Nonequilibrium Statistical Mechanics
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Lecture No 06
Linear response theory (Part 1)

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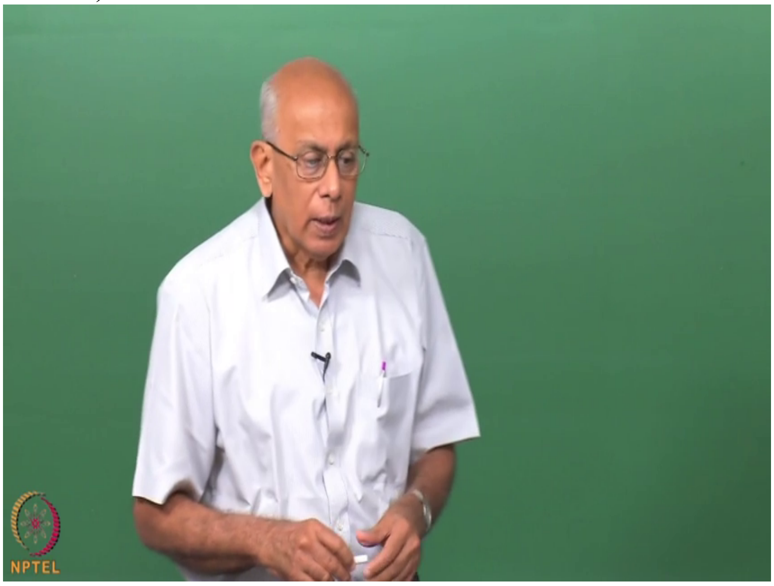

In the last lecture I made some preliminary remarks about linear response theory, a topic which we will study in some detail and today I would like to set the stage for it by discussing how time evaluation can be viewed, of dynamical observables can be viewed both in classical and quantum mechanics in a kind of unified manner at least as far as the formalism is concerned and then we can proceed with linear response theory itself.

Now remember that our target in linear response theory is to try and understand how observables change with time to first order of perturbation under finite temperature conditions in general, so both in the presence of thermal fluctuations as well as in external perturbation, we would like to find out how dynamical observables change on the average under this perturbation to first order in the external force or perturbation.

Now it turns out to be extremely convenient to recast the usual Hamiltonian dynamical evolution in terms of the operator called the Liouville operator, the advantage of which we will be that we have at least formally way of writing dynamic evolution which is independent of whether the system is classical or quantum mechanical.

So let's start with the following observation and I will do both the classical and the quantum mechanical evolution kind of side by side so you begin to see what the commonalities are. Although of course we know the classical dynamics and quantum dynamics are very different things altogether, so time evolution and the Liouville operator is L, Ok...

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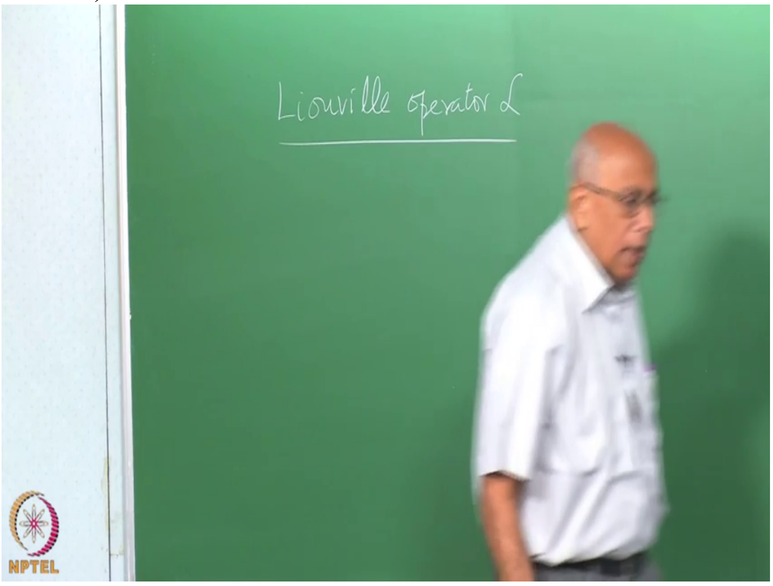

We shall have in mind always the Hamiltonian system. So the evolution we are talking about is Hamiltonian evolution and the Hamiltonian as you know is function of set of generalized coordinates and generalized momenta, conjugate momenta. In classical physics we would write this as Hamiltonian H of q comma p where I use q and p

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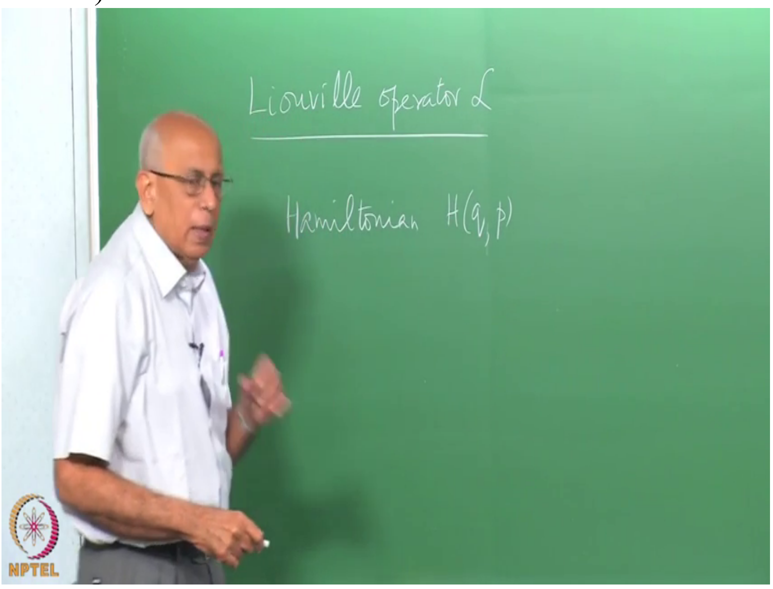

as symbols to stand for full set of generalized coordinates and the full set of corresponding conjugate momenta.

And as you know in classical mechanics, I use the abbreviation C M the evolution of this dynamical variables is given by Hamilton equations. So you have q dot is delta H over delta p and p dot is minus delta H over delta q, Ok and

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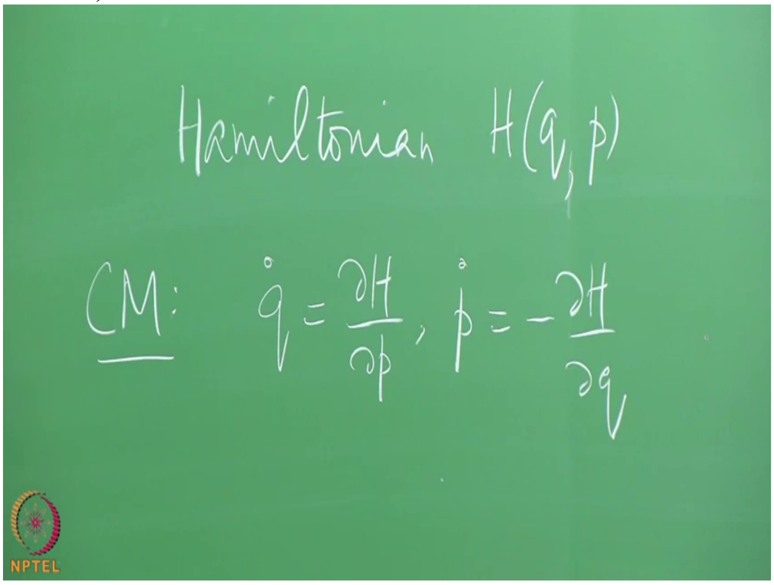

in principle, in principle if you specify the initial values of all the qs and all the ps, one is supposed to solve this set of equations to get the values of q and p at any arbitrary instant of time.

So for instance the solution of this would be q t at time t will be some function of the initial values q naught p naught and of course time itself

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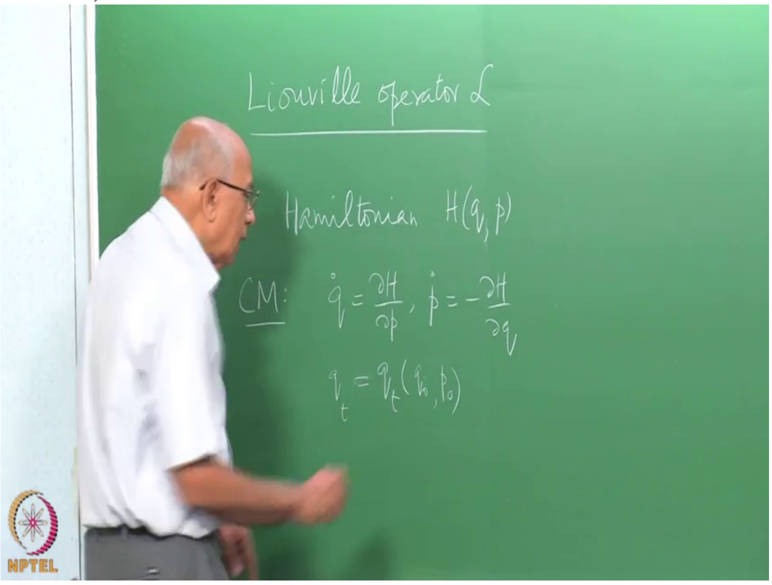

and similarly for p, some t this is p t of q naught and p naught. So given the initial

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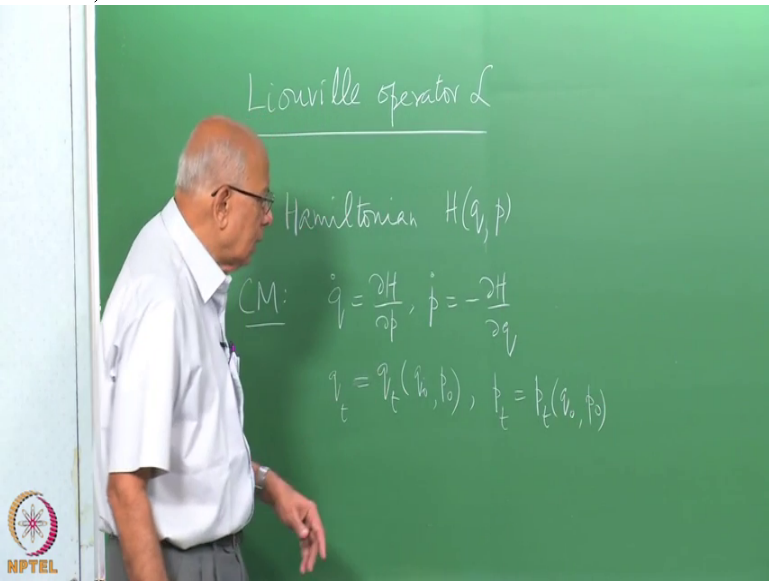

conditions, notionally one is supposed to solve the equations so that you can write what the qs and ps are at any instant of time subsequent to that, Ok.

Quantum mechanically this is not how things go. Quantum mechanically this becomes an operator so in Q M, you again have a Hamiltonian operator q and p.

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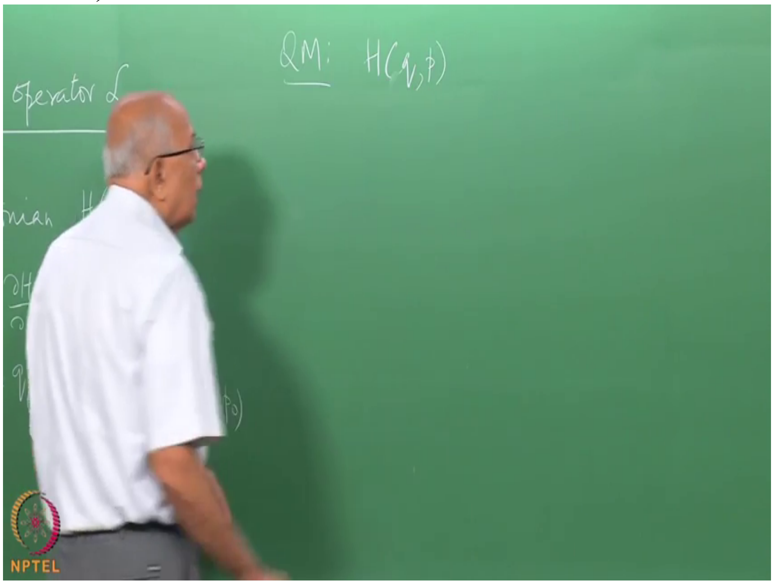

I won't bother to write operator symbols on all these objects but it is understood to be the case and then one asks, what is the equation of motion is for any dynamical variable, any function of all the qs and ps

For instance if you had some function a of qs and ps, then observable which is the function of the qs and ps, then we know that Heisenberg equation of motion says i h cross d A over d t is equal to the commutator of A with H.

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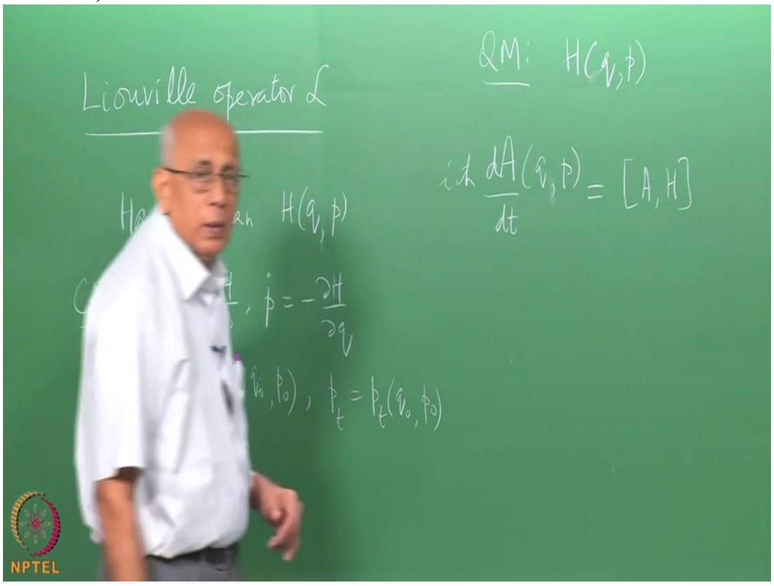

Classically the analog of the Heisenberg equation of motion of course, is the equation for the Chang variation of any A which is a function of q and p, this quantity is equal to the Poisson bracket of A with H.

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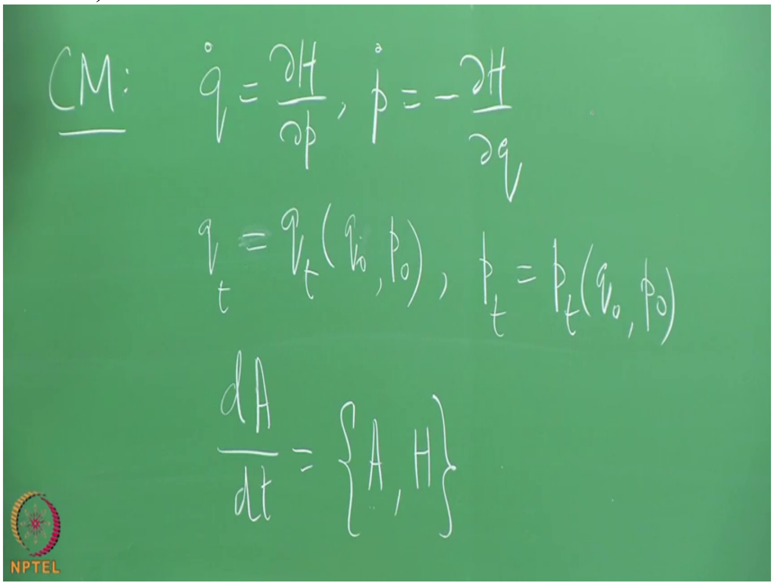

So this is the active picture of quantum mechanics where we say that the observables are changing with time and the time rate of change is given by this Heisenberg equation of motion which is the quantum analog of this equation of motion in terms of the Poisson bracket here, Ok.

Now is there some way in which we can write both these equations in exactly the same form? The answer is yes. So we introduce an object called the Liouville operator L which says that d A over d t in this case, is equal to i times L in C M and Q M. In both classical mechanics and quantum mechanics

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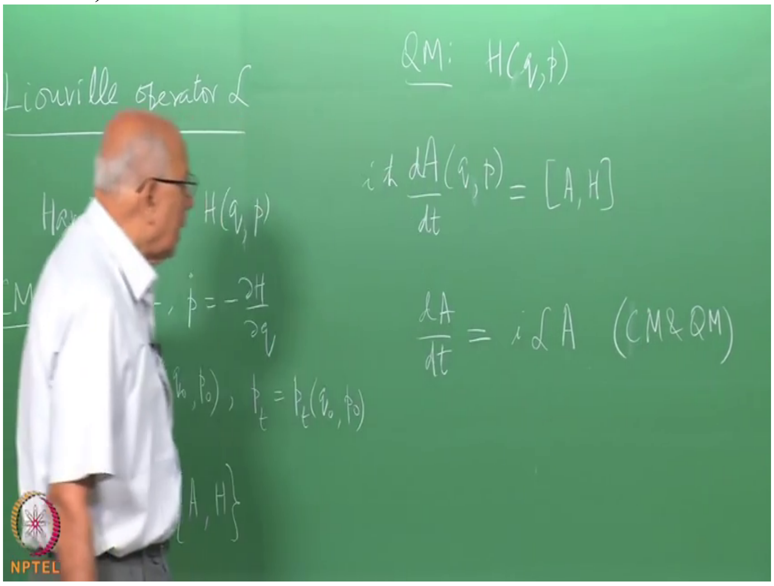

we write it in this form.

Because you can see here that the equation is linear in A and it is linear in A here too, so one could write it in this form with an i here for a purpose which will become clear in a few minutes. And this operator L is called the Liouville operator. By definition this i L A is equal to A Poisson bracket with H out here, so it is immediately clear that L acting on any A is equal to, I bring the i down out here to write d A over d t is i L A.

So I want i L A to be A with H and therefore L A is A with H divided by i and I get rid of a minus sign so it is i times H with A. This is true in classical mechanics and the quantum analog of this is again from this equation.

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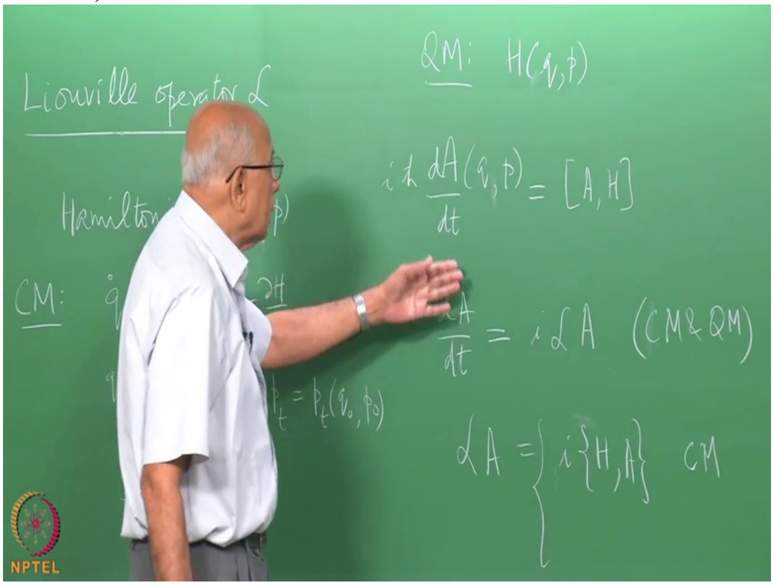

I write this as i L A on the right hand side and therefore, in quantum mechanics, d A over d t equal to A H divided by i h cross and if this is equal to i L A then it says

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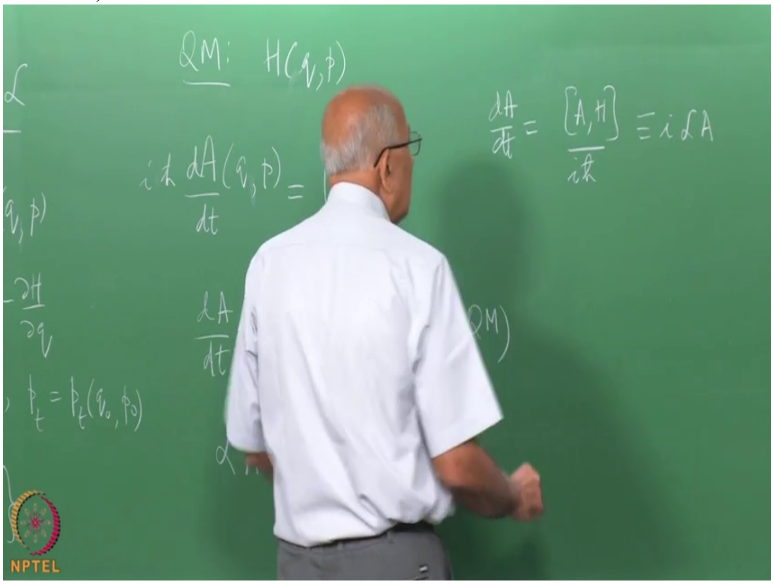

L with A is equal to 1 over whatever it is.

So L with A is equal to 1 over h cross, Poisson bracket of, commutator of H of A, quantum mechanics. So formally I introduce

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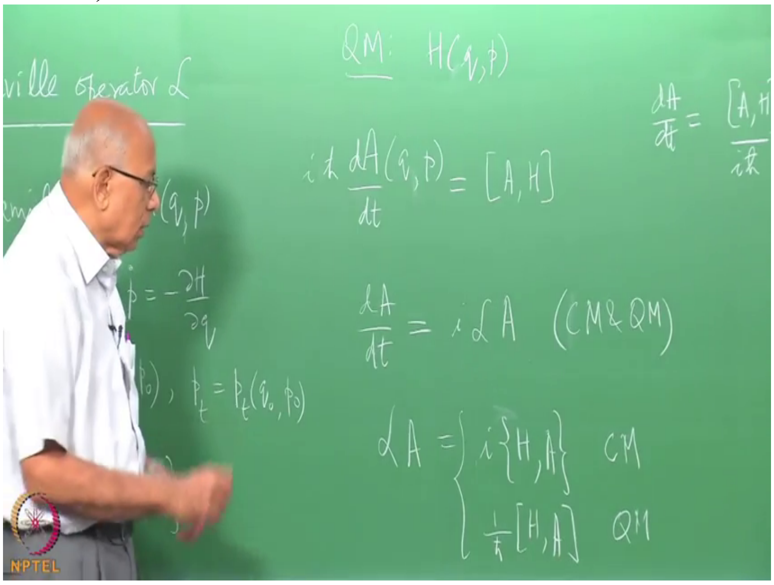

a super operator, this L should be regarded in quantum mechanics as a super operator because it says you perform something, you take the operator A which acts on state vectors in the Hilbert's space concerned and what you do is when L acts on this operator A it is the same thing as commuting H with A, A with H in this fashion, Ok.

So once we have this written down in this form then the formal solution to these equations, the formal solution is like this. Formally A of t equal to e to the power i L t A of zero. That's what this equation says

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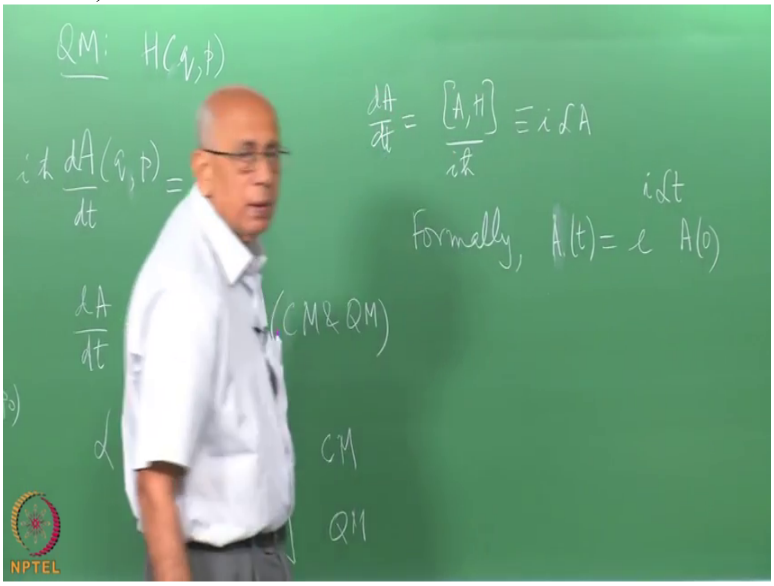

here. What do I mean by A of zero?

Well, you already familiar with this in quantum mechanics more than in classical mechanics. Because we are working in the Heisenberg picture here and as you know the solution to this, this thing explicitly is simply that A is a Schrodinger picture operator and this fellow is equal to, for instance e to the power i H t over h cross A of zero e to the minus i H t over h cross in quantum mechanics.

That's the formal solution

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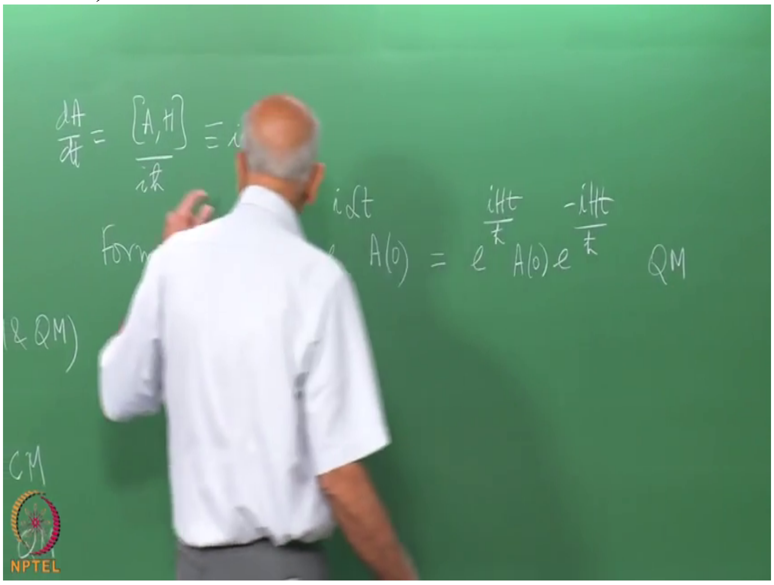

to the Heisenberg equation of motion. So it is really saying, now you see why it is a super operator, it says either the i L t acting on the Schrodinger picture operator A of zero is equal to operating with this operator on the left of it and that operator on the…, it is conjugant, unitary, its Hermetian conjugate on the right of it, Ok.

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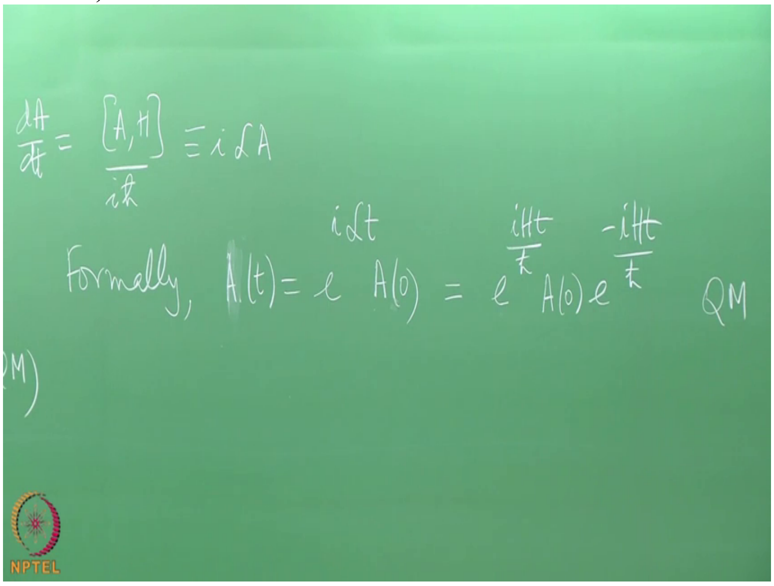

In classical mechanics, in classical mechanics, the formal solution to this equation would again be, this is Q M, so in classical mechanics it would correspond to saying that A of t which is really A q t p t where you are supposed to solve the Hamilton equations of motion for the qs and ps and then substitute those as the arguments in this A.

So by definition, I call that A of t, this quantity here is again equal to e to the i L t A of zero, oh this is the function of q zeroes and p zeroes here.

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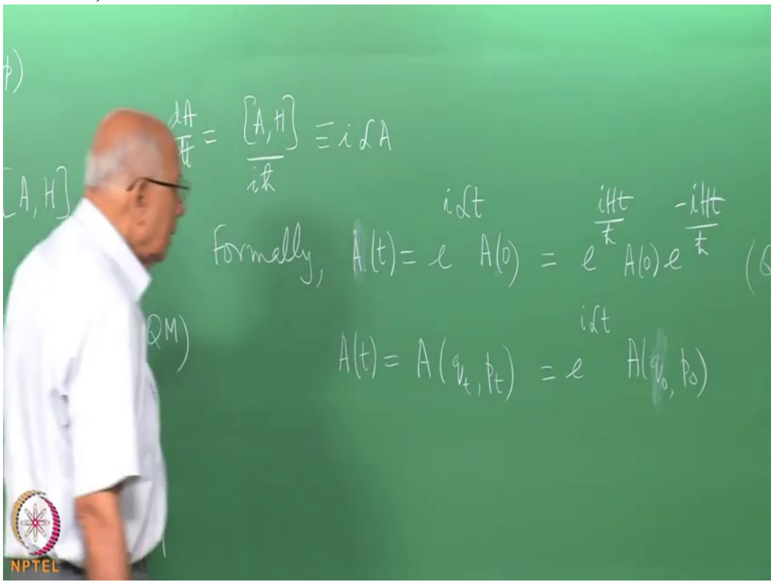

And by this I mean the exponentiation of this Poisson bracket operation.

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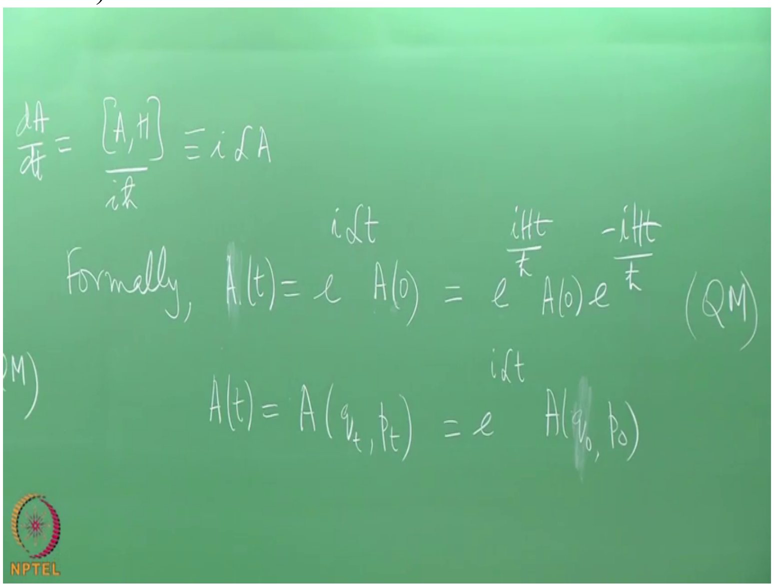

So that is why it is so formidable looking in classical mechanics because you are supposed to take this operation, the exponential of a Poisson bracket and act on that, of the Poisson bracket operation and act on this function here.

So in principle one can write the solution down formally very simply but in practice it is very complicated as you can see. Whatever it is, the properties we are going to need in what follows are that L, this thing here is a Hermitian operator and once you established that it is a

Hermitian operator then matter becomes, matters become very simple because the exponential of i times the Hermitian operator is a unitary operator.

So, while we are familiar with the fact that Hamiltonian evolution in quantum mechanics with a Hermitian Hamiltonian is a unitary evolution, in classical mechanics that is not so familiar in this language but it is still a unitary evolution all the same in a sense which would become clear. So let me first try to establish that this L is a unitary operator, is a Hermitian operator both in classical and in quantum mechanics, Ok.

Now as you know when you define, when you have a Hilbert space and you want to define a Hermitian operator on it, you would like the following. So we are going to establish the Hermiticity of L, in both classical and quantum mechanics,

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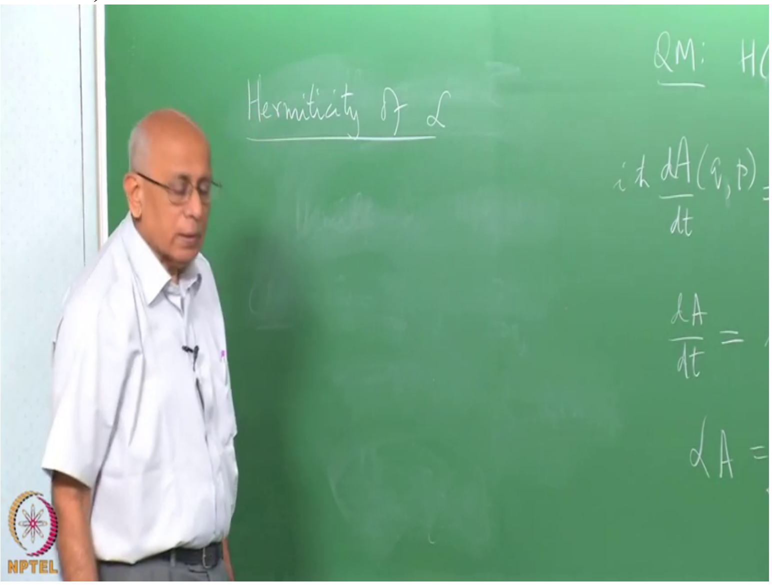

Ok. Just to remind you in quantum mechanics in the usual cases when you have a linear vector space with element psi, phi and so on which are ket vectors, then you would say that an operator is Hermitian, so let me, this.

If for any pair of

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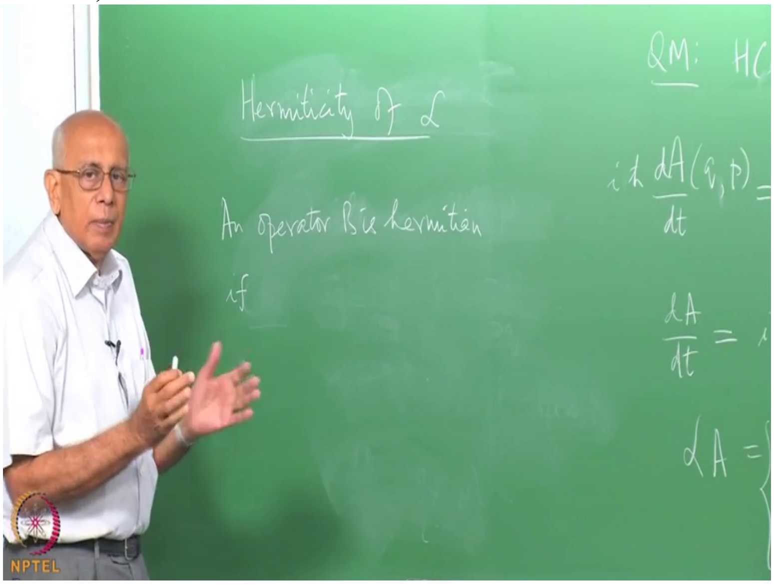

elements of the space, Hilbert space you have d psi on phi equal to psi d phi, where this is an

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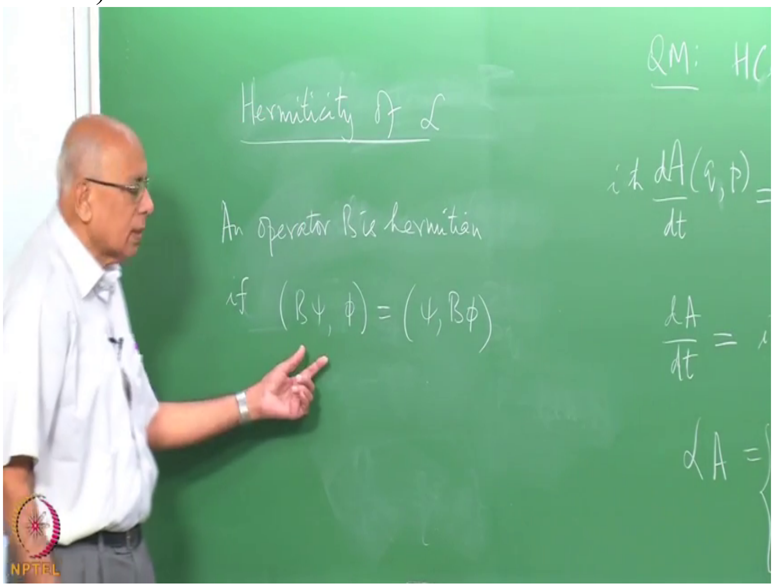

inner product defined in that space. Now we have to answer 2 questions right away. What do I mean by scalar product or

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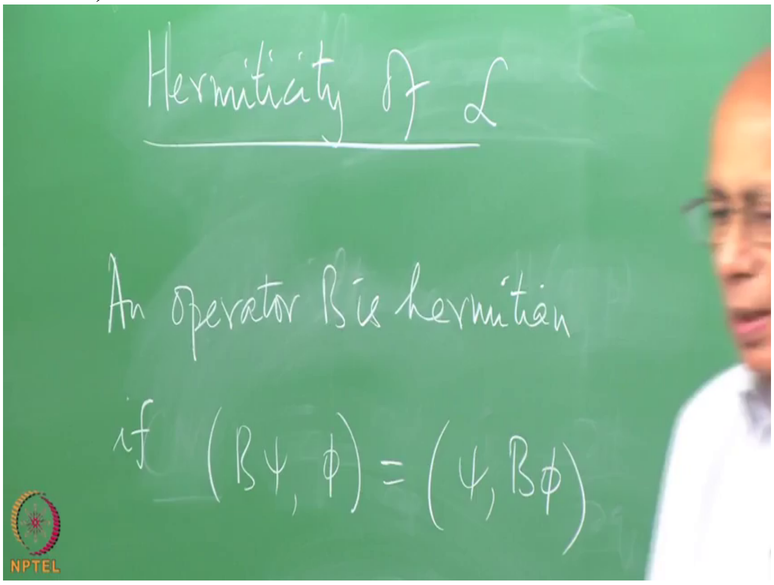

inner product of, in a, from space of operators? Because remember in quantum mechanics we are talking in the Heisenberg picture so the elements are actually observables, they are operators. So first thing I have to do is define a suitable inner product, the proper inner product definition for operators and I have to do the same thing in classical physics as well, Ok.

In classical physics matters are little simpler because my dynamical observables are functions of the phase, of the independent phase space variables here. So they really are space of functions. In quantum mechanics we have a space of operators. Now how do I define an inner product in this and once I do that, then I would impose this condition to show that an operator like L

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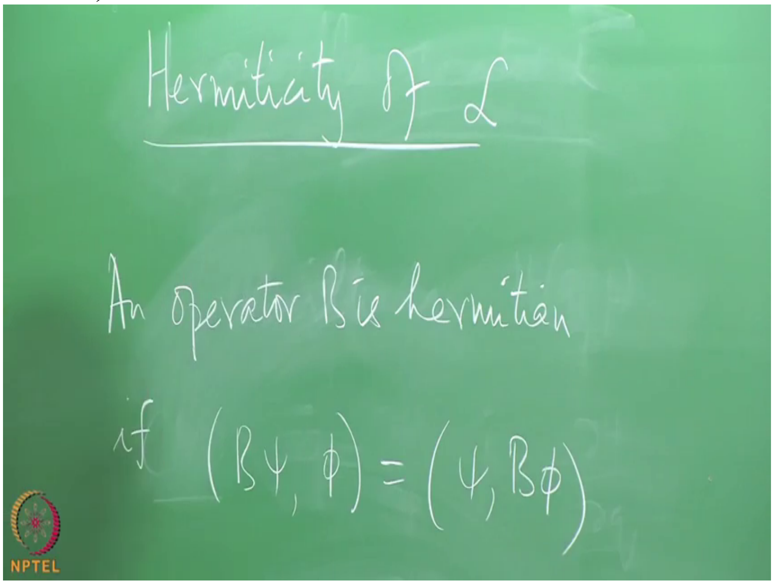

is a Hermitian operator.

So what's the definition of an inner product here? So let's do classical mechanics. The observables in this problem are functions of phase space. So let's call these functions f of q, p, g of q, p and so on. And then

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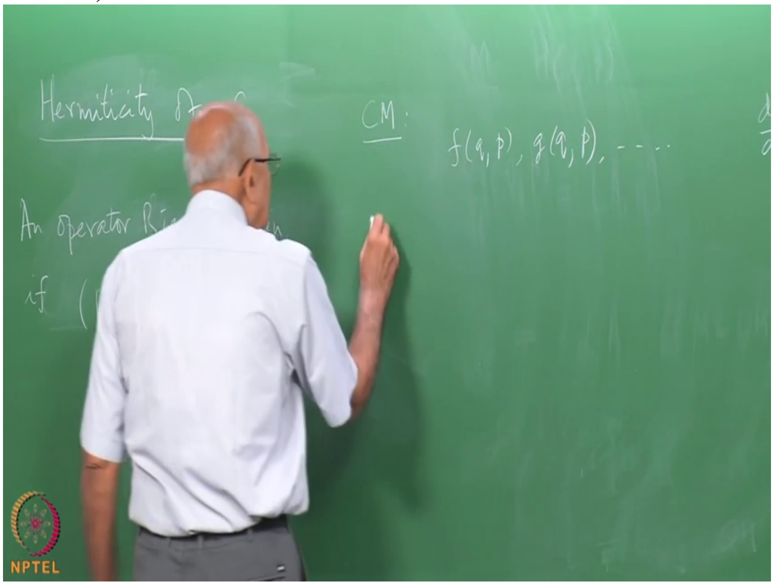

the natural definition of the inner product f with g is a summation or an integration over all the independent dynamical variables d q, d p, f star of q p with g of q and p. That's the definition.

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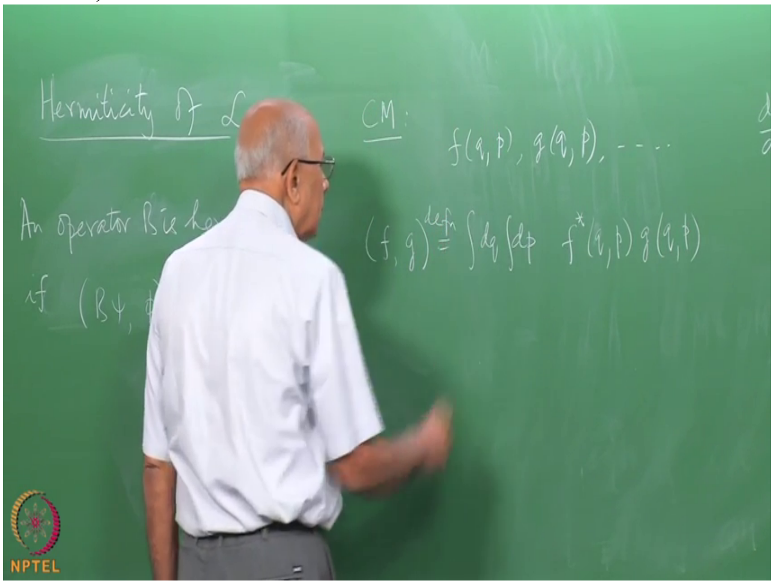

So it's a normal, usual kind of function space

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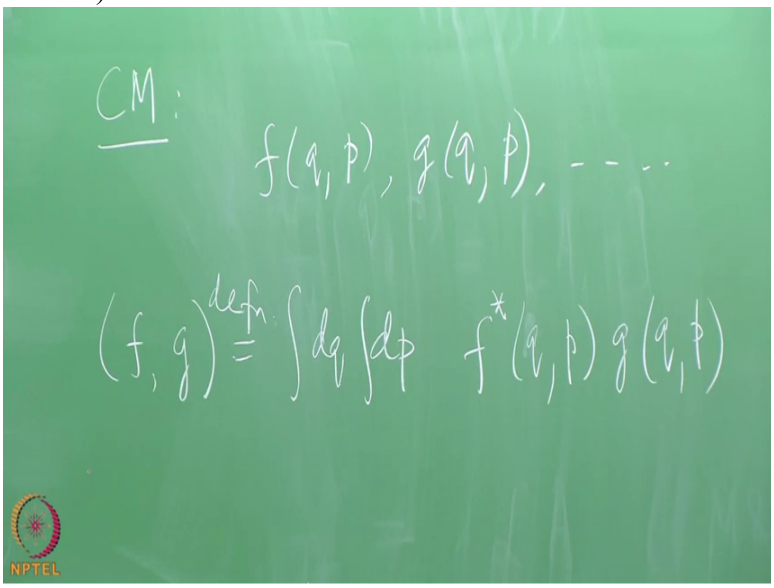

and in this function, for instance the same sort of thing applies when we talk of wave functions in quantum mechanics. They are representatives of the state vectors in some basis like the position or momentum basis and then you impose inner product or the scalar product of two such states, by, in the position basis by integrating over all positions f star g.

But here we are talking classical mechanics in phase space so q and p are both independent observables and therefore the definition involves an integration over all q and p in this fashion. We need the corresponding definition in the space of operators in quantum mechanics and here is what it is.

So in quantum mechanics, the inner product of 2 operators A B by definition, remember these are operators which act on a Hilbert space of states, of state vectors and you can find the basis set of vectors in that Hilbert space. Then the inner product is defined as the trace with respect to that basis or any basis of this quantity A dagger B.

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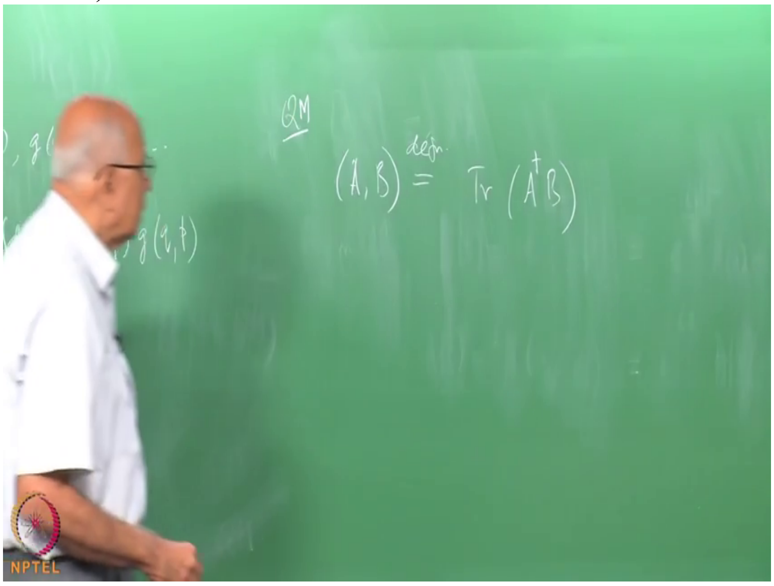

This has all the required, desirable properties of an inner product. One can check that these inner products have, satisfy whatever is needed from inner product in linear vector space theory, Ok.

Now given this, we have to establish that this operator L is a Hermitian operator namely it satisfies this condition, Ok. So let's do that. In classical physics we therefore had to show that L times f g must be equal to, I put a question mark here, we need to show this, must be equal to f with L g.

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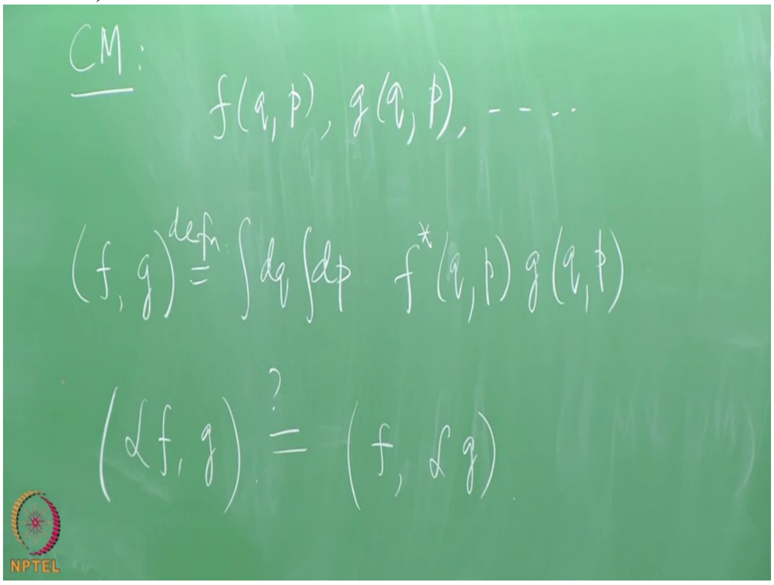

That's what has to be shown.

And out here, we have to show that L is a Hermitian operator which means that we need to show that L A with B is equal to A with L with this definition of the inner product.

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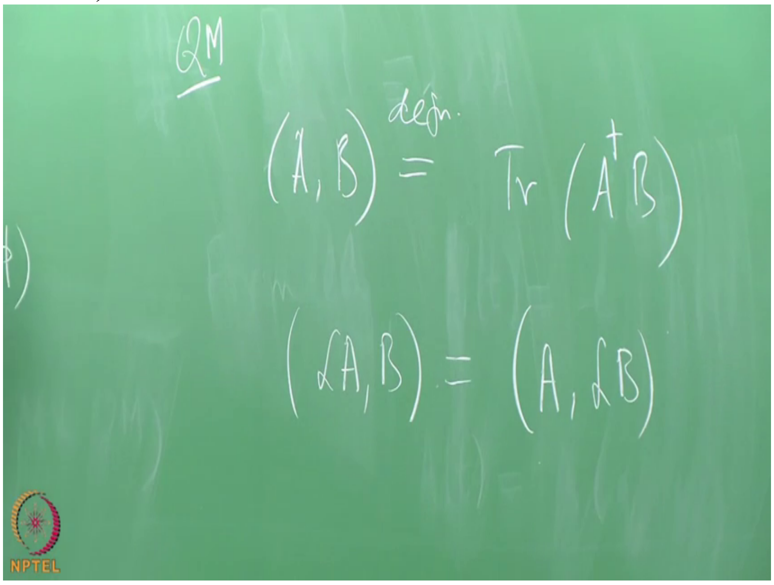

And if we do that, then L is a Hermitian operator and e to the power i L t which governs time evolution both in classical and in quantum mechanics is a unitary evolution with conservation of probability and so on, Ok.

Now let's start with this, we would like to show this. Let me do that by the following, so f with L g is equal to integral d p, d q, integral d p, f star of q and p, L with g, but remember that L with g in classical mechanics,

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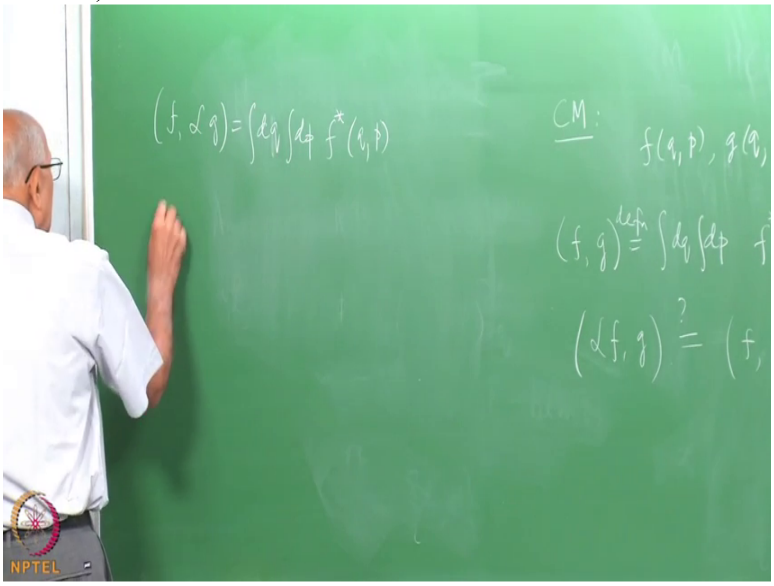

L on g is equal to the i times the Poisson bracket of H with g. That was our definition

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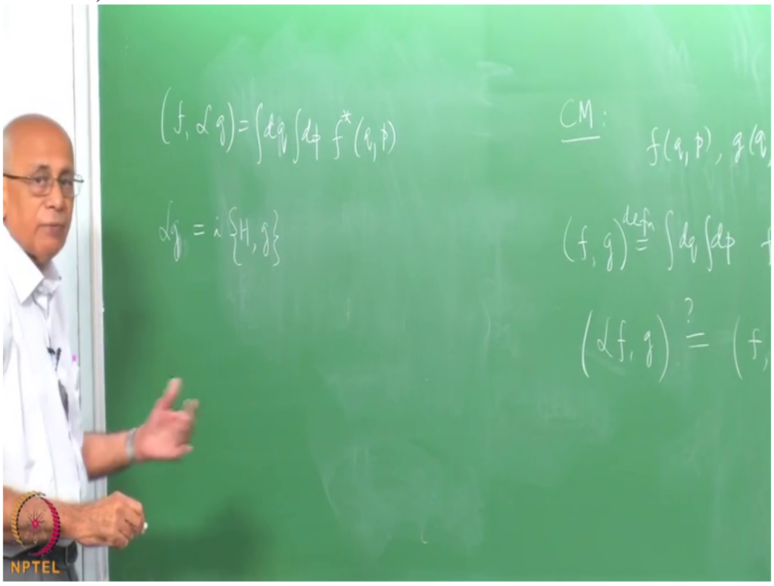

of L times g.

So we need to put that in here and you are going to get an i outside,

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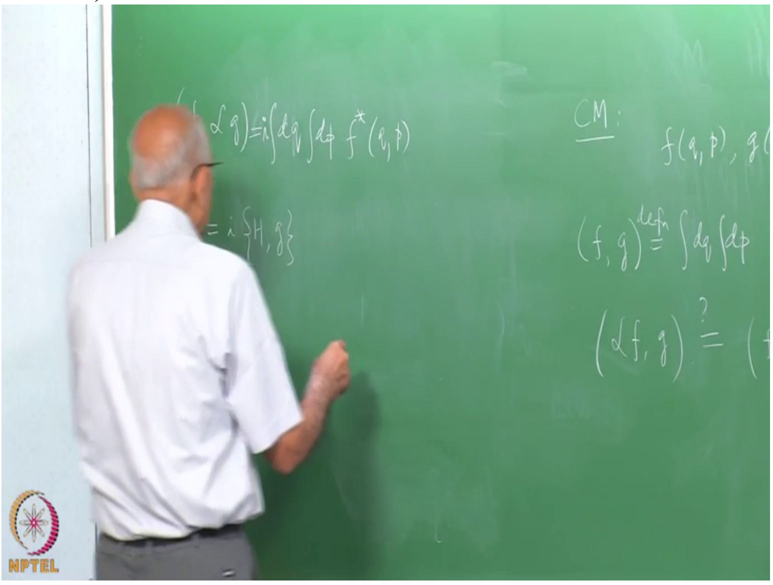

the Poisson bracket of H with g which is equal to delta H over delta q, delta g over delta p minus delta H over delta p delta g over delta q, Ok. This is over all the phase

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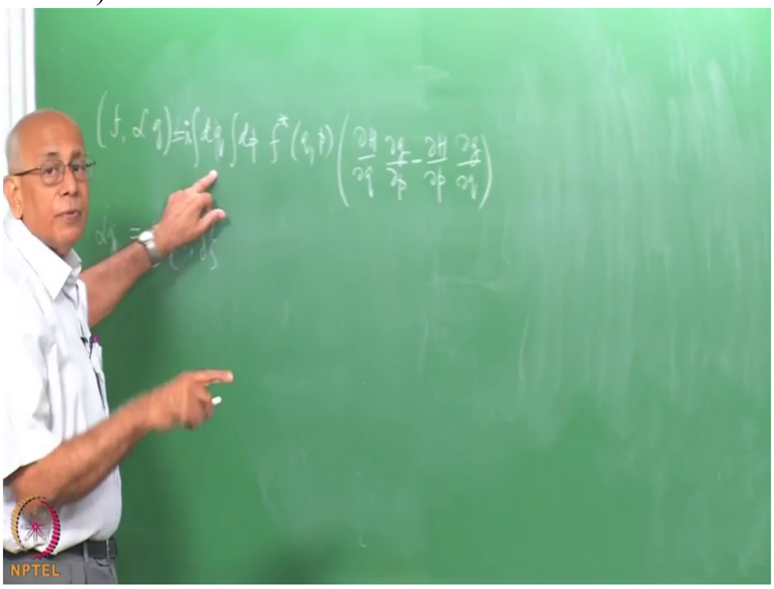

space, n degrees of freedom, on all the n qs and n ps and let's assume the simplest case that all the qs and ps run over the entire real line namely minus infinity to infinity in all the variables, although it is not important in this case.

So this thing here becomes equal to i times, in the first integral integrate over p. You use this fact to integrate over p. So you have a d q but then inside you have, let me not use a curly bracket because it is confusing, f star of q p delta H over delta q times g so let me not write the arguments of these functions, f star delta H over delta q times g. I have integrated over p, so that's gone. And I have this over the boundary values.

So limits in p, so let me notionally write this as p equal to minus infinity to infinity, the boundary

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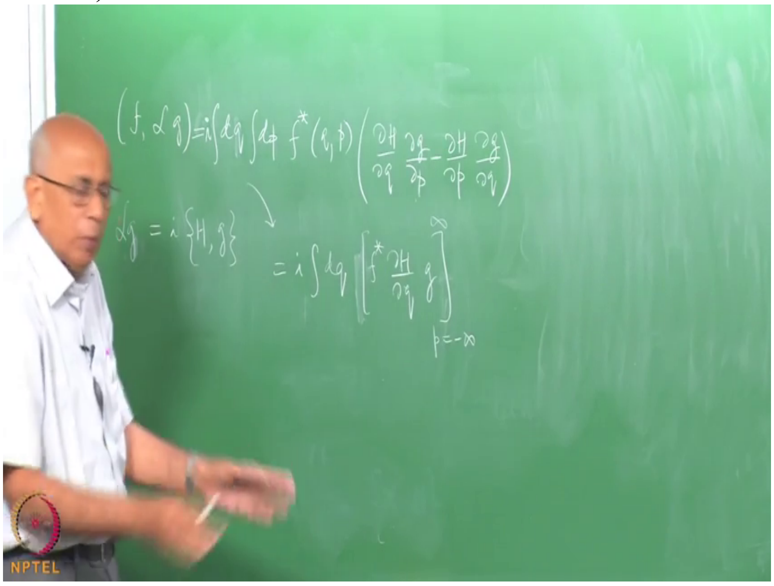

points the range of p Ok, minus, I know the whole thing is inside the bracket, minus integral d p, that's still sitting there and then the derivative of this thing with respect to p. So we have, this thing has been integrated.

So we differentiate this, delta over delta p of delta H over delta q times g, 0:20:43.0 f f star sorry, derivative of f star, that is this thing, delta H over delta q and then a g, because that's been integrated over. So much for the q integration of this term.

And in this term, do the integral over q. So you are

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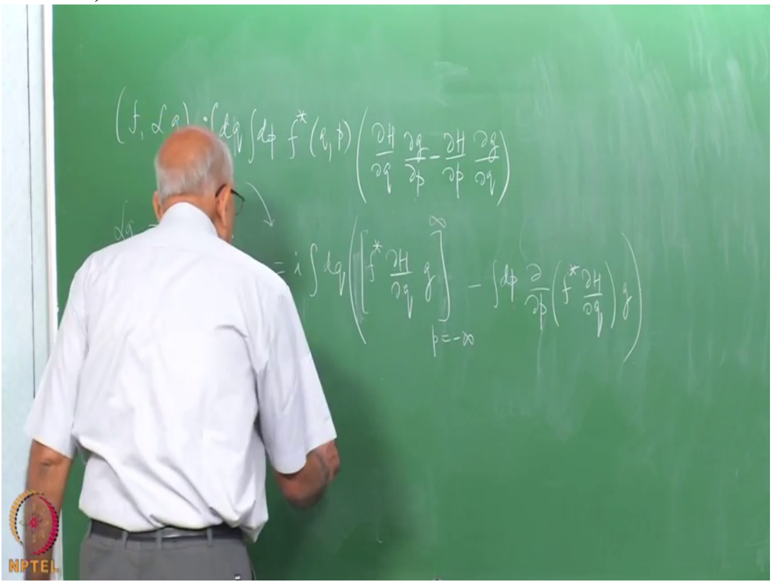

left with minus i times integral d p and then a boundary term which is equal to f star delta H over delta p, this time it still remains, times g, I should write it like this, q equal to minus infinity to infinity, minus and now comes the integral again over q, delta over delta p since we integrate it over q in this term, so differentiate with respect to q, sorry, q differentiate f star delta H over delta p and then multiply it by g and put a bracket outside, ok.

Now we

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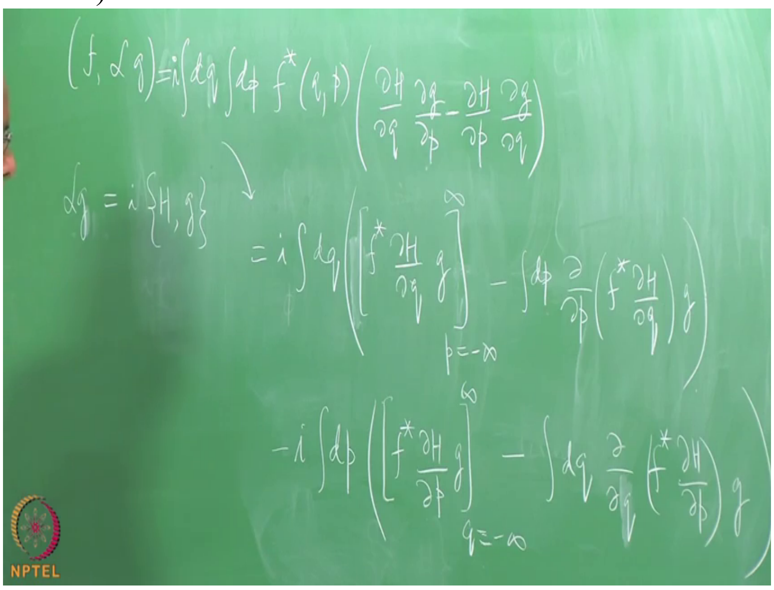

expect our functions to be normalizable functions, to be well-behaved, to be member of some function space perhaps, L 2 or something like that. So the functions, these things would vanish at spatial infinity, plus or minus infinity both in p and in q in all the variables. So the surface terms drop out in normal conditions and you are left with

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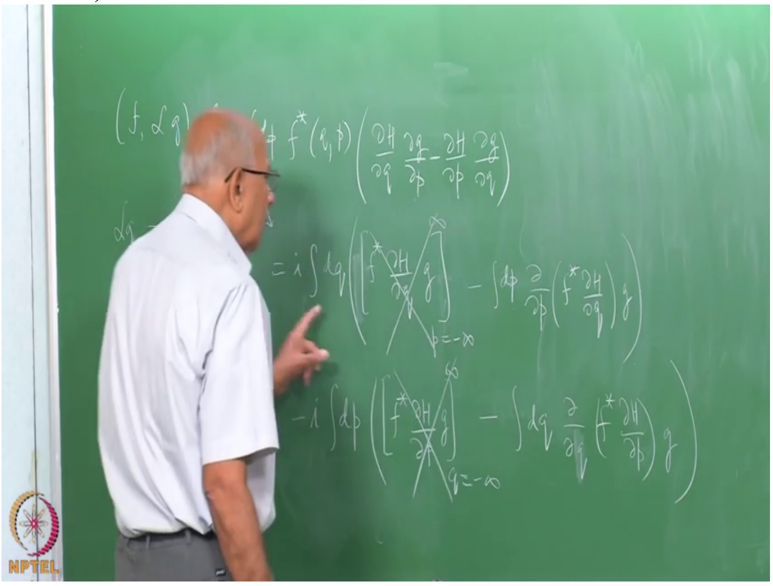

this term and this term.

And of course here you can see, if I differentiate this, I get delta f star over delta p delta H over delta q and then a second term which is equal to f star times delta 2 H over delta p delta q. But exactly the same term appears when I differentiate this term here with respect to q. And those two cancel out because there is a minus sign, Ok. So I might as well replace this term by delta p, delta f star over delta p delta H over delta q. So I am going to write it like this.

And the

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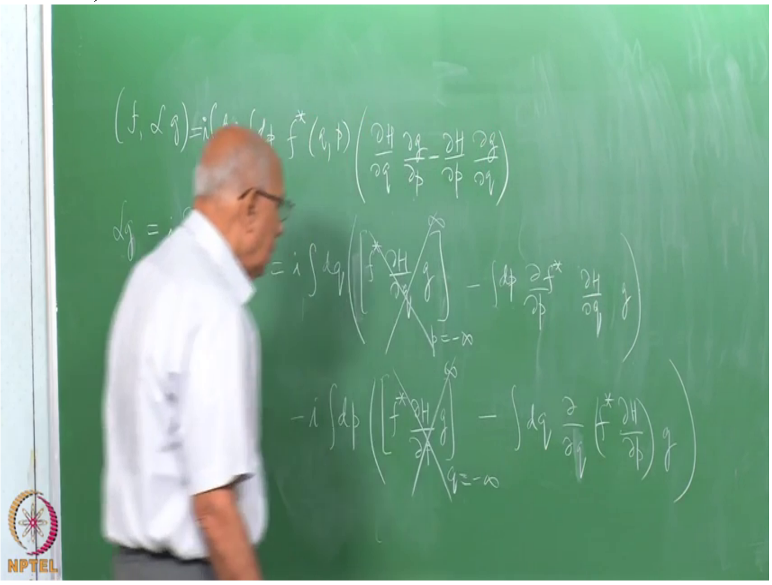

same argument applies here and this is delta f star, this is delta H over delta p times g in this fashion. And you are

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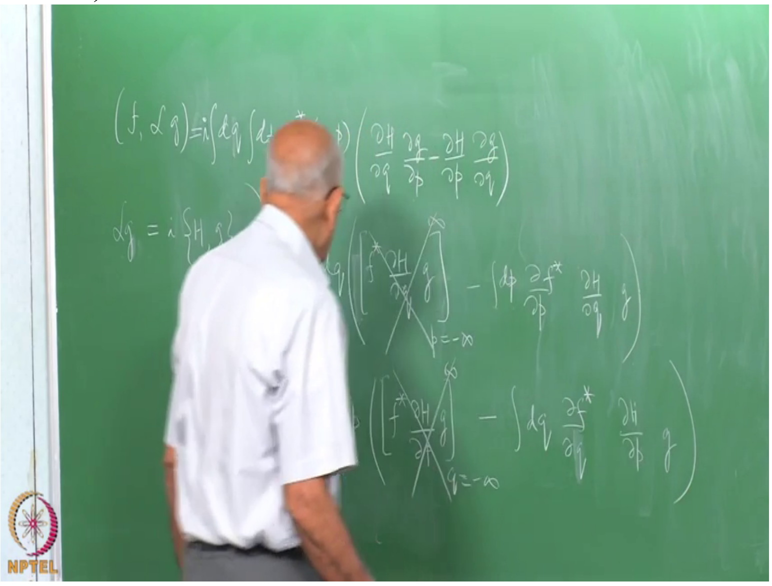

left with this minus that and as you can see, this is straightaway equal to i times an integral over d q, integral over d p 0:23:36.2 and then you have delta star over p, H over q with a minus sign and with a plus sign you have f star over q, H over p.

So it is equal to the Poisson bracket of f star with H. And then there is a g outside.

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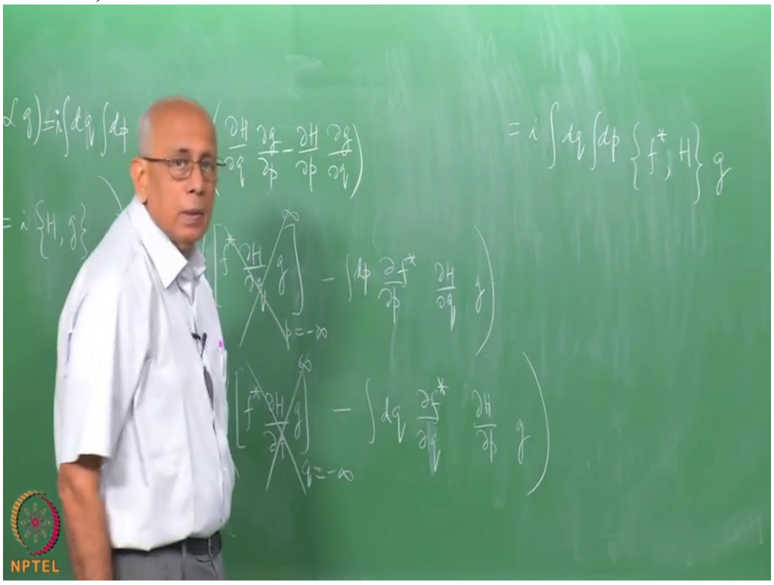

But this is equal to integral d q integral d p, let's put a minus sign and put H with f star 0:24:16.6 times this.

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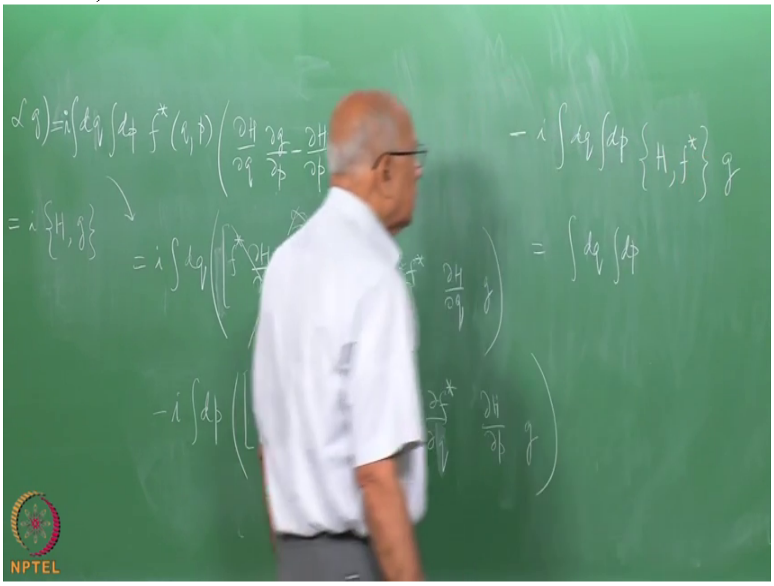

So this whole thing is equal to that, which is equal to i times H with f whole thing star on g.

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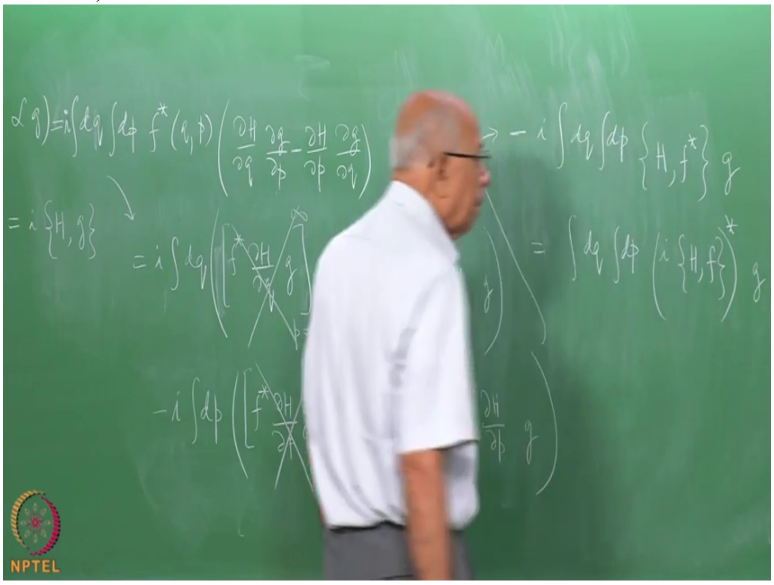

And by definition, this guy here is L on f. So this is equal to integral d q integral d p L f star g which by definition

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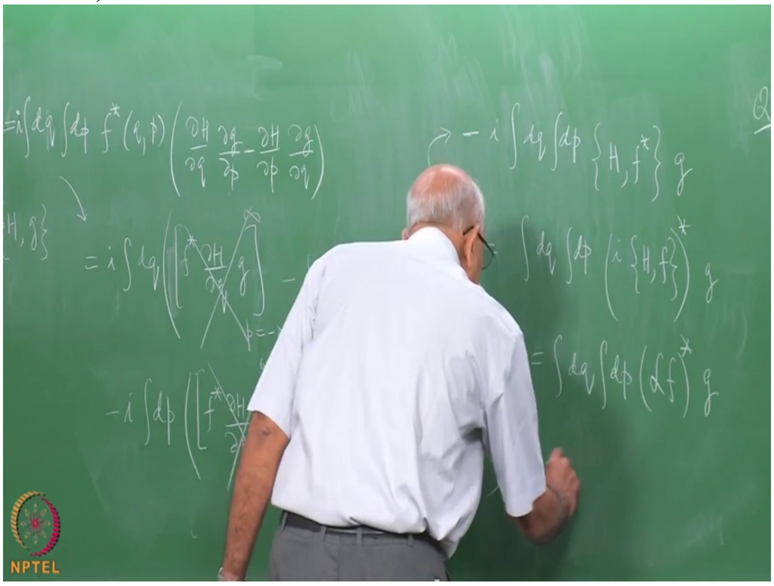

is equal to L f with g.

So we started with

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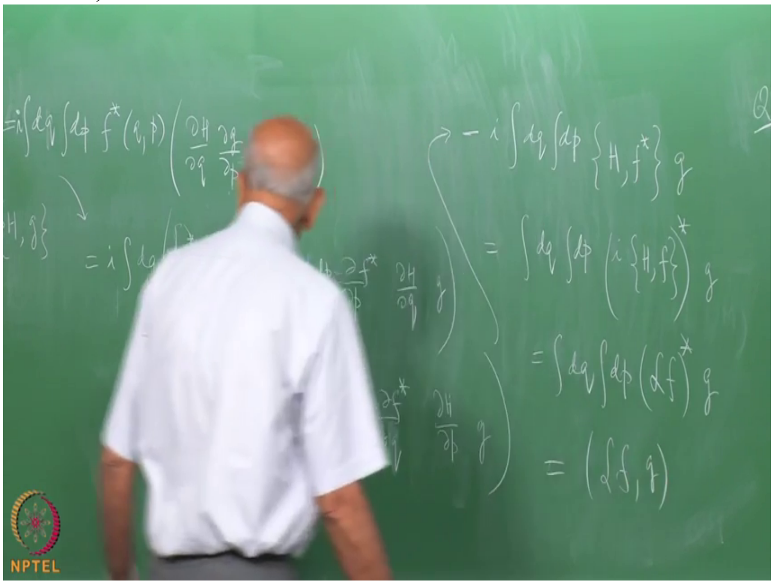

f with L g and we have ended up by showing that it is exactly the same for all f and g with L f and g. So this immediately implies that L equal to L dagger. In other words,

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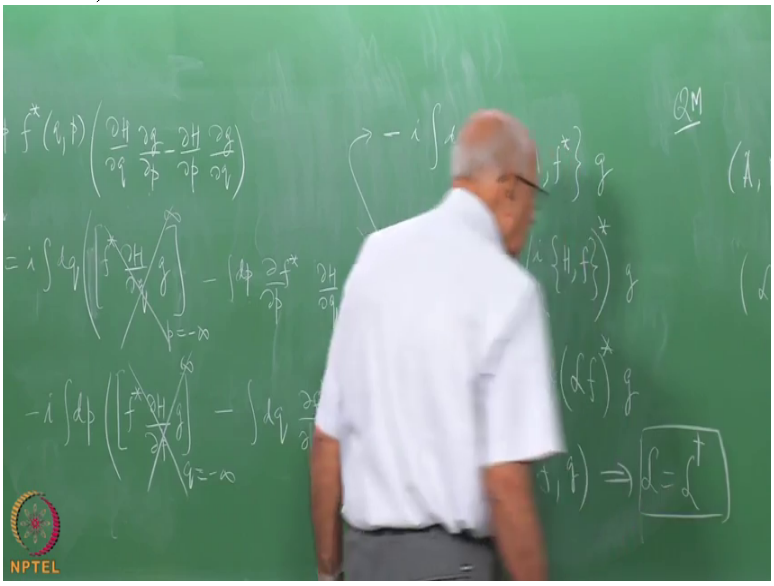

L is self-adjoint. I have been rather loose in saying things are Hermitian, one has to distinguish in these infinite dimensional spaces in general between Hermitian, symmetric and self-adjoint operators.

What we have really shown is the self-adjointness and I haven't explicitly said so but I have used this loose terminology that it is Hermitian because in quantum mechanics we very often use that in lieu of more rigorous statement that it is self-adjoint. This is really shown it is self-adjoint but for that you have to show what domain of L dagger is and as compared to that of

L and show that they both have the same domain. I was slurring 0:25:53.5 over some of those niceties but L is a Hermitian operator or a self-adjoint operator in the sense we wanted to be.

What about quantum mechanics? This looks something totally different establishing this but not so because all we have to do is to use this expression here. So if you took the left hand side for example, in quantum mechanics L A with B by definition equal to trace of L A dagger with B in this fashion. So let me use this bracket to put everything inside for the trace,

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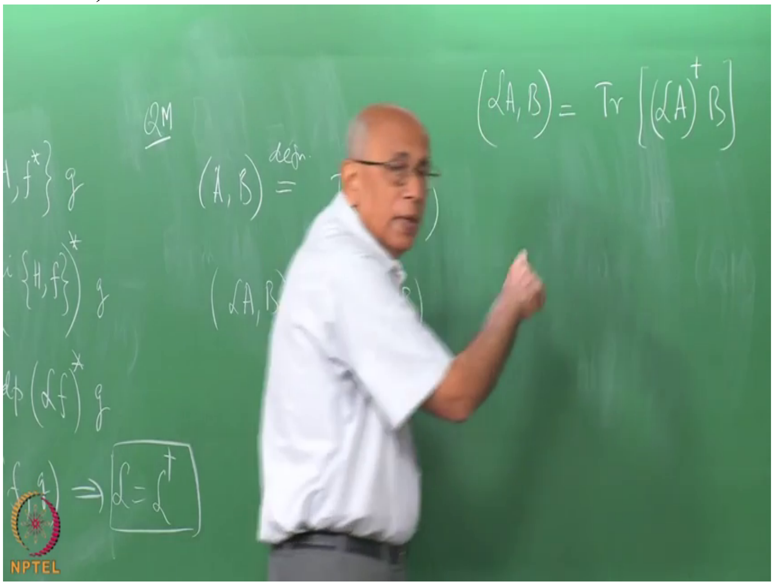

the argument of the trace, this is equal to the trace of, now L with A we already had a formula for this, it was 1 over h cross Poisson bracket of H with A.

So that 1 over h cross comes out and you had the Poisson bracket of H with A dagger, let's put a round bracket

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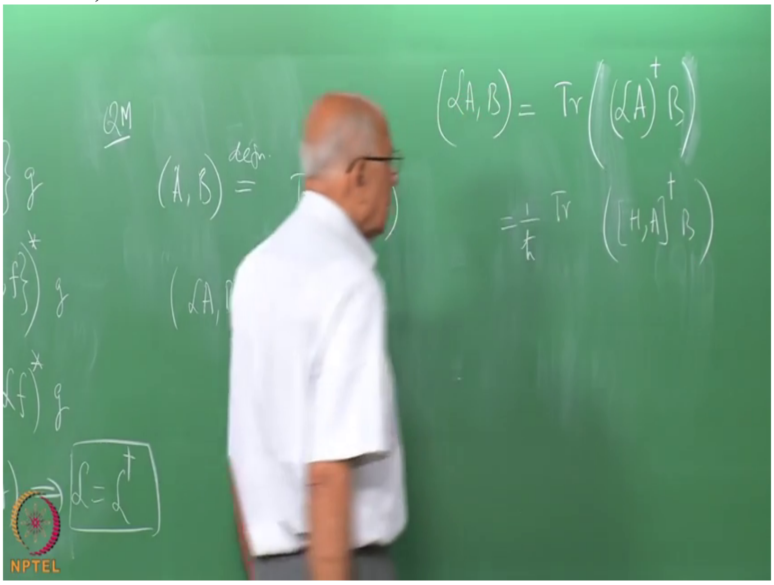

Ok. So that is the quantum mechanical definition of the Liouville operator. But this is equal to 1 over h cross trace of, the dagger of H A so this is equal to the trace of H A minus A H dagger, bring the whole thing inside, this is equal to 1 over h cross trace of, well, H A dagger is A dagger. H is Hermitian and I multiply it by B, that is here minus the trace of, 1 over h cross is outside, A with H, Hermitian conjugate is H dagger A dagger but H dagger is the same as H, so A dagger B.

So you have this and you have this

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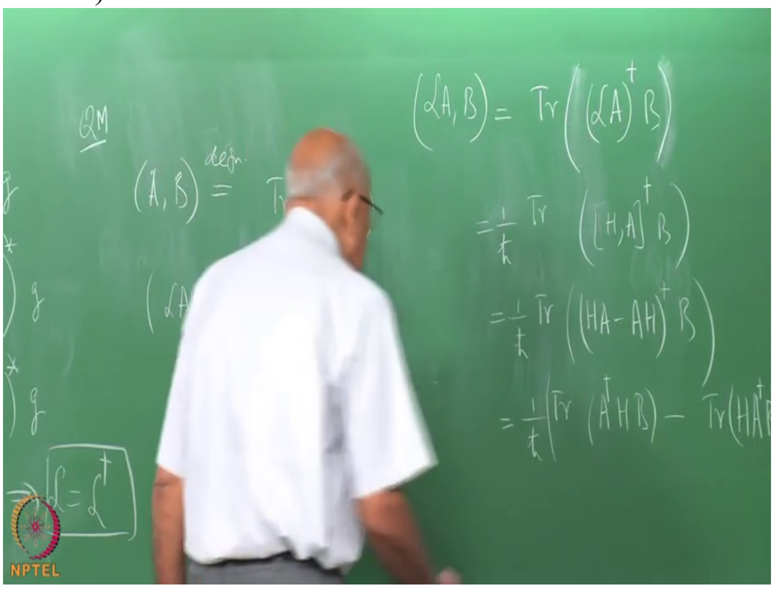

which is equal to 1 over h cross A dagger H B minus trace of, now I use the cyclic property of the trace, so I argue this is the block and can be moved to the right and therefore you have B H A dagger. Did I miss something?

Or sorry write this more simply A dagger, I use the cyclic property to move this to the right and therefore this is A dagger B H by

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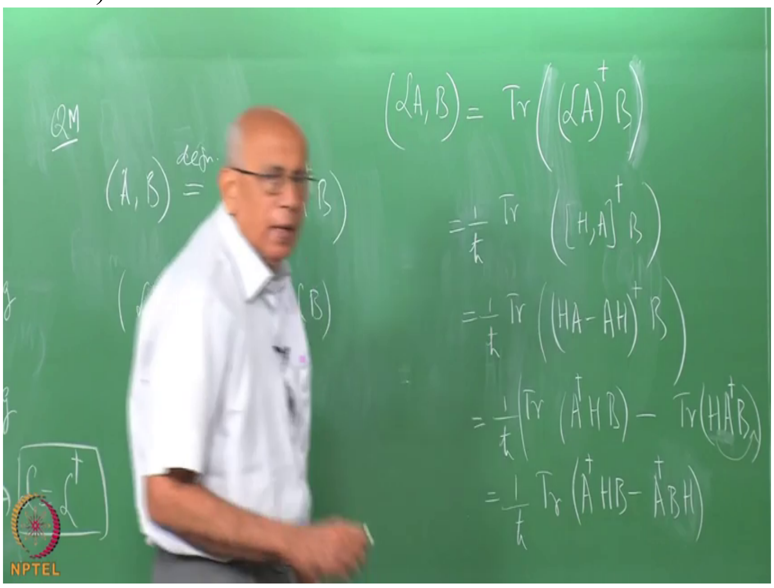

the cyclic property of the trace. But this is the trace of A dagger with the commutator of H with B. So we have this whole thing, therefore L A with B is equal to 1 over h cross the trace of A dagger the commutator of H with B.

That by definition is equal to the trace of A dagger L B. That was the definition. 1 over h cross

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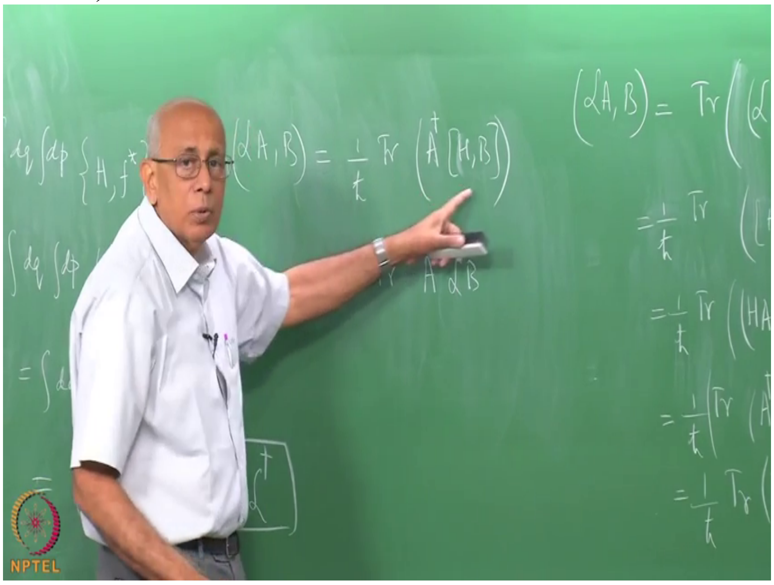

H with B is the definition of Liouville operator

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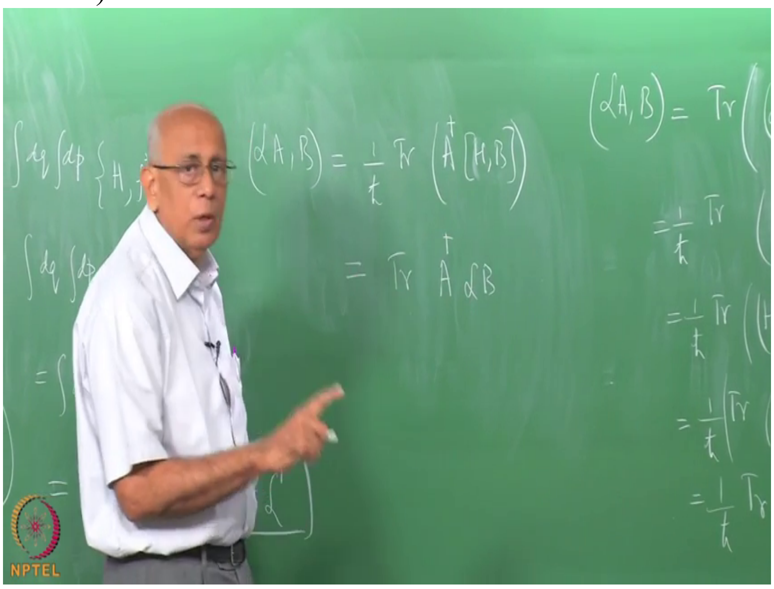

acting on B. So it is this, which again by definition is equal to A with L.

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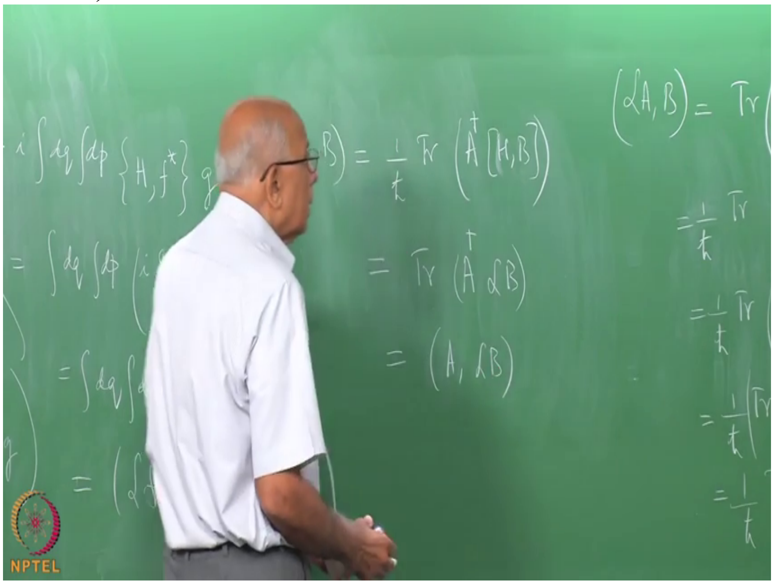

We started with L A comma B and we have ended with, showing that it is equal to A with L B. So again it follows that L is L dagger.

This establishes the unitarity, or it establishes the Hermiticity of the Liouville both in classical and in quantum physics, quantum mechanics, Ok. What does that gain us? That tells us immediately, it says immediately e to the power i L t which if you remember is in fact the time development operator U which takes you from the state at t equal to zero to the state at time t under this evolution governed by the Hamiltonian H, this thing here is such that since this is Hermitian, this is equal to, implies that U dagger U is equal to the identity which is also equal to U U dagger, Ok. I have slurred 0:30:45.2 over details here, U is unitary; this implies

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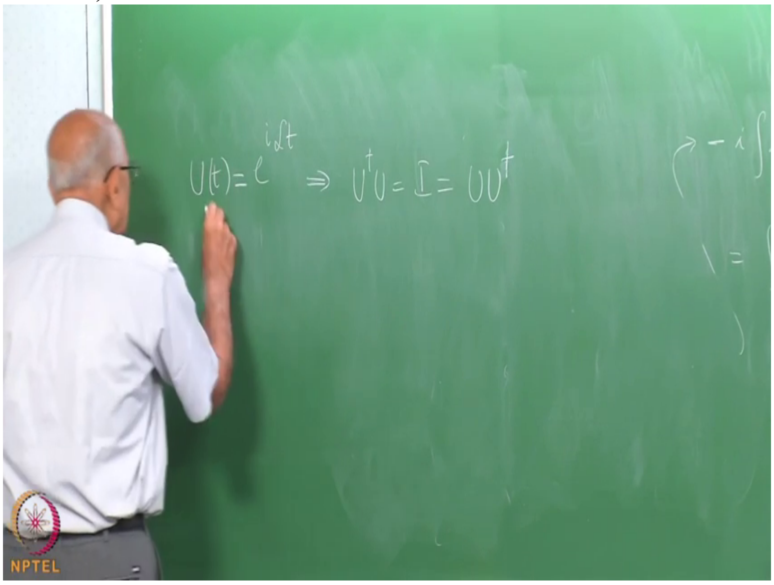

this thing here, is of unitary evolution, Ok.

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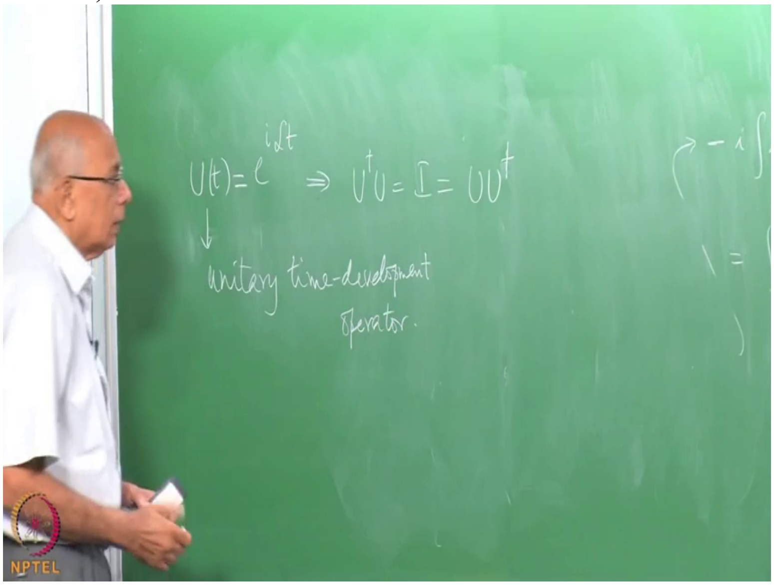

Now it has got consequences, the fact that this is unitary is essentially in quantum mechanics the statement of the fact, if you like, that the Schrodinger and Heisenberg pictures are unitarily equivalent to each other. You go from one to the other by unitary transformation generated precisely by this, governed by this U, the transformation time development operator, access the transformation operator, Ok.

Now can we say this in a slightly more precise manner? Well for this, we need to have the notion of a density matrix. We need to have the notion as to what the expectation value of quantum mechanical or classical function of the dynamical variables? So let's get to that, expectation values. You see in classical mechanics, when we have deterministic Hamiltonian mechanics; we are not used to writing down things in terms of distribution functions in phase space.

But you could equally well regard classical evolution as evolution according to a phase space distribution function where the distribution function satisfies an equation called the Liouville equation which is essentially the way the dynamical variables change. In other words you have a phase space distribution rho of q p and t, which is, if you like a delta function at the values given, of qs and p is given by the solutions of Heisenberg, of Hamilton's equation of motion.

What I am trying to say is that whatever you say in quantum mechanics, you could say equivalently in classical mechanics as well and you could define the expectation value of a dynamical variable A of q p you could write A in classical mechanics as equal to, as equal to the integral d q d p of some distribution function rho q p, let me call it zero here of A of q t p t, this would be the analog of the Schrodinger picture in classical mechanics,

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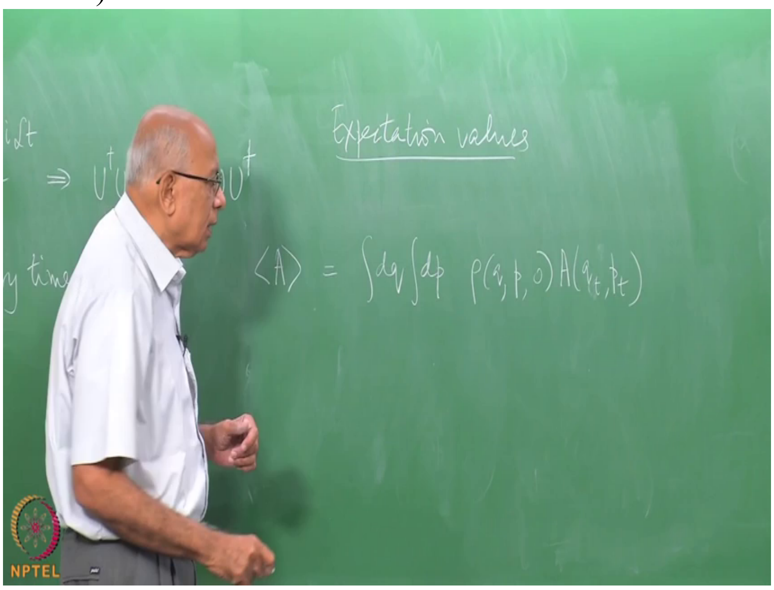

once I tell you what this quantity is which tells you how this variable changes, the expectation value changes as a function of time, is given by averaging over all phase space with this weight function, this distribution function which is fixed once and for all, it is like the Schrodinger picture in quantum mechanics where the state vector evolves, I am sorry, the other way about, the Heisenberg picture where the state vector does not evolve and the dynamical variables evolve but you could also equally well put the blame of time evolution on the distribution function and leave these alone.

So you could also write these as d q d p rho of q p t A of q zero p zero. But you need an equation of motion for this rho to do this.

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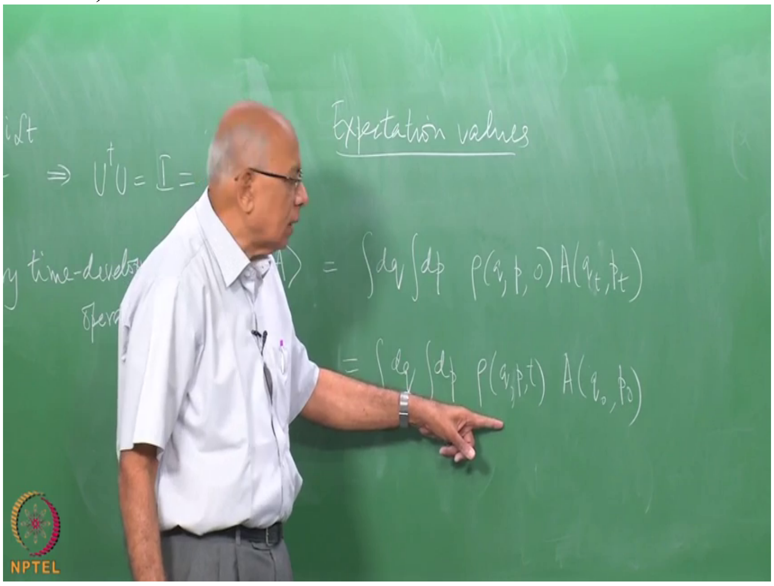

We have an equation of motion for this. It says d A over d t is the Poisson bracket of A with H. But what about this thing here? Well that is called the Liouville equation in classical mechanics and it says delta rho over delta t is equal to minus the Poisson bracket of rho with H which is the same as plus H with rho.

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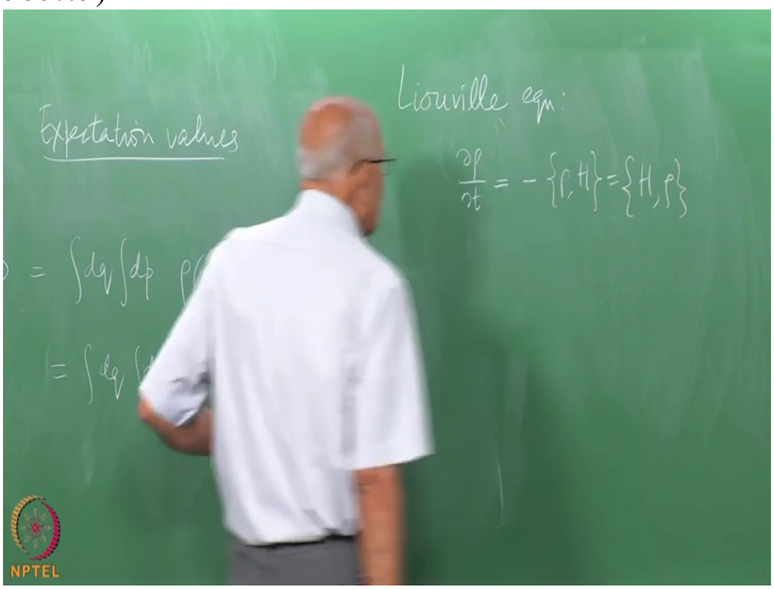

This thing here, it is a probability distribution; it is not a physical observable, so it doesn't satisfy the same equation of motion as physical observables do. There is an important, crucial minus sign here which makes this equation different from that for any normal dynamical observable like A or B or whatever.

Similarly in quantum mechanics, you would replace these formulas by writing a trace formula because this is like an inner product as you can see. So the whole thing can also be written as equal to rho, let me write it inner product of rho with A, so I should really be precise, rho of zero with A of t or rho of t with A of zero. It doesn't matter,

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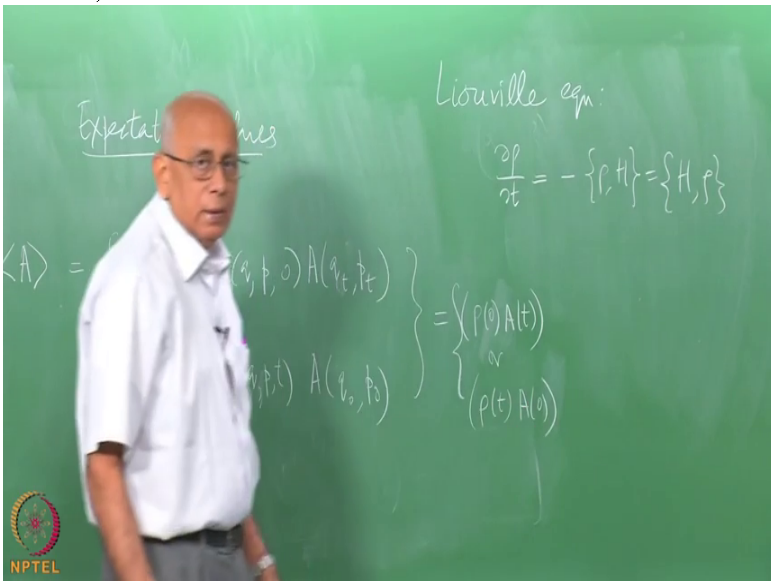

they are equivalent of each other, whether I take an active viewpoint and say that dynamical observables change for a given distribution function or the distribution function changes by this rule, Liouville's equation keeping the dynamical observables unchanged under time.

They give exactly the same result. Now what is the corresponding statement in quantum mechanics? As you know when you have pure states, when you have states described as state vectors, this thing here, this rho would be given by very specific form which I will come to in a minute, and you have here on this, in this case you have the Heisenberg picture and in this case, you have the Schrodinger picture, doesn't matter how you evaluate this average here.

Now the quantum mechanical equivalent of it is again a trace, so you have precisely the same thing so in all cases, Q M and C M, the expectation value of A can be written as trace rho A where this quantity

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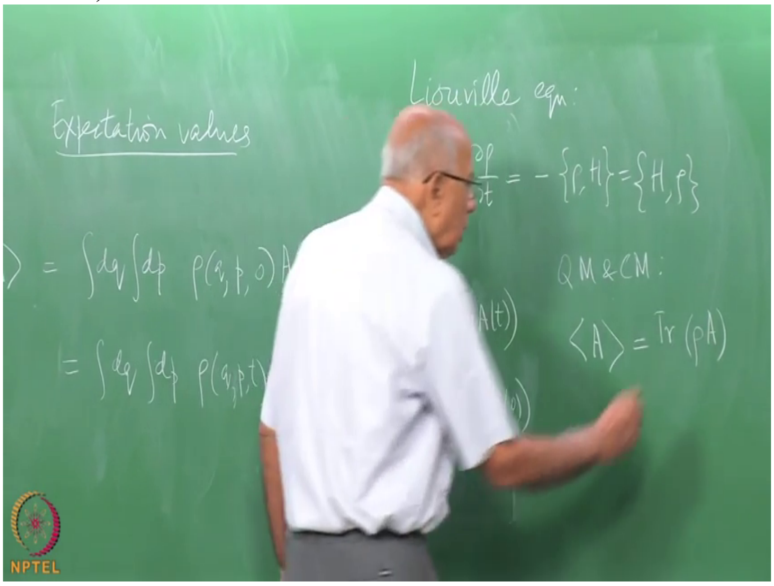

is called as density matrix or density operator and it is Hermitian

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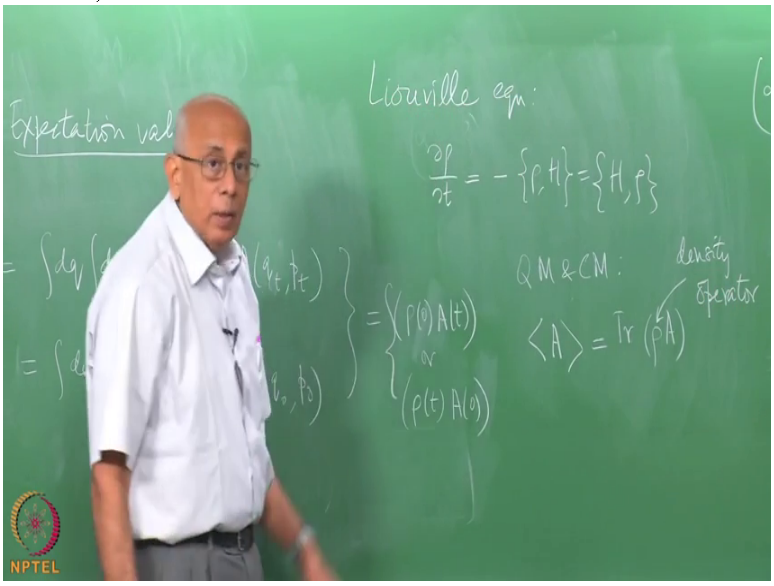

as we will see in a minute, I will assert this, we will show that this is Hermitian, this operator here so this is the definition of the inner product assuming that this is normalized to unity otherwise you have to put this trace rho in the denominator, Ok.

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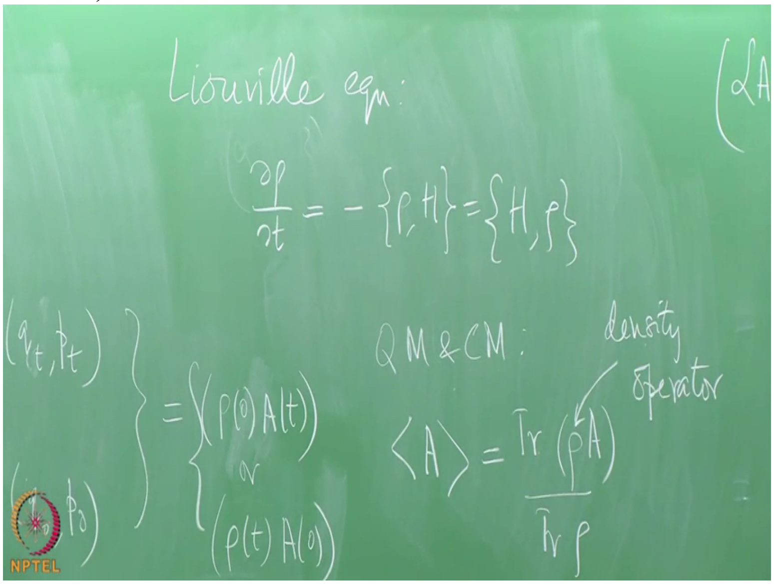

We will see in a second that this is the, corresponds to the classical, usual formula in quantum mechanics for what do you write by, mean by an expectation value of an operator in a given state. But this is the classical equation and the corresponding Liouville equation is this fellow here. Now in quantum mechanics it changes slight.

In quantum mechanics, you are used to writing a thing like A of t is equal to, in the conventional, simplest form of quantum mechanics where the system is described by a state vector in a Hilbert space at any instant of time which you can normalize, this thing here is psi of t A psi of t divided by this quantity psi of t psi of t.

I will assume this to be equal to 1, this denominator, the state is normalized, you don't have that, the denominator factor, it is just the matrix element of this A between state vector on either side. Ok. This is the Schrodinger picture but in the Heisenberg picture

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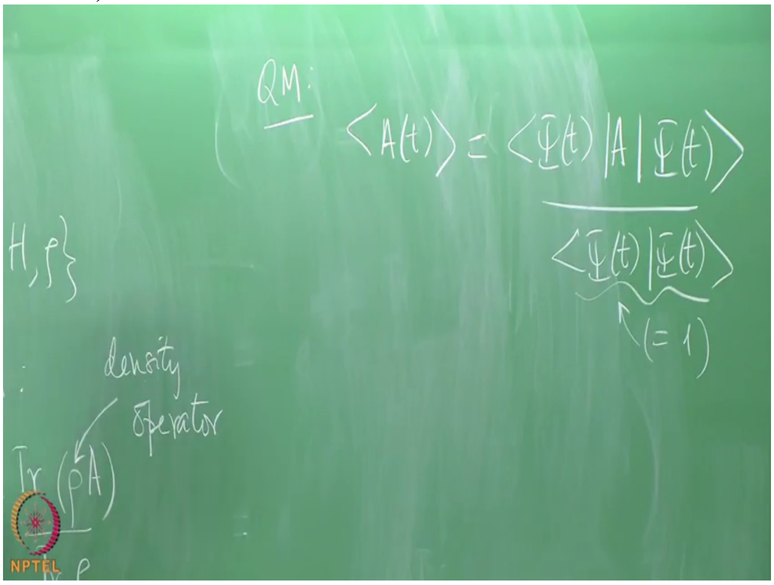

you really write this as equal to psi of zero A of t psi of zero and we know what psi of t is. If you solve the Schrodinger equation for the psi of t, this is equal to e to the power minus i H t over h cross psi of zero.

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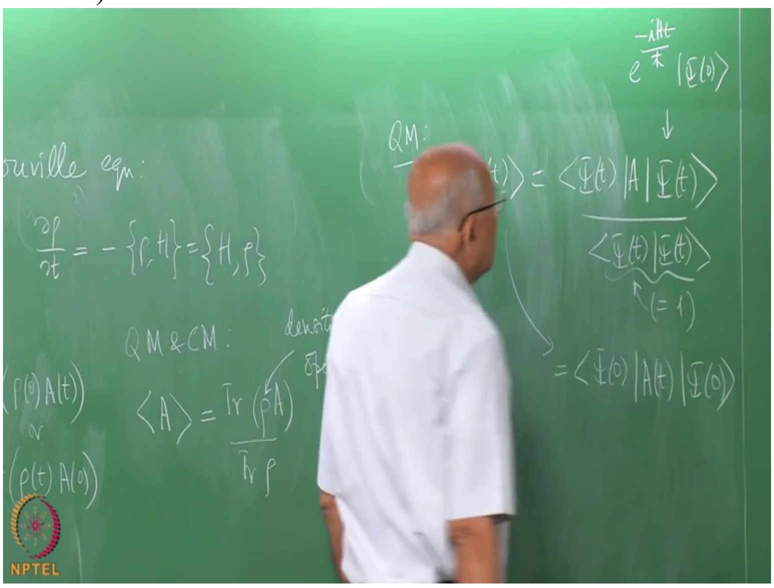

So if you put that in here, on this side it becomes psi of zero bra e to the power plus i H t over h cross, so A in between and this is what you are used to calling as A of t in the

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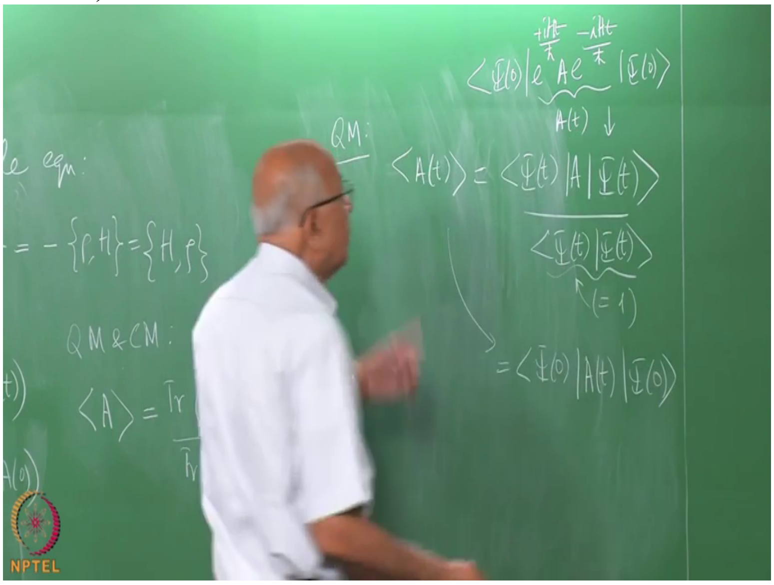

Heisenberg picture. So that's this statement here, Ok. So it doesn't matter which picture you use but the point is

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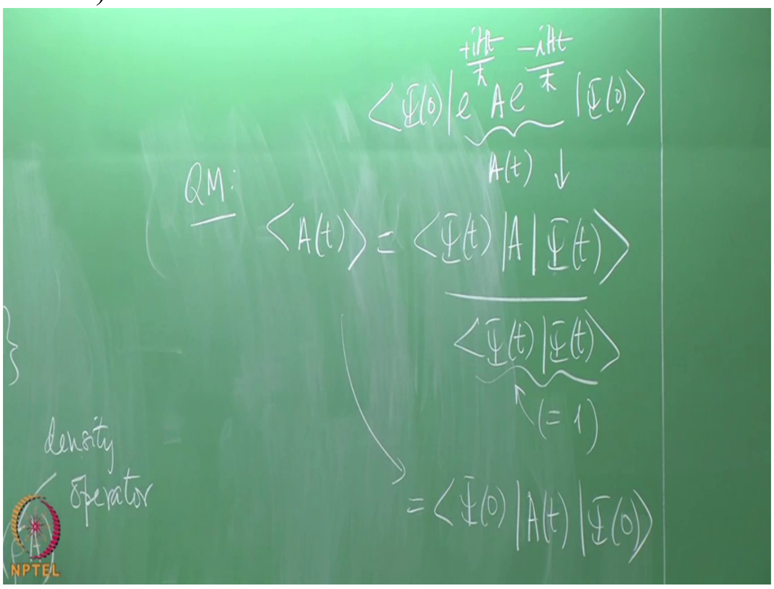

you need to use a density matrix in a more general context where you have temperature fluctuations and therefore the system need not be described by a state vector.

What does one do in this case? The answer is obvious which is known to you perhaps, you use a density matrix which is not writable necessarily in the form of state vectors but has a certain, there is a Hermitian matrix which describes the analog of this quantity here and that is the following. This formula is still valid but in quantum mechanics so this is C M and in quantum mechanics you have an equation which says delta rho over delta t equal to, once again a thing like this, this is equal H with rho with an i h cross.

And this is called the von Neumann equation for the density matrix,

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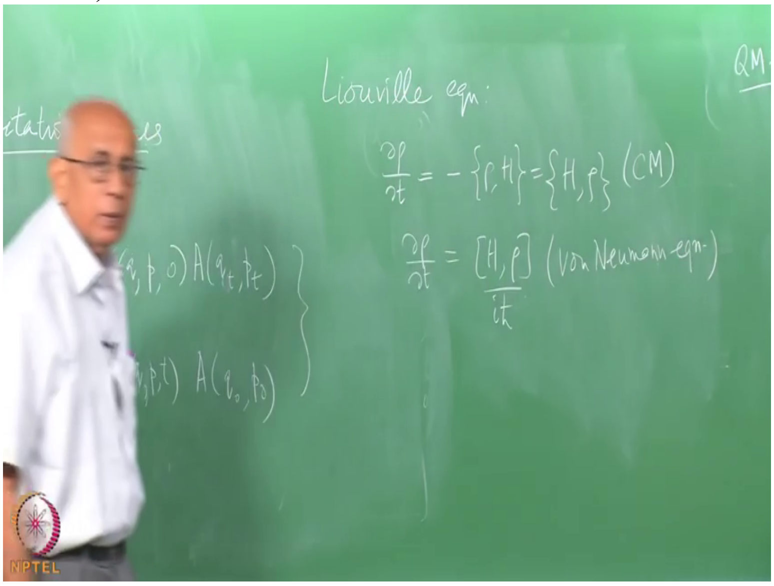

Ok. In the case in which you have state vectors describing the state of the system then density matrix rho in that case is just psi with psi. And this is called a pure state, where this is some state vector in the Hilbert space of the system, not necessarily an energy eigenstate or anything like that,

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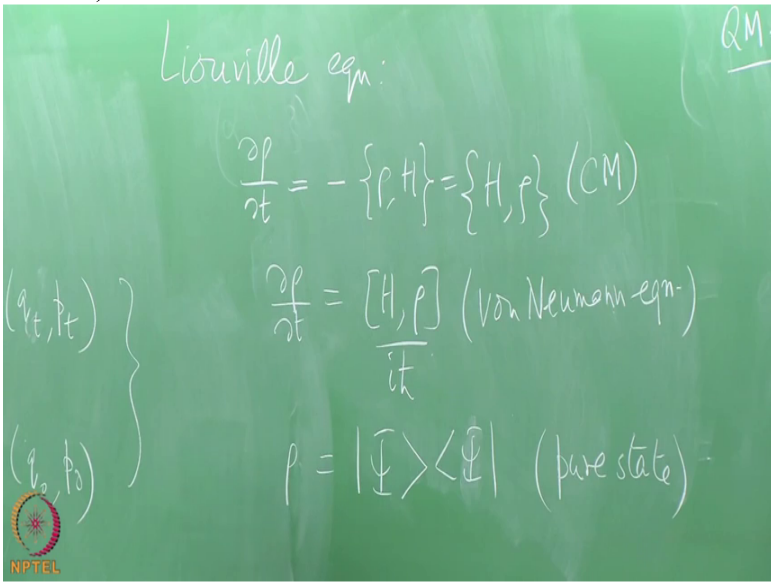

some state vector which could be expanded in a basis of energy eigenstates in general.

But more generally when you have statistical fluctuations like thermal fluctuations, what you really must do is to use a matrix which is a superposition of various possible states with different prescribed probabilities and that's done as follows. We start with the following.

What you do for a single, pure state is to write psi as equal to summation over n C n phi n where these states of a basis in the Hilbert space for instance, and then it is very clear what this expectation value is in terms of rho. If you were to write this rho in that fashion then it is clear

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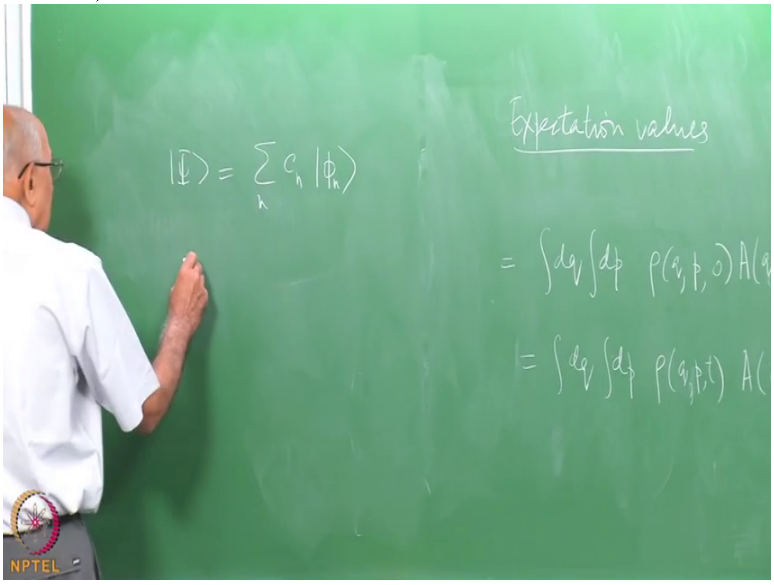

that, let me see the simplest way of writing this, yes, I would like to write it as trace whatever it is.

So what happens to psi A psi, this is equal to summation over m, summation over n C n C m star, well let us put this, let us expand this in terms of m, so it is C m star is equal to summation over m, summation over n C m star C n so I have these two and then I have A sandwiched in between phi m A phi n, that's the expectation value when you normalize

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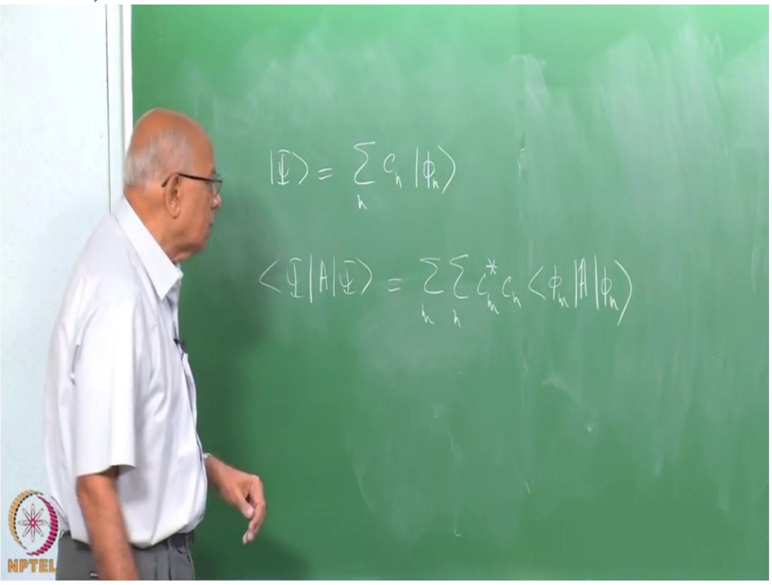

the whole thing, this quantity is what you call A m n, Ok

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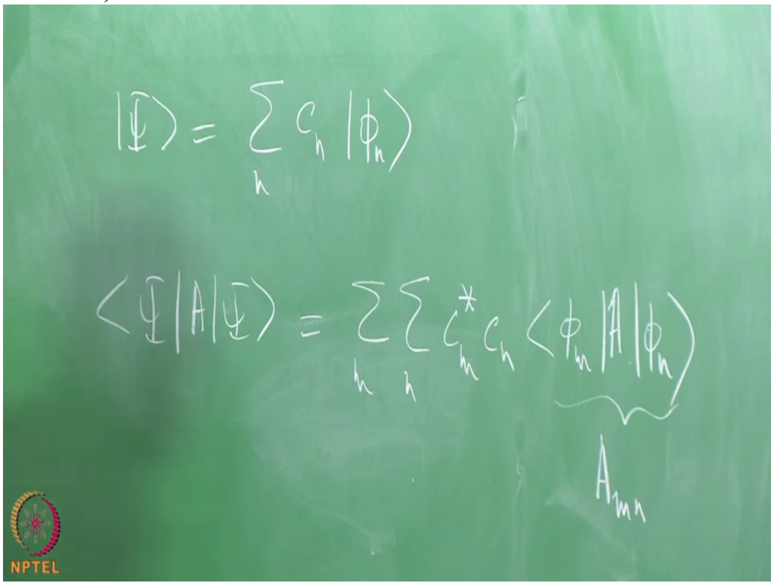

with an m on the left and n on the right and this quantity, if I call this, so I can write this as summation over m, summation over n A m n rho n m where rho n m is equal to C n C m star some m n,

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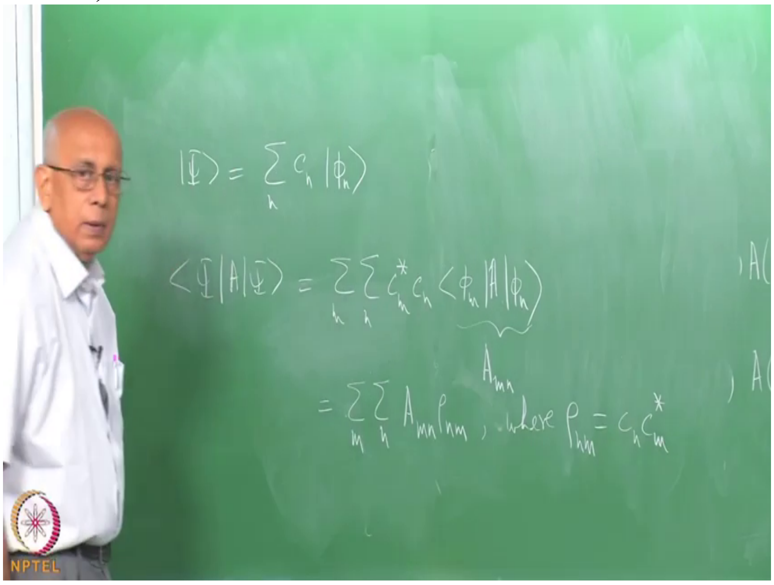

Ok which is equal to, I sum over n, and then I sum over m as well, so this is equal to trace A rho.

That is precisely the formula that I wrote down first saying that you can express the expectation value

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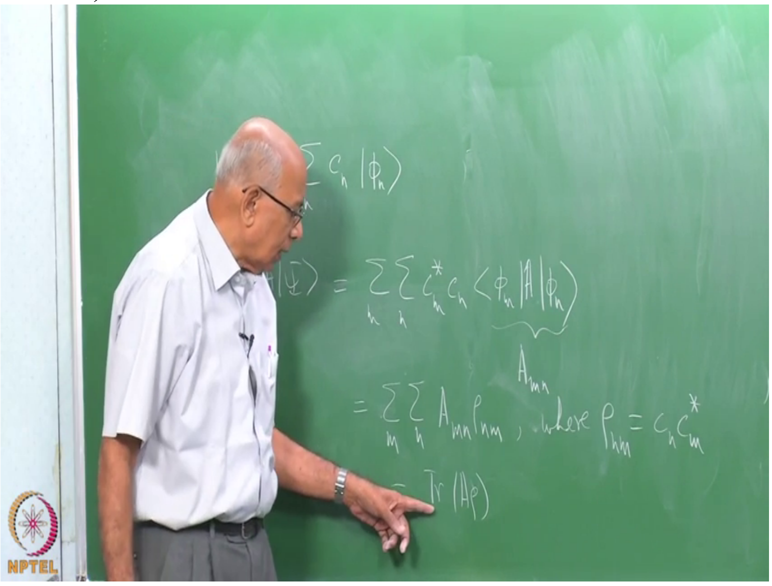

as the trace of A times the observable times the density operator here. Well this density operator has these matrix elements in the basis concerned, Ok.

Now when you have a mixed state, so called mixed state, the whole thing goes through as it stands, except that if you have a superposition of mixed states labeled by some quantity j, some number j, this is equal to C n j here

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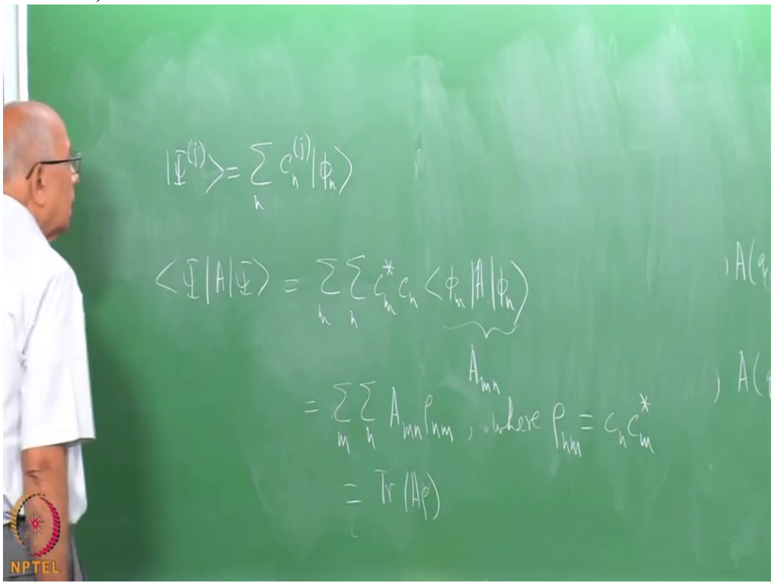

then your density matrix in general would be of the form, rho would be of the form summation over this j and if the state j, pure state j appears with the probability p j which you specify may be from statistical mechanics, may be in the canonical ensemble then this is p j psi j psi j in this fashion and for psi j,

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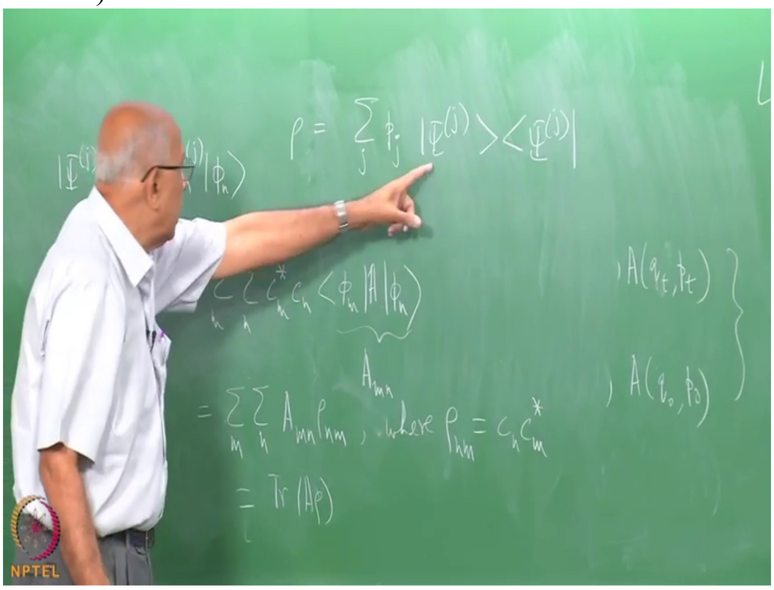

each of the psi js you have to make an expansion of this kind and now it is easy to see that you have exactly the same kind of thing going through except that rho n m.

So once again expectation A is equal to trace rho A, that is the same as trace A rho by cyclic invariance of the trace where rho n m is not equal to C n alone, it is C n for the pure state j, C n j star times summation over j with the probability factor p i, p j.

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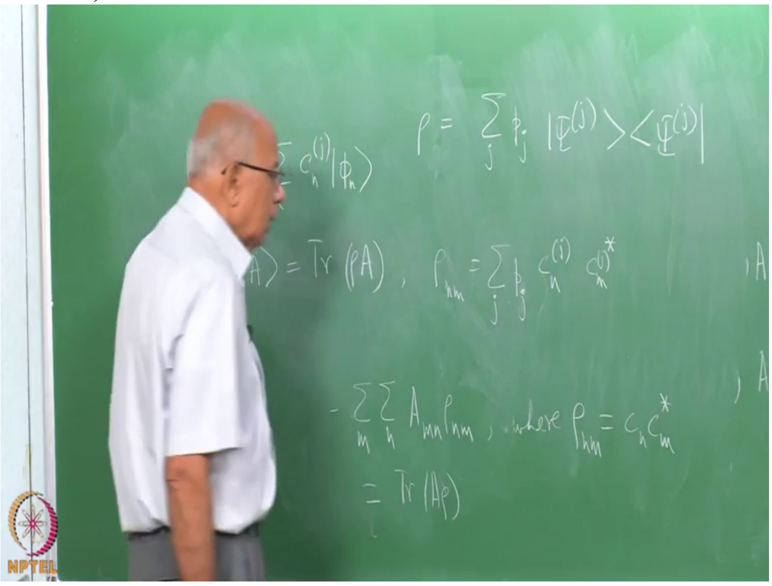

So instead of just one term like this, one product you have a whole superposition of such products. And this quantity is called the density operator or the density matrix here.

So this is a slightly more general formalism than the usual one that you have in quantum mechanics because you are going to allow for the fact that these quantities may be specified say, with finite temperature in the canonical ensemble by may be e to the power minus beta times some appropriate energy or that kind. So to allow for that one needs the more general foundation, formulation and this is the general formula here.

Now the equivalence between the Schrodinger and Heisenberg pictures is exactly this. It is like saying either I compute A of zero in a density matrix which goes like e to the minus i L t rho of zero, this is rho at times t. So either I do this with respect to this density operator or by unitary transformation I can also write this as equal to expectation of e to the i L t A of zero with respect to rho of zero.

So this is the Heisenberg picture and that is

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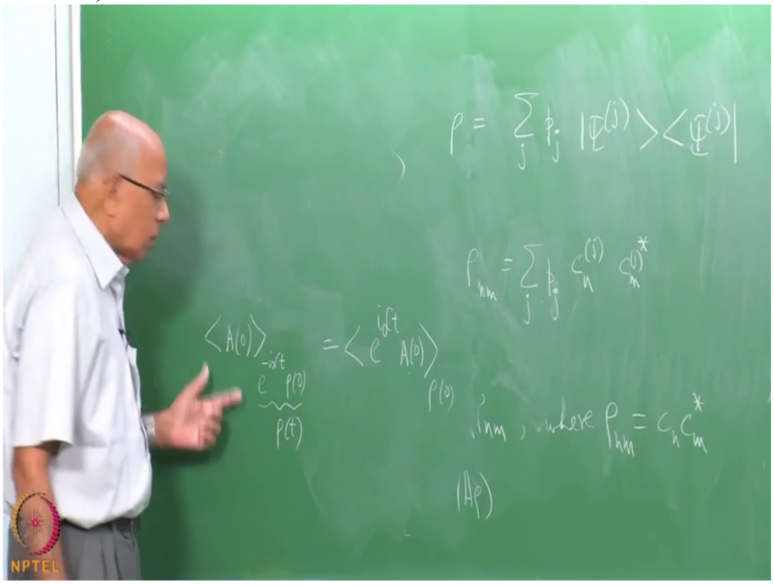

the Schrodinger picture and the two are equivalent by unitary transformation. And this kind of puts both classical and quantum mechanics, at least the formalism of time evolution formally on the same footing and we will see next what happens when you introduce the Liouville operator in the presence of the perturbation. That will be the content of linear, the responsibility of linear response theory which we will take up next time.