Quantum Physics

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Lecture No. # 06

Let's our formalism of quantum mechanics but today, let me start by comparing classical physics with quantum physics and write down what the differences are between the two and how you make a transition from one to the other. So let's go back and look at Hamiltonian mechanics because the whole of quantum mechanics also presumes that you have a Hamiltonian for the system and quantum mechanics is really concerned with evolution in the presence of a Hamiltonian.

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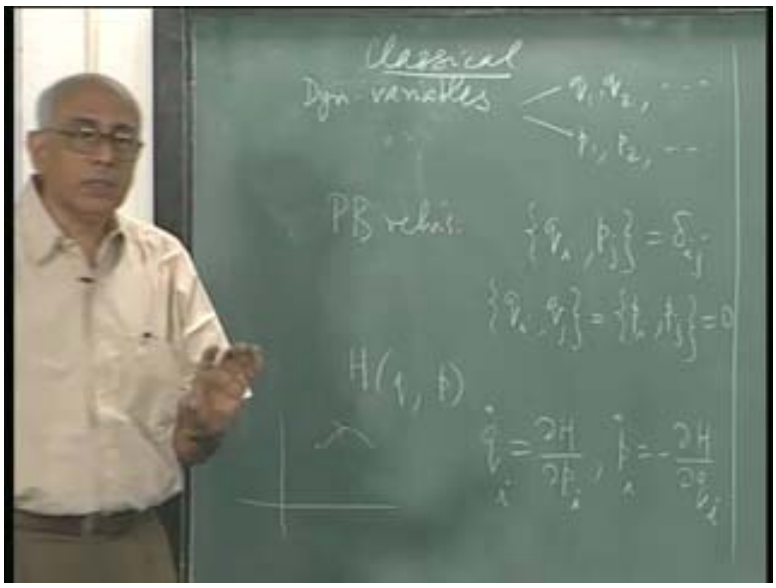

So classically you start by defining dynamical variables. And these dynamical variables are of two kinds. There are q 1 q 2 etc and then there are p 1 p 2 etc. so they go in canonically conjugate pairs. And then these dynamical variables satisfy Poisson bracket relations. The Poisson bracket relations are $\{q_i, p_j\}$ = delta $_{ij}$ and $\{q_i, q_j\}$= $\{p_i, p_j\}$ = 0. Now of course no dynamics has been put in. so far, it just says you have a set of variables and they obey these relationships among each other. The dynamics comes in prescribing the time evolution equations. So you introduce a Hamiltonian which is a function of q and p. There exists a Hamiltonian which is a function of the dynamical variables such that q_i dot is delta H over delta p_i and p_i dot is - delta H over delta q_i.

This is the Hamiltonian formalism in classical mechanics. the statement is that in phase space, in the space of the q's and p's, specifying initial data corresponds to specifying a point in this phase space after which you are supposed to solve these equations and if this is autonomous Hamiltonian, then the trajectory of the point that you started with in phase space will tell you what the future values of the dynamical variables are.

And therefore use this information together with initial conditions to find out what happens to dynamical variables as time evolves or elapses. Now the important thing to note here is that there are two pieces of information. One of them is this dynamical piece of information which tells you what the equations of motion and how things evolve in time.

The other piece of algebraic information is the input. It tells you a basic algebraic relation in this phase space between the q's and the p's. And it is not hard to see that these relations are valid at all times. in other words at any instant of time, q_i at time t with p_j at time t is delta $_{ij}$ if you start with that, it continues so. So the Poisson bracket relations themselves remain preserved as time goes along. The q's and p's adjust themselves such that they always obey the Poisson bracket relationship which is why you could use any of the points as the initial state. So this is very important to understand there are two sets of relations. One is the structure, the Poisson bracket, the canonical variables and the other is the evolution equations.

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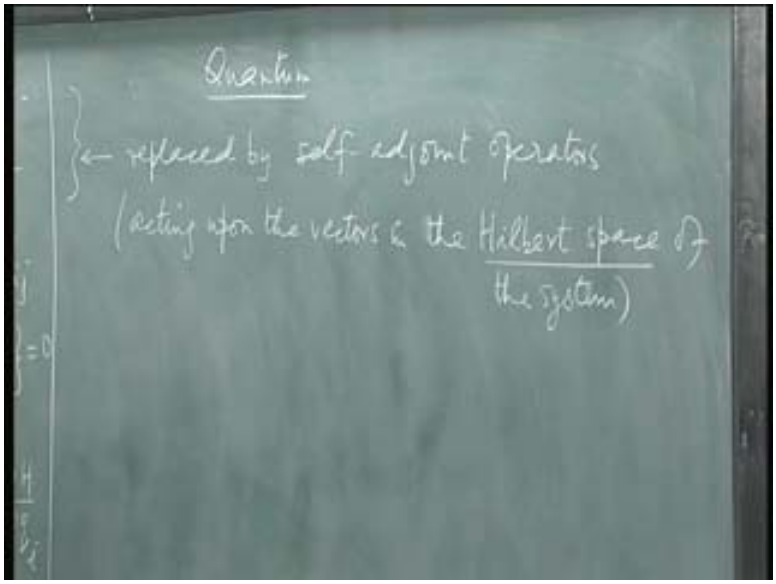

Now when you come to quantum mechanics, our assumption is going to be that the algebraic information is replaced by self-adjoint operators acting on the vectors of some Hilbert space. So, just as you had phase space in classical physics, in the quantum version it's no longer a phase space. It's meaningless to talk about points in phase space due to the uncertainty principle. So this is replaced by the Hilbert space. So the appropriate space in

which things happen in quantum mechanics is the Hilbert space of states. We still got to say where a state fits into this. But the dynamical variables are replaced by self –adjoint operators.

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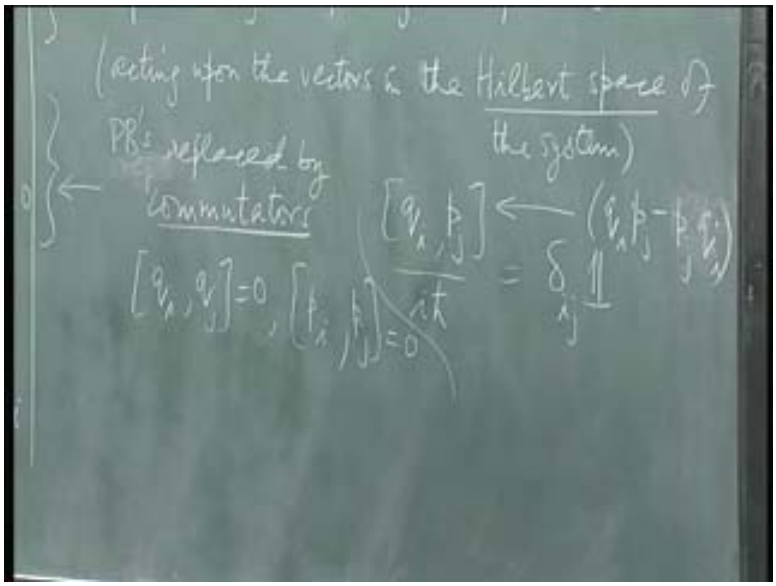

There an analog of Poisson bracket relations here and that is a relationship between the operators and they are replaced by commutator brackets. Then a commutator of two operators is the difference of operating with the two operators, one on the other in different orders. So the commutator here would be $[q_i\ p_j]$ which is a shorthand for $(q_i\ p_j - pj\ q_i)$. If these are matrices, then it says you have two matrices A and B and the commutator AB - BA is also a matrix. So what happens in quantum mechanics is the Poisson brackets are simply replaced by the commutators divided by ih cross. We need that factor there for a reason i will come to it.

And this is equal to delta ij but then these are operators. So there must be an operator on the right hand side and the appropriate operator here is the unit operator. It doesn't do anything just acts on a state and leaves it as it is. But the i and j are the labels which specify the dynamical variables. They could be Cartesian components, labels of the dynamical variables, the phase space variables in the classical case or the canonical variables.

So of course the other two commutators are 0. So [qi, qj] = zero and [pi, pj] = 0. These two are also part of the algebra. So algebraic relationships between the operators replace the algebraic relationships for a canonical variable. The Poisson brackets are replaced by commutators. The answer why i need that ih cross is technical. These quantities are physical quantities which are real variables. The corresponding thing here would be self-adjoint operators. But you see the commutator of two self-adjoint or Hermitian operators is not Hermitian itself.

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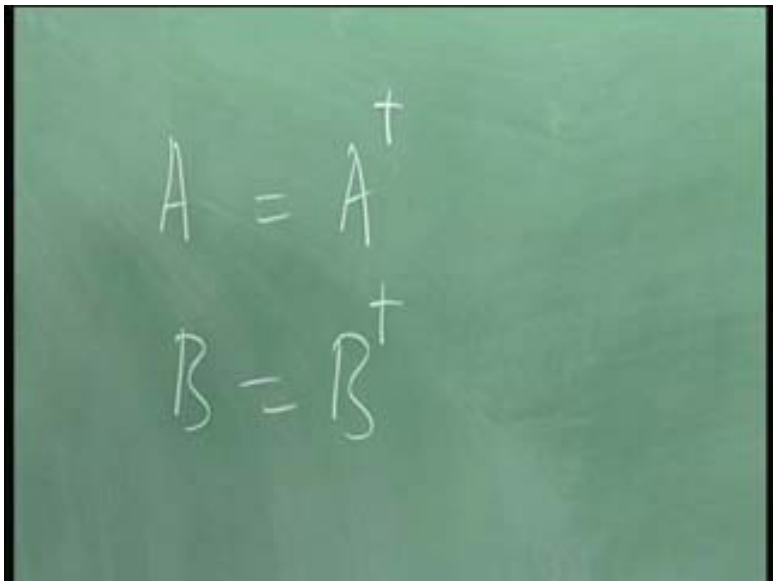

Suppose you have a matrix A and B which are Hermitian, they both would represent some physical operator physical quantities.

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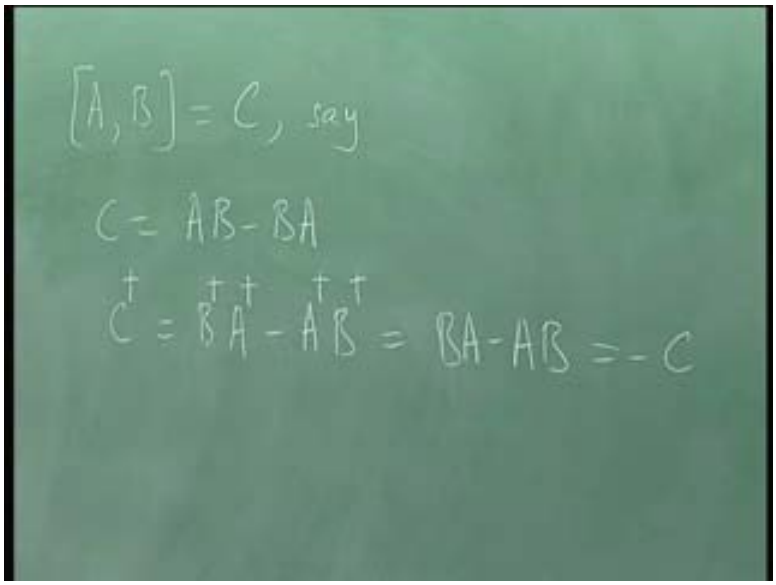

Then [A, B] =C, which is some other operator. Then C is AB – BA. But C dagger = B dagger A dagger - A dagger B dagger. But that's equal to BA - AB because B and A are themselves Hermitian. But this is equal to- C. so a commutator becomes anti-Hermitian. On the other hand, if it's a physical quantity, the combination AB - BA is also an observable.

Then you must make it Hermitian. That's the reason why you need this i here (refer Slide Time: 11:11) because the moment you put the i, that also changes sign and it makes this quantity a Hermitian quantity. The h cross is there for dimensional reasons. Because you can see that the product of any generalized coordinate and the corresponding conjugate momentum has always got the dimensions of energy multiplied by time. And there is a fundamental quantum constant called Planck's constant which has the same dimensions. So this makes it dimensionless here. You could ask why not minus ih cross. + ih cross turns out to be the right prescription and we will see as we go along what would happen if you had a minus here.

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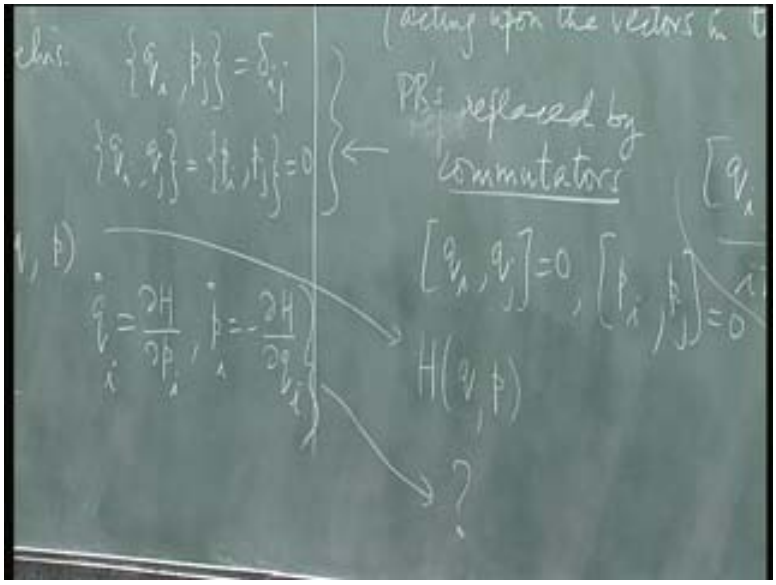

So the algebraic structure in classical goes to the algebraic structure in quantum. The next question is what about these equations. You again have a Hamiltonian. The presumption is you again have a Hamiltonian which is a function of q's and p's, except these are operators and therefore the Hamiltonian is also an operator. And you can immediately know that if q and p are complicated operators like derivatives and so on and then you take functions of these derivative operators, you can get fairly complicated operators.

Suppose q and p involves differentiation of the state vector, this H would be some function of this derivative operator, perhaps e to the power d over dx and so on. But they are not the analogs of the classical equations. There are no direct analogs of these equations. As it stands, the equations are going to be slightly more complicated and we will see what these equations become. So what's the time evolution of a quantum system and how is it described?

Now keeping this in mind, let's go back and look at what we said about expectation values and then we are going to get a hint as to what's going to happen.

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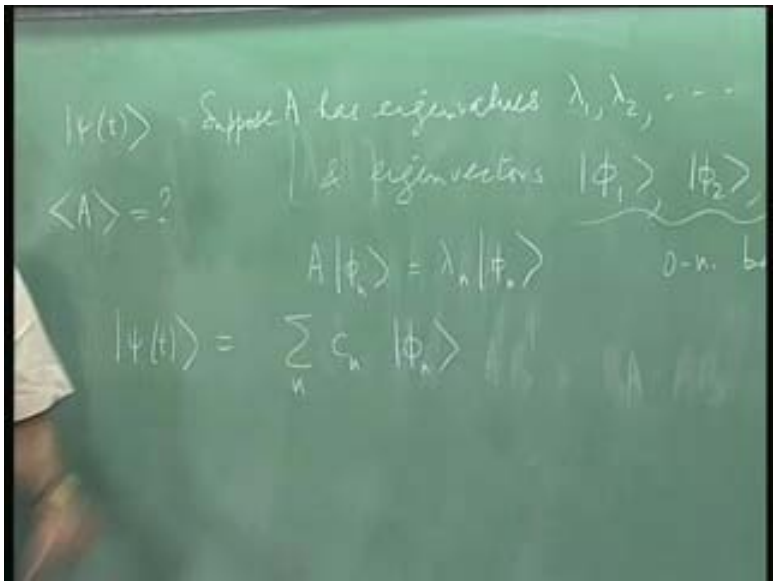

I pointed out that if you took a physical observable and I asked what is the expectation value or average value of this observable at some instant of time in a quantum system specified by a certain state, then we asked the following question. The state of the system psi of t is given to you at some instant of time and now i ask the following question, what is A at that instant of time. I explained yesterday that if you make a measurement on this system to measure this physical quantity A, you are guaranteed to get one of the eigenvalues of the system. Which one it is you can't say a priory depends on the state of the system.

So now lets assume for simplicity of notation that A has eigenvalues lambda 1, lambda2, etc possibly an infinite number. Let's called them lambda $_i$. Eigenvectors phi 1 phi 2 etc form a bases set in this Hilbert space of the system. This is an assumption. There would be operators for which you may not be able to justify this but just to set the formalism, let me assume this for the moment. It's a Hermitian operator or a self-adjoint operator. It has these eigen values and these eigen vectors. In other words A acting on phi $_n$ is lambda $_n$ times phi $_n$ and they form an orthonormal basis. That immediately implies that i can expand psi of t at any instant of time in the form summation over n, all the allowed values of n, some coefficient c_n times phi $_n$.

Now this operator A is perhaps like position, angular momentum etc. It's supposed to be made up of the dynamical variables of the q's and p's. To start with we assume there is no explicit time dependence in A. After all, if I want to measure the position of a particle, that position x has no explicit time dependence. It may depend on time after you solve the

equations of motion but there is no explicit time dependence. On the other hand, say let me measure x squared + y squared + t times z squared divided by some tau.

So i could put in t explicitly and then this observable becomes explicitly dependent on t. But let's start by saying A is a not explicitly time dependent in which case it has some eigen values and some eigen vectors. These eigen vectors are found once and for all form a basis set and i have an expansion of this kind here. If it's an orthonormal basis, this is a unique expansion. The time dependence go into the coefficients. Imagine in three dimensions, I fix my coordinate axis x, y, z. these are the unit vectors and I take the position of a particle which is moving and I expand that in this basis. Then of course the components are the ones that carry the time dependence.

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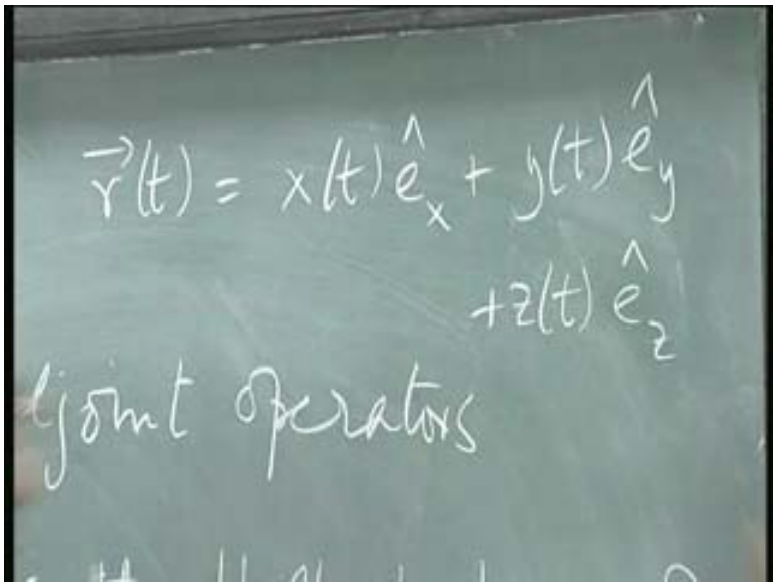

So you would say immediately that r of t = x of t times e_x + y of t times e_y + z of t times e_z.

So it's these components and not the unit vectors that carry the time dependence. In exactly the same way these components carry the time dependence here and they would change from instant to another. To start with, the basis is fixed.

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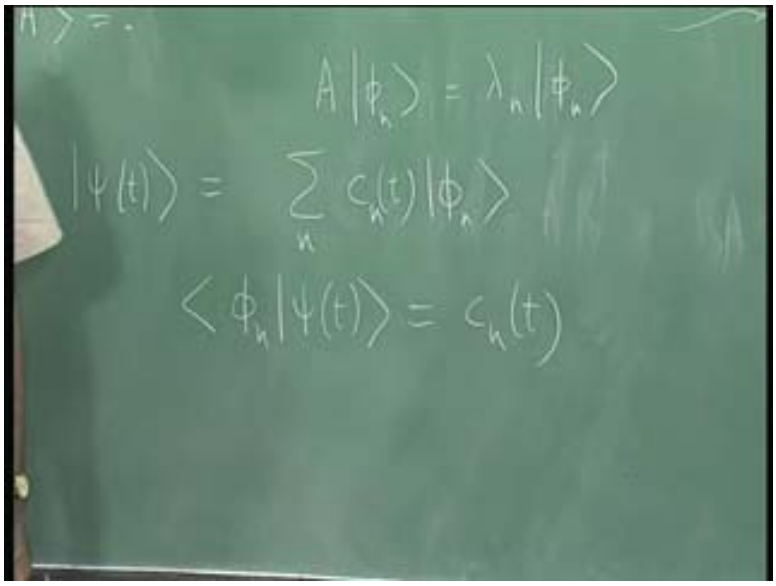

This implies that the probability amplitude that the state psi of t is in fact the unit vector phi n is given by this here (Refer Slide Time: 18:46).

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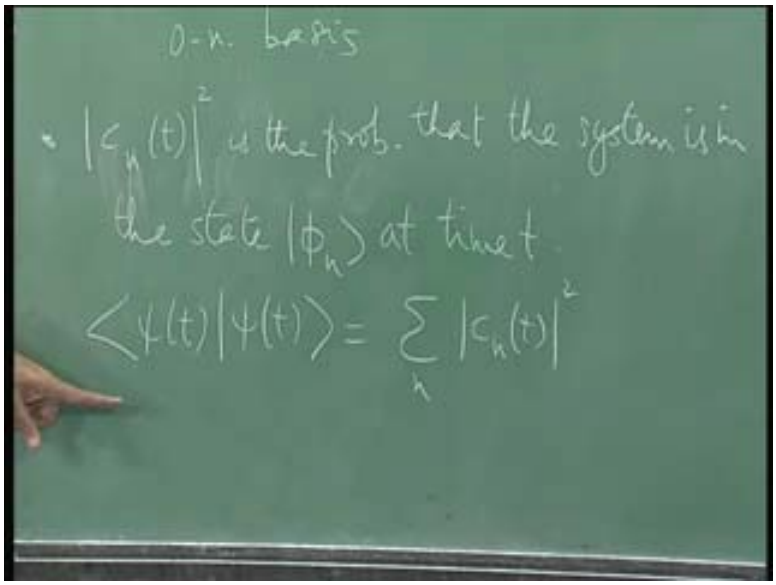

The probability interpretation of quantum mechanic says that mod mod c_n of t whole square is the probability that the system is in a state phi $_n$ at time t. This is a postulate. Now of course you may start with a state which is not normalized to unity which presumes that this state is normalized to unity. Because you immediately see that if i do a psi of t bra vector

here, then by orthonormality we know that psi of t psi of t = summation over n mod c_n of t whole squared. This follows by orthonormality immediately. Therefore this is a probability provided, this is unity (Refer Slide Time: 20:16). But i give an arbitrary state; there is no reason why it should be normalized to unity. Just as i can expand this position vector in terms of some vector along the x direction, something along the y and something along the z, it may not be unity.

Only if I make it unit magnitude, can I talk about the magnitude of this vector as exactly equal to x squared + y squared + z squared, squared root. i have to first normalize these unit vectors. I may not do it all the time. i may start with an arbitrary state and you may need to normalize it. You do exactly what you do in statistical physics. You divide by the normalization factor which in statistical mechanics was called the partition function. Because relative probability of a system having an energy e in contact with the heat power that inverse temperature beta was e to the power minus beta e. But the absolute probability was e to the power minus beta e divided by the sum over all these betas. So you have to keep track of that of the normalization all the time.

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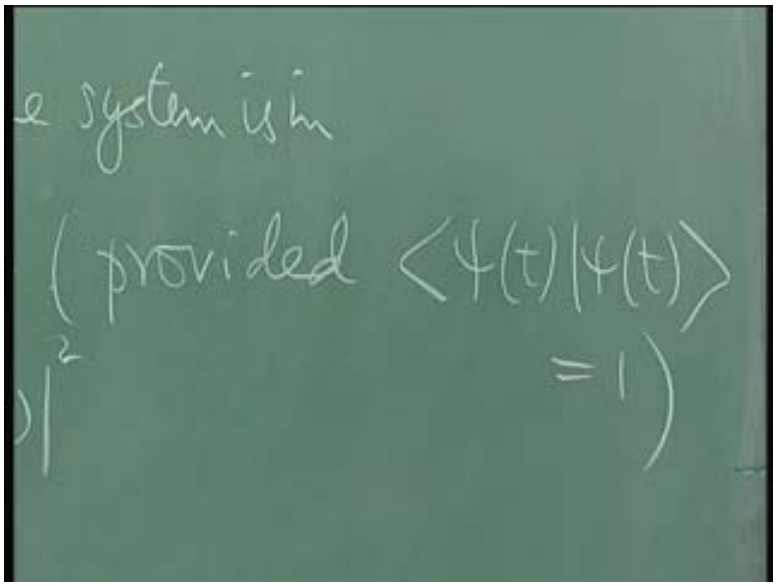

So if not divide by the norm and then you normalize. This is how you normalize any vector. You take the vector, divide by its magnitude and you get a unit vector always. So we will assume that we have normalized this state. We will see what happens if you don't normalize it. If that is the case we can write a formulary down for the average. This immediately implies that A average is equal to the weighted average summed over n of all the Eigen values of A together with the corresponding probability.

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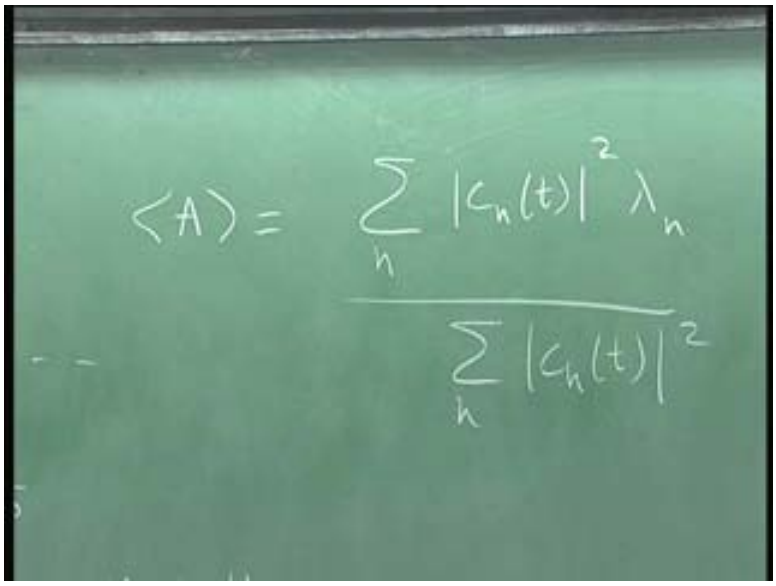

When it is in the state phi n, the value of A is lambda $_n$. you are guaranteed this is the value you will produce and now you know the probability with which it's in the state phi $_n$. Its mod c_n squared. So it's immediately clear that this quantity is mod c_n of t whole squared times lambda $_n$. that's the meaning of the average. Once you give me a probability distribution, the average is just the value at each point in this the probability distribution times the probability.

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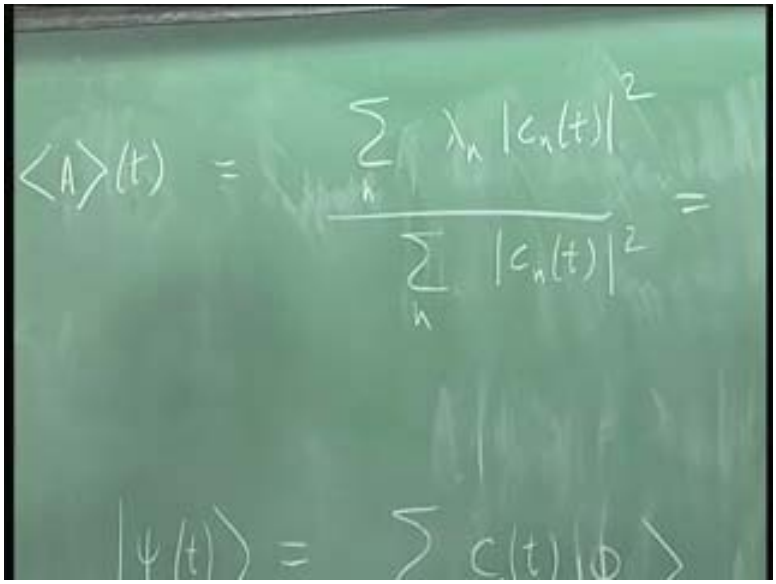

Incidentally if this were not true and it were not normalized, you simply divide by n mod c_n of t whole square in general. To normalize it later, you just divide by the total probability. So we have here a formula which says A, which is the average as a function of t and does not explicitly depend on time. So this is summation lambda $_n$ mod c_n of t the whole squared divided by summation n mod c_n of t the whole squared. I would like to go back and write it in terms of psi to get a compact formula

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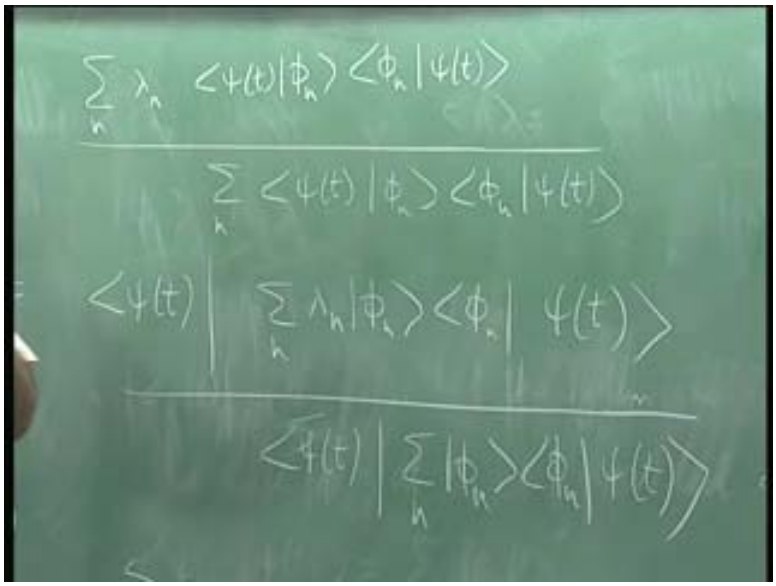

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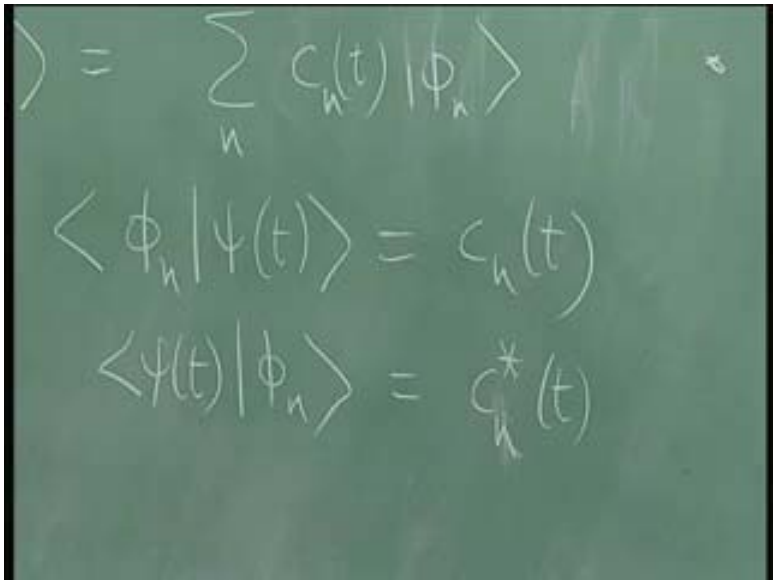

c_n of t is this (Refer Slide Time: 24:44). So I take its complex conjugate and that gives you c_n * = psi of t phi n because the complex conjugate of this is the reverse. So let's put that in. Now the average A of t is psi of t psi n phi n psi of t divided by summation over n psi of t phi n psi of t. The summation can be moved in and we write this as psi of t because that has nothing to do with the summation. A summation over n lambda n phi n phi n psi of t ket vector.

Now this is psi of t summation over n phi n phi n psi t. now you see the power of this notation. This thing here (Refer Slide Time: 26:34) is a number and must have two angular brackets. So what I have done is to move this out of the summation because we know that the sum over n of these scalar products we will take sum inside and sum one by one because it's a linear vector space.

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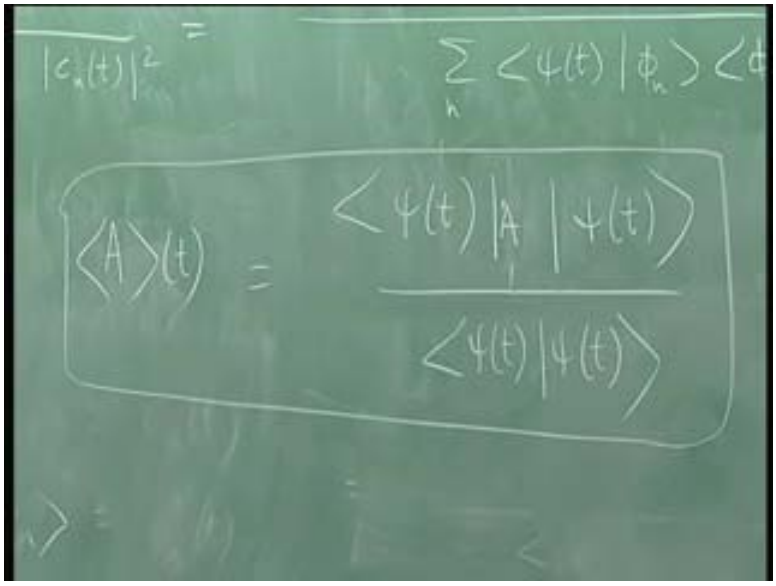

But this (Refer Slide Time: 27:48) quantity is the unit operator. So the denominator becomes psi of t psi of t, which is a normalization factor as we expected. But in the numerator, I can't take phi n phi n out and call it the unit operator because of the presence of the lambda ones.

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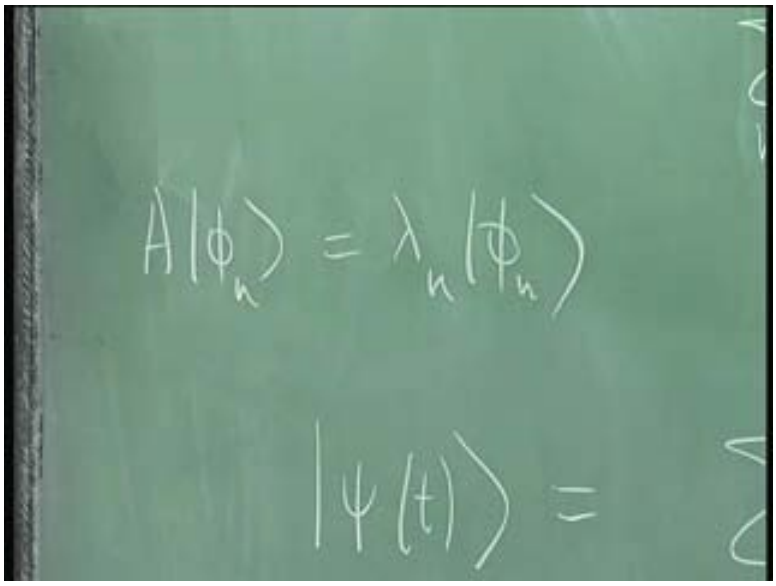

But we also know that A acting on phi n = lambda n on phi. So we use this relation in reverse. So the lambda n phi n can be written as A acting on phi n. But A is a linear operator and when it acts on a sum of states, it is as if you can sum those states first and act with A. So you can move the A out of the bracket and use the fact that this is a complete set of states. So you get a psi of t A psi of t and at the bottom, we get psi of t with psi of t. this is a fundamental formula. You have this A sandwiched between two states. This looks like a diagonal matrix element in a basis psi.

This is the reason why in quantum mechanics we say matrix elements are expectation values. It's by this little piece of rigmarole that you know that once you put in the probability interpretation, it follows that the expectation value of A apart from that normalization constant below is in fact the matrix element of A. Take the state vector psi operate with A. you get a new state vector. Take the inner product with the original state and that gives you the expectation value.

It is very important to notice that a sandwiched between the states is a very complicated object here and cannot be taken as something that can be normalized to one. So the whole purpose of everything is to find these quantities. And now this gives us a hint as to what these equations of motion would look like. Whatever they are, they should be such that when I take average values, I recover the formula here. So we will keep that in mind. Now you could ask how does the average A of t change as a function of time, i.e., dA over dt. Since every element here is a function of t, we need a rule now for how psi of t changes. So I will start with that because there are two ways of doing quantum mechanics at this stage. There is an active way of doing it which follows directly from this and its call the Heisenberg picture.

And there is another way of doing it which is called the Schrodinger picture which specifies what the state vector does as a function of time and these two are completely equivalent to each other because they will lead to exactly the same answer for these physical quantities. That is the consistency check. So without further ado, let me write the Schrodinger equation down here to show you how the state vector changes as a function of time. So we replaced dynamical variables by operators. We replaced Poisson brackets by commutators.

Next thing we do is we replace the phase space by the Hilbert space of the system. We replace knowledge of the phase space variables by knowledge of the state vector of the system. The phase space variables change with time classically according to Hamilton's equations of motion. The state vector changes as a function of time according to Schrodinger's equation and that is the input here in the Schrodinger equation.

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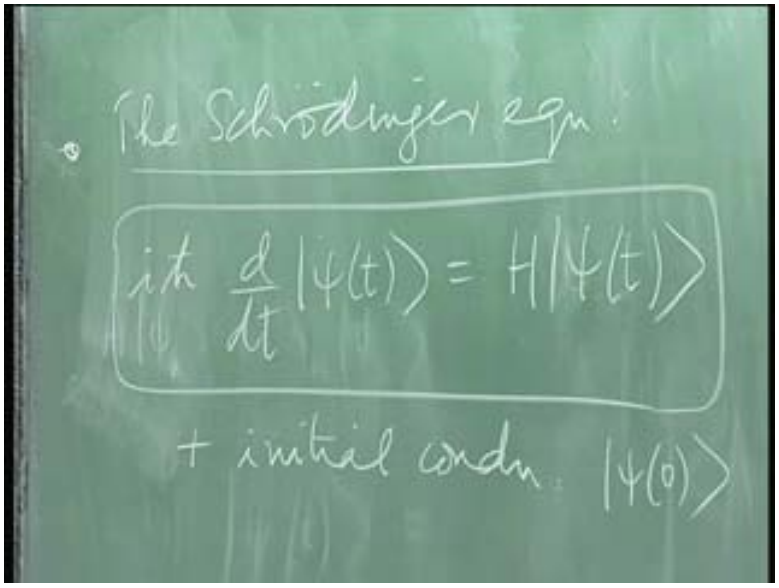

Schrödinger equation says ih cross d over dt on psi = H psi of t and it's a postulate. This is not an eigen value equation because this tells you we have to define what this (Refer Slide Time: 34:34) quantity is but intuitively we know what it is. It's the state vector at time t + delta t subtract the state vector at time t divide it by delta t and you get some other vector. This is given by the action of the Hamiltonian on this state so it takes you to some other state vector. After all this is an operator the whole point is this is an operator and it takes you to some other state all together. When we discuss eigen states of this operator, then we will see that this equation reduces to an eigen value equation but only for those eigen states. In general, it's a first order differential equation but an operator equation for vectors in a Hilbert space. Our task would be to see how to represent this Hamiltonian and solve physical problems here.

It's a first order in time. In principle if you treat this like an ordinary differential equation this together with initial an initial condition is needed to solve this equation. The unknown here is the state vector psi of t. so you have to specify state at some initial instant of time. It's an initial value problem. So we will assume that we know the state at some instant of time. We will see later how we have to specify the states along with initial condition psi of zero. If this H does not have explicit time dependence, this is an autonomous system.

Similarly if this H (Refer Slide Time: 36:49) is a function of just q's and p's, then it is very much an autonomous system. There is no explicit time dependence here in this H (Refer Slide Time: 37:02) and if I change t to (t + delta), d over dt doesn't change. So it's clear that this whole thing is time translation invariant. You could choose any instant as the initial instant of time, just as you could for an autonomous system. Now let's find the solution of Schrödinger equation. Then comes a question of whether it exists and it can be written in this form. So for the moment it helps to think of psi as a column vector in some vector.

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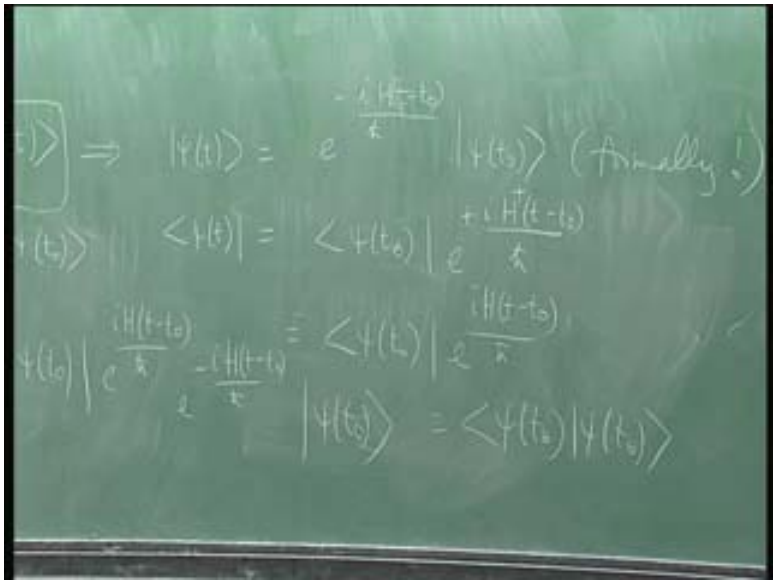

So the solution is psi of t equal to e to power Ht over ih cross. So let's put the i up and these results in e to the power - i Ht over h cross psi of 0. Please notice that you need to have a state vector at time t and therefore that initial vector is put on the right hand side and this operator e to the power minus i Ht over h cross acts on it from the left. So order starts mattering here in quantum mechanics. Suppose I choose some arbitrary number t_0. The solution becomes t - t_0 acting on psi of t_0. This is a formal solution. Now we know that Hamiltonian evolution preserves the volume in phase space. That was Liouville's theorem and that was one of the crucial inputs. So phase space flow in classical dynamics is like the flow of an incompressible fluid in real space.

The analog would have to again do with the probabilistic evolution. So this is just like saying here that points don't disappear from phase space. The fluid moves around and this volume element doesn't change. In exactly the same way, here too there is a conservation which operates. The norm will be preserved. So you can see that psi of t = psi of t_0 e to the + i H (t - t_0) over h cross. The i becomes - i but the matrix H must become H dagger and it acts from the right. H is Hermitian. It's the Hamiltonian of a system. So all the systems we are going to look at is assumed to be described by Hermitian Hamiltonians. When you include dissipation in quantum mechanics, then you may need Hamiltonians which are not Hermitian. The reason is dissipation would mean the energy is not conserved. Things would die down as a function of time, etc. But as long as the eigen values of the Hamiltonian are real, this can never happen. Damping would involve imaginary components and for the movement we look at systems with Hermitian Hamiltonians.

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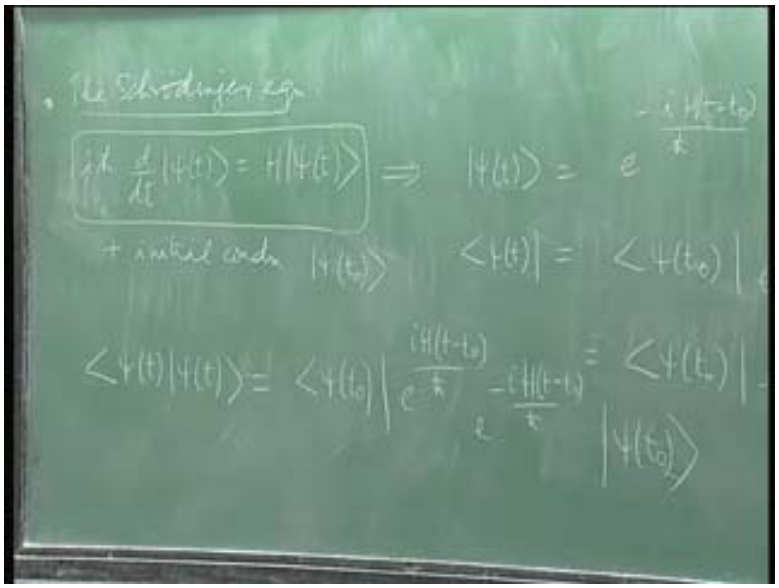

Therefore to write the norm, one can close one's eyes and put this(Refer Slide Time: 42:37) on the left and this on the right and you have psi of t_0 e to i H (t - t_0) over h cross e to the power - i H (t - t_0) over h cross psi of t_0.

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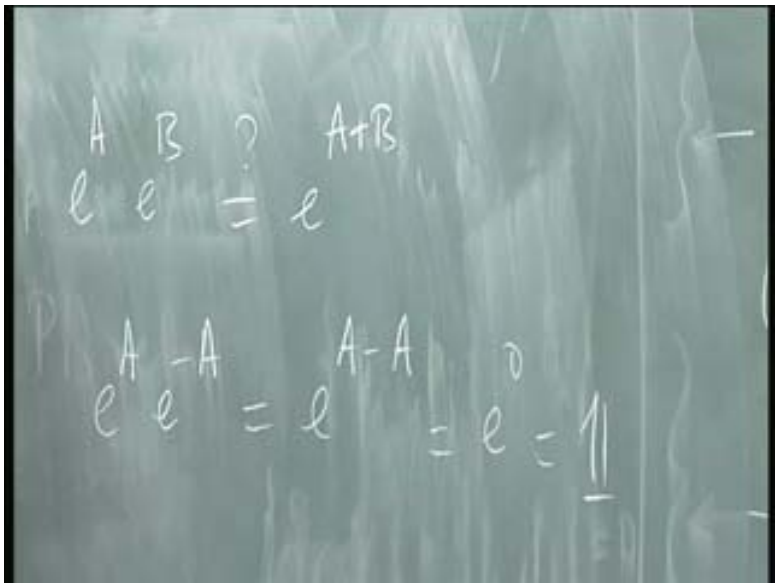

I have e to the A e to the B = e to the (A+B). This will be true if A and B commute with each other. This is a complicated formula and we are going to use this over and over again. But e to the A e to power - A = e to the (A –A) = e to the power 0= 1. This is certainly true because A and - A commute with each other. And of course if A commutes with any scalar multiple of itself and therefore e to the A e to power minus A is indeed one. And this (Refer Slide Time: 44:33) becomes a unit operator and therefore this gives us a preservation of norm. That's the analog of the Liouville theorem which says the volume element in phase space is preserved. Here the quantum evolution says the state vector preserves its norm as time goes along. That's a consequence of the fact that the Hermitian conjugate of this operator (Refer Slide Time: 45:06) is its inverse. It came out from that fact that the Hermitian conjugate of that operator was just the inverse of that operator.

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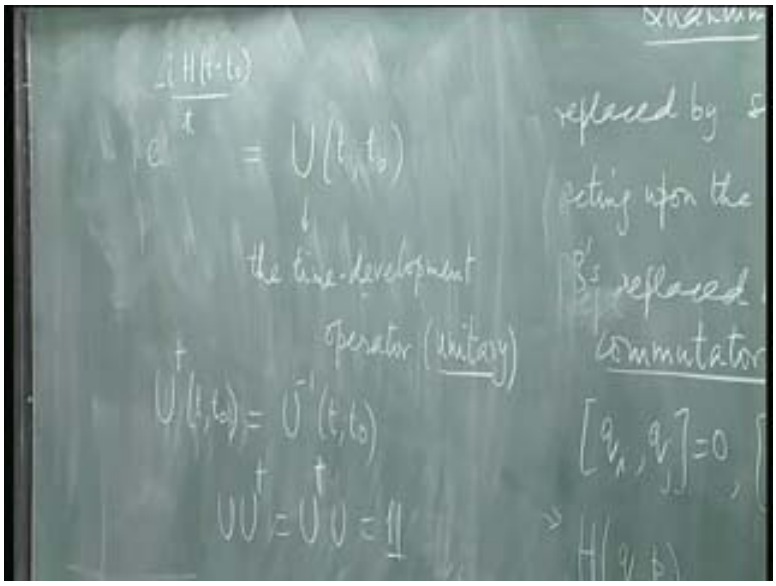

Let us consider the operator e to the power - i H (t - t_0) over h cross. Let's call it something lets call it an operator U of t, t_0. It depends on t and t_0 and happens to depend on difference in (t - t_0) in the simple case. And this operator takes the state of a system from what it was at time t 0 to what it was at time t. This operator is called the evolution operator or the time development operator. When I take its matrix elements, I will call it the propagator because that's what propagates you from one time to another.

The time development operator has some interesting properties as its stands. To get U dagger, I have to take Hermitian conjugate everywhere. So this (Refer Slide Time: 46:52) becomes + i and this becomes H dagger and of course these are real numbers and nothing happens to them. But H dagger is the same as H and therefore U dagger (t, t_0) = U inverse (t, t_0) or U U dagger is 1, which is the identity operator. I have just left out the time arguments for convenience. You call a matrix which has these properties as unitary. So the time development operator is unitary. It satisfies some important properties among which unitarity is first and foremost. The fact that it's unitary leads to the conservation of this quantity (Refer Slide Time: 48:06). If you identify this with the probability total probability then it says the conservation of probability follows from the unitarity of the time development operator.

So you find a time development operator which is not unitary. You know it's wrong so immediately you know that probability is not going to be conserved. So unlike classical physics where Liouville's theorem doesn't seem to play much of a role it just happened there that it was volume preserving evolution. At least in the elementary treatments it didn't seem to play a very fundamental role.

In quantum mechanics, on the other hand the unitarity of the evolution is very important and you have to keep track of that at all times. I will mention here that even if H is time dependent explicitly and the Hamiltonian changes from instant to instant while remaining Hermitian, the time development operator is not given by this (Refer Slide Time: 49:04) formula as you can see even in elementary differential equations, if this coefficient becomes a function of time then this is not exponential is not the solution you need some e to the power some integral and so on. The time development operator in those cases would continue to be unitary. We are going to look at some problems where it becomes explicitly time dependent.

For instance I take an atom and I switch an electric field on and off. Then of course it's a time dependent Hamiltonian and I need to know what the time development is. This operator has the following property.

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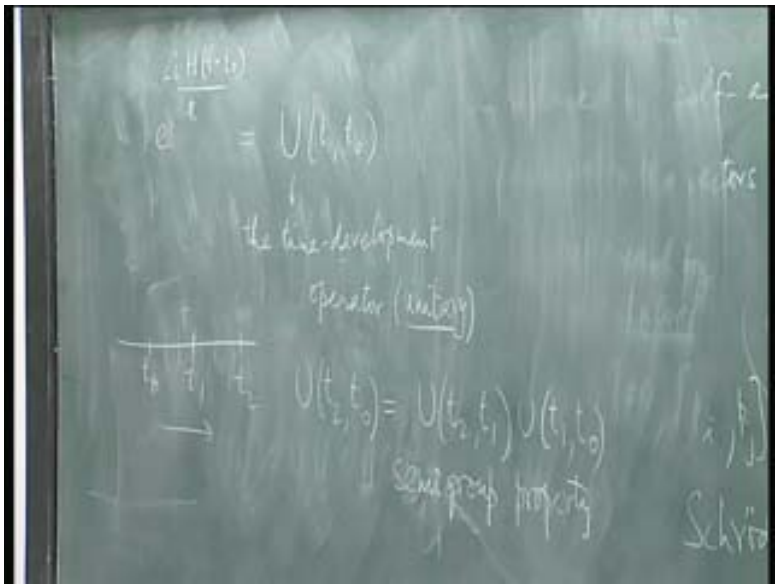

In time, suppose this (Refer Slide Time: 49:55) is an instant t_0, this is the instant t_1 and this is the instant t_2, as time elapses this direction, then you could ask what is U of t_2 , t_0 equal to. And its immediately clear from this exponential structure that it is equal to U of t_2 , t_1 and U of t_1, t_0 in that order. The order is important. Of course here (Refer Slide Time: 50:23) there is the Hamiltonian which is time independent so it doesn't really matter but in general, once again you have to keep track of this.

U (t_2, t_0) says that the system propagates from time t_0 to time t_2. The state evolves from time t_0 to time t_2. If there is an intermediate time t_1, then this evolution operator which describes the evolution from t_0 to t_2. So it goes from t_0 to t_1 first and then it starts at t_1 and goes to t_2 in this order. You can't interchange these orders except in the simplest of cases and this is called a semi-group property. It's called a semi-group because you know when

you have a set of elements and you multiply them together over a time, you get more elements and that forms a group. But here the order of multiplication is important. It's a semi-group it doesn't happen the other way. I emphasize this because even when the Hamiltonian is time dependent, this would still happen. Let me point out what would happen if the Hamiltonian is time dependent. Well it's a much harder problem.

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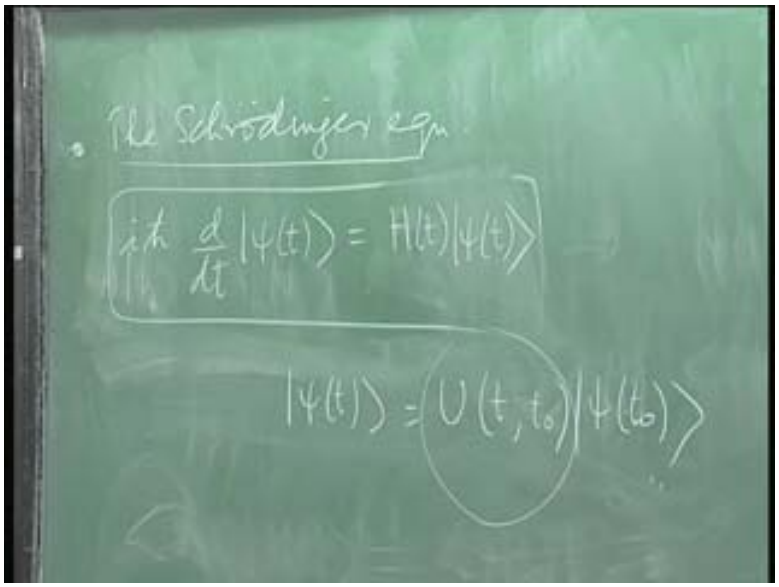

If the Schrödinger equation were given as equal to H of t, psi of t, then the solution is highly nontrivial.

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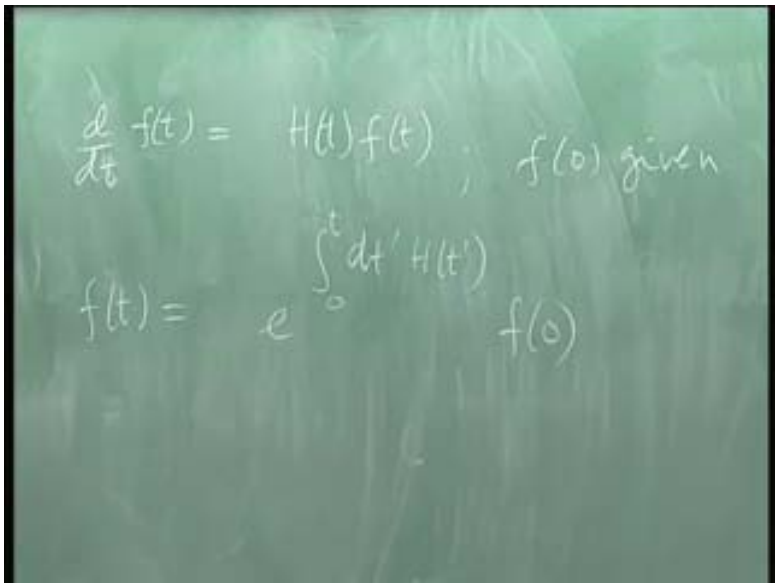

Let's look at it classically. You have d over dt, some f of t = H of t, f of t. Suppose f of t is just an ordinary function, you have an equation of this kind. If H were a constant, then you write e to the power Ht and that's the end of the story. But what's the solution now given initial condition f of zero. f of t = e to the power integral 0 to t, dt prime, H of t prime, f of 0. That's the solution. Of course if H is time independent, this integral just becomes t. but otherwise this is the solution to this differential equation.

To verify this solution, you differentiate and then you have to find the derivate of this (Refer Slide Time: 53:33) quantity as a function of t. you then use this famous formula for differentiation under the integral sign. It is not a solution for this problem here and the reason is this is a summation. So it's like writing e to power H at one instant and the following instants and adding them all up. There is no guarantee because of this property e to the A, e to the B is not e to the (A + B).

Because H, at one instant of time may not commute with itself at another instant of time. Then you immediately run into problems. So this is not the formal solution. When we look at time dependent Hamiltonians, I will point that out. But the evolution still is unitary. Its still is true that you can write psi of t as U of t, t_0, psi of t_0 with this (Refer Slide Time: 54:58) being a unitary operator with the semi-group property. It is a much more complicated formula it's called a time ordered exponential and we will look at that a little later. So the formal solution to the Schrodinger equation looks fairly simply but it's not all that simple because it involves exponentiation of the Hamiltonian and this is always a nontrivial task. You have to take a matrix and exponentiate it which is simple. But if you take a differential operator and exponentiate it, it becomes much more complicated. So that's the basic problem in quantum physics that you need to find the exponential of the Hamiltonian. But that is nothing new because even in classical statistical physics or in any statically physics,

you have to find e to the power - beta H. So exponentiation of the Hamiltonian is in fact the fundamental problem both in equilibrium statistical physics as well as in quantum mechanics and it continues to be case in quantum physics theory. This is the reason for the mathematical commonality that you need to exponentiate the Hamiltonian theory. What I will do next time is to start with this equation here and show you why the Hamiltonian plays such a fundamental role it's called the time infinitesimal generator of time translations and we will see why it is so fundamental.

It's analogous to what it does in classical physics but in quantum physics, there is an even more fundamental role because it really controls the entire state of the system as you can see and we will see why. We still have to make contact with the classical Hamilton equations and see what are they are going to be replaced by. We replaced it by the Schrodinger equation but I would like to show that for physical observables there exist differential equations called the Heisenberg equations of motion. They are true analogs of the Hamilton equations of motion.

Thank you!