeds  $V(x)$  on one side (or both), then the particle Comes in from "infinity", slows down or speeds up under the influence of the potential, and returns to infinity. We call this a scattering state.

$$E > \min(V(\infty), V(-\infty))$$

Some potentials admit only bound states; some allow only scattering states); some permit both kinds

# Scattering and Tunnelling

Thus, to study the simplest scattering problem, we will study the potential

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases}$$

# Scattering and Tunnelling

Let us first consider  $E > V_0$ . Solving Schrodinger Equation in both the regions is trivial, we obtain sinusoids.

$$\phi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\phi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$$

where

$$k_1^2 = \frac{2mE}{\hbar^2}, k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$$

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First, we get  $D=0$  as there is no incidence from the right hand-side.  $D$  is the eigenstate which moves in the negative  $x$ -direction. Thus, its corresponding coefficient is 0.

# Scattering and Tunnelling

Applying appropriate boundary conditions, we obtain

$$A + B = C, \quad k_1(A - B) = k_2C$$

$$\phi_1(x) = A \left( e^{ik_1x} + \frac{k_1 - k_2}{k_1 + k_2} e^{-ik_1x} \right)$$

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Observe that there is a non-zero probability associated with the particle in region  $x < 0$  having negative momentum, a kind of reflection. Thus, we define

Reflection Coefficient  $R = \left| \frac{B}{A} \right|^2$

Transmission Coefficient  $T = \frac{k_2}{k_1} \left| \frac{C}{A} \right|^2$

And note that,  $R + T = 1$

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First, we get  $D=0$  as the wavefunction cannot blow up in the limiting case.

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Observe that there is a non-zero probability associated with the particle being observed in region  $x > 0$  having negative momentum, a kind of penetration.

Reflection Coefficient  $R = \left| \frac{B}{A} \right|^2 = 1$

Thus, the Reflection Coefficient = 1, implying that the probability of reflection is 100%. However,  $C \neq 0$  means that the particle penetrates into region II. Not meaningless, just confusing :).

# Scattering and Tunnelling

With this, we are again essentially done with the analysis of the Scattering Problem. However, we must address the fact of how do the above solutions represent any kind of motion. Scattering essentially seems like a time-dependent problem where the particle arrives, interacts and then proceeds. But our solutions don't seem to capture that. Additionally, our solutions are not normalisable as well. They are, for all practical purposes, meaningless?

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This is not an issue because we have solved for stationary states only. The incident side, on superposition will become a wave packet and on writing it in the time-dependent form, it will become incident with a velocity and undergoes scattering.

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This is not an issue because we have solved for stationary states only. The incident side, on superposition will become a wave packet and on writing it in the time-dependent form, it will become incident with a velocity and undergoes scattering.

What next? We will analyse the scattering states for a finite width step potential.

# Scattering and Tunnelling

Consider the following potential

$$V(x) = \begin{cases} V_0, & 0 \leq x \leq L \\ 0, & \text{elsewhere} \end{cases}$$

We again take cases over  $E(E > V_0, E < V_0)$ .

# Scattering and Tunnelling

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We again take cases over  $E$  ( $E > V_0, E < V_0$ ).

We proceed in a similar way and obtain the wavefunctions in the 3 regions for each of the above 2 cases and apply boundary conditions to express the result in terms of a single constant, which gets determined by normalisation (of course, once you take superposition)



# Scattering and Tunnelling

Say, in either case the wavefunction is

$$\psi(x) = \begin{cases} Ae^{ikx} + B^{-ikx}, & x \leq 0 \\ Fe^{ikx}, & x \geq L \end{cases}$$

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I leave it to you to find the functional form in the step potential and apply the appropriate boundary conditions. The important takeaway is:

$$R = \left| \frac{B}{A} \right|^2$$

$$T = \left| \frac{F}{A} \right|^2$$

Note the difference between these expressions and the ones above and how the transmission coefficient has no extra factor(Why?) and vet.  $R + T = 1$

# Scattering and Tunnelling

Simplifying the expression above for transmission coefficient leads to some interesting results (You could simplify the reflection coefficient and obtain the same result as their sum is 1)

$$T(E) = \left( 1 + \frac{1}{4} \left( \frac{V_0^2}{E(V_0 - E)} \sinh(\alpha L)^2 \right) \right)^{-1}$$

$$T(E) = \left( 1 + \frac{1}{4} \left( \frac{V_0^2}{E(E - V_0)} \sinh(k' L)^2 \right) \right)^{-1}$$

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As you can see, for certain values of  $E$ , for a given  $L$ , the transmission coefficient becomes 1 for the case  $E > V_0$ , this resonance<sup>17</sup> occurs when

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2} + V_0$$

<sup>17</sup>Check Ramsaur effect and Size Resonance from slides if present

# Scattering and Tunnelling

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Recall, we had solved the particle in a finite potential well problem for the bound states only. Such a potential also accepts scattering states. You should try to solve for them on your own. The results are rather interesting. I will state one of them here. The condition for transmission resonance is again

$$E_n + V + 0 = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

## Extra - Scattering Matrix

We will not go into much detail on the scattering matrices. However, it is interesting to note the dependence of the outgoing amplitudes in terms of the incoming amplitudes is fairly linear. Thus, we can represent

$$\begin{bmatrix} B \\ F \end{bmatrix} = S \begin{bmatrix} A \\ G \end{bmatrix}$$

The scattering matrix is a  $2 \times 2$  matrix where  $S_{ij}$  represents the Reflection and Transmission coefficients if  $i = j$  or  $i \neq j$  respectively depending on the direction as well.

Another notable fact is that The S-matrix tells you everything there is to know about scattering from a localized potential.

Surprisingly, it also contains (albeit in a concealed form) information about the bound states (if there are any).

# Tunnelling

A few interesting questions on tunnelling

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- There's no energy transfer, but we can find the particle. How do we understand this ?
- If we try to calculate the transmission coefficient, will it be zero?
- Some ideas on trying to measure the energy of the particle in region II.

## Continuity Equation

Let the probability distribution as described by the wavefunction be expressed as  $\rho(x, t)$  and the probability flux be expressed as  $j$ . Hence, consider a slice between  $x_0$  and  $x_0 + dx$ . The probability of finding the particle in this slice is  $\rho(x_0, t_0)dx$  at a time instant  $t_0$ .

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$$\frac{d\rho}{dt} + \frac{dj}{dx} = 0$$

where  $\rho = \psi^* \psi$  and  $j = \frac{d\rho}{dt} = \frac{\hbar}{2im} \left( \psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right)$

# Tunnelling

Tunnelling is a classic difference between the classical and quantum theories. It also allows us to model and explain various situations.

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<sup>18</sup>Check the tutorial problem on this

# Tunnelling

Tunnelling is a classic difference between the classical and quantum theories. It also allows us to model and explain various situations. Some of them are

- Field Emission: Electrons are emitted from a metal in presence of strong electric field
- Alpha Decay: Decay of radioactive elements with emission of alpha-particles
- Ammonia Inversion: Change in spatial Orientation of ammonia
- STM: Microscope<sup>18</sup>

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# Harmonic Oscillator

We talk about the notion of equilibrium and stable systems and the like. When we performed analysis on these systems, many a time, we would approximate it with quadratic potential which would give us a harmonic oscillator for small oscillations. It is only natural that we use our new theory to analyse this very important potential.



# Harmonic Oscillator

We talk about the notion of equilibrium and stable systems and the like. When we performed analysis on these systems, many a time, we would approximate it with quadratic potential which would give us a harmonic oscillator for small oscillations. It is only natural that we use our new theory to analyse this very important potential. Since the motion is governed by Hooke's law, we deal with the potential

$$V(x) = \frac{1}{2}mw^2x^2$$

And the corresponding Schrodinger's equation governing it is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi$$

# Harmonic Oscillator

There are 2 ways to solve the above<sup>19</sup>

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}, \quad \xi = \sqrt{\frac{m\omega}{\hbar}} x$$

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

<sup>19</sup>Extra material, not in the syllabus

# Harmonic Oscillator

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This concludes the quantum harmonic oscillator. Some standard observations are the quantisation of energy, the non-zero ground state energy and the form of the wavefunctions.

<sup>19</sup>Extra material, not in the syllabus

## Extra - Harmonic Oscillator

The analytical method to solve the Schrodinger equation involves a constructing a recursion formula which is equivalent to the Schrodinger equation. We introduce a dimensionless variable  $\xi = \sqrt{\frac{m\omega}{\hbar}}x$  and then simplify the Schrodinger wave equation to

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi, \quad K = \frac{2E}{\hbar\omega}$$

Since, at large values of  $\xi$  dominates, we can set up  $\psi = h(\xi)e^{-\xi^2/2}$ . Thus, to now solve for  $h$ , we set up a recursion and obtain

$$h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi)$$

where  $h_{\text{even}}(\xi) = a_0 + a_2\xi^2 \dots$  and similar for  $h_{\text{odd}}(\xi)$  and the recursion is  $a_{j+2} \approx \frac{1}{j}a_j$

## Extra - Harmonic Oscillator

Thus, obtaining  $a_0$  and  $a_1$  and solving the recursion is able to determine  $\hbar$  entirely. The functional solutions to  $\hbar$  are the Hermite polynomials, with a multiplicative factor (anyway handled by normalisation).



## Extra - Harmonic Oscillator

And correspondingly, if  $\psi$  satisfies the Schrodinger equation, with energy  $E$ , then  $a_-\psi$  satisfies the Schrodinger equation with energy  $(E - \hbar\omega)$ . Thus, the name 'ladder' operator is quite apt!

Thus, we obtain

$$E_n = (n + \frac{1}{2})\hbar\omega$$

and the wave function takes the form, in terms of the ladder operators

$$\psi_n(x) = A_n(a_+)^n e^{-\frac{m\omega^2}{2\hbar}x^2}$$

## 2D/3D systems

We have solved various potentials in one dimension. However, as we know, the real utility of such is limited unless we are able to solve the same potentials in multiple dimensions. Must we go through the same procedure again? Luckily, extending the solutions to multiple dimensions is quite easy. We utilise the solutions in one dimension effectively using the neat trick of variable separation.



## 2D/3D systems

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$$\psi(x_1, x_2, \dots x_n, t)$$

, we can use variable separation as we did earlier to write

$$\psi(x_1, x_2, \dots x_n, t) = \left( \prod_{i=1}^n \phi_i(x_i) \right) f(t)$$

## 2D/3D systems

Let us consider particle in a 2D box. Using variable separation, we write a stationary state as the product of 2 functions<sup>20</sup>

$$\psi(x, y) = \psi_x(x) \cdot \psi_y(y)$$

Thus, plugging in the above into the Schrodinger equation,

$$\psi_x(x) = A \sin\left(\frac{n_x \pi x}{L}\right)$$

$$\psi_y(y) = B \sin\left(\frac{n_y \pi y}{L}\right)$$

$$\psi(x, y) = C \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right)$$

where C is determined by normalisation

<sup>20</sup>Technically, we also have a time component, so 3 functions

## 2D/3D systems

A stationary state is uniquely determined by an ordered pair of natural numbers  $(n_x, n_y)$  in the case of the 2D infinite potential well. Thus, by normalisation, we obtain

$$\psi_{n_x, n_y}(x, y) = \frac{2}{L} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right)$$

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Operating the Hamiltonian on the wavefunction, we obtain

$$E_{n_x, n_y}(x, y) = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2)$$

## 2D/3D systems

A visualisation of particle in a multidimensional infinite potential box

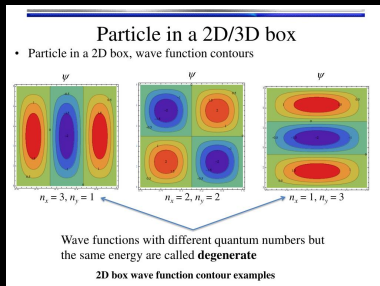


Figure: Particle in 2D Box

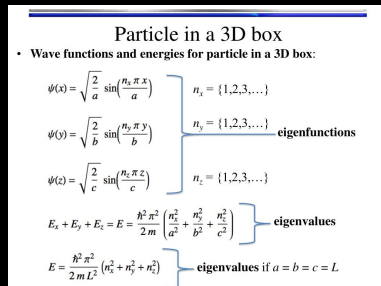


Figure: Energy calculations in 3D

# Statistical Mechanics - Motivation

We have successfully seen the need for a new theory, challenged classical theories further and find ourselves armed with a capable new theory which helps us model and analyse various potentials. Our model also fits experimental data. So, what's the next natural step?

# Statistical Mechanics - Motivation

We have successfully seen the need for a new theory, challenged classical theories further and find ourselves armed with a capable new theory which helps us model and analyse various potentials. Our model also fits experimental data. So, what's the next natural step? We now seek to model entire systems. Single particle systems can only get us so far, we must seek to extend our system model and our resolution capability to a greater beyond. Thus, we extend to multi-particle systems and eventually, a statistical number of particles. Let's dive into quantum statistical mechanics.

# Statistical Mechanics - Introduction

So where do we start?

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<sup>21</sup>state formally means an eigenstate



# Statistical Mechanics - Introduction

So where do we start? We first set up a toolbox for analysing a system having multiple particles. Then, we can construct a system with the given properties. We first want to find the number of particles between energy  $E$  and  $E+dE$ . If we model this as a function of  $E$ , say  $N(E)dE$  to capture this, then we can uniquely identify the macro-properties (large scale properties) of the system. So our problem is now reduced to computing  $N(E)$ .

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<sup>21</sup>state formally means an eigenstate



# Statistical Mechanics - Density of States

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We will first talk about  $g(E)$ , which represents the density of states.  $g(E)$  depends entirely on the potential field which determines the eigenstates. We will consider a standard Particle in an infinite potential box in 3-d. Hence, the state of the particle will be completely defined by the ordered set of quantum numbers  $(n_x, n_y, n_z)$ . Now, we have to determine the number of quantum states having energies between  $E$  and  $E + \Delta E$ .

## Statistical Mechanics - Density of States

Consider the plot in 3-d space where the axes are  $n_x, n_y, n_z$  and hence, the point  $(n_x, n_y, n_z)$  specifies a unique quantum state. Energy of a particle is given by:

$$E = \frac{n^2 h^2}{8mL^2}$$

where  $n^2 = n_x^2 + n_y^2 + n_z^2$ .

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Let us plot the graph of the region satisfying:

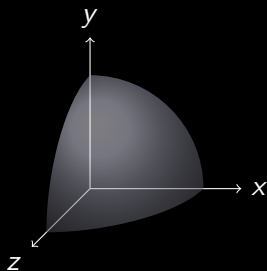
$$n_x^2 + n_y^2 + n_z^2 \leq n^2$$

$$n_x \geq 0$$

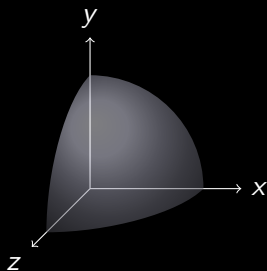
$$n_y \geq 0$$

$$n_z \geq 0$$

# Statistical Mechanics - Density of States



# Statistical Mechanics - Density of States



$$V = \frac{\pi n^3}{6} \implies dV = \frac{\pi n^2}{2} dn, \quad E = \frac{n^2 h^2}{8mL^2} \implies dE = \frac{nh^2}{4mL^2} dn$$

$$g(E)dE = \left(\frac{L}{h}\right)^3 * (2\pi) * \sqrt{(2m)^3 E} dE$$



## Statistical Mechanics - Two-particle system

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Now, we will talk about computing  $f(E)$ . But before we can talk about the statistics governing this probability, we need to analyse the simpler case of a two-particle system. For a single particle, the wave function  $\psi(r, t)$  is a function of the spatial coordinates and the time  $t$  (we'll ignore spin for the moment). The wave function for a two-particle system is a function of the coordinates of particle one ( $r_1$ ), the coordinates of particle two ( $r_2$ ), and the time ( $t$ ):

$$\psi(r_1, r_2, t)$$

and this wavefunction evolves as per the Schrodinger equation. This is the wavefunction for the entire system

## Statistical Mechanics - Two-particle system

This is where things get interesting. The above assumes that we can tell the particles apart-otherwise it wouldn't make any sense to claim that number 1 is in state  $\psi_a$  and number 2 is in state  $\psi_b$ ; all we could say is that one of them is in the state  $\psi_a$  and the other is in state  $\psi_b$ , but we wouldn't know which is which.

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## Statistical Mechanics - Two-particle system

But in quantum mechanics the situation is fundamentally different: You can't paint an electron red, or pin a label on it, and a detective's observations will inevitably and unpredictably alter the state, raising doubts as to whether the two had perhaps switched places. The fact is, all electrons are utterly identical, in a way that no two classical objects can ever be.

## Statistical Mechanics - Two-particle system

But in quantum mechanics the situation is fundamentally different: You can't paint an electron red, or pin a label on it, and a detective's observations will inevitably and unpredictably alter the state, raising doubts as to whether the two had perhaps switched places. The fact is, all electrons are utterly identical, in a way that no two classical objects can ever be. It is not merely that we don't happen to know which electron is which; God doesn't know which is which, because there is no such thing as "this" electron, or "that" electron; all we can legitimately speak about is "an" electron. Quantum mechanics neatly accommodates the existence of particles that are indistinguishable in principle: We simply construct a wave function that is noncommittal as to which particle is in which state.

## Statistical Mechanics - Two-particle system

There are 2 ways to account for this and thus, our theory accounts for 2 kinds of two kinds of identical particles: bosons, for which we use the plus sign, and fermions, for which we use the minus sign. Photons and mesons are bosons; protons and electrons are fermions.

$$\psi_{\pm}(r_1, r_2) = A[\psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_1)\psi_a(r_2)]$$

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This connection between spin and "statistics" (as we shall see, bosons and fermions have quite different statistical properties) can be proved in relativistic quantum mechanics.



## Extra - Exchange Operator

We define the exchange operator

$$Pf(r_1, r_2) = f(r_2, r_1)$$

Two things to note about  $P$ .

One is that  $P^2 = I$ , thus, it admits 2 eigenvalues,  $+1, -1$  corresponding to bosons and fermions.

Additionally, we have  $[H, P] = 0$  and hence we can find a complete set of functions that are simultaneous eigenstates of both. That is to say, we can find solutions to the Schrodinger equation that are either symmetric (eigenvalue  $+1$ ) or anti symmetric (eigenvalue  $-1$ ) under exchange:

# Pauli Exclusion Principle

Say we have  $\phi_a = \phi_b$ , then we will have,  $\phi_-$  to be 0 and thus, the wavefunction will become identically 0, which is not valid. Thus, 2 fermions cannot occupy the same state.

# Pauli Exclusion Principle

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## Pauli Exclusion Principle

Two identical fermions (for example, two electrons) cannot occupy the same state.

## Problem

Consider a system of five particles trapped in a 1-D harmonic oscillator potential.

- What are the microstates of the ground state of this system for classical particles, identical Bosons and identical spin half Fermions.
- Suppose that the system is excited and has one unit of energy ( $\hbar\omega$ ) above the corresponding ground state energy in each of the three cases. Calculate the number of microstates for each of the three cases.
- Suppose that the temperature of this system is low, so that the total energy is low (but above the ground state), describe in a couple of sentences, the difference in the behavior of the system of identical bosons from that of the system of classical particles.

# Distribution Functions

Finally, we have the requisite background to develop the distribution functions for the elementary particles.

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- Classical Particles
- Bosons
- Fermions

# Classical Particles

We will model finding the distribution function as a constrained optimisation problem. Our constraints are

$$\sum_i N_i = N, \quad \sum_i N_i E_i = E$$

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Consider the  $i^{th}$  state has degeneracy  $g_i$ . Now, we invoke The fundamental assumption of statistical mechanics which is that in thermal equilibrium every distinct state with the same total energy  $E$  is equally probable. Thus, we maximise the objective function

$$N! \prod_i \frac{g_i^{N_i}}{N_i!}$$

We obtain the Maxwell Boltzmann Statistics

$$f_{MB}(E) = A e^{-\frac{E}{k_B T}}$$



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$$\prod_i \frac{(N_i + g_i - 1)!}{N_i! (g_i - 1)!}$$

We obtain the Bose-Einstein Statistics

$$f_{BE}(E) = \frac{1}{A e^{-\frac{E}{k_B T}} - 1}$$

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$$\prod_i \frac{g_i!}{N_i!(g_i - N_i)!}$$

We obtain the Fermi-Dirac Statistics

$$f_{BE}(E) = \frac{1}{A e^{\frac{E - E_f}{k_B T}} + 1}$$

# Statistical Mechanics

Thus, we can now find out  $N(E)dE$  and analyse the macroscopic properties of the system as a whole. Let us formally mention what is a microstate and a macrostate.

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## Microstate

A microstate is defined as the arrangement of each molecule in the system at a single instant.

## Macrostate

A macrostate is defined by the macroscopic properties of the system, such as temperature, pressure, volume, etc. For each macrostate, there are many microstates which result in the same macrostate.

## Statistical Mechanics - Conclusion

This concludes statistical mechanics. There are 2 things which yet remain, but they're just computational exercises

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- One is the derivation of the Objective function. The procedure to obtain an objective function is to obtain the number of ways a certain configuration is possible.
- Statistical analysis blackbody radiation but it is very similar to the computation for a 3D box



## PH107 - Conclusion

What next, you say?

Well, the next step would be to step into and appreciate Dirac formalism. This would be followed by an analysis of more complex systems such as the Hydrogen atom and then the many-electron atoms. During the study of these or otherwise, you will also encounter Perturbation theory and Variational Method. Finally, this will allow you to reach relativistic quantum mechanics and quantum field theory.

### PH107 and Beyond

A journey of a thousand miles begins with a single step.

With this, we officially end PH107 :)

## Conclusion

# Thank you!

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Phone: 9167204954