FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

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Lecture-33

Open Quantum Systems: Quantum Trajectory Approach

In this lecture, we will talk about the quantum trajectory approach to solve the Lindblad master equation. This is a very powerful technique when we want to solve a system which is very large in dimension, so that it's difficult to solve it in the form of density matrices. So, this provides the alternate way of solving the master equation and it goes like this. Start with the Lindblad master equation. It is rho dot equals minus i H rho plus sum over n gamma n Ln rho Ln dagger minus half Ln dagger Ln and rho and numerator.

So, here H is the system Hamiltonian. I'm not writing the subscript S. Ln are the Lindblad operators. Gamma n are the coefficients of the Lindblad operators. And rho is the state of the density matrix of the system. So, first we notice that rho dot, the time derivative of the density matrix.

By definition, the derivative can be written as limit delta t tending to infinite 0, rho of t plus delta t minus rho of t divided by delta t. That is, by definition, the derivative of a function or operator can be written in this form, where delta t tends to 0. But as an approximation, we can say that rho dot that is the time derivative is approximately equal to rho of t plus delta t minus rho of t over delta t if delta t is chosen small enough. That small enough will come with experience we need to try different values of delta t and see if we are getting absurd answers or not if the answers which we are getting they are fine then probably delta t which we have chosen should be fine this way of dealing with the derivative of a function this is called finite difference method and this is used in in numerical simulations very often. Now, using this, we can see that the Lindblad master equation can be written as rho of t plus delta t minus rho of t over delta t. So, it is not same as the Lindblad master equation, but it is close to the Lindblad master equation. And this we can write as minus i H commutator rho plus sum over n gamma n Ln rho Ln dagger minus half Ln dagger Ln and rho anti commutator. So, here when we say rho this is a time t.

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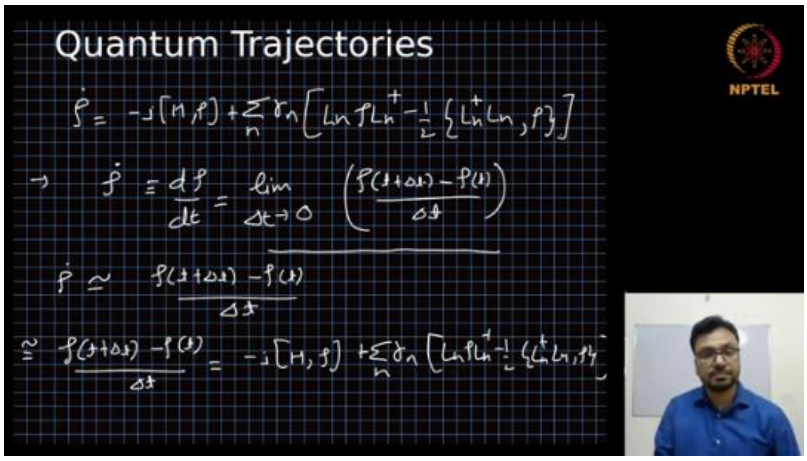

Okay we are choosing it to be at time t not t plus delta t, so, from here we can write rho at t plus delta t as rho of t plus delta t times the whole of the right hand side. Let me repeat first, what we have done is first we replace the time derivative with the finite difference method finite difference derivative and then we write rho of t plus delta t in terms of rho of t and delta t from here we can see that this right hand side can be written as rho of t plus delta t that is minus i delta t H commutator rho of t, so, on the right hand side everything is rho of t so we don't need to write it again and again this will just make the expression cumbersome so we just write rho so on the right left hand side we have rho of t plus delta t and on the right hand side we have rho of t plus sum over n delta t gamma n Ln rho Ln dagger minus half delta t ln dagger Ln n to the power delta rho.

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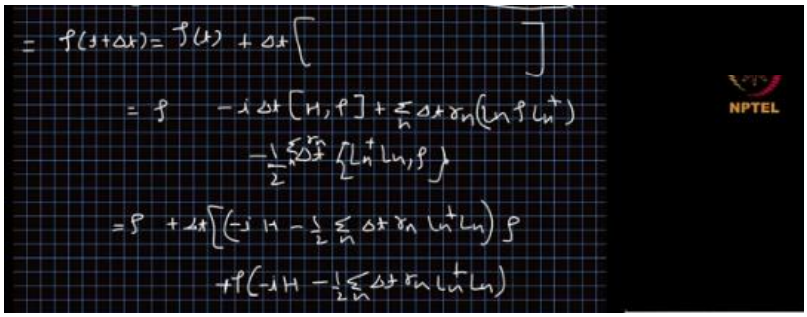

This thing can be written as rho plus delta t minus i H plus or minus half sum over n delta t gamma n Ln dagger Ln rho minus i H minus rho times minus i H minus half sum over n

delta t gamma n Ln dagger Ln. Is that correct? No, there is a plus sign. So, plus and there is a minus sign here.

So, you see a minus i H rho and rho i H that is the commutator of H with rho with minus i outside and minus half sum over n delta t gamma n Ln dagger Ln rho minus half rho delta t gamma n Ln dagger Ln is the anticommutator of rho with Ln dagger Ln. Plus we have delta t times sum over n gamma n rho Ln dagger. So, our rho of t plus delta t can be written in this form. And we can call this term here as minus i times H effective. So, that H effective becomes H plus or minus i over 2 sum over n delta t gamma n Ln dagger Ln.

This is a non-Hermitian Hamiltonian. This is a non-Hermitian Hamiltonian which characterizes the evolution of the open quantum system including the dissipation. Here in the Hamiltonian, this part is the imaginary part. This is the non-Hermitian part and this is causing the damping or the dissipation in the system. In the similar spirit, here we can say that this is a non-Hermitian Hamiltonian which characterizes the dissipative dynamics of the open quantum system.

With that we can write rho of t plus delta t as rho of t minus i delta t H effective rho minus i delta t rho H effective dagger plus sum over n gamma n Ln rho Ln dagger. So, in this way, our Lindblad master equation looks like this in the finite time step evolution, discrete time evolution. In fact, we can actually write rho of t plus delta t as sum over n, n is from 0 to capital N, kn rho of t kn dagger, where kn depends on t and delta t. So, at the time when we are applying this kn, it depends on that time and the time step delta t. So, in that way, we can write the evolution, the infinitesimal or small time evolution of the state as a in terms of operator sum representation. Operator sum representations, we have discussed it in In quantum maps also and in measurements also.

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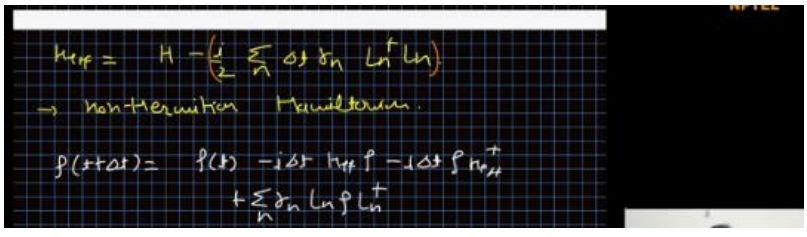

So, this is a completely positive map and we can see one step of evolution, one discrete time evolution delta t from t to t plus delta t in terms of this K n's where K 0 is identity minus I delta t times H effective and K n is square there is a delta t also here square root

of delta t gamma n Ln and in this representation we are discarding the delta t square term. So, what we have done now is we have represented the Lindblad master equation or the solution of that in terms of a small time step evolution and that evolution is governed by the cross operators Kn where n is from 0 to N, capital N and they are given by the effective Hamiltonian which is non-Hermitian Hamiltonian and the Lindblad operator. Now, how does this help us solve the dynamics of the quantum system? We can use it to solve the dynamics of a quantum system in a stochastic in a numerical method, in a numerical way as follows.

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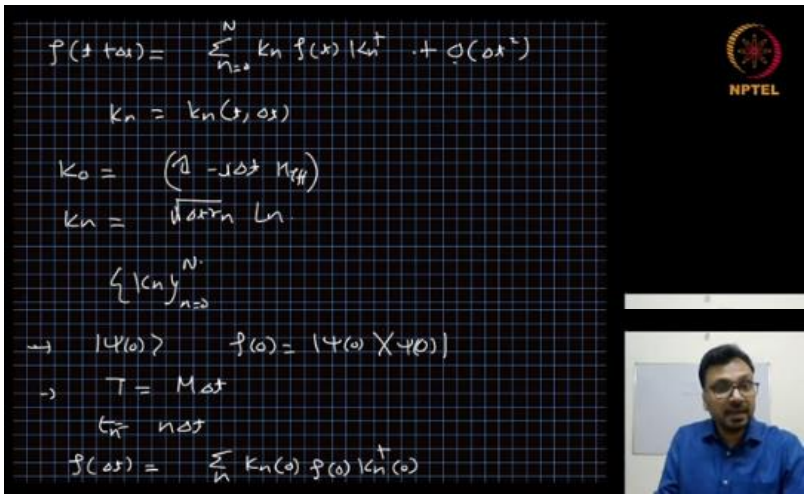

Let us say our initial state is psi of 0. It is a pure state. So, the rho at 0 is psi 0, psi 0. Now, we have time, which is discretized. So, we have total time t, which is capital N or some m times delta t, where m is some integer, large integer.

So, now we will just talk about time t, which is tn, which is n times delta t. So, state at time delta t will be sum over n key n at zero rho at zero kn at zero dagger so we will find kn for at time t equals zero since our ln let us take a simple case where ln is time independent gamma n is time independent so kns are constant throughout. And the H effective also is time independent so K0 is also independent of time in the whole dynamics. So, this KN will not change. So, this is sum over N. KN, there is no time dependence here, rho of 0, KN dagger.

And from there, we can have K of 2 delta t, which is sum over N, KN rho of delta t, KN dagger. Similarly, rho of n delta t will be sum over n, m delta t sum over n, Kn rho of m minus 1 delta t, Kn dagger. In that way, we can evoke the state in the discrete time from the start to the end. But here still we are using the density matrix at every instance of

time. So, what we can do is let us say we have the initial state is the pure state psi of 0, we have discretized the time, so we have t equals 0 1 2 3 4 5 and so on now in the beginning our state was psi of 0

And at the time step 1, our state will be rho 1, sum over n, k n, psi of 0, psi of 0, k n dagger. But what we can do is we can say that the psi of 0 pure state goes to another pure state, psi bar of delta t in this evolution and this state psi of delta t can be any of those, any of the states, kn acting on psi of 0 and the probability of this. This is not normalized state, this is the probability. And the probability Pn is given by psi of 0, kn dagger, kn psi of 0. So, let me repeat again, instead of Solving or instead of evolving the density matrix of the system in this fashion, what we can do is we can say that our initial pure state goes to another pure state after one time step evolution.

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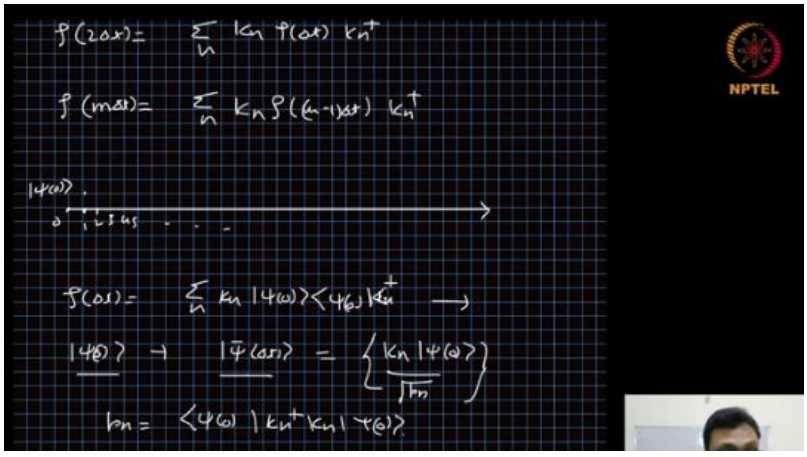

And this pure state is one of the states given by Kn psi of 0 after normalization. And the probability of this happening is given by Pn, which is the expectation value of Kn dagger Kn. The numerical simulation algorithm from here can be derived as follows. We start with the state psi of 0, initial state. And then from here, we calculate the probabilities pn given by psi of 0, kn dagger kn, psi of 0.

Now, these psi of 0s are such that, the pn's are such that sum over n, pn is 1. So, if we have a line between 0 and 1, then up to some point we will have p0. So, this space will be p0 and then next space we have will be p1 and then we will have p2 and p3 and p4 and p5 and so on. We can divide the line between 0 and 1 into segments of size given by pn. Next, what we do is we find the random number r in the range 0 and 1 uniformly distributed.

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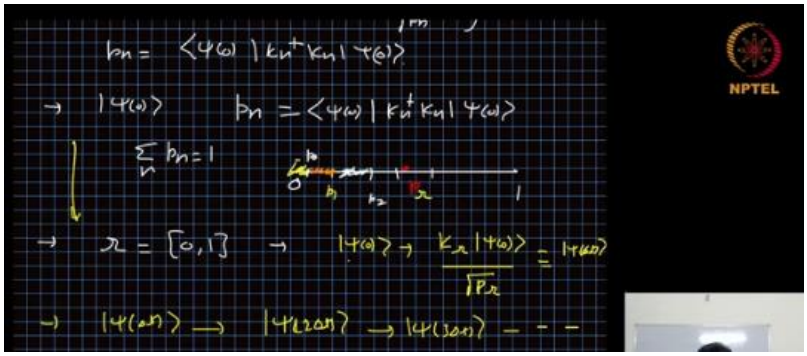

So, we get a random number between 0 and 1 uniformly. And that random number will be somewhere on this line. And let us say this correspond to p of k, the segment corresponding to p of k, that means in this trial, we got the outcome k of i shouldn't say k, let me say r here, r also, yes that is better. p of r so it means we our state psi of 0 went to k of r acting on psi of 0 divided by sum of square root of p of r. So, in this attempt our state psi of 0 went to psi of r which is k r acting on psi of 0. We repeat this process and then we our psi of delta t that was delta t we got and then we evolve it using the same method.

And we get psi of 2 times delta t. In this also we will draw a random number. Our probability distribution will change because our initial state has changed now for this attempt. So, we will rewrite the probability distribution. We draw a random number. We get a random number uniformly between 0 and 1.

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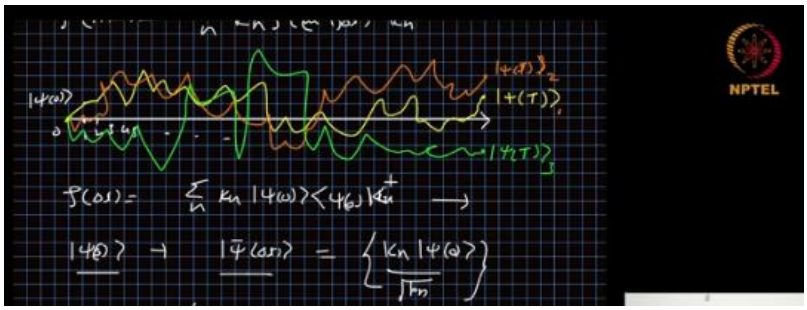

We find which, it corresponds to which probability and accordingly we apply the cross operator or K, on the state and we get psi of 2t from there we get psi of 3t and so on. In

that way we will get a sequence of states. So, we started from psi of 0, we got some state then we got some other state then some other state some other state at each other time and then will be a trajectory because of this and we end up getting some state psi of capital T. If we repeat this again from the beginning, in the next time, we may not get the same trajectory, we might get some other trajectory and some other final state. Let me put outside the attempt, this is the first attempt, this is the second attempt, then we can have another trajectory starting from the beginning. And we get psi of capital T in the third attempt and so on.

We can repeat this thing for a large number of times. And what we do at the end is, we start from psi of zero we get psi of t in the nth attempt and we construct rho of n which is psi of capital t out of product psi of capital t and we sum over it so rho final will be sum over n, psi of t, psi of t and divide by n, that number of trials, total number of trials. Let us say we had r number of trials. So, n is from 1 to r, r is the number of trials we have.

So, our final state will be the mixture of all the possible outputs we got in all the trials. And the claim is if delta t is small enough and r is large enough then rho final will be rho of t, what we were expecting from the exact solution, from the proper solution of the Lindblad equation. Let me repeat that if our initial state is a pure state, then we can solve the Lindblad equation using the finite difference method by evolving the pure state to pure state probabilistically. The probability of the jump is probability of the delta t evolution is determined by the Kraus operators we are using KN. And that can be used in a computer program to evolve the state psi of t to psi of t plus delta t. And if we repeat this thing, each sequence of this step will result in a trajectory in the phase space, in the state space giving us a different state at every time and we have a final state in this process.

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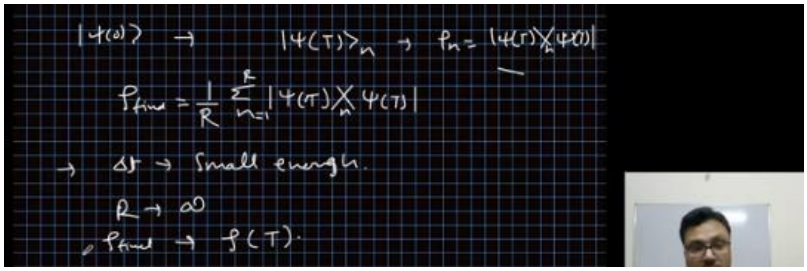

If we repeat this thing, this operation, this method multiple times starting from the same state, we will end up getting many, many final states. If we take the mixture of those final

states, then we will get a final density matrix. When we say mixture, we convert the pure state into a mixed state and then we add all the mixed states and divide by the total number of trials. Doing this thing you can see that our final state is positive, it has trace one, so it's a valid density matrix. Now if our delta t the time step is very small, ideally, if delta t tending to zero and r tending to infinity, the number of trials, then our final state will converge to the exact solution we were expecting.

If it is not chosen appropriately, if delta t is too large or r is too small, then there can be significant difference between the final state and rho of t. But in all this process, what we have done is we started with a pure state and we were getting pure state at the end. And if you want to calculate not the state but some other quantities like the average or expectation value of some operator, let us say we want to calculate expectation value of operator at time t. Then the idea, the expression for it is A times rho of t and trace in our quantum trajectory method, it will be 1 over r, n is from 1 to r and psi at time t, the nth attempt and psi at time t at the nth attempt and this becomes 1 over r n from 1 to r and psi of t A psi of t in the nth attempt. So, it means it is the expectation value of A, this is the average of the expectation value of A in each trajectory at every time, okay, so if you want to calculate the expectation value of observable A at every time t, then this can be written as the average of the expectation value of A in each trajectory at every time t. In that way, we do not need to store any state or anything. We can just keep track of all the expectation values of any observable we are interested in.

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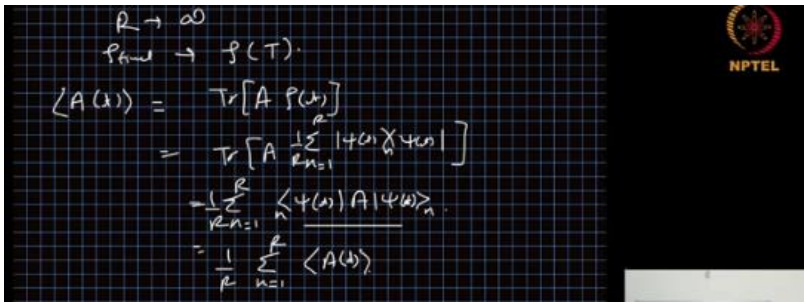

So, this technique is the whole method of solving the master equation this way is called quantum trajectory approach. Here k 0 which is identity minus i H effective delta t, this corresponds to the time evolution governed by the non-unitary, non-Hermitian Hamiltonians. And Kn where n is not equal to 0, they are called jump operators. Jump operators are quantum jump operators. So, here generally the probability of getting K0

that is p0, K0 dagger K0 is generally much, much larger than all the other p ns in a typical time evolution.

So, generally the system experiences only the evolution caused by the non-Hermitian Hamiltonian. Once in a while, we see a jump happening. So, at that time, the whole process can be seen as we start from a state and we are getting some evolution because of the non-Hermitian Hamiltonian. And once in a while, there will be a jump. So, it will suddenly jump and it will go to some other state and then it will start the evolution again from there using the non-Hermitian Hamiltonian. Then again there will be some jump at some point and then it will start the evolution from there.

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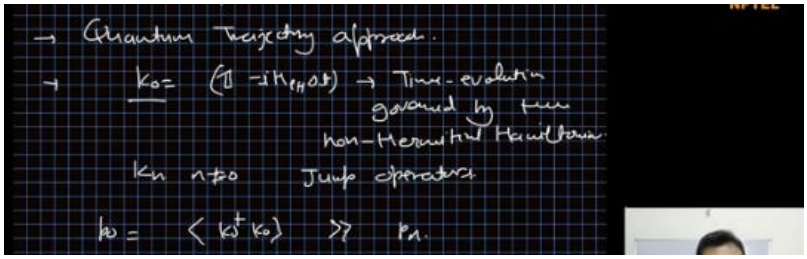

So, if you want to understand it, it will be like this that mostly the evolution of the system is governed by the non Hermitian Hamiltonian and once in a while there will be a quantum jump and the state abruptly will change and the evolution will start again from that point. And this can be a very powerful technique to find the evolution of a quantum system if the quantum system has a very large dimension.