Quantum Physics
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Lecture No. # 31

Let's look at perturbation theory in slightly more formal way.

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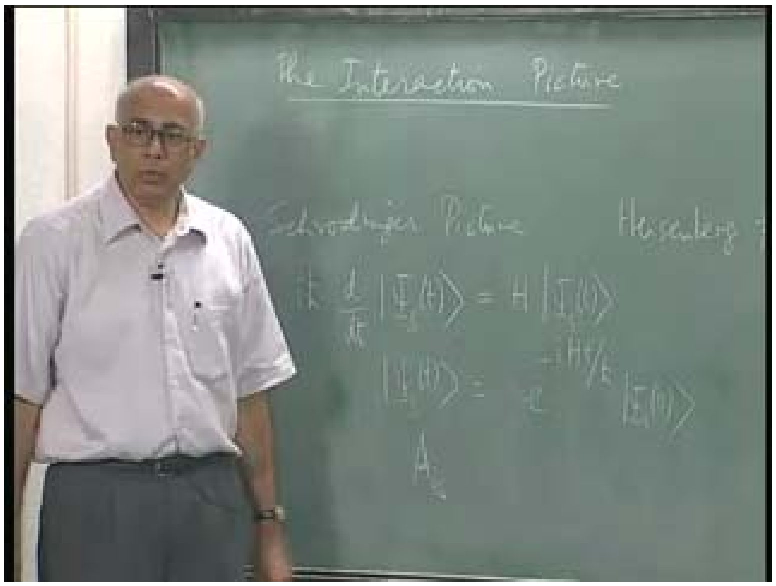

recall that we were looking at Hamiltonians of the form H_0 + some perturbation and my idea was to show you how you could find the eigenvalues and eigenfunctions of the new Hamiltonian as a perturbation series and powers of this lambda for the simplest case of non-degenerate perturbation theory with H_0 has discrete levels which are non-degenerate. And then we looked at simple formalism for handling cases when H_0 has some levels which are indeed degenerate and that was the portion where you went into the substate of this degenerate states and then you found the exact eigenstates and after that proceeded as before. Now today what I'd like to do is to put this whole thing on a slightly more general frame work so that even if H prime has explicit time dependence which is what we would like to handle, we can still handle the problem. and after we set up of the formalism i will apply it to simple cases such as 2 level systems or what happens when you switch on a time dependent magnetic field for an electron whose spin couples to the magnetic field and so on because this will have implications for both quantum optics as well as magnetic resonance and many other areas. So that would be our last topic. Now formal way of handling this was evolved long ago by the Dirac himself in the early days of quantum mechanics. He introduced a way of writing a transformation which goes from the original Schrodinger representation, not to the Heisenberg picture which we already studied but something in between the Schrodinger and Heisenberg pictures called the interaction picture. I would like to introduce that. It was a clever trick which tells you natural way how to handle problems of kinds of perturbations including time dependent once. So just to the call to you what we have done, recall the original situation for a minute where we had a Hamiltonian H and we had the Schrodinger picture. We had on the other side, the Heisenberg picture and for the moment let me just look at a Hamiltonian H_0 which is time independent. So in the Schrodinger picture, we started with Schrödinger's equation which is ih cross d over dt, the Schrodinger wave function or state vector this was = the Hamiltonian H on psi$_S$(t). This was the total Hamiltonian of the system and that's the equation satisfied by the state vector in the Schrodinger picture. In the case where H was explicitly time independent, you could write a solution which was psi s (t) was e to the - i Ht over h cross psi s (0) for any given state vector. And physical observables which didn't have explicit time dependence in them were represented by Hermitian operators of the form A_S. There was no time independence here. So just you recall to your memory observables didn't have explicit time dependence. They were hermitian operators and the state vector carries the burden of time dependence and it evolves according to this (Refer Slide Time: 05:34) rule given, an initial state you could say what the state was at any time t. this is for Hamiltonian which doesn't have explicit time dependence.

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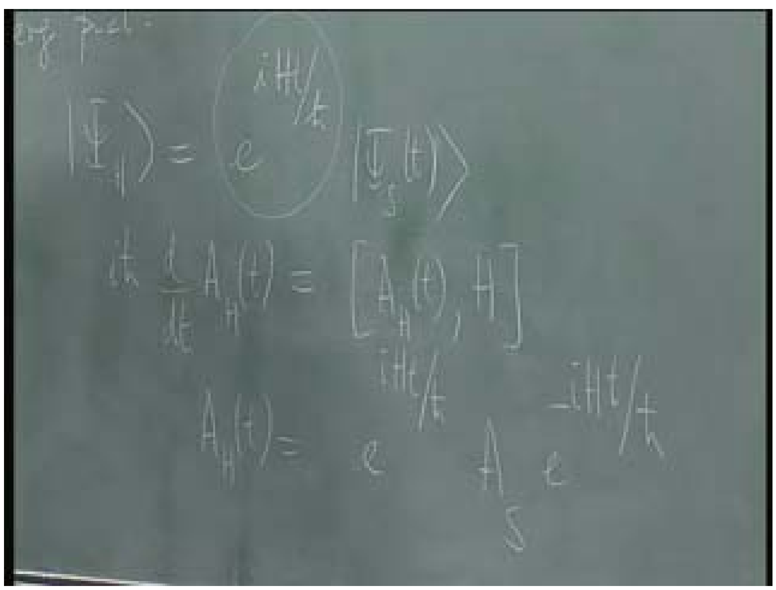

The Heisenberg picture was a unitary transformation on the Schrodinger picture and it corresponded to saying that psi H was geared in a such away as to coincide with the Schrodinger state vector at some fiducial instant of time which we took to be 0. so psi Hwhich didn't have explicit time dependence was essentially this (Refer Slide Time: 06:11) vector or if you want to write in terms of the Schrodinger state vector, its e to the i Ht over h cross psi S (t). In a sense what happened was that the time dependence of this in the time dependence of this (Refer Slide Time: 06:30) canceled l out and you had a time independent state vector. The Schrodinger equation was replaced by the Heisenberg equation of motion and the Heisenberg equation of motion says ih cross d over dt A_H(t) was = the commutator of A_H(t) with the Hamiltonian. And the solution to this, again in the simple case of time independent H was simply A $_H$(t)of t = e to the power i Ht over h cross A $_H$ at 0 which we said the same as Schrodinger operator A_S. So to repeat what I have said in the Schrodinger picture, the state vector carries the burden of time dependence and evolves in this fashion. Operators don't have any explicit time dependence. In the Heisenberg picture, the state vector doesn't have any time dependence but the operators have explicit time dependence. You go from 1 picture to another by a unitary transformation because if H is hermitian, e to the power i times H times a real number is a unitary operator. so this (refer Slide Time: 08:09) is a unitary operator, U for example and then psi H is the unitary operator acting on psi $_S$. similarly, the Heisenberg operator is a unitary operator A $_S$ U dagger or U inverse on this side. So we are justified in saying that the Heisenberg and Schrodinger pictures are unitarily equivalent.

They are just unitary transformations of each other. Now we are going to what is it for time independent Hamiltonian. But I define for time independent Hamiltonians by the Heisenberg picture by this trick. Now what we have to do is to ask what happens if there is time independence in the Hamiltonian. you could still continue to say at some fiducial instant of time, even if this has time dependence, you could say that the Heisenberg operator is defined as this operator A_S at 0 and then this operator again here (Refer Slide Time: 09:12). But you can still make a unitary transformation. There is no problem but you can see that is not very effective to do this if H has explicit time dependence. so what Dirac did was to say the cases we are going to look at are generally going to have a Hamiltonian.

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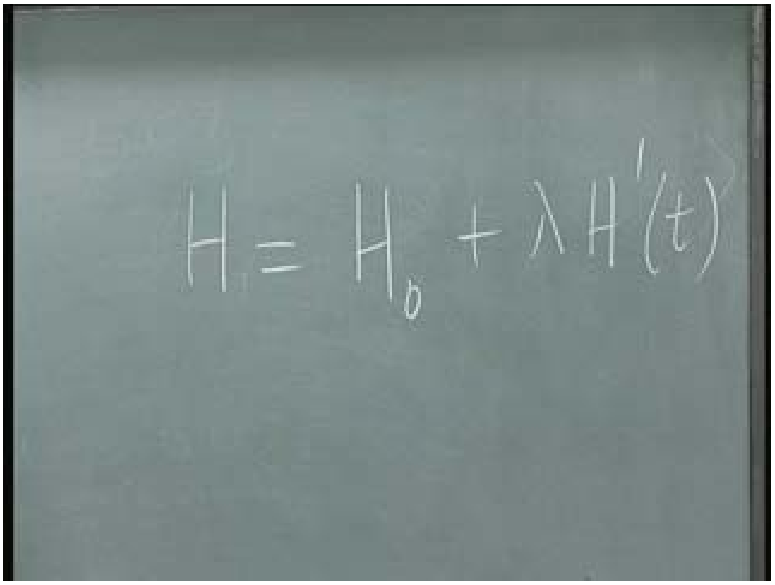

This total Hamiltonian is of the form H_0 which is time independent and which you presumably can solve + the perturbation which we have been writing down as H prime and it's possible that it is time independent. What kind of unitary transformation do you do? This is the problem that you would like to address. Of course there are lots of cases where H prime is time independent and you would like know what's the perturbation series, etc but we would like to address the general problem of this kind. Dirac's idea was the following. He said after all, whether the Hamiltonian has time dependence or not the Schrodinger state vector is going to evolve by some unitary operator acting on whatever is the initial state that you are given. now if the Hamiltonian consists of 2 parts which don't commute with each other of this kind (Refer Slide Time: 10:43), there is always going to be unitary evolution due to H_0, even if you switched off the other term, you still have this all the time. So why carry the time dependence around? Let's get rid of the time independence and therefore he said lets go to a in intermediate picture between these 2 pictures called the interaction picture.

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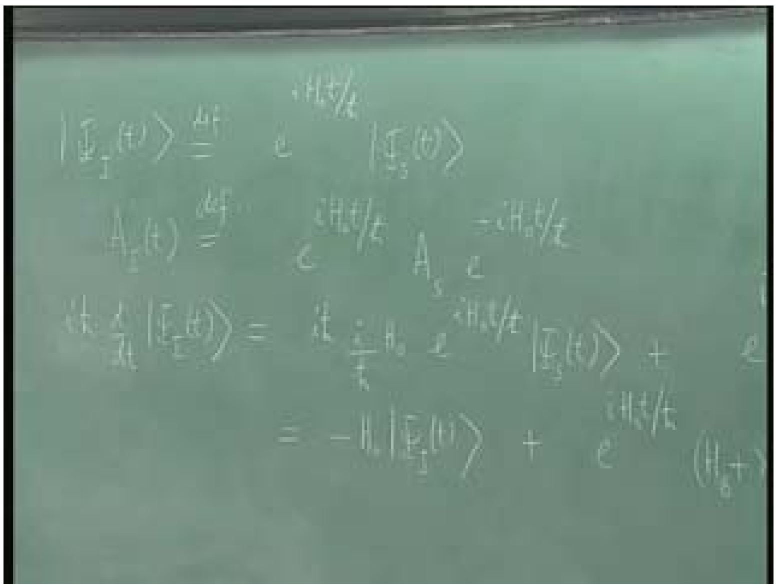

I define |psi $_I$ (t)> in this form, just as the Heisenberg picture you define this to be e to the power iH $_0$ t over h cross psi $_S$(t). If you did not have H prime in the Hamiltonian, then the interaction state vector psi I (t) is identical to the Heisenberg. But now I might have an interaction, H prime. Now what's the equation satisfied by this (Refer Slide Time: 12:07)?

For any operator A, i define A_I (t) = e to the power iH $_0$ t over h cross A_S. If you didn't have H prime, then the i subscript the interaction is same as going to the Heisenberg picture. Notice that you switch on an H prime but you still make the unitary transformation using only H_0, the portion of the Hamiltonian that you know. And then what happens? Well, if i write ih cross d over dt psi I (t) = the first term is going to give me ih cross i over h cross H $_0$ e to the i H $_0$ t over h cross psi S (t). That's the derivative of this (Refr Slide Time: 13:41) term, i bring down on iH $_0$ over H cross and it commutes with e to the iH $_0$. So it doesn't matter which place i write it + ih cross e to the iH $_0$ t over h cross d over dt psi S (t). now this (Refer Slide Time: 14:10) is ih cross times is d over dt but ih cross d over dt psi S (t) is the total Hamiltonian acting on psi s of t by definition. so this = - H $_0$ this h cross cancels e to the i H $_0$ t. By the way, psi S of t e to the iH $_0$ t over h cross is by definition psi I of t.

So let me write this (Refer Slide Time: 14:45) as psi I (t) with a - sign here + e to the i H $_0$ t over h cross H $_0$ + lambda H prime psi S of t by definition. This is the Schrodinger equation written in the Schrodinger picture. The total Hamiltonian is H $_0$ + lambda H prime.

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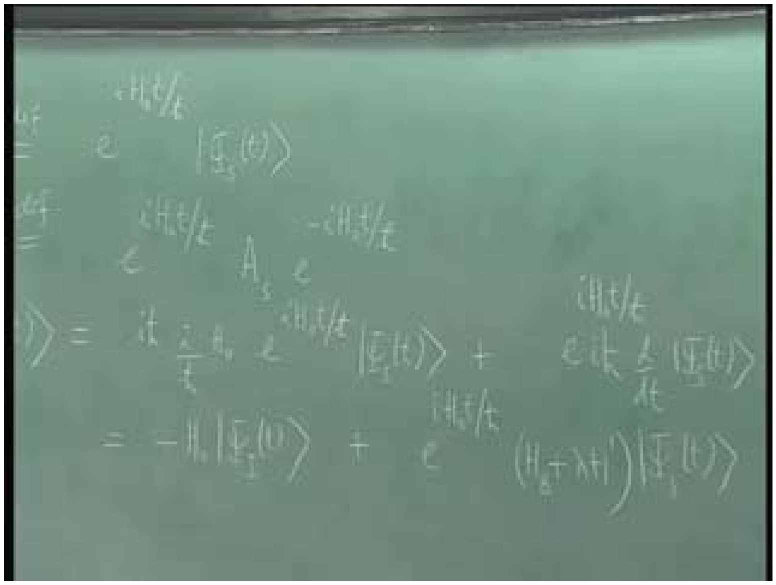

You still have to be careful to note that this H prime need not comminute with H $_0$ in general and therefore you can't move this in. that but certainly this (Refer Slide Time: 15:52) H $_0$ can be brought to this psi because it comminutes with itself. Once you do that, this H $_0$ comes here and you got e to the iH $_0$ t over h cross psi $_S$ but that psi I and that would cancel with this term completely.

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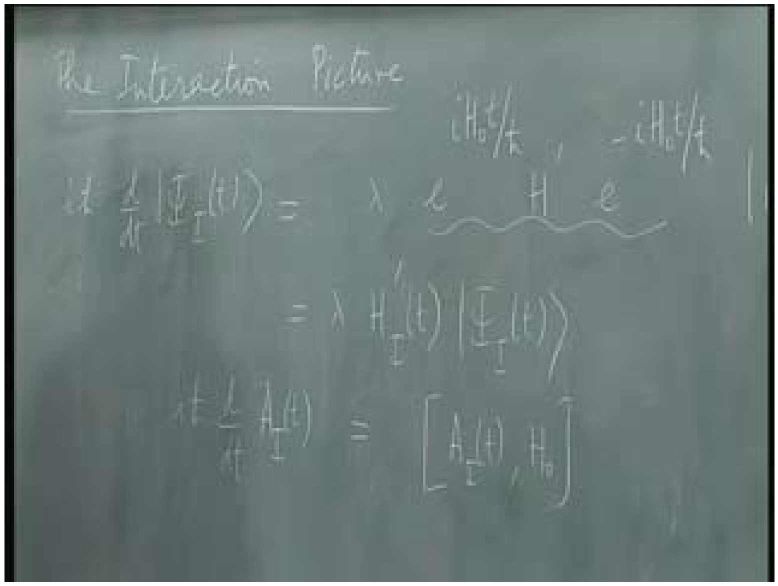

so it gives us an equation it says ih cross d over dt psi I (t) = it just leaves the lambda H prime term. Nothing more than that. therefore its + lambda e to the i H_0 t over h cross H prime acting on psi S (t) but psi s (t) is e to the - iH_0 t over h cross. I am going to substitute for psi S of t by bringing this (Refer Slide Time: 17:05) exponent to this side here and its - here and then psi I of t. but by definition, this quantity here (Refer Slide Time: 17:21) is the interaction picture operator H prime. So finally we get lambda H I prime of t psi I of t. so we have arrived at a situation where the evolution of this state vector in the interaction picture is governed entirely by the perturbation which might be time dependent explicitly. In this Hamiltonian, this (Refer Slide Time: 18:10) is the perturbation in the interaction picture. So whether H prime is explicitly time dependent or not, we don't care. This is the equation. What about operators? Well, look at an operator which doesn't explicitly dependent of time otherwise you include partial derivatives. What does this equation give you?

This immediately says if I differentiate and put an ih cross d A_I by dt, it's the commutator with A_I and the Hamiltonian H_0. So it says ih cross d over dt $A_{I (t)}$ is = the commutator of A_I (t) with H_0 and not H because we when differentiate it, we are going to get this H_0 coming on this side and then the H_0 on the other side (Refer Slide Time: 19:12). We have achieved the intermediate picture where both the state vectors as well as the observables or the operators representing the observables are time dependent unlike the Heisenberg or Schrodinger the pictures. But the time evolution of the state vector is governed entirely by the perturbation or potential that you apply and the time evolution of the observables is governed entirely by the free Hamiltonian. So it's in between the 2 pictures here and it turns out this problem is much easier to tackle because this (Refer Slide Time: 20:06) is very straight forward. You don't have the problem that we had earlier of this being sum of 2 operators we don't commute with each other. There is just one operator. Of course, it maybe time independent. We will see what to do about it but this is now a neater way of doing things because you have separated the problem. You have got rid of the systematic evolution due to H $_0$ which appears anyway, whether or not you have a perturbation. The task now we use to actually try and solve this equation. Now how would one do that? Well, there are many ways of doing this. But if you specify psi$_I$(t) at some initial instant of time, this (Refer Slide Time: 21:06) is a hermitian operator still. Therefore, you still have unitary evolution of system. Then you can write down, given this vector at some initial instant of time, you could chose that to be the Schrodinger state vector at t = 0, this becomes an initial value problem and you could try to solve this initial value problem by systematic expansion as follows.

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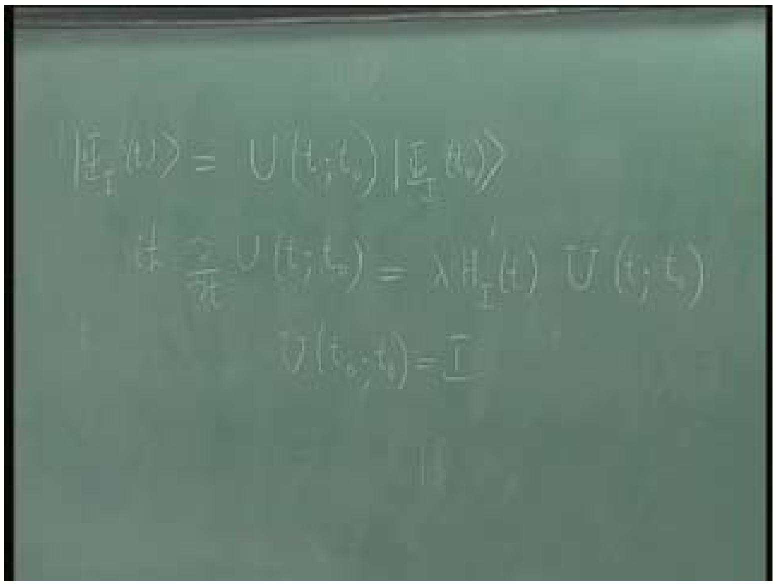

Let’s write psi I (t) = U(t) given some initial state vector at t 0 acting on psi I at time t 0. And this t 0 need not be chosen to be t = 0. All you have to do is to specify the initial state which could be a prepared state. I could prepare the system and switch on the perturbation. So we have given ourselves a little more freedom now. We match the Schrodinger and Heisenberg pictures at t = 0 but we would match Schrodinger and interaction picture ket vectors at the instant at which you switch on your perturbation which could be anything. So with some initial ket vector t 0, here is a unitary operator. And now the question is what’s the equation satisfied by this operator here and it is not hard to see that this is just H I on U.

So this immediately says ih cross partial derivative d over dt U (t, t 0) HI. The reason i use a partial derivatives is because i have introduced this initial time a label t 0 and i want to make sure that I differentiate it with respect to t. now what’s the initial condition that you would impose on this? Clearly U (t 0, t 0) = the identify operator because it’s clear that if you set t = t 0, we want the identity operator. We have to solve that equation for the operator U. after that i plug that in into this first line and i tell you what the state vector is at any instant of time. Since the way have do this is by developing things in power series, its clear there is lambda sitting here. This will help me keep track of the first order, second order, third order terms etc. but as it stands, this is not a trivial equation to solve. Therefore the first thing is do is to convert this into an integral equation satisfying this differential equation.

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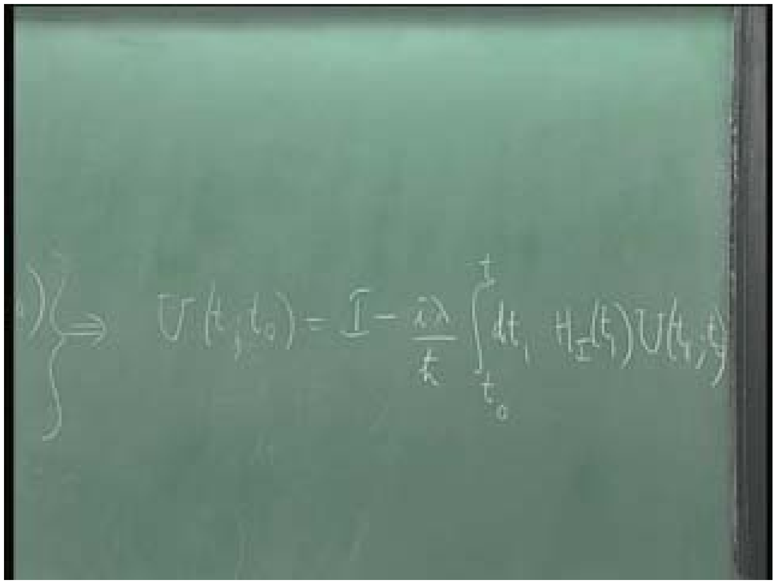

This is entirely equivalent to saying that U (t, t 0) = I - i lambda over h cross and integral t 0 up to t dt1 say some fiducial time H_I (t1) U(t1,t 0) because if you differentiate this equation both sides after multiplying by ih cross, if you differentiate I, it is a constant, so it gives you 0 here. When you multiply by ih cross, you get lambda HI (t) U (t, t 0) by using the formula for differentiation under the integral sign. the upper limit of integration is a variable and therefore you would write integral at that with time multiplied by dt over dt which is1. so this differential equation together with this initial condition is equivalent to this inhomogeneous integral equation for U. that integral equation can now be solved by the method of iteration because to order lambda to the 0, U is I, so you put that in here (Refer Slide Time: 26:38). That’s the first order correction. If we want the next order correction, you put a U to order lambda which is this formula and so on.

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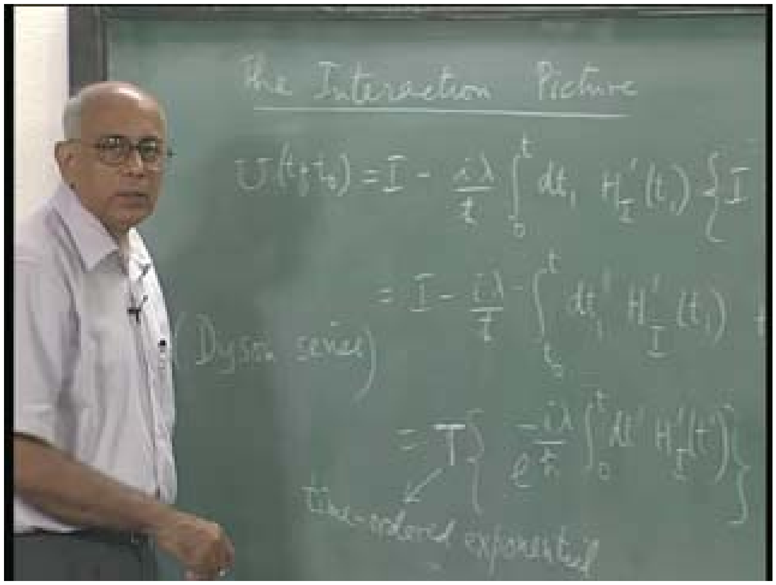

So you end up with series which says U(t, t 0) = I - i lambda over h cross and integral 0 to t, dt1 HI prime (t1) times I - i lambda over h cross and if you substitute for U (t1,t 0) inside , it would be exactly the same formula t 0 to t1 dt 2 and then you end of with a U (t 2). So this would be integral t 0 some t1 dt 2 HI prime (t 2) U(t 2,t 0) for which i again put I and so on. so it's clear that this exact equation gives you an infinite series which is I - i lambda over h cross 0 to t dt1 HI prime (t1) + (- i lambda over h cross whole squared) t0 to t dt1 integral t0 to t1 dt 2 H_I prime (t1) H_I prime (t2) + etc. notice very carefully that H_I prime(t1) and H_I prime(t2) need not comminute with each other. They have time dependence and there is nothing to say that they comminute with each other. But, they are automatically time ordered because it's evident from this that 2 is always less than t1 and t1 goes up to time t and the next term would be the order term and so on and so forth.

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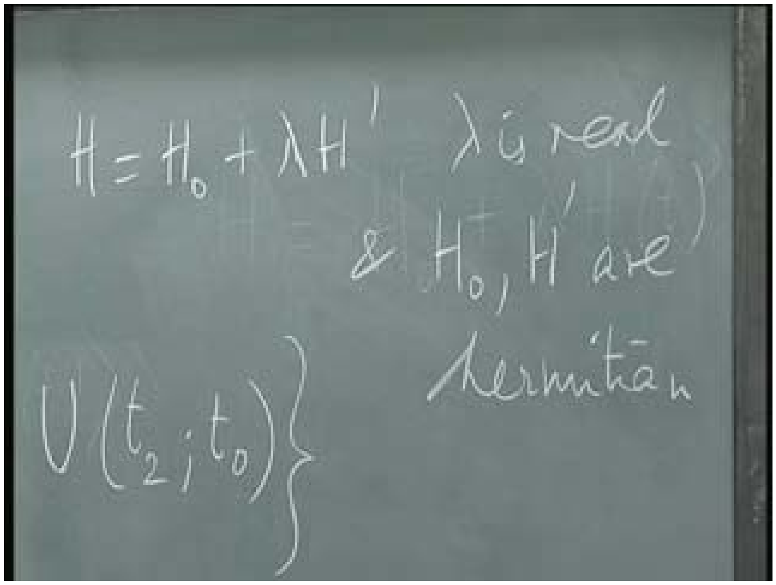

We started off by saying H is H $_0$ + lambda H prime and H $_0$, H prime are Hermitian and lambda is real. We started with the Hermitian Hamiltonian. So we have conservation of probability because we don't know anything about it at all. But the fact is, if the Hamiltonian is hermitian, its eigenvalues are guaranteed to be real, whatever the consequences of that be. So in such a situation you can never look at dissipation. so what would happen however is, if you switch on the perturbation, the total probability would be conserved but the system, if you start in given state of H $_0$ would not remain in that state. It will go to some other state. It would make transition back and4th but it doesn't disappear. If we are talking about a particle in some external field, the particle doesn't get absorbed or disappear. It just makes transitions from one state to another. There are situations where you might want to put in a complex or non-hermitian Hamiltonian to explicitly put in friction or put in dissipation, loss or absorption. We aren't looking at that class of problems. This series is called the Dyson series. It's in a little greater a generality than we need to solve our problems in ordinary quantum mechanics.

But the advantage is that this is precisely the series that we use in quantum field theory for instance, because we haven't any made any assumption about what kind of system we have, except that it has a hermitian Hamiltonian. The way to get the perturbation series explicitly is to convert this differential equation for unitary operator U into the integral equation and then it follows by iteration. Now of course, you could ask, does the series converge and you have exactly the same problems have convergence which we brush under the carpet without really looking at it. So you really have to again prove explicitly that this Dyson series converges formally. We not going to get into that technical question here because this is outside the purview of what I want do here. But the fact is that this is exact and there is no approximation being made here. In that sense, this is the formal power series and i am assuming that it makes sense.

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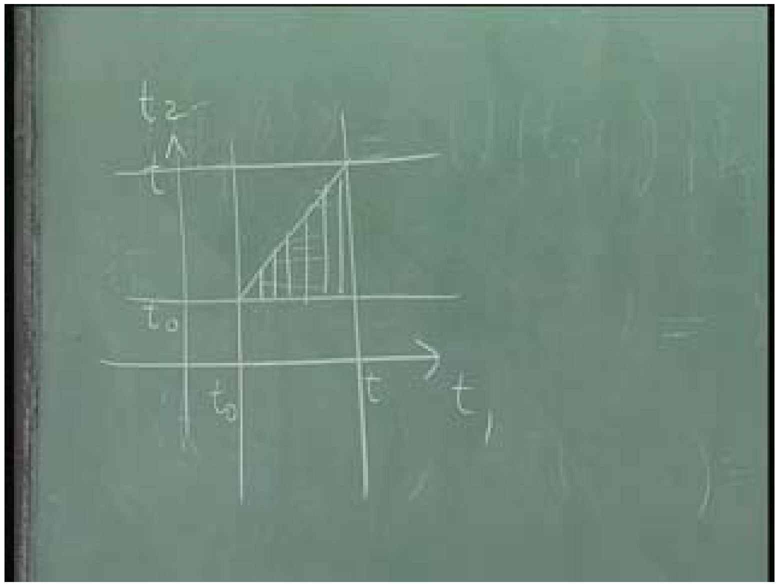

I pointed out that these operators, HI prime (t1) and HI prime (t2) at different instants of time don't commute. if they did, if you could freely mix this around, then it's clear that each of these integrals, for example take the second order integral here, it runs over 2 variables, there is a t1 and there is t 2 and each of them runs from some t_0 up to t. and the integration is being done in such a way that t 2 is always less than t1. So it's being done over this triangle here (Refer Slide Time: 34:32). So what you are really doing is fix a t1 between t_0 and t and integrate over t2 along this line from t_0, up to the current value of t1 and you add up these and you end of with this integral. Now if you didn't have the problem of convergence for anything like that, then this integrand (Refer Slide Time: 35:03) is symmetric under the interchange of t1 and t 2.

Therefore, the value of integral here (Refer Slide Time: 35:10) is the same as the value of the integral reflected about this 45 degree line. So you could write this as half the value of the integral over the full square divided by 2 factorial. So you write this as over 2 factorial integral 0 to t, 0 to t. The next one would be 1 over 3 factorial 0 to t for all of them. Because, if we took 3 numbers t1, t 2, t 3 and ordered them, there is exactly one way in which you have t1 less than t 2 less than t 3. You have several other ways of permuting. Out of 6 combinations we, have1 of these. So each time you put a 1 over n factorial and you do the integral for each of the variable from t_0 to t. And then, it's just the exponential e to the power - i lambda over H cross t_0 2 t dt prime H prime (t). You can't quite do that her because of this lack of commutativity. But you could still time order it.

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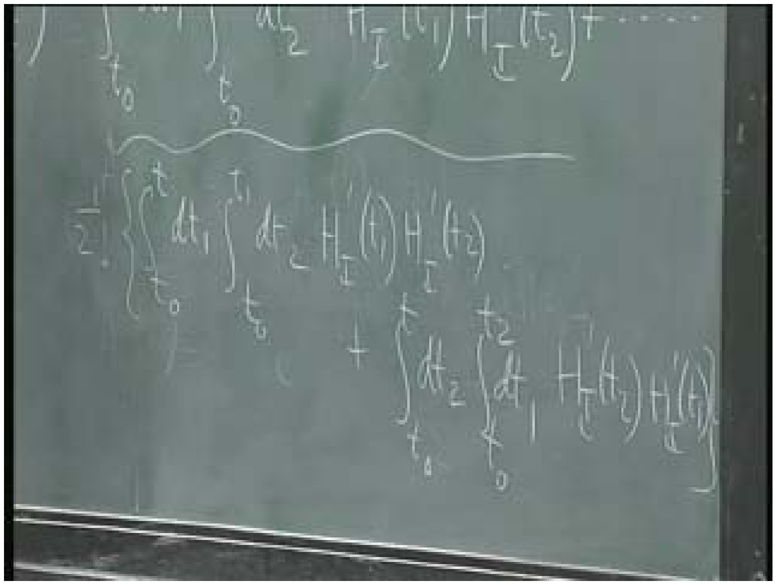

So I would still write this as =1 over 2 factorial, an integral t $_0$ to t dt1, t $_0$ to t1 dt 2, HI prime (t1) HI prime (t 2) + integral t_0 to t dt 2 integral t_0 to t_2 dt1 HI prime of t 2 HI prime of t1. That's exactly the same as before because all I have done is to interchange the labels t1 and t 2 and i have taken care of the commutation problem because the earlier time is on the left and the later time is on the right. I could call this sum as the time ordered product in which the rule is, put the earlier time argument on the left and the later time on argument on the right.

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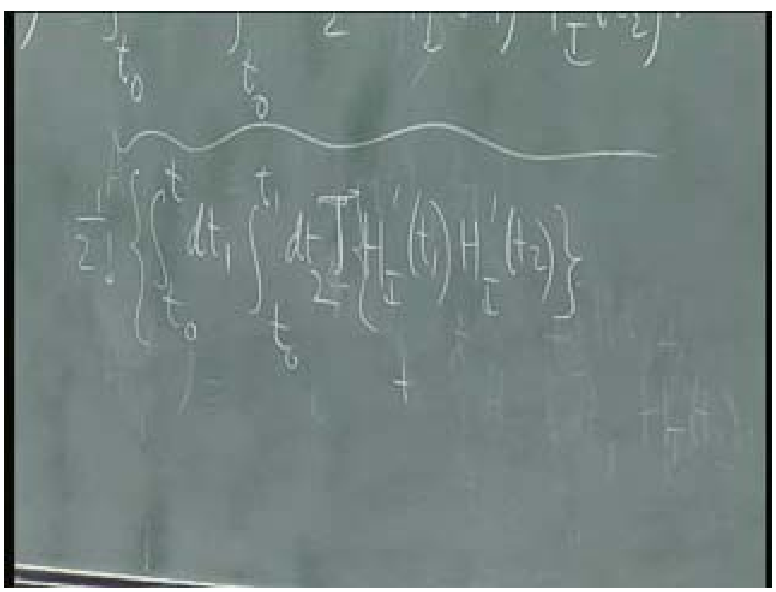

So I could write this as the time ordered product t of this and erase this. Then I have 1 over 3 factorial, the time order product etc.

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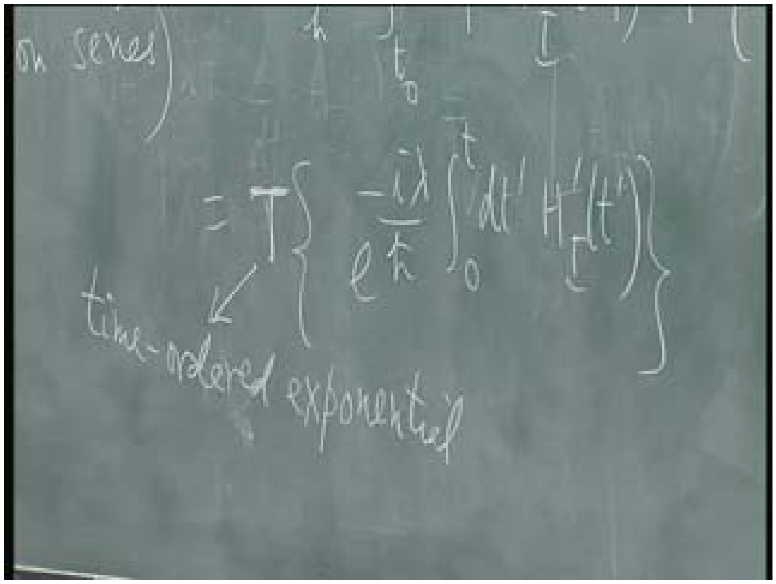

The whole thing can therefore be written as T, the time ordered exponential - i lambda over h cross integral 0 to t dt prime H_I prime (t prime). So, this is of great use in quantum field theory. When you write down perturbation expansions, you must remember that the formal solution to the Schrodinger equation for the time development operator in the interaction picture is a time ordered exponential. When you do relativistic quantum field theory, the question of can you order time, etc comes in and this can be done for the physical processes we are interested in. there are intervals which are placed like where the question of ordering doesn't make sense. So causality is brought in and so on forth. But for the kind of problems we are looking at here, this is a little too powerful. We don't need this but I thought we should know the formal expression. Now let's do the following.

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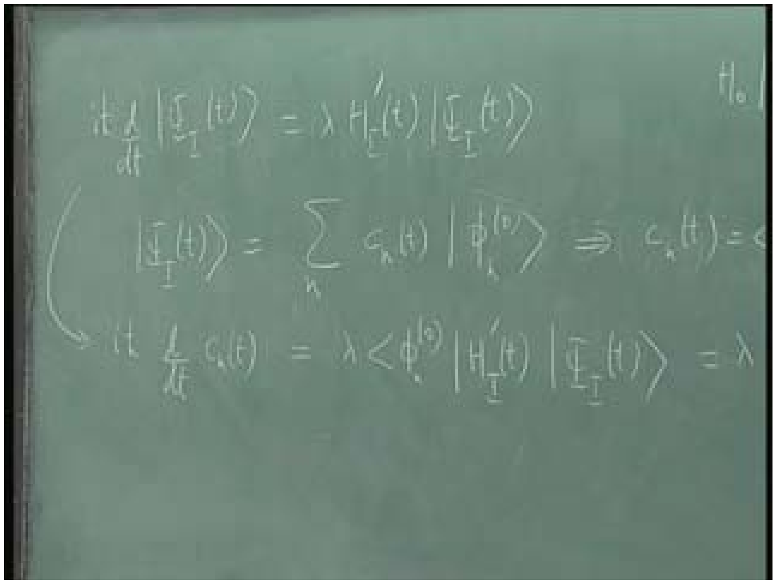

Our task is to find out what is psi i at time t. as usual, we assume that the unperturbed Hamiltonian H $_0$ has eigenvalues and eigenstates which we know. We call them phi n 0's and En 0's. So let's expand it in that bases I know that this equation satisfies HI (t) psi I (t) in this fashion. So let's write psi I (t) as = a summation over n, some coefficient which will be time dependent, in general and then phi n 0.

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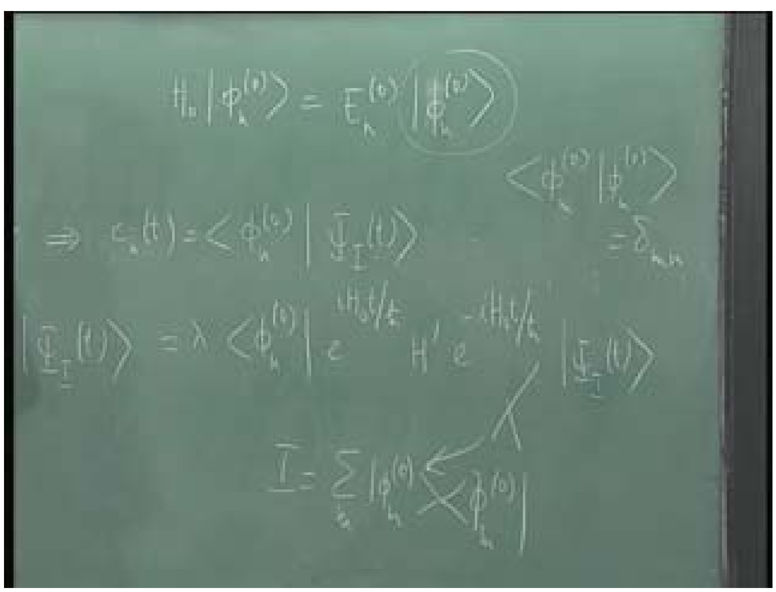

The assumption is that H_0 on phi n 0 is = E n 0 phi n 0 and that they form a complete set. Now, i can still use the system bases and that's like fixing a coordinate system once and for all. so i use the same bases and in this Hilbert space, the assumption is the perturbation is such that the states are not taken out of this Hilbert space. They could be transitions but they not taken out of this space. And then I can expand any arbitrary state vector in whatever picture you like in that bases with coefficients which would be, in general time dependent. So this is a completely general statement here and i am going to put that into this here (Refer Slide Time: 41:41) and see what happens. So how do i find out what the is Cn (t)? This implies that phi m 0 phi n 0 = delta mn. So it forms an orthogonal basis.

Then Cn (t) is just this amplitude phi n 0 psi I (t). Once you have an orthonormal basis, this coefficient is just the overlap of this state vector with the corresponding bra. So let's put that in and write ih cross d over d t C_n (t). So I take the scalar product on both side with phi n of 0 and phi n of 0 is the time independent bases vector. So it becomes d over dt Cn (t) on this side. That is = phi n 0 HI (t) psi I (t). this is = lambda times phi n 0 and if you recall our definition of this operator HI prime (t), it was = e to the i H_0 t over h cross H prime in the Schrodinger picture, e to the - iH_0 t over h cross and then a psi I (t). what should i do next? Well, what i am trying to do is to take this equation expanding the unknown ket vector in this bases set and converting the differential equation for this ket vector to a differential equation for the coefficients (Refer Slide Time: 44:25 to 44:40). And of course this is going to be an infinite set of equations for the coefficients. On the right hand side, since it's a linear equation you expect a linear combination of the same coefficient with some factor in front. So, what would you do next? I would like to get an equation which involves the Cn's on this side. I'm almost there but i need to convert this state vector into a coefficient. What should I do? I insert a completed of states. Insert inside here (Refer Slide Time: 45:30), I = summation over m |phi m 0> < phi m 0|.

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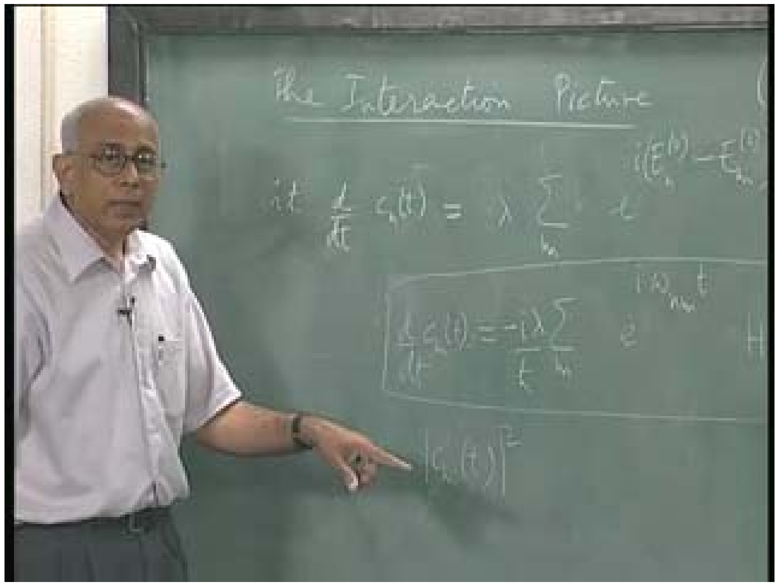

So that gives us i h cross d over dt Cn (t) = lambda times summation over m phi n 0 H prime. what is this operator acting on phi n (0) ? Well, we know that it's just e to power i En 0 t over h cross. that comes out as the factor this side. So you get the first term which is e to the power i En 0 t to the over H cross that comes out as the factor but what remains inside is phi n 0 H prime. and notice that once again, H_0 t acting on phi m 0 is going to you the same e to the i Em 0. So this becomes (Refer Slide Time: 47:33), - Em 0 t power h cross and then phi n 0 H prime phi m 0. So both the phase factors have come out and you have this matrix element and it's multiplied by phi m 0 bra vector psi i of the ket vector but that's Cm of t. now what would you like to call this (Refer Slide Time: 48:10)? Well, these are the unperturbed levels; E1 (0), E 2 (0), E 3 (0) and so on and what we have here is an energy difference Em 0 - En 0 divided by h cross. So it has dimension of frequency.

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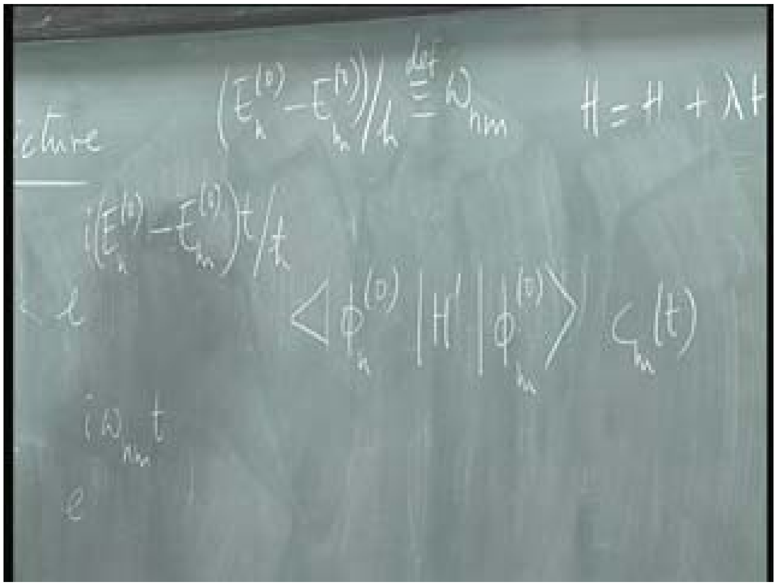

So En 0 - E m 0 over h cross = omega nm. omega could be negative, if En is less than Em. So it's e to the power i omega nm t times this (Refer Slide Time: 49:20) but what is this? This is just the matrix element of H prime in the original basis. So this is H prime nm, some complex number and Cmt, in general. All we do know is that H prime nm is a complex conjugate of H prime mn. So we have a set of linear ordinary differential equations for the coefficients.

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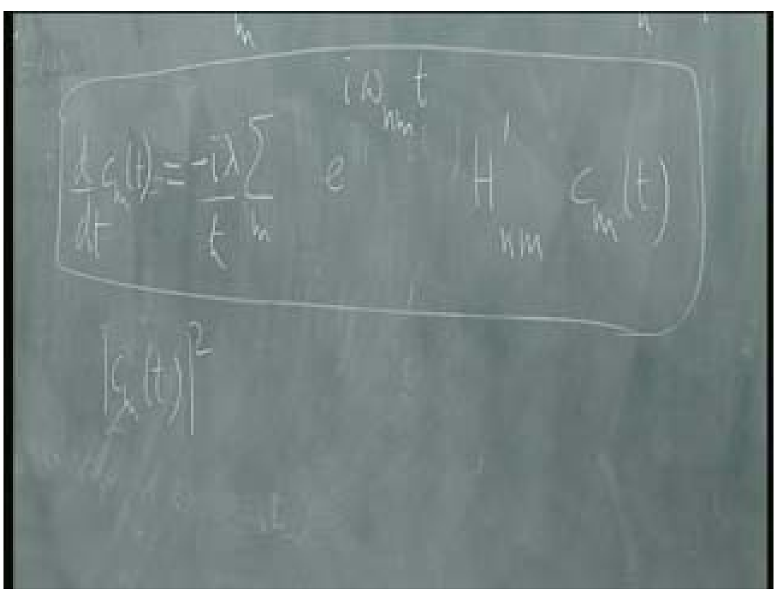

And now if you give me the perturbation, these quantities and frequencies are supposed to be known. What we are doing is solving a matrix equation. It could be infinite dimensional in general. But this would depend on how big these matrix elements are. So it you turns out that H prime doesn't have a connection between levels which are very far separated, then you could drop it and truncate it. In any case, there is a lambda sitting here. So you can solve this set of equations again iteratively. So the next trick would be to say let Cn of t = Cn 0 th order + Cn first order + etc, plug it in sequentially and solve these equations. So I put in the 0 th order here. That will give me the first order term, i solve it and then i put it back here, solve it and so on. This is an operational way of solving the Dyson equation series, in general. But this quantity here is some kind of time dependent matrix acting on this coefficient (Refer Slide Time: 51:43).

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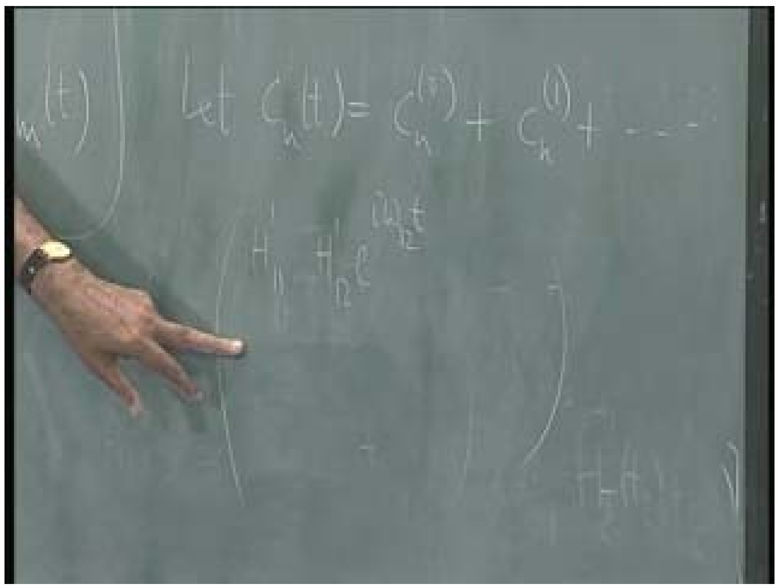

This time dependent matrix would look like, for example, if you write down the 11 element, this would be just H prime1 1 but the 1 2 th element would be H 1 2 prime e to the power i omega1 2 t. on this side, you would get H prim 21 e to the - i omega1, 2, 3. So it will be in fact, the complex conjugate of that. Then you could use iterative methods once again to see whether you can write the solution and series in lambda. So what we are going to do next time is to take this equation (Refer Slide Time: 52:40) and apply it to the simplest possible case and the case I am interested in applying it to, is the following. I have a spin half system or i have an atom in which I assume that there is extra ground state and an existed state. It doesn't matter. I end up with 2 ket vectors.

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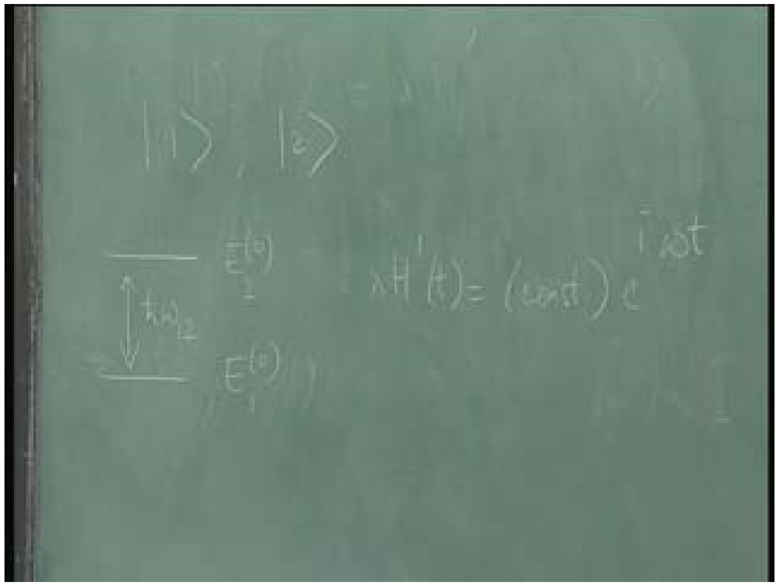

One of which is |1>, |2>. That's it. It's just a 2 level system with 2 levels, either the ground state or the exited state of an atom or if i put it inside a magnetic field, this would correspond to spin down and spin up states, for example. Whatever it is, this has some energy E1 (0) and this has energy E 2 (0). so that's my unperturbed system. I prepared a system in one of these 2 states. Then, i switch on a time dependent field. The field I have in mind is the following. So this separation is natural frequency with some energy difference h cross omega. This is omega 21 if you like, and I switch on ta perturbation at a different frequency. So I add an H primary of t = some lambda, some constant e to the power i omega t. And I switch on a field at some other frequency and then i would like to know what happens as I tune omega over different values. For instance, if omega exactly equals omega1 2, what happens when it's in resonance? So this is the problem we are going to look at. I will show you that there occurs what are called Rabi oscillation in this problem which is of significance in many physical applications. The one I am going to look at, specifically is magnetic resonance.

So the idea is I apply a huge field on the z direction so that i have 2 possible states of the system. After that I apply a field in that transfer direction as a perturbation which would cause flips between up and down. But now I am going to apply a time dependent field. This is typically what's done in an NMR experiment where you align with the static field and then you apply a transverse radio frequency field and watch what happens to the system. We will see that there is rich amount of physics involved in this. So this I will do it tomorrow and that would be our last application. I will also mention the connection with the similar model for atoms in the presence of a radiation. It's essentially the same physics once again.

So each time we need to write down the model Hamiltonian, a model for the perturbation and then ask what happens to the transition rates. In particular, we will be interested in calculating what these quantities are because modulus Cm of t whole squared is the probability that, remember this whole thing is with some given initial condition, so this is the probability that at time t, the system is in the eigenstate phi m of 0. That will change and we would like to see how it oscillates. Now we saw this a little bit earlier when we took the spin half system and just apply the static external field in the transverse direction. But now we would like to apply a time dependent external field. There are now 2 time scales to play with in this problem. One of which would be the energy difference h cross omega that gives a natural frequency as the system but there is second time scale coming in from the frequency of the driving force. We would like see with interaction between these 2 time scales and see which one dominates. So that will be the next topic. Let me stop here today.