F Fundamental of Spectroscopy

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Lecture – 02
Introduction to Quantum Mechanics – I

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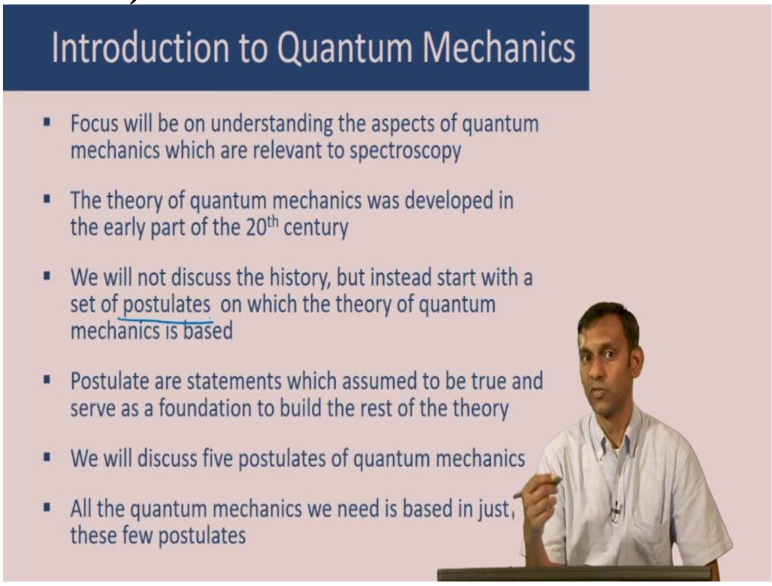

Introduction to Quantum Mechanics

- Focus will be on understanding the aspects of quantum mechanics which are relevant to spectroscopy
- The theory of quantum mechanics was developed in the early part of the 20^{th} century
- We will not discuss the history, but instead start with a set of postulates on which the theory of quantum mechanics is based
- Postulate are statements which assumed to be true and serve as a foundation to build the rest of the theory
- We will discuss five postulates of quantum mechanics
- All the quantum mechanics we need is based in just these few postulates

In the last lecture, my co instructor Sayan Bagchi mentioned that you need to understand the basics of quantum mechanics to understand light matter interaction or spectroscopy. So, that is what we are going to do in this lecture. Our focus while studying quantum mechanics will be to understand those aspects of quantum mechanics which are relevant for spectroscopy. Now, this theory of quantum mechanics was developed in the early part of the 20th century.

Above 100 years back and before that, in the late part of the 19th century, there were certain experiments like blackbody radiation, photoelectric effect, the discrete spectrum of atoms like hydrogen, which could not be explained by the existing theory of that type and that prompted the development of this theory. However, in the interest of time, we will not discuss this history but instead take postulation approach to understand quantum mechanics, which is that we start with a set of postulates on which this theory is based.

Now, a postulate is nothing but a statement, which we can assume to be true and then use that to build the rest of the theory. So, we will start with 5 such statements or postulates and then developed the theory of quantum mechanics just based on those statements. Now, these 5 postulates themselves may appear very non intuitive to you, because they are not like the postulates of classical mechanics which we are very used to.

However, we see that there is a parallel between the postulates of classical mechanics and that of quantum mechanics. All of quantum mechanics that we study is based on just these few postulates.

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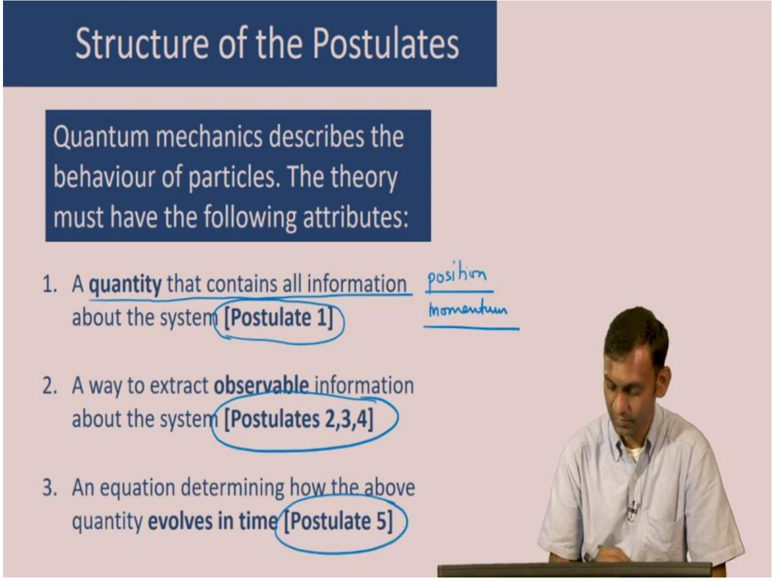

Structure of the Postulates

Quantum mechanics describes the behaviour of particles. The theory must have the following attributes:

1. A **quantity** that contains all information about the system [Postulate 1]
2. A way to extract **observable** information about the system [Postulates 2,3,4]
3. An equation determining how the above quantity **evolves in time** [Postulate 5]

position

momentum

Let us look at the structure of the postulates As you know, quantum mechanics describes the behavior of particles, just like classical mechanics describes the behavior of particles. So, we will see that classical mechanics and quantum mechanics have some parallels. And you can see the parallel by looking at the structure of the different postulates. So, the first thing that a theory which describes the motion of particles should have is that there should be a quantity, which contains all information about the system.

So, this quantity in the case of classical mechanics is the position and the momentum of the different particles. In the case of quantum mechanics, there is a different quantity because as you will see that, in the case of quantum mechanics, the position and momentum of a particle is not really well defined, or at least it means not be well defined, there would be a distribution and there is a different quantity that contains information about the system or contains information about the state of the system that will be discussed in postulate 1.

The second thing that a theory that describes motional particles requires is a way to extract observable information about the system. This means that you need to connect the theory with what you can observe like a property like energy or angular momentum. And in the case of classical mechanics, these observable quantities are just functions of the position and the momentum. We will see that that is different in quantum mechanics.

And that will be the content of postulates 2, 3 and 4. Finally, a theory describing emotional particles requires an equation to tell you how this how the state of the particle or how the system evolves in time. And this in the case of classical mechanics is just Newton’s equation of motion. There is a different equation, which tells us how the state of the system or the wave function in quantum mechanics evolves in time. And that will be the content of postulate 5.

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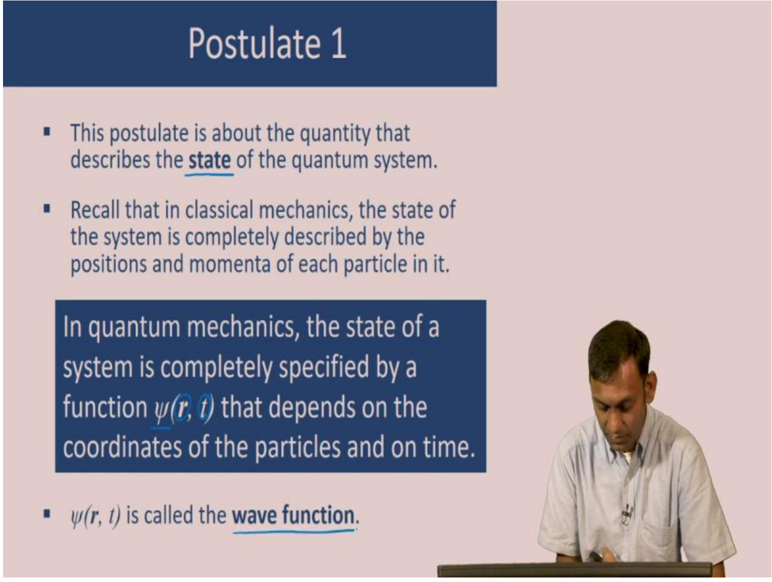

Postulate 1

- This postulate is about the quantity that describes the state of the quantum system.
- Recall that in classical mechanics, the state of the system is completely described by the positions and momenta of each particle in it.

In quantum mechanics, the state of a system is completely specified by a function $\psi(r, t)$ that depends on the coordinates of the particles and on time.

- $\psi(r, t)$ is called the **wave function**.

Let us begin with postulate 1. This postulate is about the quantity that describes the state of the quantum system. Now, recall that in classical mechanics, the state of a system is completely described by the positions and momenta of each particle in it. So, if there is just one particle, if you know its position and you know its momentum, then you know everything about the state of that particle. Now that is different in quantum mechanics.

And in quantum mechanics, we postulate that the state of a system is completely specified by a function, which is denoted as psi here, and it is a function of the coordinates of the particle, which is denoted as this little vector r and on time, so, this function depends on position and time of the particle. This function looks like the function which describes the equation of a wave and therefore it is called wave function.

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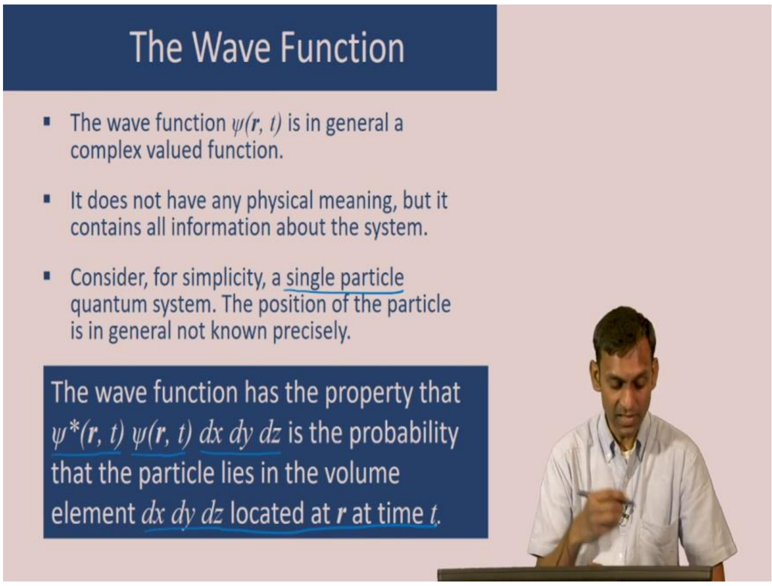

The Wave Function

- The wave function $\psi(\mathbf{r}, t)$ is in general a complex valued function.
- It does not have any physical meaning, but it contains all information about the system.
- Consider, for simplicity, a single particle quantum system. The position of the particle is in general not known precisely.

The wave function has the property that $\psi^*(\mathbf{r}, t)\ \psi(\mathbf{r}, t)\ dx\, dy\, dz$ is the probability that the particle lies in the volume element $dx\, dy\, dz$ located at $\mathbf{r}$ at time t.

The wave function in general is a complex valued function. That means it can have a real part and an imaginary part. So what is this wave function? It turns out that the wave function itself does not have any physical meaning. It is just a function of position and time, but it itself does not correspond to anything observable. However, it contains all information about the system. So, let us look at this.

So the first thing we would want to know is what is the position of the system. And for that, let us consider a simple situation first, where our quantum system consists of a single particle. And as I have mentioned, the position of a quantum particle is in general not known precisely, but the wave function tells us something about the position of the particle, not its precise position, but something which tells us where the particle can be found. So, let us look at this.

The wave function has a property that if you take the wave function and take the complex conjugate of the wave function, multiply by the way function, and then multiply by a small volume element at the position or then this entire quantity is the probability that the particle lies in that volume element located at r at time t. So, this tells us that there is a distribution of positions of the particle, but the distribution is given by this psi star psi.

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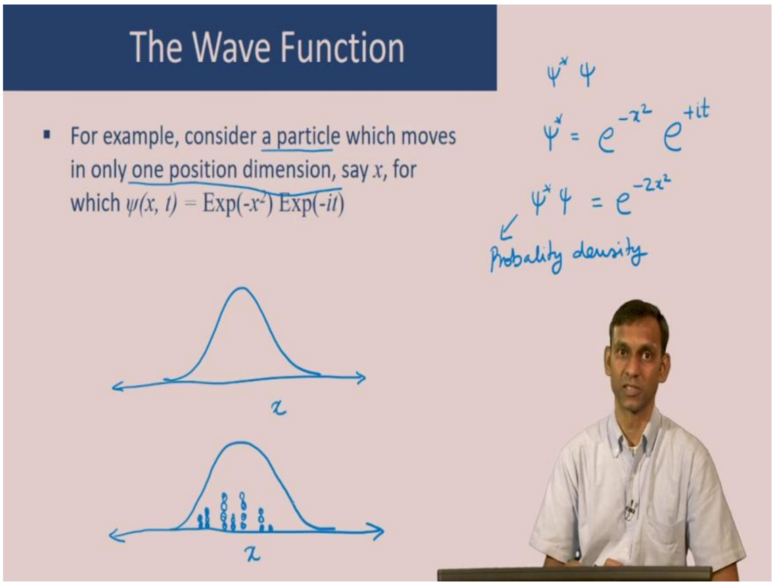

The Wave Function

- For example, consider a particle which moves in only one position dimension, say x, for which $\psi(x, t)$ = Exp($-x^2$) Exp($-it$)

$\psi^* \psi$

$\psi^* = e^{-x^2} e^{+it}$

$\psi^* \psi = e^{-2x^2}$

Probability density

Let us try to understand this more precisely by taking an example of a simple system where this system contains 1 particle, which moves in one position dimension, say the x direction. So, let us draw that let us say this is the x direction along which the particle can move. And it is wave function is given by psi x, t = exponential - x square and exponential - it. So, we have said that it is probability depends on psi star psi.

The probability of finding the particular to certain point depends on psi star psi, psi star in this case, is e to the power of minus x square, multiplied by e to the power of minus it, the complex conjugate of e to the power of minus it is e to the power of minus it. So psi star psi is e to the power of minus 2 x square. And the part which depends on time gets cancelled. Now, this psi star psi, if you plot on this axis looks like this. It is a Gaussian function which looks like this.

So what does this tell us about the probability of finding the particle at a certain point? So this is how we should interpret what this tells us. If we consider that the particle is moving along this direction, let us say the x direction and we have multiple replicas of the quantum system, where you can make measurements of the position of the particle. Let us see one such measurements give gives us the position of the particle to be here, but another measurement can give us the position of the particle to be there.

And every measurement in general can give us different positions of the particle. However, suppose we keep doing experiments and put a dot every time we find a particle at a particular position and keep adding a dot every time we find the particular position and keep doing this for lots and lots of experiments. Then, as we keep on doing more and more experiments, we will find that the particle actually has a distribution of position and after we have done a lot of experiments, it will turn out that this distribution is exactly like psi star psi.

So, psi star psi which is the probability density. This is called the probability density contains information about the distribution of the position of the particles. So, clearly the wave function psi contains information about the distribution of positions of the particle. And we will see that just like information about where it you can find the particle, it contains all other information about the quantum system.

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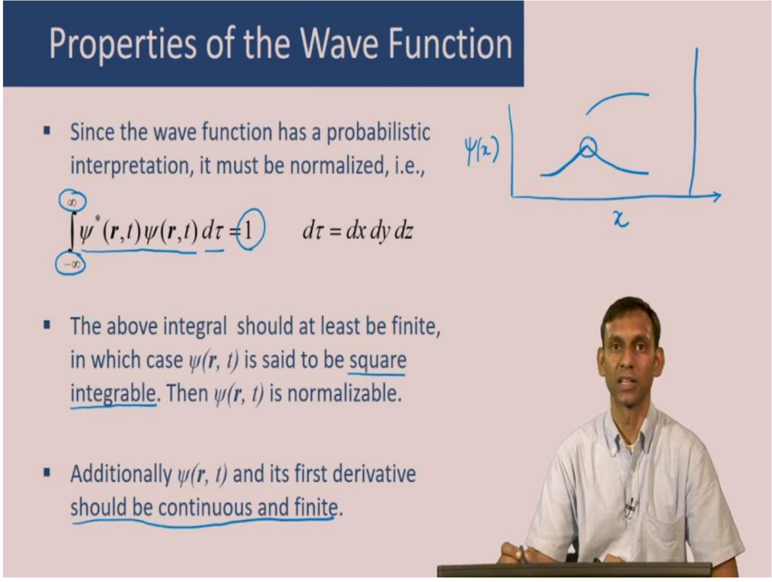

Properties of the Wave Function

- Since the wave function has a probabilistic interpretation, it must be normalized, i.e.,

$$\int_{\boxed{-\infty}}^{\boxed{\infty}} \underline{\psi^*(r,t)\psi(r,t)}\,\underline{d\tau} = \boxed{1} \qquad d\tau = dx\,dy\,dz$$

- The above integral should at least be finite, in which case $\psi(r, t)$ is said to be <u>square integrable</u>. Then $\psi(r, t)$ is normalizable.
- Additionally $\psi(r, t)$ and its first derivative should be continuous and finite.

The wave function representing a quantum system has certain properties. And let us look at those now. The first is related to the probabilistic interpretation of finding the particle which we just talked about. And this is that the wave function must be normalized. What I mean is that if you take psi star psi, which is the probability density multiply by a small volume element that gives you the probability of finding the particle in that small volume element.

But if you sum up all the volume elements where you can find the particle it has to be to make physical sense that this probability is equal to 1. So, the wave function should have this property that when you sum up or in other words you integrate in the entire space of where the particle can be found. So, in this case from - infinity to infinity, then psi star psi the probability in that entire space should sum up to 1.

So, this is just a statement that the total probability of any event is equal to 1 the above integral should at least be finite, if not exactly is equal to 1, because if it is finite, then you can always divide by a constant number and make sure that that integral becomes equal to 1. So in that case, the function is said to be square integrable and a square integrable function is normalizable. So property of the wave function is that it should be at least square integrable.

Additionally, some other property that the wave function needs to have is that it should be continuous and it should be finite. By continuous I mean that the wave function suppose this is the x axis, and I am plotting the wave function psi of x here, then I cannot have a wave function which is something like this, because this wave function is not continuous. And it also should be finite you cannot have a wave function which at some point is just going to infinity going forever, it has a value infinity that is also not allowed.

Moreover, its first derivative should also be continuous. So, you cannot have a wave function which is like this and like this, because this wave function is continuous. However, it is first derivative at this point is not continuous. So, these are some properties that the wave function needs to have.

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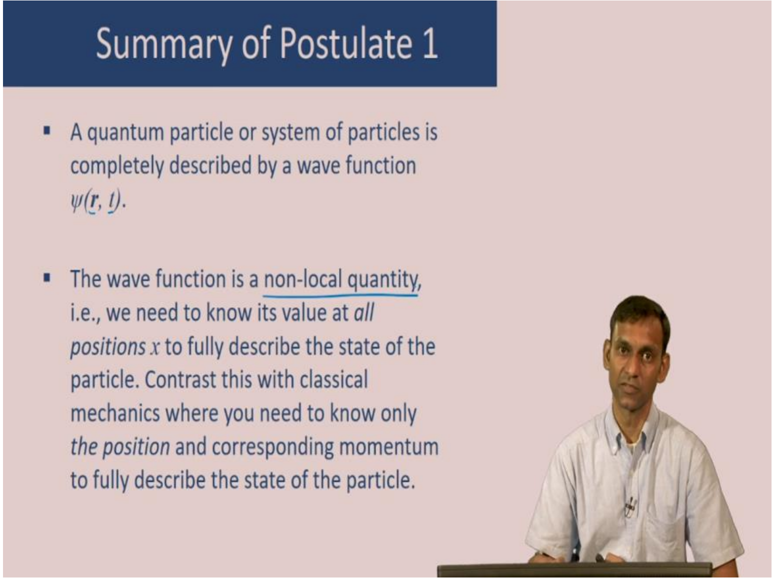

Summary of Postulate 1

- A quantum particle or system of particles is completely described by a wave function $\psi(r, t)$.
- The wave function is a non-local quantity, i.e., we need to know its value at *all positions* x to fully describe the state of the particle. Contrast this with classical mechanics where you need to know only *the position* and corresponding momentum to fully describe the state of the particle.

To summarize the content of postulate 1 is that a quantum particle or a system of particle is completely described by a wave function, which is a function of position and time. Note that we have used the letter psi here to denote the wave function and you will see that this is commonly used and that is only because of convention, this could be a function f of r, t or G of r, t also, but it is more common in quantum mechanics to use symbols like psi and fi to denote the wave function.

The other thing to note is that the wave function is a non-local quantity, meaning that you need to know its value at all positions x to fully describe the state of the particle. This is in contrast with classical mechanics, where you need to know only the position and the corresponding momentum to fully describe the state of the particle you need to know its precise position. Here on the other hand, you need to know the function at all positions to be able to describe the state of the particle.

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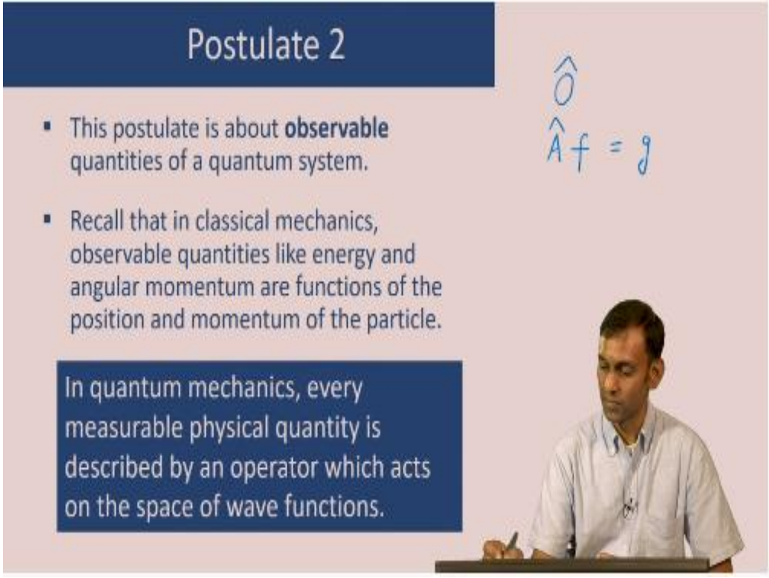

Postulate 2

- This postulate is about **observable** quantities of a quantum system.
- Recall that in classical mechanics, observable quantities like energy and angular momentum are functions of the position and momentum of the particle.

In quantum mechanics, every measurable physical quantity is described by an operator which acts on the space of wave functions.

$\hat{O}$

$\hat{A} f = g$

Let us now look at postulate 2. This postulate is about observable quantities of a quantum system. And now again let us recall that in classical mechanics, observable quantities, like energy and angular momentum are functions of the position and momentum of the particle, which are the basic variables which described the state of the particle that is different in quantum mechanics. And here, every measurable quantity is described by an operator which acts on this space of the wave functions.

Now, what is an operator it is an object which often is denoted by O hat or A hat. An operator operates on a function and gives another function in general.

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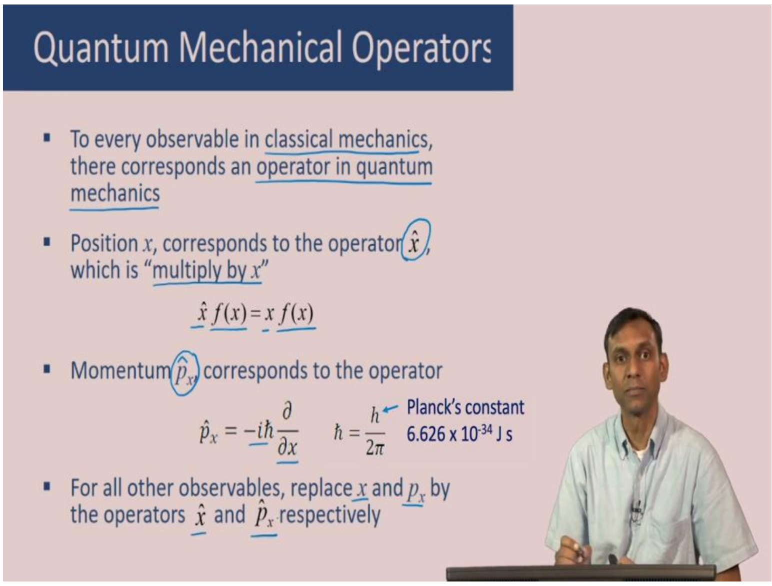

Quantum Mechanical Operators

- To every observable in classical mechanics, there corresponds an operator in quantum mechanics
- Position x, corresponds to the operator $\hat{x}$, which is "multiply by x"

$$\hat{x} f(x) = x f(x)$$

- Momentum $\hat{p}_x$ corresponds to the operator

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} \qquad \hbar = \frac{h}{2\pi}$$

Planck's constant 6.626×10^{-34} J s

- For all other observables, replace x and p_x by the operators $\hat{x}$ and $\hat{p}_x$ respectively

Let us look at the nature of the quantum mechanical operators to every observable in classical mechanics that corresponds an operator in quantum mechanics. Now, you know that every classical observable depends on the position and momentum of the particle which is in the system. So, we have to start by defining the position operator and the momentum operator in quantum mechanics. So, the position operator first we denote this position operator by x hat and this operator is simply multiply by x.

In other words, the position operator operating on a function leads to multiplying the function by x. The other important operator is the momentum operator. And we denote this by P x hat. And this operator is defined as minus i h bar del / del x. This operator operates on a function and takes the first derivative of the function with respect to the position. Now, all classical operators are just functions of position and momentum. So, to get another classical observable or to get the quantum operator corresponding to any other classical observable.

We simply need to replace the position and the momentum respectively by the position operator and the momentum operator. So, let us look at a few examples who understand this a little more concretely.

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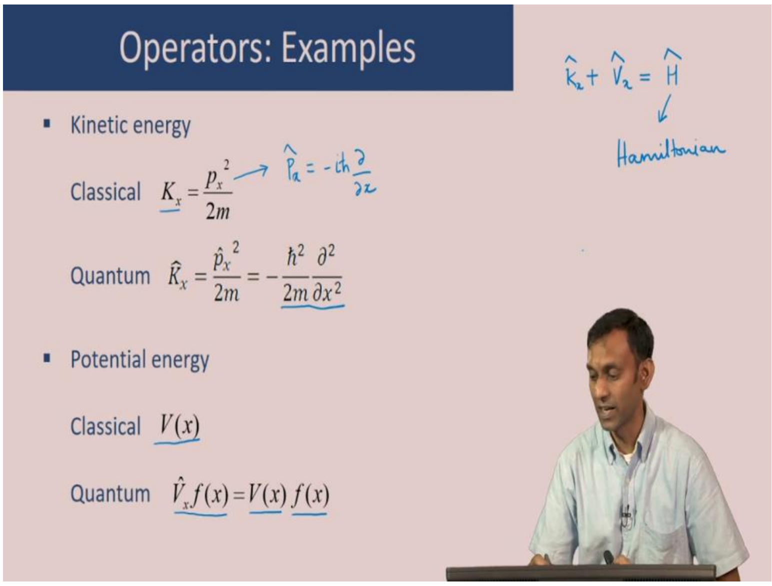

Operators: Examples

- Kinetic energy

Classical $\underline{K_x} = \frac{p_x^2}{2m} \rightarrow \hat{P}_x = -i\hbar \frac{\partial}{\partial x}$

Quantum $\hat{K}_x = \frac{\hat{p}_x^2}{2m} = -\underline{\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}$

- Potential energy

Classical $\underline{V(x)}$

Quantum $\underline{\hat{V}_x f(x)} = \underline{V(x)}\, \underline{f(x)}$

$\hat{K}_x + \hat{V}_x = \hat{H}$

$\downarrow$

Hamiltonian

So, the first observable we consider is the kinetic energy. And in classical mechanics, the kinetic energy in one dimension is momentum square / 2 m to get the corresponding quantum mechanical kinetic energy operator, we need to replace this the momentum here by the momentum operator, which is P x hat is equal to minus i h bar del / del x. And when we take square of that operator and write it out, we see that the quantum mechanical kinetic energy operator is - h bar square / 2 m del square / del x square.

Let us now look at the potential energy operator. And the classical potential energy is just observable, which is denoted by V x the corresponding quantum mechanical operator, which we denote as V hat of x operating on f x is a multiplication of the potential energy by the function f of x. now taken together the kinetic energy and the potential energy K x hat + V x hat is the total energy operator and that is usually denoted by h hat and is called the Hamiltonian operator. This Hamiltonian operator will be very important in the study of quantum mechanics and will come again and again.

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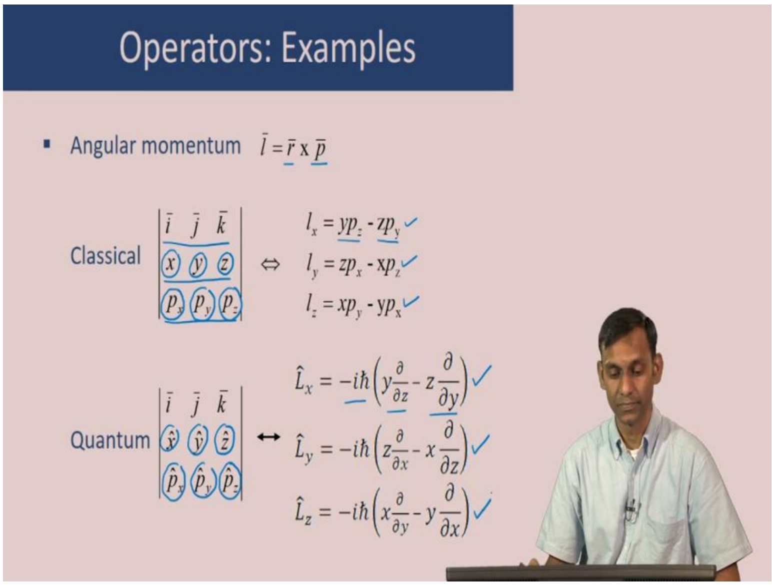

Operators: Examples

- Angular momentum $\bar{l} = \bar{r} \times \bar{p}$

Classical $\begin{vmatrix} \bar{i} & \bar{j} & \bar{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \Leftrightarrow$

$l_x = yp_z - zp_y$ ✓

$l_y = zp_x - xp_z$ ✓

$l_z = xp_y - yp_x$ ✓

Quantum $\begin{vmatrix} \bar{i} & \bar{j} & \bar{k} \\ \hat{x} & \hat{y} & \hat{z} \\ \hat{p}_x & \hat{p}_y & \hat{p}_z \end{vmatrix} \leftrightarrow$

$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$ ✓

$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$ ✓

$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$ ✓

Let us know take another example of a classical observable and find its quantum operator. So, let us look at the angular momentum operator. The classical angular momentum is just cross product of the position vector and the linear momentum. And using determinants, this can be written as 3 by 3 determinant where the top rows are just the unit vectors i j and k. The second row are the position variables x, y and z and the last row are momentum variables p x p y and p z.

And we know that if you expand out this determinant, you will get the 3 vector components of the classical angular momentum, which are l x is equal to y p z - z p y. And similarly, you can get l y and the l z component of the classical angular momentum. Now, to get the quantum angular momentum operator from the classical angular momentum observable. We need to replace the position variables x, y and z by the corresponding position operators x hat, y hat and z hat.

And the momentum variables p x, p y and p z by the momentum operators, p x hat p y hat and p z hat. And when you expand out this determinant, then you see that the operator also has 3 components and the x component is denoted as L x hat, which is written here as – i h bar y del / del z - z del / del y that is the x component of the angular momentum operator in quantum mechanics. And similarly, you have the L y component and the L z component.

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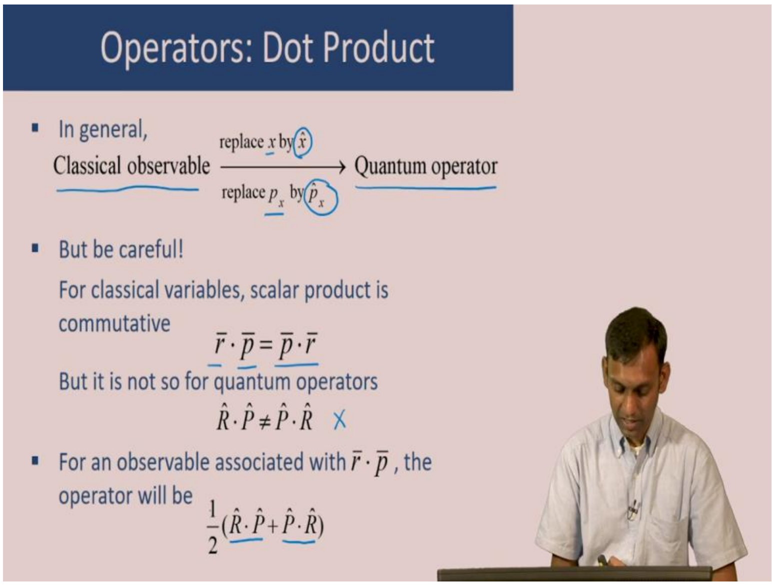

Operators: Dot Product

- In general,

  Classical observable $\xrightarrow[\text{replace } \underline{p_x} \text{ by } \hat{p}_x]{\text{replace } \underline{x} \text{ by } \hat{x}}$ Quantum operator

- But be careful!

  For classical variables, scalar product is commutative

  $$\bar{r}\cdot\bar{p}=\bar{p}\cdot\bar{r}$$

  But it is not so for quantum operators

  $$\hat{R}\cdot\hat{P}\neq\hat{P}\cdot\hat{R} \quad \times$$

- For an observable associated with $\bar{r}\cdot\bar{p}$, the operator will be

  $$\frac{1}{2}(\hat{R}\cdot\hat{P}+\hat{P}\cdot\hat{R})$$

So, in general to get a quantum operator from a classical observable, you need to replace position by the position operator you need to replace momentum by the momentum operator. Now, you have to be a little careful with this in certain situations. For example, if you have a classical observable, which is given by a dot product, let us say a dot product of r and p. Now, you know that a scalar product is commutative, so, r dot p is the same as p dot r.

No that is not the case in the case of operators. So, R dot P is not equal to P dot R in quantum mechanics. And then we have to do something little different. So, here we postulate that foreign observable associated with a dot product, the operator will be a sum of the 2 commuted dot product. So, if the operator is R dot P you have to take R dot P and P dot R and the average of that. So, that is why you have this half is the corresponding quantum operator.

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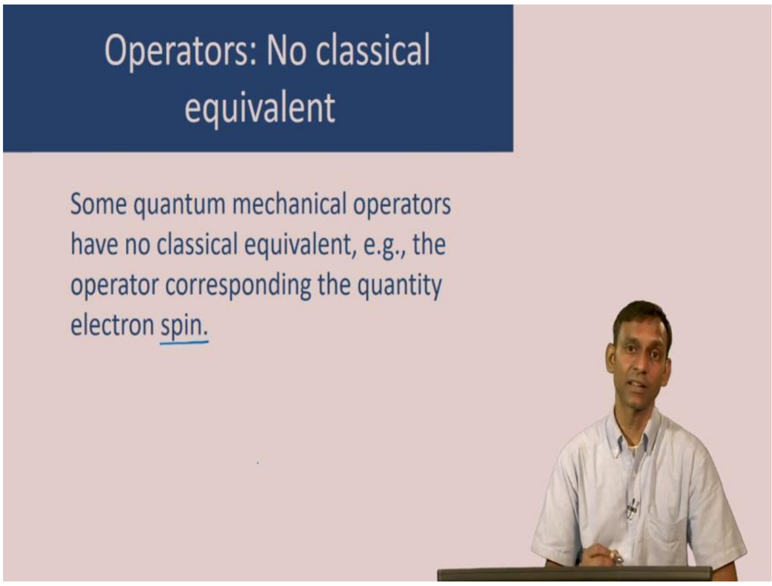

Operators: No classical equivalent

Some quantum mechanical operators have no classical equivalent, e.g., the operator corresponding the quantity electron spin.

There are some operators in quantum mechanics, which have no classical equivalent. For most operators, like we discussed, there is a operator in quantum mechanics corresponding to a classical observable quantity and there you just have to replace the position by the position operator, the momentum by the momentum operator. However, there are some operators which do not have a classical equivalent and a very important operator of that type is the spin and this is relevant because we will encounter spin in spectroscopy.

When we talk about ESR spectroscopy, which is electron spin resonance spectroscopy. And you will see that this quantity of spin does not have any classical equivalent.

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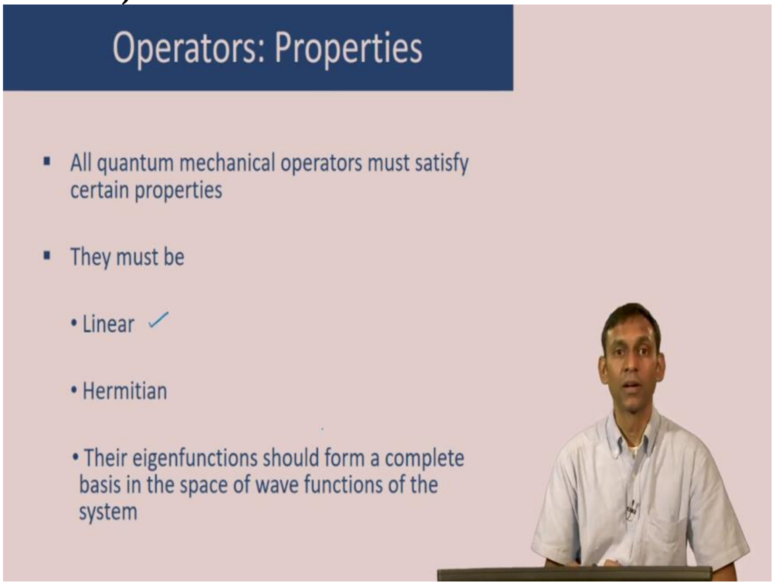

Operators: Properties

- All quantum mechanical operators must satisfy certain properties
- They must be
  - Linear ✓
  - Hermitian
  - Their eigenfunctions should form a complete basis in the space of wave functions of the system

Now, all quantum mechanical operators must satisfy certain properties. So, let us look at those. These operators must be linear, they should be Hermitian. And their eigenfunctions should form a complete basis in the space of the functions of the system. So, let us look at each of these separately, we will start with linear with the linearity property of quantum operators.

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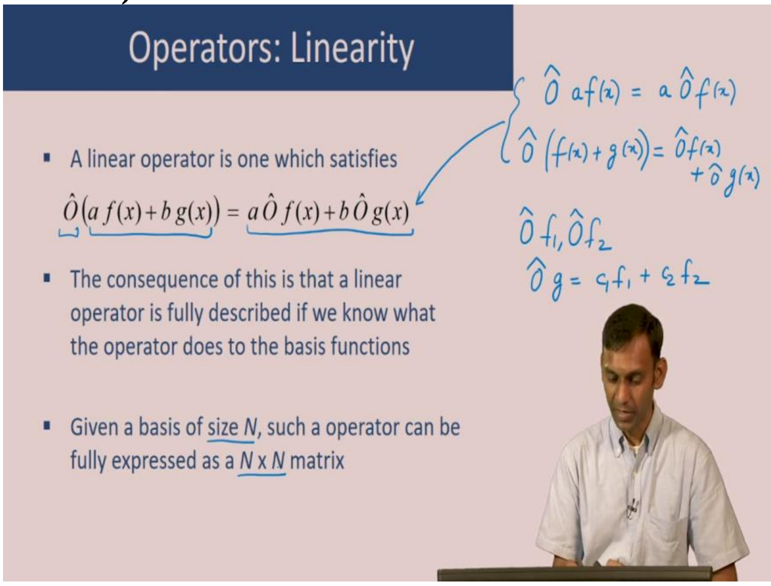

Operators: Linearity

- A linear operator is one which satisfies

$$\underbrace{\hat{O}}\big(\underbrace{a\,f(x)+b\,g(x)}\big) = \underbrace{a\,\hat{O}\,f(x)+b\,\hat{O}\,g(x)}$$

- The consequence of this is that a linear operator is fully described if we know what the operator does to the basis functions
- Given a basis of size N, such a operator can be fully expressed as a N x N matrix

$$\begin{cases} \hat{O}\, a f(x) = a\,\hat{O} f(x) \\ \hat{O}\left(f(x)+g(x)\right) = \hat{O} f(x) + \hat{O} g(x) \end{cases}$$

$\hat{O} f_1, \hat{O} f_2$

$\hat{O} g = c_1 f_1 + c_2 f_2$

A linear operator is one, which satisfies the following condition where an operator O acts on a function of the psi and gives what you see on the right hand side. Let us break this down a little bit. So a linear operator O has a property that if it acts on a function, which is a constant times of function, f of x, then you get the constant multiplied by the operator acting on f of x and if you have to operator acting on sum of functions.

Let us say a f of x + b g of x, then you get this as a sum of the operator acting on the function x f of x + the operator acting on the function g of x. And these 2 have been combined in the statement that is written here. So, what is the significance of the linearity of an operator? Suppose, you have a space of functions, which is spanned by just 2 basis function, let us say f 1 and f 2. This means that you can write any general function g as some linear combination of f 1 and f 2.

Now, the linearity property helps in that if you know what the operator does on f 1 and you know what the operator does on f 2 then you will automatically know what the operator does on a general function in that space of functions. This is why linearity is special and is an important property that an operator can have. If instead of just 2 functions like f 1 and f 2 the space of functions was banned by a basis of size in then such an operator can be fully expressed by n / n matrix which will contain all information about what the operator does in that space of functions. So, there is an intimate relationship between matrices and linear operators.

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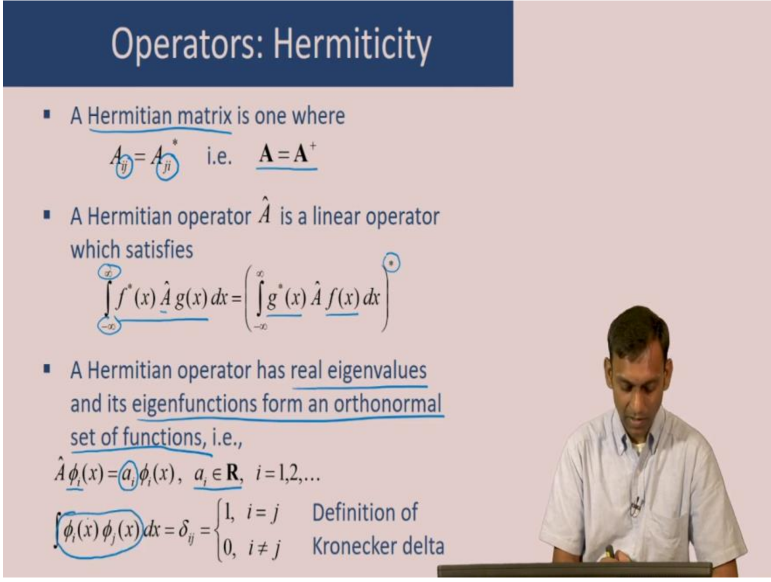

Operators: Hermiticity

- A Hermitian matrix is one where

$$A_{ij} = A_{ji}^* \quad \text{i.e.} \quad \mathbf{A} = \mathbf{A}^+$$

- A Hermitian operator $\hat{A}$ is a linear operator which satisfies

$$\int_{-\infty}^{\infty} f^*(x)\,\hat{A}\,g(x)\,dx = \left(\int_{-\infty}^{\infty} g^*(x)\,\hat{A}\,f(x)\,dx\right)^*$$

- A Hermitian operator has real eigenvalues and its eigenfunctions form an orthonormal set of functions, i.e.,

$$\hat{A}\,\phi_i(x) = a_i\,\phi_i(x), \quad a_i \in \mathbf{R}, \quad i = 1,2,\ldots$$

$$\int \phi_i(x)\,\phi_j(x)\,dx = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Definition of Kronecker delta

The other property that an operator needs to have is that it has to be Hermitian. Now, to understand that, let us consider first of Hermitian matrix and Hermitian matrix which is denoted as A = A star has a property that its matrix element A i j is equal to the complex conjugate of the matrix element ji. In other words, the elements of the matrix when reflected across the diagonal are related by being complex conjugates of each other. Keeping this in mind, we can understand what a Hermitian operator is.

So, a Hermitian operator, A is a linear operator which satisfies a condition which is similar to the one which you see in the case of matrices. So, if you take function f star operator A, multiplied by function g and you integrate this from - infinity to infinity. If this operators Hermitian it needs to have the property that now if you take g star instead of f star, so you have interchange g and f. And you again take the integral and you take the complex conjugate then these two are equal, this is the permittivity condition of operator.

It turns out that if the operator has this condition, then you can prove that such an operator has real eigenvalues. And further, its eigenfunction form orthonormal set of functions. They are written here symbolically that the operator acting on a set of functions gives a corresponding eigenvalue and all these eigenvalues are real. And the eigenfunctions which you see here, they are orthogonal. This is the condition of orthogonality.

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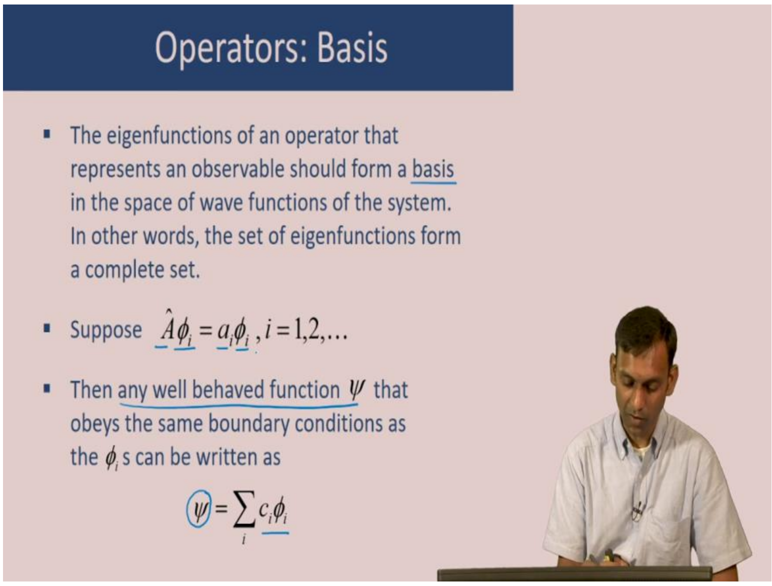

Operators: Basis

- The eigenfunctions of an operator that represents an observable should form a basis in the space of wave functions of the system. In other words, the set of eigenfunctions form a complete set.
- Suppose $\hat{A}\phi_i = a_i\phi_i$, $i = 1,2,\ldots$
- Then any well behaved function ψ that obeys the same boundary conditions as the ϕ_i s can be written as

$$\psi = \sum_i c_i\phi_i$$

The other property that operator corresponding to a observable quantity in quantum mechanics should have is that it is eigenfunctions should form a basis in the space of wave functions of the system. In other words, the set of a eigenfunctions should form a complete set. So, suppose these phi i is eigen functions of the operator A and the corresponding eigenvalues or A i. So, you will have several eigen functions because i = 1, 2 and so on.

And if this forms a complete set, we mean that any well behaved function psi can be written as a linear combination of these eigenfunctions. So, you see here this is the linear combination and by writing that any wave function can be expressed in the eigenfunctions of this operator corresponding to a quantum observable.

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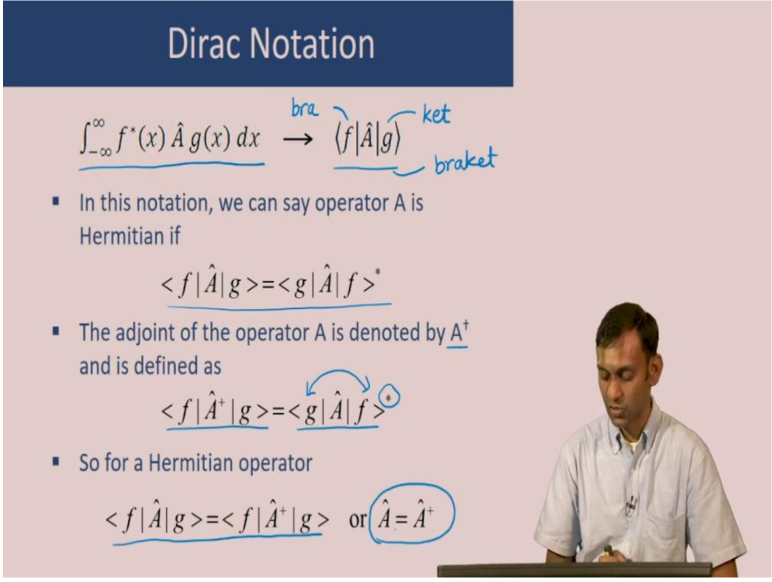

Dirac Notation

$$\int_{-\infty}^{\infty} f^*(x)\,\hat{A}\,g(x)\,dx \longrightarrow \langle f|\hat{A}|g\rangle$$

bra

ket

braket

- In this notation, we can say operator A is Hermitian if

$$< f|\hat{A}|g> = < g|\hat{A}|f>^*$$

- The adjoint of the operator A is denoted by A^+ and is defined as

$$< f|\hat{A}^+|g> = < g|\hat{A}|f>^*$$

- So for a Hermitian operator

$$< f|\hat{A}|g> = < f|\hat{A}^+|g> \quad \text{or} \quad \hat{A} = \hat{A}^+$$

Let me introduce you to some notation that we are going to use. So, the integral that you see here f star A g x - infinity to infinity will be is a very, very common form that will appear again and again in our study of spectroscopy. So, to write this in a shorthand manner, we introduce a notation where this integral is written in shorthand like this. This is called the Dirac notation or sometimes the bracket notation. This on the right part is called the ket vector or the ket function and this is called the bra vector or the bra function.

Taken together this whole thing is the bracket. Let us look at the utility of this notation by expressing Hermiticity property of the operator A. In this statement using Dirac notation or bracket notation, we are saying that the operator is Hermitian. So, what we saw in the previous slide can be written in a much shorter manner using this notation that we have in this slide. The adjoint of the operator A is denoted by A dagger and is defined using Dirac notation in the following manner.

So, the matrix elements of that adjoint operator is equal to the matrix element of the regular operator, but with g and f interchanged with respect to the left hand side and by taking a stuff. So, for a Hermitian operator or a quantum mechanical operator, if we combine these 2 statements, we get the following statement here, which is essentially implying that a Hermitian operator is self adjoint. So, A = A daggered.

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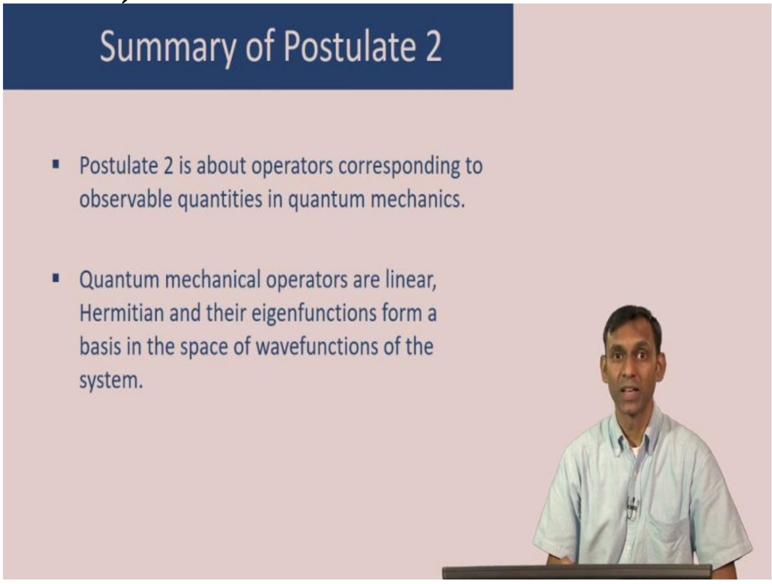

Summary of Postulate 2

- Postulate 2 is about operators corresponding to observable quantities in quantum mechanics.
- Quantum mechanical operators are linear, Hermitian and their eigenfunctions form a basis in the space of wavefunctions of the system.

To summarize, postulate 2 is about operators corresponding to observable quantities in quantum mechanics. We have seen that starting with the classical variable and replacing the position momentum variables by the corresponding position and momentum operators, we can get the operator corresponding to any observable in quantum mechanics. Furthermore, we have seen that the quantum mechanical operators have certain properties and they are that they should be linear.

It should be Hermitian and then eigenfunctions should form a basis in the space of the functions of the system.