Implementation Aspects of Quantum Computing
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Lecture – 12
Modern Look at Quantum Mechanics

In the last lecture we came up to the point of the Bohr model of the atom, and we were able to see how this quantum mechanical principle that he introduced to explain the atomic spectra of hydrogen atom in terms of line spectra.

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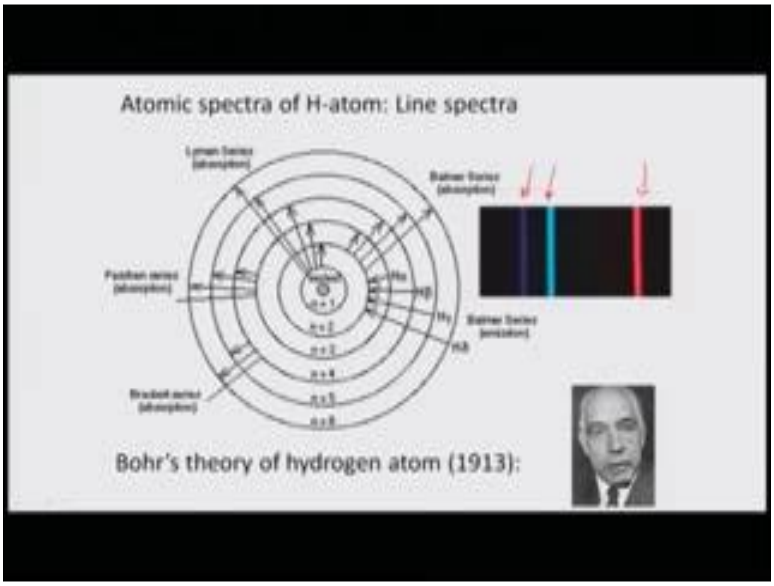

Atomic spectra of H-atom: Line spectra

Bohr's theory of hydrogen atom (1913):

So, this idea of energy quantisation was the critical one in terms of quantum mechanics, and modern approaches to quantum mechanics develop from the idea that this quantisation is possible.

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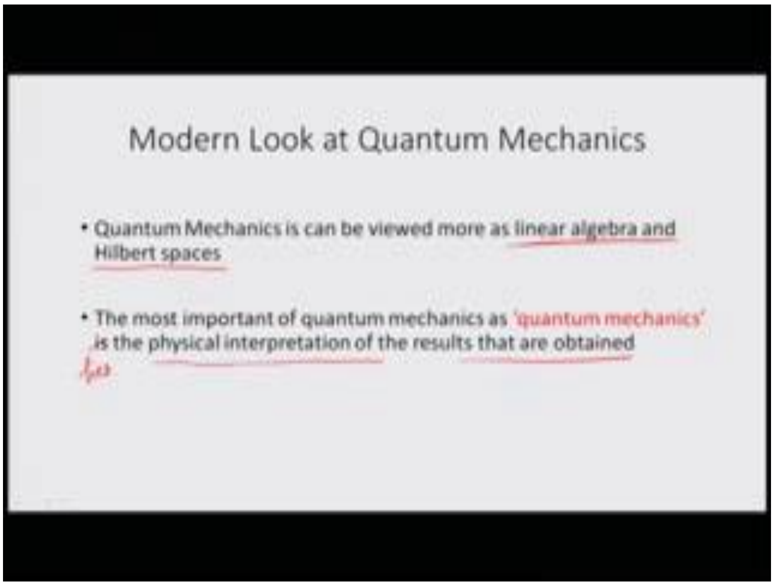

Modern Look at Quantum Mechanics

- Quantum Mechanics is can be viewed more as linear algebra and Hilbert spaces
- The most important of quantum mechanics as 'quantum mechanics' is the physical interpretation of the results that are obtained

lies

So, a modern look at quantum mechanics can be viewed from the fact that quantum mechanics is more like liner algebra of variables and Hilbert spaces. The most important part of quantum mechanics as quantum mechanics lies in the fact that the physical interpretation of the results that are obtained.

So, is the physical interpretation which is very important in terms of the way of looking at quantum mechanics which is otherwise mostly liner algebra Hilbert spaces, and some of it can be simultaneously done by using mattresses and others. So, those are the tools that we have mathematical.

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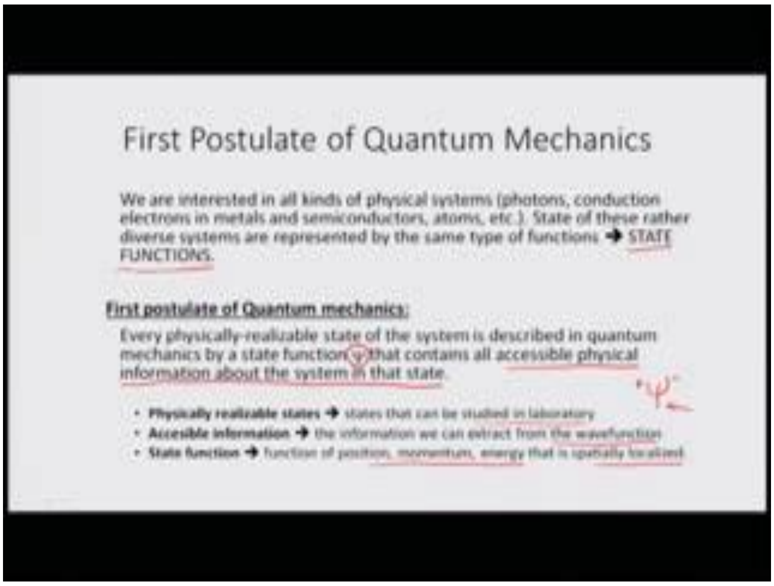

First Postulate of Quantum Mechanics

We are interested in all kinds of physical systems (photons, conduction electrons in metals and semiconductors, atoms, etc.). State of these rather diverse systems are represented by the same type of functions ➔ STATE FUNCTIONS.

First postulate of Quantum mechanics:

Every physically-realizable state of the system is described in quantum mechanics by a state function ψ that contains all accessible physical information about the system in that state.

ψ

- **Physically realizable states** ➔ states that can be studied in laboratory
- **Accesible information** ➔ the information we can extract from the wavefunction
- **State function** ➔ function of position, momentum, energy that is spatially localized

The more important part to understand in this is the laws as in the Newtonian picture. Also we knew that in classical mechanics we had certain basics from where we started the problem, here also there are a few laws which are known as the Postulate. So, the first postulate of quantum mechanics is basically to do with the state of the system.

Since we are all interested in the kind of physical systems that we have which have photons, conducting electrons in metal semi conductors, atoms really the small once microscopic once states of these rather than the diverse system represented by the same type of functions are the state functions. So, we are trying to look for fundamental properties which can defined the principle of quantum mechanics

So the first postulate defines that every physically realisable state of the system is described in quantum mechanics by a state function psi that contains all accessible physical information about the system in that state. So, this definition of psi is roughly the first postulate of quantum mechanics. It leads to the principle of physically realisable states that can be studied in the laboratory. It has all the accessible information that we can extent from the wave function. And, this is the state function is a function of position momentum energy that is spatially localised.

Now the principle of psi in general is mathematical. There are waves to make it observable and that is the part which will look into.

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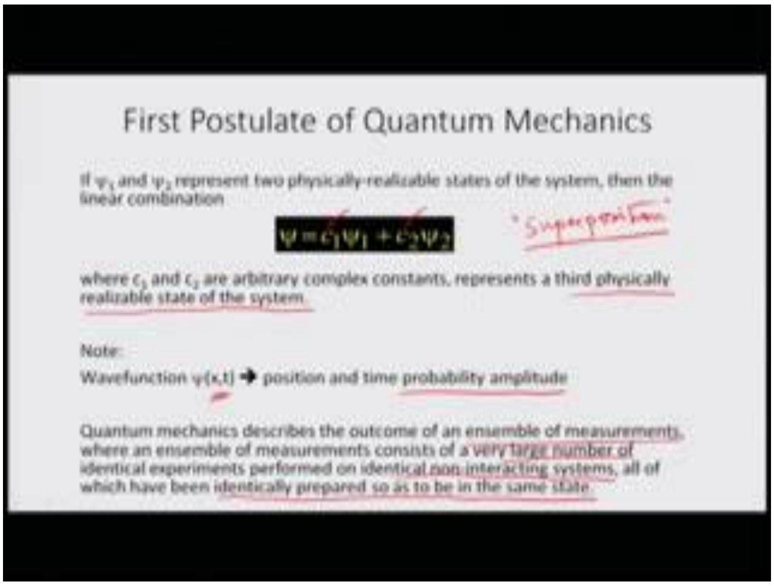

First Postulate of Quantum Mechanics

If ψ_1 and ψ_2 represent two physically-realizable states of the system, then the linear combination

$$\psi = c_1\psi_1 + c_2\psi_2$$

"Superposition"

where c_1 and c_2 are arbitrary complex constants, represents a third physically realizable state of the system.

Note:

Wavefunction $\psi(x,t)$ ➔ position and time probability amplitude

Quantum mechanics describes the outcome of an ensemble of measurements, where an ensemble of measurements consists of a very large number of identical experiments performed on identical non-interacting systems, all of which have been identically prepared so as to be in the same state.

If psi 1 and psi 2 represents two physically realisable states of the system then they are linier combination psi, whereas c 1 and c 2 are arbitrary complex constant represents a third physically realisable state of the system.

So, this principle that any number of wave functions can combined to give rise to a final wave function which is the principle of super position is extremely important in quantum mechanics. So, the wave function psi x and t which is the function of position and time probability amplitude is the one which can be put together through super position of many many more wave functions which can come together with certain amount of the contribution, which can have arbitrary complex forms is what we are looking at. In some sense quantum mechanics is probability having complex numbers associated with it.

So, quantum mechanics is describing the outcome of an ensemble of measurements or a large number of measurements, where an ensemble is the measurement consisting of very large number of identical experiments performed on identical non interacting system; all of which have been identically prepared so has to be in the same state. So, if each of them could be measured they sum together is also the result which can be looked at. That is the basic premise of this entire picture.

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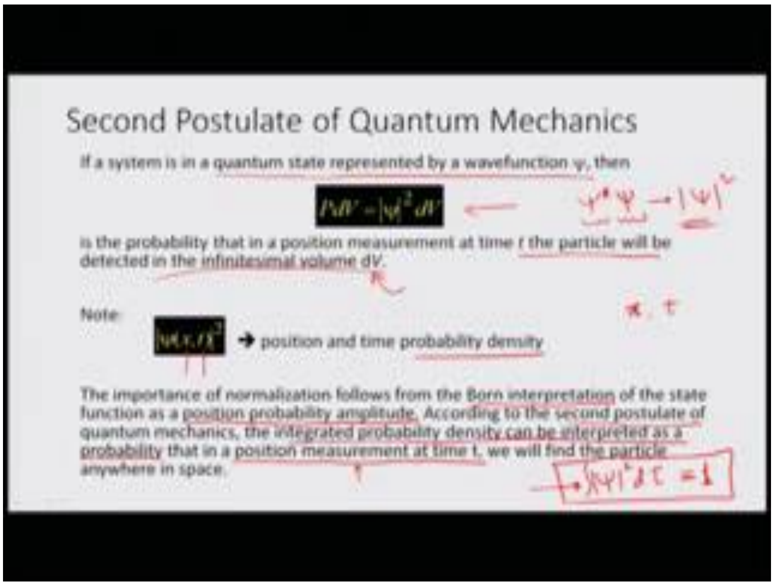

Second Postulate of Quantum Mechanics

If a system is in a quantum state represented by a wavefunction ψ, then

$$P dV = |\psi|^2 dV$$

$\psi^* \psi \rightarrow |\psi|^2$

is the probability that in a position measurement at time t the particle will be detected in the infinitesimal volume dV.

Note:

$|\psi(x,t)|^2$ → position and time probability density

x, t

The importance of normalization follows from the Born interpretation of the state function as a position probability amplitude. According to the second postulate of quantum mechanics, the integrated probability density can be interpreted as a probability that in a position measurement at time t, we will find the particle anywhere in space.

$$\boxed{\int |\psi|^2 d\tau = 1}$$

However, if a system is in a quantum state represented by a wave function psi then there is a probability of its observation which comes because of the observable in nature. So, the probability of a position measurement at any time t of the particle will be detected with the infinitesimal volume of dV. And that is why the probability can be defined in terms of the square of the wave function.

Since the wave functions are complex the observable has to be a real value it is a probability after all. So, it is the complex conjugate measure is the product of the conjugate with the respect to itself which gives rise to the mod psi squared value. Whenever these two coordinates are given position and time then this is the probability density associated with both position and time. One of the things to note here very importantly is that we are only quantifying in terms of the coordinate space and time space, and we are not mixing momentum at the same time because that is what we had already started in the very beginning showing that probability was measure of momentum and space cannot be done simultaneously in the same dimension.

The importance of normalisation follows from the Born Interpretation. So, this is the Born Interpretation of the state function as a position probability of amplitude. According to the second postulate of quantum mechanics which is what is, it is the integrated probability density can be interpreted as a probability that results in a position measurement at time t. Since the particle has to be always found we can always represent this with the fact that, if we take the measurement the total integral of that over the entire time then we are going to always find the probability; the total probability as 1, because where at a given time or at the entire time period where the time has been integrated out then the particle over the entire space will definitely give rise to its probability of find.

So, the total probability of finding a particle is absolute and that is what is represented here.

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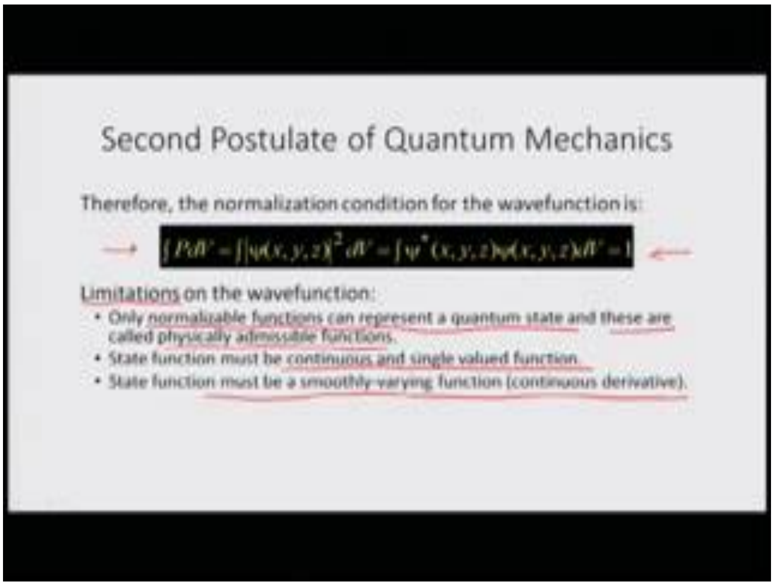

Second Postulate of Quantum Mechanics

Therefore, the normalization condition for the wavefunction is:

$$\int P dV = \int |\psi(x,y,z)|^2 dV = \int \psi^*(x,y,z)\psi(x,y,z) dV = 1$$

Limitations on the wavefunction:

- Only normalizable functions can represent a quantum state and these are called physically admissible functions.
- State function must be continuous and single valued function.
- State function must be a smoothly-varying function (continuous derivative).

So, the normalisation condition which I just wrote for the wave function can be written as total integral in terms of the entire volume space which becomes equal to 1. So, the limitations on the wave functions as a result of this requirement lie on the fact that; only normalizable functions can represent a quantum state. And these are physically admissible functions, otherwise the particles existence becomes questionable and that is the reason of this limitation which is required as per the postulate. The state function must be continuous and single valued. State function must be smoothly varying function which means that it should have a continuous derivative.

Now these are requirements which make sure that the waves we are looking at this probability make sense.

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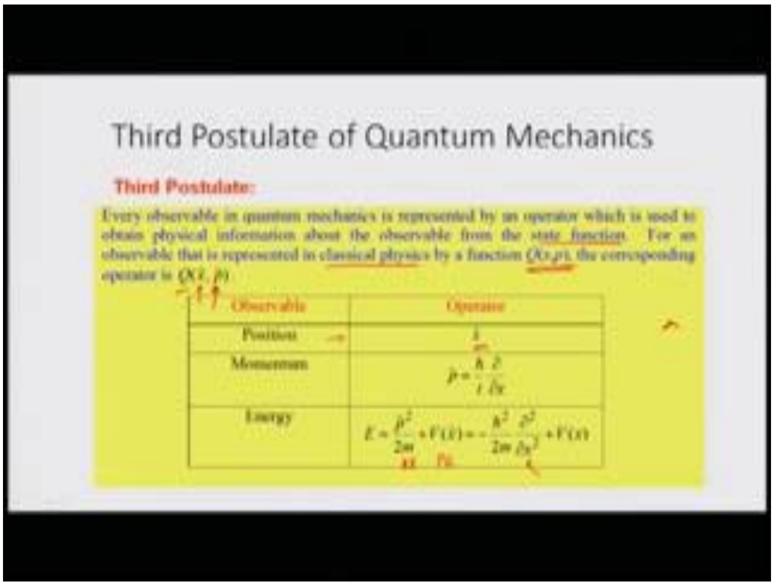

Third Postulate of Quantum Mechanics

Third Postulate:

Every observable in quantum mechanics is represented by an operator which is used to obtain physical information about the observable from the state function. For an observable that is represented in classical physics by a function $Q(x,p)$, the corresponding operator is $Q(\hat{x},\hat{p})$

Observable	Operator
Position	$\hat{x}$
Momentum	$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$
Energy	$E = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

The third postulate of quantum mechanics lies in the fact that every observable in quantum mechanics is represented by an operator which is used to obtain the physical information about the observable from the state function. For an observable that is represented in classical physics by a function say q x and p, the corresponding operator is q x cap t cap. For instance, proposition we write x with the cap; little cap on top, little hat which represents its operator state. Similarly, for a momentum operator we have t with hat which is h cross over i derivative of space coordinate. Similarly, for energy we have the Hamiltonian operator which is essentially a sum total of potential energy and kinetic energy. And for a single coordinate space x axis is just the double derivative, is the momentum space p squared and p squared over 2 m and the potential.

So, this is how the operators are connected to the observables and that is the third part postulate of quantum mechanics which tells how to get the observable values from the state function.

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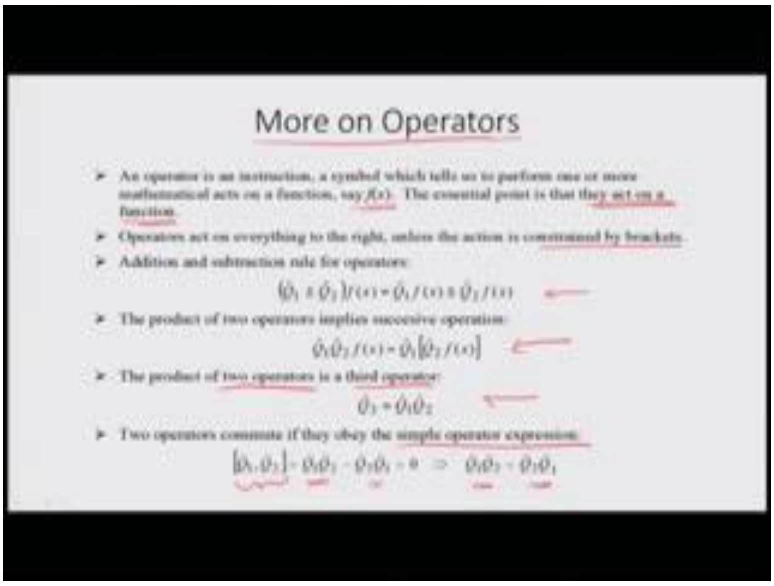

More on Operators

- An operator is an instruction, a symbol which tells us to perform one or more mathematical acts on a function, say $f(x)$. The essential point is that they act on a function.
- Operators act on everything to the right, unless the action is constrained by brackets.
- Addition and subtraction rule for operators:

$$(\hat{O}_1 \pm \hat{O}_2)f(x) = \hat{O}_1 f(x) \pm \hat{O}_2 f(x)$$

- The product of two operators implies successive operation:

$$\hat{O}_1\hat{O}_2 f(x) = \hat{O}_1\left[\hat{O}_2 f(x)\right]$$

- The product of two operators is a third operator:

$$\hat{O}_3 = \hat{O}_1\hat{O}_2$$

- Two operators commute if they obey the simple operator expression:

$$\left[\hat{O}_1, \hat{O}_2\right] = \hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1 = 0 \Rightarrow \hat{O}_1\hat{O}_2 = \hat{O}_2\hat{O}_1$$

So, this principle of operative math which is also be in put to use by many including Dirac in his later develop into quantum mechanics. States that an operator is actually an instruction, a symbol which states or tells us to perform one or more mathematical acts and a function say f of x. The essential point is that they act on a function. Operators act on everything to the right unless the action is constrained by brackets. Addition and subtraction rules for the operator follow the same kind of principle as the associative low or the distributive low. As we can see at these two operators can act on the function based on these principles, and their action is determined by the principle as of mathematics as we are showing here. The product of two operator's employee's successive operations and the product of two operators with the third operator can be great in this term.

Basically, two operators coming together this essentially a third operator; now the two operators commute if they obey the simple operator expression were this is shown by this commutative bracket as they call it essentially the product of the two in one direction versus the other, if the two are equal then the commutative bracket gives rise to 0. In the case where this is not 0 then you will get a situation where the operators do not commute.

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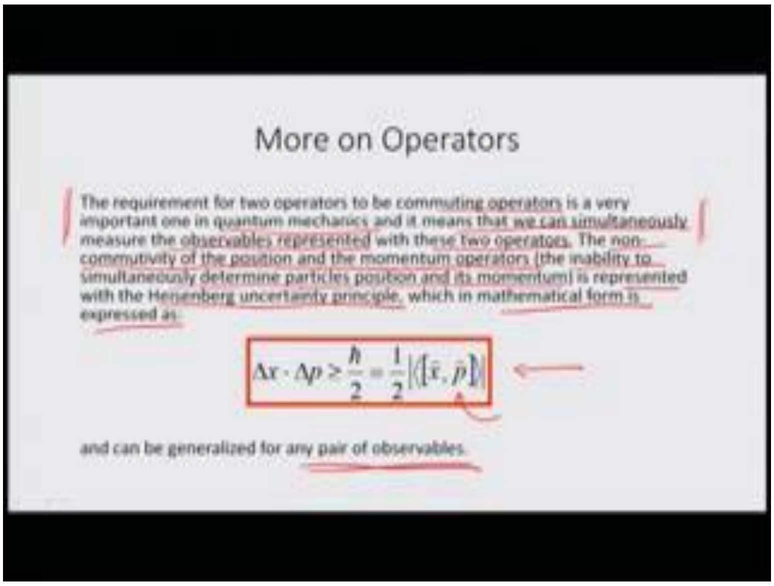

More on Operators

The requirement for two operators to be commuting operators is a very important one in quantum mechanics and it means that we can simultaneously measure the observables represented with these two operators. The non-commutivity of the position and the momentum operators (the inability to simultaneously determine particles position and its momentum) is represented with the Heisenberg uncertainty principle, which in mathematical form is expressed as

$$\boxed{\Delta x \cdot \Delta p \geq \frac{\hbar}{2} = \frac{1}{2}\left|\left\langle\left[\hat{x}, \hat{p}\right]\right\rangle\right|}$$

and can be generalized for any pair of observables.

The requirement for the two operators to be commuting operator is a very important one in quantum mechanics and it means that if we simultaneously measure the observable represented by these two operators. So, that is essentially the principle behind finding out weather two operators can be simultaneously measured or not, the observable represented by them.

The non commutivity of the position and the momentum operators that is the inability to simultaneously determine the particle position and its momentum is represented with the Heisenberg uncertainty principle which in mathematical form is now expressed simply like this, in terms of the commutative operator. And this can be journalised to any pair of observables to show that whenever there is commutator and they are commuting then you can measure them simultaneously, if they do not commute then you cannot measure them simultaneously.

So that is the crux of this entire problem. So, the development of the modern theory enables understanding of this quantum mechanics in a very nice mathematical form as I had mentioned initially.

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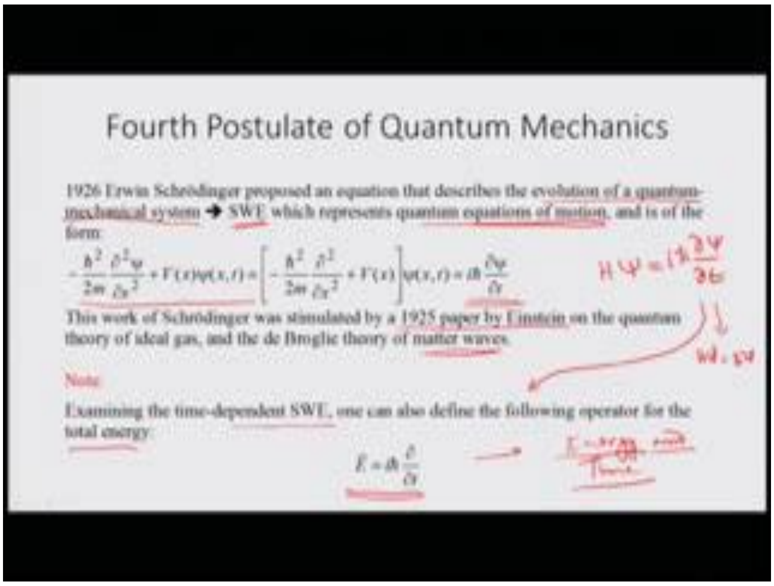

Fourth Postulate of Quantum Mechanics

1926 Erwin Schrödinger proposed an equation that describes the evolution of a quantum-mechanical system ➔ SWE which represents quantum equations of motion, and is of the form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi(x,t)=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi(x,t)=i\hbar\frac{\partial\psi}{\partial t}$$

$H\Psi = i\hbar\frac{\partial\Psi}{\partial t}$

This work of Schrödinger was stimulated by a 1925 paper by Einstein on the quantum theory of ideal gas, and the de Broglie theory of matter waves.

$H\Psi = E\Psi$

Note:

Examining the time-dependent SWE, one can also define the following operator for the total energy:

$$E = i\hbar\frac{\partial}{\partial t}$$

[illegible]

The fourth postulate of quantum a mechanics shows discusses about the evolution, the equation of motion of these wave functions. In 1926, so in the wave equation which represents a quantum equation of motion and is of the form this which is for a single dimension x coordinate at a given time with a Hamiltonian which is a Bohr kinetic and potential terms that is equated to the change of the wave function with the respect to time. This work of Schrodinger was stimulated by a 1925 paper by Einstein on the quantum theory of ideal gas and the de Broglie theory of matter waves.

So, on examining this time dependent Schrodinger wave equation one can also define an operator for the total energy as time evolution operator like this. And that can give rise to the principle of the fact that; so energy and time do not commute because this is a corollary of the way of looking at the time evolution. So, this Schrodinger wave equation is sort of the principle behind the idea of equation of motion of quantum states, and that gives rise to the fact that it is possible to get the equation of motion of the wave function with respect to the Hamiltonian which is what is written on the left hand side.

In other words can be written in terms of H psi is equal to i h cross psi d t, and this essentially has led to the idea that there can be a definition of an total energy operator which can be of this form, because when you do a time integration of this particular Schrodinger equation it becomes H psi is equal to E psi.

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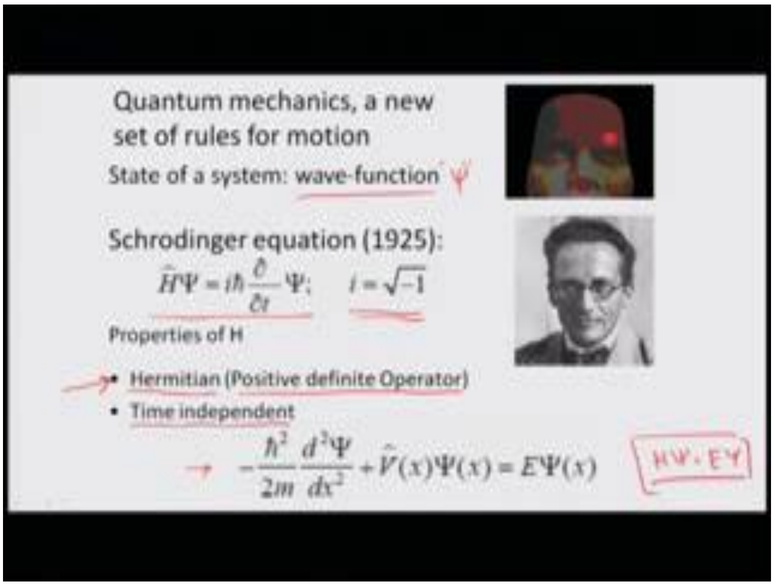

Quantum mechanics, a new set of rules for motion

State of a system: wave-function ψ

Schrodinger equation (1925):

$$\hat{H}\Psi = i\hbar\frac{\partial}{\partial t}\Psi; \quad i = \sqrt{-1}$$

Properties of H

- Hermitian (Positive definite Operator)
- Time independent

$$\rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + \hat{V}(x)\Psi(x) = E\Psi(x) \qquad \boxed{H\Psi = E\Psi}$$

So, quantum mechanics has a new set of rules promotion where the state of the system the wave function psi gives rise to an equation of motion which is the Schrodinger equation of motion H psi is of this kind where i is the complex number which represents that it is a negative square root of 1.

The properties of h have to be defined also in a certain way so that the results are observable. So, the Hamiltonian has to be hermitian. So, that a positive definite operator is the result of this hermitian nature. The time independent part is a result of this integration which gives rise to the Schrodinger equation which has the Hamiltonian and the energy equated in this form E psi is equal to H psi.

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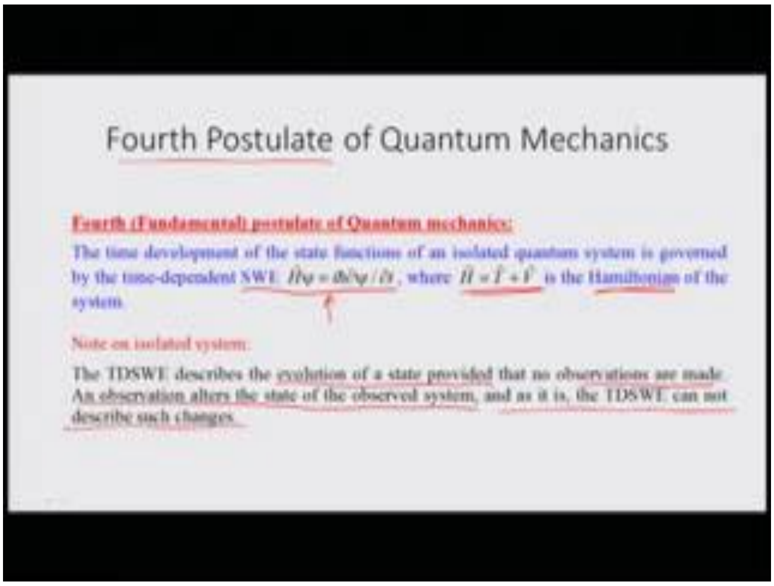

Fourth Postulate of Quantum Mechanics

Fourth (Fundamental) postulate of Quantum mechanics:

The time development of the state functions of an isolated quantum system is governed by the time-dependent SWE $\hat{H}\psi = i\hbar\partial\psi/\partial t$, where $\hat{H} = \hat{T} + \hat{V}$ is the Hamiltonian of the system.

Note on isolated system:

The TDSWE describes the evolution of a state provided that no observations are made. An observation alters the state of the observed system, and as it is, the TDSWE can not describe such changes.

As a result of the fourth postulate of quantum mechanics we just saw that the state function of an isolated quantum system is governed by the time dependent Schrodinger wave equation it is i H cross d psi by d t. Where, H is as we defined as the Hamiltonian of the system. On the isolated system is also means that the time dependent Schrodinger wave equation describes the evolution of a state provided that there is no observation that have being made.

Now this is the very important point to remember because whenever you make measurements you part of the system and that is going to change the way you look at the system. And so it is just stated here on observation alters the state of the observed systems and as it is the time dependent Schrodinger in the wave equation cannot describe such changes. So, that is built into the fourth postulate of quantum mechanics.

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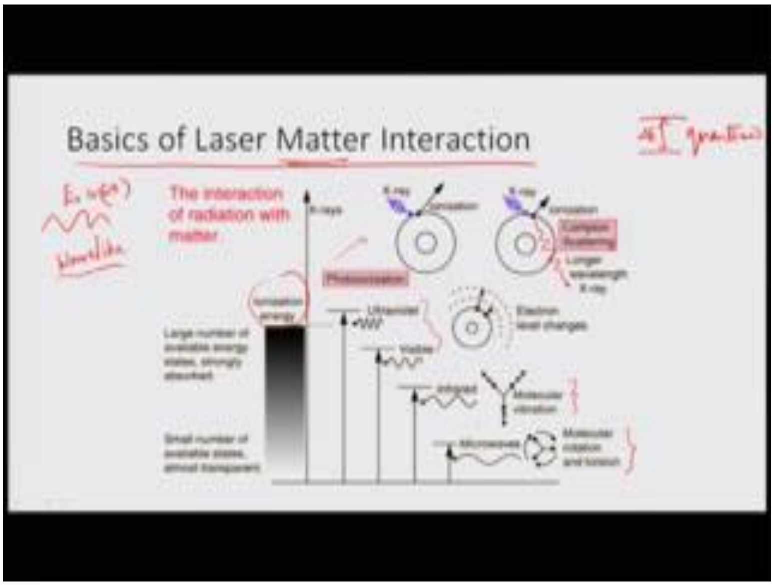

Basics of Laser Matter Interaction

The interaction of radiation with matter

In order to make measurements, one of the other very important things which are necessary is to be able to understand the basics of laser matter interaction. So, in this case the interaction of radiation with matter often is considered under the condition that the radiation is consider to be wave like, accepting totally well that the photo electric effect does not consider the wavelike picture alone of the photons. But still in typical processes were we are considering the particle or the matter as a practical which is quantised, we consider the radiation as wavelike and the matter as quantised. So, as long as the energy of the wavelike electromagnetic radiation matches with the energy of the gap between the matter states say delta e transitions or changes can occur.

So, there are many different levels of this interaction. There can be very low energy waves which are micro wave radiation; it can lead to molecular rotation and torsions. The next level up when it is of the region of infrared radiation that would be leading to molecular vibrations. And then there is this visible region where it is often electronic and definitely the ultra violet region is changing the energy of the electrons. So, beyond a certain point ultimately the electron will be separated from the atom and that is basically the idea of ionization. So, there have various different ways these interactions happen, and depending on the energy of the electromagnetic radiation that we are using we will be seeing different levels of interactions.

So, we will deal with this a little bit more detail later. This is just in terms of ionization these are some examples somehow an x-ray which is very high energy can actually lead to. Ionization it could also lead to other kinds of effects like Crompton scattering, longer wavelength generations ionization in all of that as we just mentioned. But in most are the cases this is the case where it is the photoionization principle.

In the case that we are looking at typically are the electronic transitions are ultra violet and visible where the electronic jumps into different states that we are talking about, these are the quantised states. And in the other cases where we look at by vibrations and rotations, they required much lesser energy and that is the case were we have different places to look at.

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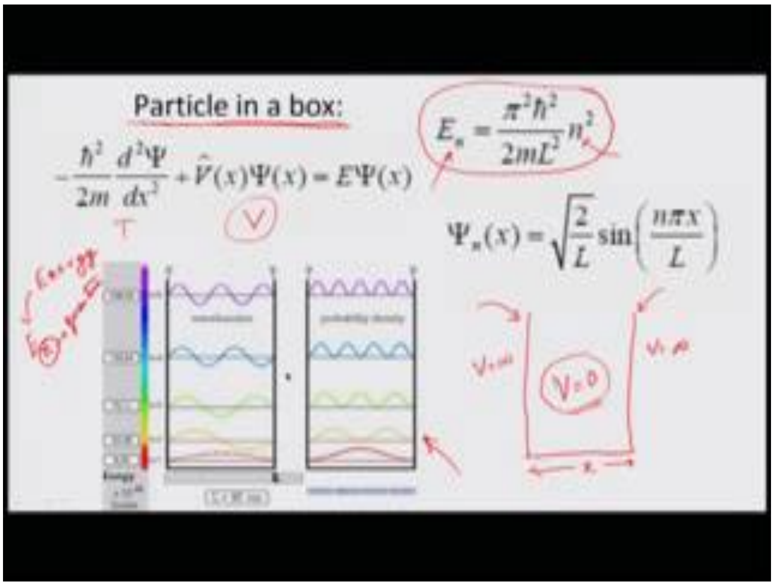

Particle in a box:

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

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

$$\Psi_n(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

Now one of the popular models to test out, quantum mechanics lies in the principle of particle in a box. So, this is actually a very interesting case because this is the first case where quantised systems come up if in this Hamiltonian for the simplest case which is kinetic part often represented by t or t e and the potential part. If the potential part goes to 0 then it is a free particle. And if you solve the Schrodinger equation assuming that the phi is never there which is basically meaning the d equal to 0 then it just becomes a wave equation and then continuous solution are possible in this integrated form. And the energy and everything else follows the continuous picture.

However, the movement this constrains that perhaps the potential goes to 0 within the certain range, but beyond that particle in a box is based on the idea that you have infinite barriers at two ends of a zone where there the particle will have 0 potential in a certain point, in a certain coordinate space and beyond which it just goes to infinity. So, this principle of having constrain on the potential at two edges beyond a certain length is the idea behind this principle of particle in a box. And the interesting part is that at the movement this particular problem is solved with the idea that we have imposed free practical nature only within a certain region in space leads to the situation were the energy available to the particle changes from being continuous to discreet as if been shown here. And correspondingly the wave functions will have discreet shapes or forms as you are going through the different energy levels.

So, these energy states that we talk about n equal to 1 2 3 4 as the energy is keep on increasing these are known as Quantum Number. So, this is the energy quantum number e of n; where n e of n is the total energy and n is the quantum number essentially telling us the state or the positions or the energy level that we are looking at where the different energies are going to be there for a given wave function. So, this is the principle behind looking at quantise system.

So, practical in a box is one of the first cases of simplest cases of looking at a quantised system. At steady state which means time dependency is integrated out and we get these results, where the total energy of the system can always be computed at any given quantum state and they keep on changing as he go to different higher n values. As the n changes it is quadratically increasing, so this spacing goes up as we go higher in this particular case. So, that is the principle of particle in a box which is the first example that is always taken in terms of quantum mechanics.

In the next class will be going towards few more of the examples of quantum mechanics and then will take it from there further.

Thank you.