ELEMENTS OF MODERN PHYSICS

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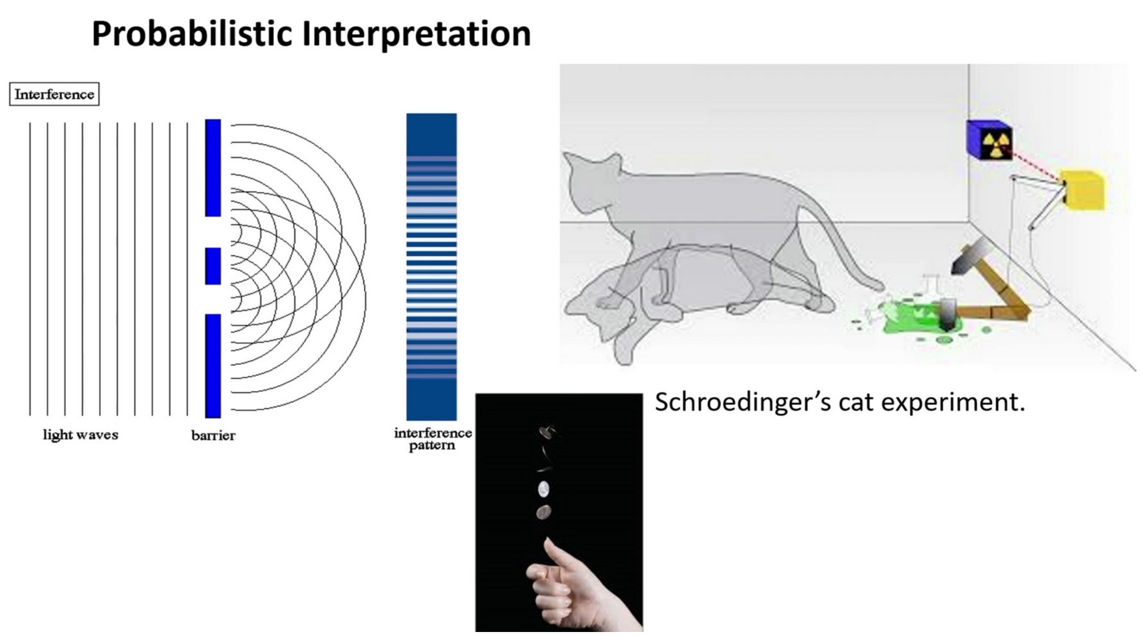
Lec 6: Wavefunction, Operators, Representations in QM

Welcome to this discussion on quantum mechanics that we have been engaged in. So, we will talk about wave function as a linear superposition of basis sets, we will talk about the postulates of quantum mechanics, the properties of the wave function, we will tell you what operators are in particular the Hermitian operators, the commutation relations, expectation values, the quantum dynamics, how the wave functions evolve with time and the operators evolve with time. And finally, we will talk about different representations, which are known as the Schrodinger representation, Heisenberg representation and interaction representation. To start with, we once again remind you of the probabilistic interpretation. The first picture on the left has been shown to you. It is an interference pattern of two slits. This is called the Young's double slit experiment. And what you see on the right is the interference pattern on a screen which comprises of alternate dark and bright bands.



And these two slits, they are taken as coherent sources or they are considered as coherent sources. And that's what creates the interference pattern on the screen because of the path difference that the light has to travel from the slits to the screen. And this path difference will give rise to phase difference. And this phase difference being, you know, sort of even integer times lambda or odd integer times lambda that will decide whether you have the bright fringe or the dark fringe and so on. That's the classical explanation coming from optics. What we have used it is to make sure that the photons are allowed to go through both the slits with certain probability with in fact half probability such that they can interfere on the screen. And if you block one screen, which means that you are trying to make sure that the photons have gone through only one slit, and that would not give rise to an interference pattern, which is what we have discussed earlier, okay. The right picture is about a cat, okay. And it's called as a famous Schrodinger's cat experiment. The cat is kept in a room and there is this green colored cat.

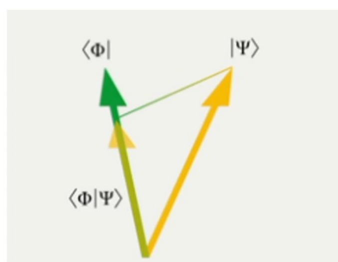
apparatus that you're seeing or that's a container that container contains poisonous gas or a poisonous liquid and there is a hammer kept in the vicinity of that so if this cat goes and breaks the container the poisonous liquid will spill out and that will cause the cat to die and if the cat is itself it desists from doing such a mischief then the cat will be alive. And you lock the room and then you come back after some time to find, let us say, the cat is alive, which means that he has not done anything, any mischief or it has not broken the poison vial. Now, that tells us that before you have made this measurement, that is you have gone and opened the room, in your mind, it is the state of the cat is in a superposition of dead and alive states, just like the two slits that we see here, it is dead and alive. These are the two states of the cat. And once you make a measurement, the measurement will force the system to assume one of the eigenstates of the system. That is, suppose it's alive. And so we are talking about probabilities. So the probabilities would exist as long as the measurement is made or before the measurement is made. So as long as the measurement is not made, it is in a probabilistic state. For example, you see that a coin being tossed and the coin goes up in the air and till it comes down and falls on the hand or on the ground, one doesn't know that whether it's going to be a head or a tail.

And it's important that we keep it that way in order to have the probability interpretation persisting. But it's also important that once when the measurement is made, that is the coin lands either on the palm or on the ground, you are sure that either its head or its tail. So, there is an observer which is making this measurement to collapse to one of the states of the system and these states are called as the eigenstates. Let us talk about that in more details. So, the outcome of this measurement will make the system collapse onto one of the possible outcomes. For example, the cat being alive. For example, the result of the coin toss gives you head and so on. So the observer really plays an important role in this whole thing. So, this possible outcomes have a technical name and they are called as the eigenstates of the system or the states of the system that I said state means the state of being dead or the state of being alive is the state for the cat and for a given quantum system this states will be called as the eigenstates and here in all these examples that we have given there are only two possible eigenstates namely the dead and alive namely the you know, the head or tail and so on. But in general, in a quantum system, there could be many eigenstates that are possible, okay.

Dirac’s bra-ket notation

The notation used by Paul Dirac in quantum mechanics as a way to make linear algebra operations more appealing. It consists of a rewriting of your usual inner products in a style that gives out more information.

$$\langle\Phi|\Psi\rangle = \int_{-\infty}^{+\infty} \Phi^{*}\Psi dx$$



So, as you make a measurement, the system collapses onto one of its available eigenstates or possible eigenstates. In this connection, we will extensively use a notation that I simply introduce here. It's called a Dirac's bracket notation. The word bra and ket, they are used by Dirac just to, you know, have a split of the word bracket. That word C is not there. The letter C is not there. So you have a bracket notation. and you just remove this and this is how he represented these two states of the system and these are the eigenstates of the system. So, the notation used by Paul Dirac in quantum mechanics as a way to make linear algebra operations more appealing and simpler too and it consists of rewriting the usual inner product in a style that gives out more information. What is an inner product? The inner product, if you look at the picture that's given, say psi is a vector which is pointing in the direction that is shown by this yellow line and phi is also a vector which is shown here in green color.

And an inner product that is phi psi is simply the projection of psi on this phi and it is given by this line that you see here. And so that's the projection or that's the inner product of two vectors. And the inner product of two vectors is written technically as an integral from minus infinity to plus infinity and a phi star psi and integration over all the coordinate variables. And we are writing it x here, but it could be r, a three-dimensional integral. But here, we are talking about just one-dimensional vectors. That is, say, psi and phi both depend only on x. So how are these postulates of quantum mechanics that are proposed? How are they helpful? What do they convey? Let us see this. There are many postulates. Some of them may be very trivial for you, but they were postulated at a time when quantum mechanics was just developing. It's been developed. And in those days, these postulates were very helpful and they lay down the guiding principles of the development of quantum mechanics. The wave function psi is the solution of the Schrodinger equation.

Postulates of Quantum mechanics

- The wavefunction $\psi(\vec{r},t)$ is the solution of the Schroendinger $H\psi(\boldsymbol{r},t) = i\hbar\frac{\partial\psi}{\partial t}$ is a function of space-time, and obeys $\int_{-\infty}^{+\infty}|\psi|^2 d^3r = 1$. $\forall t$
- To every observable, there exists a linear Hermitian operator. The observable has real eigenvalue.
- In the measurement of an observable, the correspond operator will only yield the eigenvalue. The operator A satisfies: $A\psi = a\psi$. $A|\psi\rangle = a|\psi\rangle$
  ψ: eigenfunction, a: eigenvalue
- The expectation value of an operator is expressed as: $\langle A\rangle = \int_{-\infty}^{+\infty}\langle\psi|A|\psi\rangle d^3r$
- The wavefunction is symmetric under exchange of particles for bosons, and is antisymmetric for fermions. **Pauli's exclusion principle** is a direct consequence of the antisymmetry. $\psi(x_1,x_2) = \pm\psi(x_2,x_1)$ $\psi(x) = \psi(-x)$ $\psi(x) = -\psi(-x)$

So, this is a wave function is what we are talking about and it is in general a function of r and t and then we will see that it is not only a function of r and t, we can go to another space in which it is a function of momentum and you know energy or k and omega or p and omega and so on so forth. So, it is the solution of the Schrodinger equation which is nothing but H psi equal to I h cross del psi del t. From some plausibility argument, these have been derived. In fact, they are just consistent with the energy quantization and the de Broglie relation. So, de Broglie relation is p equal to h over lambda and E equal to h nu is the energy quantization that has been used by Planck and Schrodinger. later on employed in the study of photoelectric effect by Einstein, okay. So, psi is a function of space and time as I told and it obeys, you know, the psi mod square integrated over all space. Now, we have shown it in a three-dimensional space. If you want, you can write in one dimension as dx. So, this dx and d cube are, they mean the same thing. And this is for all t. So, at each t or at all time, this normalization condition will be satisfied.

The second postulate says that to every observable, there exists a linear Hermitian operator. And these are very important things. One is that it's a linear, it's a linear operator and it's a Hermitian operator. And what we mean by Hermitian operator, we'll see that. But what it really means at this level is that the Hermitian operators are associated with the observables and which should yield real eigenvalue. So these Hermitian operators are real eigenvalues. We haven't defined this eigenvalue or, you know, an eigen equation, which will shortly do it. Before that, I thought it's more useful and relevant to put down the postulates. In the measurement of an observable, the corresponding operator will yield only the eigenvalue. And this is just to bring context from the discussion that we had earlier that the measurement is to see whether the cat is dead or alive. And psi has two states or rather psi comprises of two possibilities. One is that it is dead or it is alive and A is this measurement of observing it. So, that is the operator that observes that what is the status of the cat if you have left it say for some time and this is the eigenvalue.

So, the eigenvalue corresponds to whether the cat is dead or it is alive. Suppose if it is dead then let us call it as that as 0 and if it is dead alive, let us call it as 1 or if it is head, let us call it as 1 and if it is tail, let us call it as 0 and so on so forth. So, where psi is called as the eigenfunction and A is known as the eigenvalue and this one is called as the eigenvalue equation and it can also be written in terms of this Bra and ket notations as A psi, okay. And so there's another postulate that comes over here. That's the expectation value of an operator. And this expectation is expressed as inside this angular brackets right on the left angular bracket or left and right angular brackets. So it's like this, okay. So any operator O here we have written A. is really the integration of this coordinate variables from minus infinity to plus infinity and they are squeezed between the wave function or the eigenstates of the particle.

So these are the states, size of the states of the wave function and A is taken between the two or squeezed between the two that is between the left eigenvector and the right eigenvector. And so this is the definition of the expectation value. The wave function is symmetric under the exchange of particles for if the particles are bosons. Remember that we are talking about indistinguishable particles. They are identical and indistinguishable. But while they are identical and indistinguishable, they have two possibilities. One is that they can be either bosons or fermions and bosons are characterized by even wave function. Even means that if you have psi of x, I'm just ignoring the t for the moment. If you change this x to minus x, that's called as an even function. And if this thing changes from If you change this, it is called as an odd function. That is not exactly what we mean as symmetric. So, this is called the symmetric and this is called the anti-symmetric. We just gave you an example, but what we mean to say is that we have two particles, say for example, X1 and X2 and you change that to, you swap the two particles or interchange the position of the two particles. And whether you get a plus sign or a minus sign will decide that whether they're bosons or fermions. And the plus sign is reserved for bosons and the negative sign is reserved for fermions.

And in fact, you might have heard of the Pauli's exclusion principle, which the electrons have, you know, they are bound to obey that. And in that, it says that the no two particles can actually be in the same state, okay. And this can be understood if you write down, say, for three particles, if you write it down in terms of a Slater determinant and the Slater determinant would say that if you write any determinant and make either two rows or two columns to be identical, the same. then the determinant is equal to zero, which means that if the positions of the two particles are same, we are not talking about spin here. If you allow for spin, then, of course, a spin up and spin down can still occupy the same position. And in that case, the wave function will be equal to zero, which means that this is strictly prohibited for the electrons here. for two of them to occupy the same quantum state with all their quantum numbers to be identical. This is just a table of certain observables and their corresponding operators and this what kind of operation should you do is stated here. So, if you are talking about a position variable, we denote it by R or by X and the operators are written with a hat usually. But in most of these cases, when we write, the operators will neglect that hat.

But if you want to be very sort of strictly correct in these notations, then you should write it with a straight hat that you see here. And that is the hat that we are talking about. So, position variable is the symbol is R and then the operator will come with R cap, momentum is P, P cap, kinetic energy is T. It is T cap. And it's important to see that the momentum has is, of course, a vector operator, which has a form in the coordinate space equal to minus i h cross del del x in the x direction, del del y in the y direction and del del z in the z direction. The kinetic energy has a form minus h cross square over 2m del square by del x square plus del square by del y square plus del square by del z square. The potential energy is V of r. It has no form. I mean, if it is, say, for a particular problem, say, for example, the linear harmonic oscillator, this has a form half m omega square r square. It just simply multiplies this half m omega square r square by the, I mean, that's multiplied with the wave function and so on.

Observables and Operators

Observable	Classical Symbol	Quantum Operator	Operation
position	$\mathbf{r}$	$\hat{r}$	multiply by $\mathbf{r}$
momentum	$\mathbf{p}$	$\hat{p}$	$-i\hbar(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z})$
kinetic energy	T	$\hat{T}$	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$
potential energy	$V(\mathbf{r})$	$\hat{V}(\mathbf{r})$	multiply by $V(\mathbf{r})$
total energy	E	$\mathcal{H}$	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) + V(\mathbf{r})$
angular momentum	l_x	$\hat{l}_x$	$-i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})$
	l_y	$\hat{l}_y$	$-i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})$
	l_z	$\hat{l}_z$	$-i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$

The total energy in the time independent case is given by, so the symbol is H, which is the Hamiltonian, which is what we will see very extensively. And the eigenvalue of that is called as the energy or the total energy. And in the time independent form, it's written as minus h cross square over 2m del squared del x squared plus del squared del y squared plus del squared del z squared plus V of r. Then there are angular momentums. They're often written with a capital LX, LY, LZ, and they have these forms that are said there, I mean, that are written here. So it's, basically, you can get it as r cross p and the x component of r cross p where r is given by, you know, so, this is x i cap plus y j cap plus z k cap. So, if you write that R here and P as these ones that are said here in this particular line, then you would get this x component of the angular momentum to be like this, y component to be like this and z component to be like this.

All right, so let us do some preliminary linear algebra in order to sort of note down the properties of this wave function and what kind of information do they give and what are their derivatives. Derivatives means what else can we infer from them. So, we have this psi r t or you can call it in one dimension, we can call it x of x and t or in another space, we can call it as k and omega, okay? And k, if you are talking about a three-dimensional vector, k has to be written as a vector, but you can, if it is, you are dealing with one dimension, then that is a scalar. So, what is k? k is nothing but p is equal to h cross k. and p of course, is the momentum of the particle which has a relationship with the wavelength that is p equal to h by lambda and all these are embedded into the Schrodinger equation that we have talked about whose solutions are all these size and so on. So, what is the eigenvalue equation and the eigenvalue equation is an equation like this that the Hamiltonian, it was written with a curly H. If you look at this earlier figure, it is curly H, but we will write it with a straight H. So, H of psi, that is a ket psi, this is equal to E of psi.

And this psi is a wave function and this wave function can be expanded in terms of the basis sets. So, wave function and what I mean by that there is an important statement and this basis sets are all these different states, possible states of the particle which are, you know, which were there, like, for example, the dead or alive or the head or tail or the top slate and the bottom slate and so on. So that's written as, so the wave function is really written as some C n phi n where C n's are the coefficients of this expansion and in general complex. So the C n's are in general complex and phi n's are the basis sets. So as soon as you make a measurement and you find the cat to be alive, the C n corresponding to it being alive, that will become equal to 1 and the C n corresponding to or the coefficient corresponding to that it being dead goes to 0. So this is now this psi is normalized. This is what the normalization means. And if you write it in terms of the integrals, it means that it is just the inner product that we have said. So, the inner product of any vector with itself has to be equal to 1, right?

So, this is, I am writing it in one dimension, this is equal to 1 and this is what it should be because this is also the probability because psi star psi is the probability density, this is called as a probability density and this probability density is integrated over all space that should give us one for all time. So, psi is a function of in general a function of x and t. So, this is true for all time. So, we are not writing time here explicitly, but in terms of the linear vector space or in terms of this vector algebra, the inner product of one vector with its own self is equal to 1 and that would be giving us this relation that is inner product of psi with itself that is bra psi and ket psi that is equal to 1. So, if you put that here, you have a psi and a psi that let us call it as equation 1, this is equation 2. And this is equal to, you know, n and then we have these C n square and we have a phi n. Okay, let me write it a little more sort of explicitly. So when I take the inner product of two vectors and each of the vector is actually can be decomposed as the C and phi n, I should write it with two indices with the C m star C n and phi m star.

Phi m bra and a Phi n. And now this for these each of these vectors are orthogonal to each other and they form a complete set. And if it's an infinite dimensional space, that is, each of these Phi n and Phi m are the labels corresponding to them. I mean, they sort of represent infinite number of such states. We just talked about two of them like being alive and being dead. But suppose we are talking about another system, there are very large number of possibilities that the system can actually go to in principle infinite of them. Then these phi n and phi m, they belong to a linear vector space with a special name. This special name is called as a Hilbert space, okay. And because I said that they are orthogonal, so this has to be equal to 0 if m is not equal to n. So, this is written as a Kronecker delta, which is delta m n. So, delta mn is equal to 1 for m equal to n and it is equal to 0 for m not equal to n. And this is exactly what we said about these their orthogonality. So, which means that if you think in terms of vectors, these basis sets are also vectors as well. That is what it gives. I mean, the vector property of this psi is, is given by this vector form of the the phi's. And so this is they are orthogonal and also normalized. So that is why they are called as this psi is called as an orthonormal function.

And this if m is equal to n then only it survives then this becomes equal to n and C n mod square because m and n are same otherwise it is of course equal to 0 then it does not make sense to write this and so, this is equal to 1 because that is what is obtained from 2. So, equation 3 says that sum over n C n square is equal to 1. So, if you apply that to the to the coin tossing problem, say, for example. And in that case, you have the half probability to be equal to find it in the head state and another half probability that you would find it in the tail state. I am saying state because these are really the states of the system and so they would add up to equal to 1 and that is why 1 by root 2 is equal to C n. So, the probability is C n mod square which is half. So, the coefficient when if you want to write it for this head and tail. So, the wave function for this coin will be in this 1 by root 2 and it will be in the head state. So, I am writing a head with a h and 1 by root 2 in the tail state. And when you make a measurement, one of them will, one of the, you know, possible outcomes you will get.

$\psi(\vec{r}, t)$, $\psi(x, t)$, $\psi(\vec{k}, \omega)$. $\vec{p} = \hbar \vec{k}$

Eigenvalue equation $H|\psi\rangle = E|\psi\rangle$.

Wavefunction can be expanded in terms of the basis sets.

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle \quad (1)$$

c_n : Coefficients (in general complex).

$|\phi_n\rangle$: basis sets.

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} \underbrace{\psi^* \psi}_{\text{probability density}} \, dx = 1 \quad (2)$$

"Hilbert space"

$\delta_{mn} = 1$ for $m = n$

$= 0$ for $m \neq n$

$$\langle\psi|\psi\rangle = \sum_{n,m} c_m^* c_n \underbrace{\langle\phi_m|\phi_n\rangle}_{\delta_{mn}} = \sum_n |c_n|^2 = 1. \quad (3)$$

And when you get a possible outcome, then, of course, one of the cn's goes to 0 and the other cn, that is, this coefficient becomes equal to 1, okay. All right, so we have said some basic preliminary properties of these basis sets, and these phi n's are also linearly independent, or even, you know, these phi n's are linearly independent. And that is why if you have a psi, say prime, we can write it as psi prime is equal to some constant into psi. So, in that case, psi prime and psi are linearly dependent, okay. So in that case, they are not independent. So what we mean by independent is that suppose there are three, you know, we're just talking about a three-dimensional space. So there are C1, C2, and C3. So there is this C1, phi 1, plus a C2 phi 2, plus a C3 phi 3 is equal to 0, okay. So, then if this is true, then C1 equals C2 equals C3 equals 0. So, that tells you that the vectors or these basis sets are linearly independent, okay.

So, let us, you know, try to understand more about these basis sets because this will give you a more in-depth understanding of what we are trying to, you know, sort of relate to and what they mean. So, let us talk about an outer product of this and this outer product unlike the inner product inner product is a scalar the outer product would be still a vector. So, outer product and what we call a change in basis, okay, and we want to a priori talk about a property that is the trace of an operator or the expectation value of an operator is independent of the basis. So, this expectation value we have talked about already, they mean that this A is equal to psi A psi. So, which means that they are taken between the two sides. And you are talking about these as the matrix elements, and these matrix elements. And we are really talking about the diagonal matrix elements because these two sides are the same. And so this is actually called a trace. Okay, so trace of A.

And this trace is the sum of the diagonal elements, and the trace is independent of the basis chosen because the trace of a variable or rather of an operator should be independent of which basis you write because that corresponds to a sort of physically observable quantity. So, we can write this down as the outer product as there is a Cn and a phi n, which is what we have written, and we introduce now a different basis, which is n. So, that is like a Cn and a chi m, a different basis, and we have to use a chi m and then a phi n. So, this we could introduce because the outer product of these two vectors is equal to 1. So, we have not done anything, but we have just introduced a 1 inside. But in that case, you know, what we have done is that we have gone from an old basis phi n to a new basis chi. And what we can write down is that this, so this C, this can be like m and C m prime and chi m, where this C n and chi m and phi n, all these are scalar quantities, in general complex quantities, is written as m. C prime m. I mean, it is not the prime is not with m, but the prime is with C, which is a new coefficient that depends on the new basis. So, we have gone from a basis of phi n to a basis which is chi m.

ϕ_ns are linearly independent.

$|\psi'\rangle = a|\psi\rangle$ $\quad |\psi'\rangle$ & $|\psi\rangle$ are linearly dependent.

$c_1, c_2, c_3.$

$c_1|\phi_1\rangle + c_2|\phi_2\rangle + c_3|\phi_3\rangle = 0$

$c_1 = c_2 = c_3 = 0$

$\langle A\rangle = \langle\psi|A|\psi\rangle.$

$= \mathrm{Tr}\, A.$

outer product : change in basis.

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle = \sum_{n,m} c_n \underbrace{|\chi_m\rangle\langle\chi_m|}_{1}\phi_n\rangle. \qquad \underbrace{c_n\langle\chi_m|\phi_n\rangle}_{c'_m}$$

$$= \sum_m c'_m|\chi_m\rangle \qquad |\phi_n\rangle \rightarrow |\chi_m\rangle$$

And now, we will show that the trace is invariant of the basis that is chosen. So, its trace is invariant of the basis. And let me show that. And why it is so physically, you know, the trace actually means that these are some of the diagonal elements, or it's basically the matrix elements of the operator between the like states. That is, when you have the same states, you know, the same states are used here. So, this is the definition of the expectation value in terms of the trace. So, phi n's are some basis that we are using. Now, we will show that we are going from a basis which is phi n to something else, and we will see that this expectation value does not change. So, what we do is that we use this n, and let us use n, m, and p, and let us introduce this phi N, say for example, chi m. And chi m here, and then you have a, and then let's use another basis, let's call it gamma p, and then use this gamma p, and then phi n. So, what I've done is that,

There was a sum over n in the initial expression, and then I've introduced two dummy sums, which are m and p, and use this chi m, chi m, the outer product of which is equal to 1, and the outer product of gamma p is again equal to 1, sum over p. So I've just introduced two 1s there, 1s means these identity matrices. And then what we do is that we can write this down as N, M, and P and bring this at the front. So we have these because all these are inner products, which means that they basically talk about the length of the vector. So that's a scalar quantity. So we can swap its position. So this is bringing it to the front here will tell you that this becomes equal to phi n, then we have A gamma m and A gamma m A, and so this chi m, and then there is A gamma p, okay. So, this gamma p, phi n, phi n, chi m, chi m A, gamma p, where all these phi n is a basis, chi m is another basis, and gamma p is another basis, and they all come with different indices, which has been shown here. Now you see that we can use this sum over n and these outer product of the phi and the original basis that we have written, we can make that equal to 1 and this will go away, and then we have m and p because we have taken these n into account, and then we have a gamma p and we have a chi m.

And then we have a chi M and then A and then gamma P, and now what we can do is that again this is an expectation value that can be brought here, so this can be written as M and P, we have this chi M A gamma P, and then we have a gamma P chi m. Once again, I can use this outer product to be equal to 1 that along with this summation over p. So, that leaves me with a m and a gamma m A gamma m. So, we have indeed gone from a basis which is phi n to a basis which is gamma m, and we are still writing the expectation value in terms of sum over n and these A, the operator A is taken between these I m's, and that's what is going to be important for us. So, that tells you that the trace is invariant and it does not depend upon the basis that we choose to express. So, the trace is, as you know, that is the sum of the diagonal elements. And so, okay, let us look at this, say, for example, the Hamiltonian operator and how it looks like and so on. And I will give you a simple example to construct this Hamiltonian operator. And remember that each of these operators are nothing but matrices. And when you talk about a matrix, you need to talk about a basis.

Trace is invariant of basis.

$|\phi_n\rangle$, $|\chi_m\rangle$, $|\gamma_p\rangle$

$$\langle A\rangle = \sum_n \langle\phi_n|A|\phi_n\rangle$$

$$= \sum_{n,m,p} \langle\phi_n|\chi_m\rangle\langle\chi_m|A|\gamma_p\rangle\langle\gamma_p|\phi_n\rangle$$

$$= \sum_{n,m,p} \langle\gamma_p|\phi_n\rangle\langle\phi_n|\chi_m\rangle\langle\chi_m|A|\gamma_p\rangle \qquad \left(\sum_n |\phi_n\rangle\langle\phi_n| = \mathbb{1}\right)$$

$$= \sum_{m,p} \langle\gamma_p|\chi_m\rangle\langle\chi_m|A|\gamma_p\rangle = \sum_{m,p} \langle\chi_m|A|\gamma_p\rangle\langle\gamma_p|\chi_m\rangle \qquad \left(\sum_p |\gamma_p\rangle\langle\gamma_p| = \mathbb{1}\right)$$

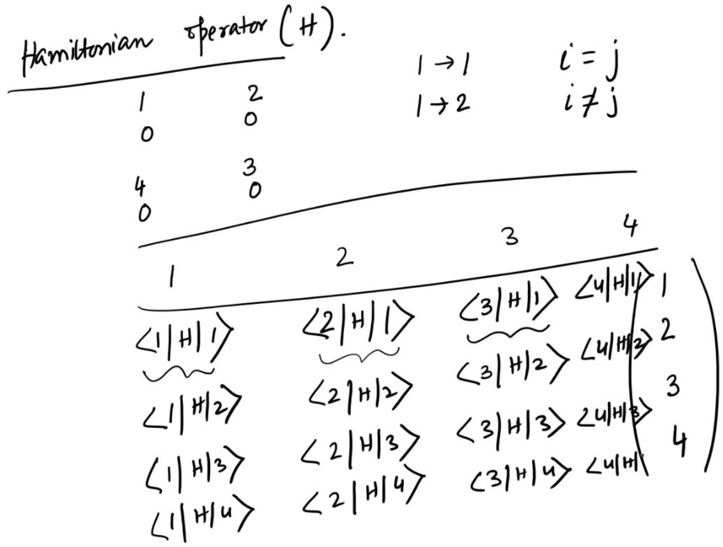
$$= \sum_m \langle\chi_m|A|\chi_m\rangle \qquad |\phi_n\rangle \longrightarrow |\chi_m\rangle$$

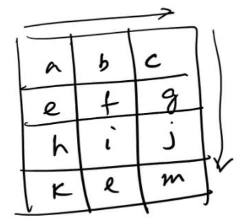
Like if I give you, for example, some data here on the X and Y axis, some data are written there, say A, B, C, E, F, G, H, I, J, K, L, M. So, it is a 3 by 3, and we have written down some numbers or just some letters. And these letters do not mean anything to you if we do not say what is recorded on the X axis and what is recorded on the Y axis. On the X axis, we can record, you know. the marks of various students and in the y axis we can note down their role number and then that will make sense that a particular student with a given role number has gotten so much in some subject and has got some other number in some other subject. So, this is called as a basis. A basis is the representation, or this makes the description of an operator complete. And we need such a description for all the operators. In particular, let us talk about the Hamiltonian operator, which forms one of the major points of discussion for us in this study of quantum mechanics, because the eigenvalue of the Hamiltonian operator gives you the energy.

And this energy is an important quantity because the energy will tell you whether the system is in a bound state or in an excited state, and what the different energy levels are. Those different energy levels will decide whether transitions are possible from one state to another, and if they are, what kind of energy is required. For example, if a particle falls from one energy state to a lower energy state, then a photon or gamma ray is emitted. What is the frequency of the photon, and so on? So, we need to know the total energy of the system. And, as I said, very importantly, if the total energy is negative, it corresponds to a bound state. For example, we will see that the hydrogen atom is in a bound state—the electron is bound to the atom and cannot escape unless you give it a sufficient amount of energy. So, let us talk about, say, four sites, and these four sites are numbered as 1, 2, 3, and 4. Now, I am going to write the Hamiltonian operator in terms of this. So, we can have terms connecting 1 to 1 itself, 2 to 2, 3 to 3, and 4 to 4. There could be on-site terms which can contribute to the energy, say, for example, the chemical potential or some other kind of on-site energy. Usually, these on-site energies are called the chemical potential.

And there could be cross terms, like 1 to 2, 1 to 3, 1 to 4, and so on. So, one can have terms where i is equal to j in the Hamiltonian matrix, and one can also have terms where i is not equal to j. And it is very easy to see that I can write this down as 1, 2, 3, 4. So, this will form my basis, which is nothing but the positions in real space in this particular case. So, we have these 1 H 1, where the Hamiltonian is written as H, as I said earlier, and then this would be like 1 H 2. And well, I mean, you can write it as 1 H 2, or you can also write it because you want to consider this as a bra. So, it's 2 H 1, and then 3 H 1, and then there's 4 H 1, and so on. So, these are the matrix elements of the Hamiltonian operator, depending on what kind of rules you set. If there is a connection between lattice sites 1 and 2, then this term will be non-zero. If there is no connection between 1 and 2, then it will be 0. For example, this is very easy to see that this can be 0 because it is not a nearest neighbor—it is a diagonal neighbor, and so on. So, this can be written as 1 H 2 and so on so forth. 1 H 2 and this is like 2 H 2. Let me write down all of them so that, so this is 3 H 2. And this is 4 H 2.

Then there's 1 H 3. Then it is 2 H 3. Then it is 3 H 3. That's the diagonal element for this. And then there is a 4 H 3. And finally, we have a 1 H 4. And we have a 2 H 4 and a 3 H 4. and finally, the diagonal term 4 H 4. So, this is the Hamiltonian matrix written in this basis. If you know the rules of connecting one lattice site to another, then you can calculate these matrix elements and you can construct the entire Hamiltonian matrix, diagonalize it, you will get the eigenvalues or the energies of that system comprising of say these four particles or four lattice sites, okay. All right, so let me tell you that what are these eigenvalues because if you make a measurement of a system by an operator that corresponds to an observable, you will always get this eigenvalue as A. Say for example, if A psi, so we will call it as eigenvalue, the discussion If you have A psi, this is equal to a psi, where A is the operator, psi is the eigenfunction, a is the eigenvalue returning back the eige function. So, an operator operates on the eigenfunction, returns the eigenvalue corresponding to this eigenfunction and returns the eigenfunction itself.





And so, this if I want to calculate the expectation value, then this is equal to psi A psi and I have simply psi a psi, but this a is just a number. So, this becomes a psi psi and because psi psi is provided is properly normalized, this is equal to a. So, that tells you that A square is equal to a square. And if I want to calculate what is A square psi, then that means that it is equal to A A psi and then it is equal to A square psi. And if you want to calculate the eigenfunction of A square or rather the trace of A square or the expectation value of A square, then this is equal to A square. So, this fluctuation in this A is now given by a square root of A square average or expectation minus A average this. And both are a square. So, this is equal to 0. So, which means that there is no fluctuation in the these the value that is obtained by the measurement of a. Of course, we are not showing that delta A has to operate on something. But if you just write delta A. acting on a state, this will give you a 0 into psi, which means that delta A has eigenvalue equal to 0.

Eigenvalue

$$A|\psi\rangle = a|\psi\rangle$$
$$\langle A\rangle = \langle\psi|A|\psi\rangle = \langle\psi|a|\psi\rangle = a\langle\psi|\psi\rangle = a$$
$$\langle A\rangle^2 = a^2$$
$$A^2|\psi\rangle = A A|\psi\rangle = a^2|\psi\rangle.$$
$$\langle\psi|A^2|\psi\rangle = a^2.$$
$$\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2} = 0$$
$$\Delta A|\psi\rangle = 0|\psi\rangle \rightarrow$$

So, this means, of course, two things that psi is an eigenstate of A and no matter how many times you make this measurement, you will still get it, this fluctuation to be 0, which means that this is the only measurement, the result of the measurement that you get. So, let us check out the Hermitian properties of matrices. I mean matrices means operators and in particular, we will show that the momentum operator is a Hermitian operator. And why is this question being raised? Because you have seen it earlier that P is equal to minus i h cross and d d x. Of course, you can write it del del X. And if you want to put a cap on that, because these are operators and we are writing it only in one dimension. If you write it in three dimension, of course, there are del del. d d y d d z that will be there and because it looks like that there is a this term which is I and how in that case this becomes a Hermitian operator which means that it will return real eigenvalue. If it retains or rather returns real eigenvalue then of course it is a it is a Hermitian operator. So, a Hermitian operators generally you know they are recognized by this relation that your A dagger i j this is equal to it is equal to A j i. So, that means that, so what is the meaning of taking a dagger?

Dagger is that you take a complex and a transpose. Transpose is the operation by which you interchange rows and columns of a matrix. So, this is the test of Hermiticity. So, let me show this for the momentum operator. So, we take this momentum operator between two eigenstates of the system, which, let us say, are psi 1 and psi 2. And we write it in the good old notation, introducing these integrals. So, this minus infinity to plus infinity, because there is a bra psi, we will have to write it as star. And then the operator, which we have decided to write in one dimension, such that this integral is just one dimension. There is no loss of generality because you can trivially extend it to more than one dimension. And this is equal to minus iħ minus infinity to plus infinity and psi 1 star and d psi 2 dx. That is d dx acting on psi 2; whatever is on the right of d dx will act on that and this. So, now how do we evaluate this integral? We can do it by using integration by parts, which gives us that minus iħ is equal to psi 1 star.

And psi 2 minus infinity to plus infinity and minus of psi 2 d psi 1 star dx dx, okay. So, that is the result for this. So, you take psi 1 star as the first function and d psi 2 dx as the second function. So, integral of u v dx is equal to u integral v dx minus du dx and integral v dx the whole dx. That is the form for integration by parts. And this is equal to 0 because, for the finiteness of psi, the product of these two cannot oscillate or cannot be finite at infinity at plus infinity or minus infinity. That takes away this, absorbing the negative sign there. So, it is iħ psi 2 d psi 1 star dx and dx. So, this is nothing but psi 2 and p and psi 1 star. So, psi 1 p psi 2 is equal to psi 2 p psi 1 star. So, this tells you that you have taken transpose because you have interchanged the row and the column and then also have taken this star, and this is exactly what I said: that is the test for the Hermiticity of an operator, and this Hermiticity ensures that it will return real eigenvalues and should correspond to an observable.

So, in simple notations, you can say that for any operator, if A is equal to A dagger, this is called a Hermitian operator, okay. There is another thing that one should be familiar with. If you take AB dagger, it is taken in from the other way. So, it is equal to B dagger A dagger. So, this is because these are matrices, and you have to be careful while multiplying these matrices because matrix multiplications usually do not commute. So, AB is not equal to BA. So, AB whole dagger that is equal to a first you have to take it is on the it is called as a cyclic property of the matrices. So, let us talk about the commutation relation between operators, okay. So, and again, we show it with two specific operators.

Hermitian properties of operator

Momentum Operator is Hermitian

$$\hat{p} = -i\hbar \frac{d}{dx}$$

$$(A^{\dagger})_{ij} = A_{ji}^{*}$$

$$\int u v\, dx = u \int v\, dx - \int \left(\frac{du}{dx} \int v\, dx \right) dx$$

$$\langle \psi_1 | p | \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_1^{*} \left(-i\hbar \frac{d}{dx} \right) \psi_2 \, dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \psi_1^{*} \frac{d\psi_2}{dx} \, dx$$

$$= -i\hbar \left[\psi_1^{*} \psi_2 \Big|_{-\infty}^{\infty} - \int \psi_2 \frac{d\psi_1^{*}}{dx} \, dx \right]$$

$$= i\hbar \int \psi_2 \frac{d\psi_1^{*}}{dx} \, dx = \langle \psi_2 | p | \psi_1 \rangle^{*}$$

$$A = A^{\dagger} \longrightarrow \text{Hermitian Operator}$$

$$(AB)^{\dagger} = B^{\dagger} A^{\dagger}$$

So, when these two operators for two general operators, if A and B equal to 0, it tells you that A and B have the same eigenfunctions, but they of course do not mean that they have the same eigenvalues. They can have different eigenvalues, but they have the same eigenfunctions. It is sometimes said that they can be simultaneously diagonalized, so they mean the same thing. And of course, the commutation of two operators plays an important role in all of quantum mechanics because If this is true, then AB equals BA because this commutation means that the commutation of two operators can be written as AB minus BA (written in reverse form). If this is equal to 0, then AB equals BA. So, you can actually interchange the order in which you write these operators. And as I said, they are matrices. Usually, matrices do not commute, but these operators, if they commute with each other, then their corresponding matrices will commute as well. So, let us consider the position and momentum operators. Again, we will write it in one dimension. So, position and momentum—what kind of relationship do they have?

So, let us check out this famous commutation relation x and p and this x and p commutation is not equal to 0 which means that x and p cannot be simultaneously diagonalized and the reason that they both are infinite dimensional matrices. So, how do we show that, and what values do they have if they do not commute? That is an important thing. So, this is equal to x p psi minus p psi x and this is equal to x minus ih cross d dx psi and minus, so this is minus ih cross d dx psi x. Remember, ψ is, of course, a function of x and t, and this is the position operator. So, in principle, one should put a hat on this, as I said earlier, but we are neglecting all these hats. If you feel more comfortable denoting these operators explicitly for your own understanding, please go ahead and do that.

And so this is equal to minus ih cross x d psi d x e minus ih cross is just a scalar quantity. And then so this is equal to a plus ih cross. And now I have two terms. I have a d psi d x and plus i h cross x d psi dx, right? Because there are two functions, psi and x, and I have to take a d dx of that. Both psi and x, they depend on x. Of course, x depends on x. So, d dx of x is equal to 1. That gives rise to this term and the other term keeping x to be constant and taking a derivative of psi with respect to x. So, the first and the last term they cancel giving rise to plus ih cross not minus ih cross and d dx of I mean it is I am sorry I have written it. So, this is equal to psi not d psi dx. Because you keep the psi constant and then take a d dx of x, which is equal to 1. So, this is simply equal to ih cross psi. So, that tells us that x and p commutation acting on psi gives ih cross psi. You can treat this as 1. This eigenvalue equation which tells you that x and p, this is equal to ih cross.

Commutation relation between operators.

$[A, B] = 0 \Rightarrow$ A, B have same eigenfunctions. $\quad [A, B] = AB - BA$

$AB = BA$

Position (x), Momentum (p).

$$[x, p]\psi = xp\psi - p\psi x$$
$$= x\left(-i\hbar \frac{d\psi}{dx}\right) - (-i\hbar)\frac{d}{dx}(\psi x).$$
$$= -i\hbar x \frac{d\psi}{dx} + i\hbar\psi + i\hbar x \frac{d\psi}{dx}$$
$$= i\hbar\psi$$

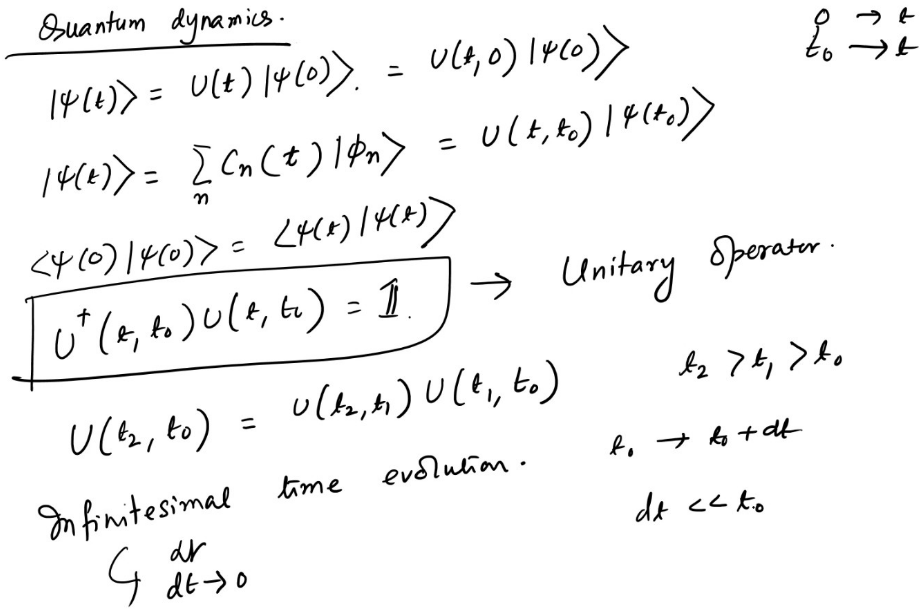
$$\boxed{[x, p] = i\hbar}$$

So, that is the commutation relation between x and p and this has been told earlier that because they are canonically conjugate variables, they do not commute. Okay, so let us, you know, next step, let us look at how we can actually talk about the quantum dynamics or rather how do we, you know, sort of talk about the time evolution of operators.

Because we have so far talked about how these psi depends, I mean its dependence only on x and we have not talked about the time evolution. So, this is called as quantum dynamics or we can just talk about the time evolution of psi. And this quantum dynamics can be obtained if you are this psi at a later time t can be obtained by multiplying it by a unitary operator and on the wave function at time t equal to 0 or you can write it because usually it is not only evolving it from time t equal to 0 to a time t equal to t, it could be from a time t equal to t1 to time t equal to t2. So, let us use two indices here in this case one of them is t, the other is 0 and this psi of 0. So, we will actually find a form for U of t0 and we will do it in two different ways. So, one is that, so a psi of t, which we have already written earlier in terms of its basis states. So, there was a c n and a phi n. We just kept it vacant for a while. Now, these phi ns are the basis states.

And it is usually sort of chosen, these basis states are chosen such that they are independent of time and the whole time dependence really goes into these coefficients Cn of t. And so this is nothing but U t of 0, say for example, or let us just take a t0 so that it is not always 0, so psi of t0. So, you are evolving it from a time t0 to a time t or you can evolve it from a 0 to a time t, it does not matter just to make it more general that we have written it that way. So, you know that at all times, this Psi of 0, Psi of 0 should be equal to Psi of t, Psi of t and which means that the normalization would hold at all times, this is what we have said. Now, that gives you a property of these matrices where you say that your U dagger t t 0 is equal to U t t 0, this is equal to 1. So, this is called as a unitary operator and this tells you that the time evolution operator is a unitary operator where you have considered that psi at a later time t can be obtained from a psi at an earlier time either say at t equal to 0 or t equal to some t0. By operating it by an operator U t t0 where U t t0 is a unitary operator which has got a form which is U dagger U equal to 1.

And why did I write it as a 1 with a bold sign or with a sort of double strand and the reason is that this is not just 1 but it is a identity matrix or it has all the diagonal elements equal to 1 and all the diagonal elements equal to 0. And the dagger has already been told that the dagger means that you take a transpose and you take a complex conjugate. of this. So, U dagger U is equal to 1 is an important property. And this, there could be another important property that you can think of is that this can be successively. So, you can do it like t2 to t0. So, it is from an initial time t0, you can go to t2 to a final time t2 in two steps where you do it as t2, t1 and U t1, t0 and so on. So, you can really successively build up this time evolution from initial time t equal to t0 to then to t1 and then to t2 and to t3 and so on so forth. So, here of course, it is understood that t2 is greater than t1 is greater than t0. Okay, so we will have to find a form for this and how do we find a form for this? You have to note that, so this, let us talk about an infinitesimal time evolution. So, it goes, so limit dt tending to 0, so it sort of evolves from t0 to t0 plus dt.



And if that is true, then so dt tending to 0, so that is called as an infinitesimal time evolution, okay? Or dt going to 0 means that dt is much, much smaller than t0, okay? And let us see how that can be handled. So, you have psi of t0 plus delta t, this is equal to U t0 plus delta or dt I am writing it as you can write it as dt they mean the same thing it is a small thing. So, either delta or d does not matter and t0 this is psi acting on t0 and So, now in the limit dt going to 0, you can take that t0 plus dt, t0, this is equal to 1. 1 means again, you know, you have to be careful that this is equal to an identity matrix. And so, if these requirements would be, you know, satisfied if you have this U t0 plus dt, and t0, this is equal to 1 minus some I omega dt. We do not know what omega is, but then we can figure it out later. So, this as dt goes to 0, then we have this U t0 t0, which of course would be equal to 1, because you are not evolving the system at all. So, psi of t0 and if you want it to be connected to be psi of t0, you simply should put a 1 here and this 1 is nothing but a U t0 t0. So, U t0 t0 equal to 1.

So, you going from U t0 plus dt to t0 is 1 minus i omega dt. And so, omega has to be is a Hermitian operator and why omega is a Hermitian operator because we have you know this U to be a unitary operator. So, that is why it has to be a Hermitian operator because you know you understand again this is not really one, but it is like a one identity matrix. And so, this means that omega dagger is equal to omega. So, we have these U dagger t0 plus dt t0 and u t0 plus dt t0, this is equal to 1 plus i omega dagger dt into 1 minus i omega dt. So, this is equal to 1 and if of course, we neglect terms which are of the order of dt square. So, where of course, we have used that omega equal to omega star. So, now, you know, sort of this omega can be identified. So, U t0 dt or U t t0 is really dimensionless. And if that is true between two any two times, it's dimensionless. Then, of course, your omega has to have the dimension of inverse of time or it has to be, you know, sort of which is known as a frequency.

$$|\psi(t_0+dt)\rangle = U(t_0+dt, t_0)\,|\psi(t_0)\rangle.$$

$$|\psi(t_0)\rangle = \underset{U(t_0,t_0)}{1}\,|\psi(t_0)\rangle$$

$$U(t_0+dt, t_0) = \mathbb{1}$$

dt

$dt \to 0$

$$U(t_0+dt, t_0) = 1 - i\Omega\, dt$$

Ω is a Hermitian operator. $\Omega^\dagger = \Omega$.

$$U^\dagger(t_0+dt, t_0)\,U(t_0+dt, t_0) = (1 + i\Omega^\dagger dt)(1 - i\Omega\, dt)$$

$$= \mathbb{1}.$$ if $O(dt^2)$ is neglected

$U(t, t_0) \to$ dimensionless.

$\Omega \to$ frequency $= \dfrac{E}{\hbar} \to \dfrac{H}{\hbar}$

Okay, so omega has to have the dimension of frequency. And when we talk about frequency at the back of our mind, if we use this E equal to h nu, so this is like E over h and this really in the operator notation should be equal to the Hamiltonian by h. So, that tells you that the U t t0 has a form which is equal to 1 minus ih, well, I mean, this is t0, this is for the infinitesimal operator. So, this is t0 plus dt. and t0. So, this is 1 minus h by h cross dt and if you recall that now we are talking about small time interval if we keep you know multiplying such time intervals or rather if we add more and more time interval and go from some t0 to some large time we would get these kind of factors And if you recognize that it is a 1 exponential i x is nothing but equal to minus i x is 1 minus i x plus you know i x whole square by 2 factorial and so on so forth. So, all these terms, so this is nothing but for large time intervals, this is only the, it is like an exponential minus i ht by h cross. So, u t t0. So, this is just the expansion of that. So, there are more terms that are going to be there like this i square h cross square by h square by h cross square and dt square and so on so forth. And so, this is equal to exponential minus i h square.

t minus t0 by h cross and this is what we have been saying that you know we will find out the form for that unitary operator that when which when applies or rather operates on the wave function would give me the time evolution of the operator and so on so forth. So this is that in the simple form. This is the equation. And we can actually do it in another way, which is simpler way or other. It's more intuitive. We don't have to go through this operator formalism. We can simply. So there's a second method of showing what is the form of this operator. So if this is the formalism number one and we'll just talk about a simpler formalism. Let us just, you know, your psi of r t, r and t, at least as far as non-relativistic mechanics goes, r and t are independent of each other. So, that tells you that g of r is equal to f of t. That is, there is a clear function of r and then there is another clear function of t. Let us call them as g of r and f of t. So, if I put it in the Schrodinger equation, so it is like i psi del psi del t r t, we are taking a time derivative, so this g of r will not be affected. So, it is a g of r f dot of t.

So, we have this, that is equal to, you know, so this is equal to i h cross f dot of t, and that is equal to h of psi, which is equal to h. and g of r f of t. So, now this is just like a normal algebraic equation if you treat it like this. So, you have a ih cross f dot by f this f dot which is a function of t f is a function of t as well. And this is like H, which, you know, so this for a system in which the Hamiltonian does not explicitly depend on time. So this H will give rise to a constant. And because, you know, you have two things which are, so this is really that H g r by, so this is g r, H g r by g r, okay, let us write it this way. Now, the left hand side is entirely a function of time. And this right hand side, if H does not include time explicitly, then it is a function of r. So, if they are equal to each other, then they have to be individually equal to be a constant. And this constant, we call it as E. And so, f dot of t is divided by f of t is equal to minus i E by h cross because 1 over i is equal to minus i. So, that tells you that f of t is nothing but a constant into e to the power minus i E t by h cross.

$$U(t_0+dt, t_0) = 1 - \frac{iH\,dt}{\hbar} \sim \exp\left(-\frac{iHt}{\hbar}\right)$$

$$e^{-ix} = 1 - ix + \frac{(ix)^2}{2!} - \dots$$

$$U(t, t_0) = \exp\left[-\frac{iH(t-t_0)}{\hbar}\right]$$

(2)

$$\psi(\vec{r},t) = g(\vec{r})\, f(t) \qquad H\psi = H\, g(r)\, f(t)$$

$$i\hbar \frac{d\psi(\vec{r},t)}{dt} = i\hbar\, g(\vec{r})\, \dot{f}(t) = H\psi$$

$$\frac{1}{i} = -i$$

$$i\hbar \frac{\dot{f}(t)}{f(t)} = \frac{H g(r)}{g(r)} = \text{Const.} = E$$

$$\frac{\dot{f}(t)}{f(t)} = -\frac{iE}{\hbar} \Rightarrow f(t) = (\text{Const})\, e^{-iEt/\hbar}$$

$$U(t) = e^{-iHt/\hbar}\dots$$

And if you are really looking for an operator, then this E is just the eigenvalue of some operator, which we know as H. So, this again, the operator that comes out, which is U of T, which is nothing but exponential minus I H t by h plus. So, this is how the wave function evolves with time. So, if you are given a wave function at an earlier time, you can multiply it by an exponential minus i h t where h is a Hamiltonian of the system and get the wave function at a later time. It is like saying the solving this Newton's law of motion, if you know x at a time t equal to 0, and V at a time t equal to 0, then you can generate the entire, you know, x at a later time and so on so forth. So, this is similar to that, that knowing the wave function at a certain time, one can actually build the wave function at a later time. by using this operator which is the time evolution operator so to say and which has a form which is given here. We will stop here for now and then we will carry on with some solutions of Schrodinger equation in some simple problems and in one dimension to begin with and then we have to go to three dimensions in order to do the hydrogen atom problem.

Which is like a sphere. So, we have to solve Schrodinger equation in presence of a spherical