

Foundation of Quantum Theory: Relativistic Approach
Time dependent perturbation theory 1.1
Perturbation theory 1.5
Prof. Kinjalk Lochan
Department of Physical Sciences
IISER Mohali

Lecture- 05

So, having have discussed about the time independent perturbation theory approach in this set of discussions we will discuss about time dependent perturbation theories. So, just to revise the key aspects what we learned in the previous sessions that the time independent perturbation theory effectively tells me about the exactness of the structure which we are dealing with. Having considered more and more potential terms which are could be present in the Hamiltonian that will update our knowledge of the true character of the eigenfunction and eigenvalues so therefore the time independent

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \dots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$
 But there is no dynamics viz- \rightarrow viz true eigenstates

$$|\psi(t=0)\rangle = \sum_n c_n |\psi_n\rangle$$

$$P_n(0) = |c_n|^2$$

$$|\psi(t=T)\rangle = \sum_n c_n e^{-\frac{iE_n T}{\hbar}} |\psi_n\rangle$$

$$P_n(T) = |c_n e^{-\frac{iE_n T}{\hbar}}|^2 = P_n(0)$$

perturbation theory is an approach to know the system better.

$$|\psi_n^{(0)}\rangle = |\psi_n^0\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \dots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

But there is no dynamics viz -a -viz true eigenstates

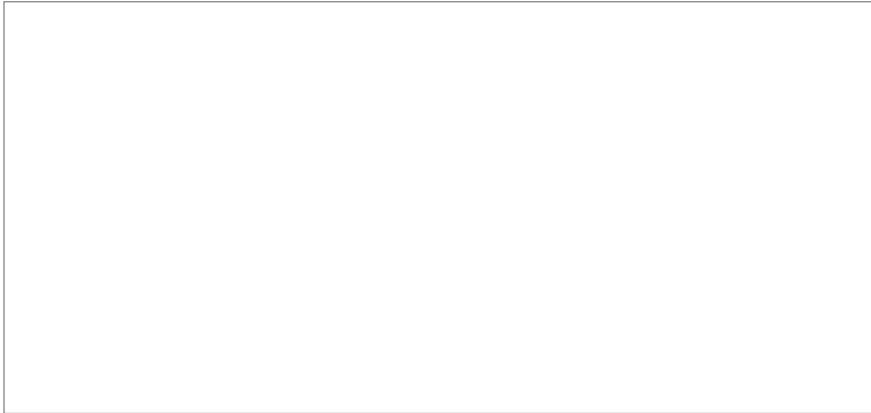
$$|\psi_{(t=T)}\rangle = \sum_n c_n e^{-iE_n \frac{t}{\hbar}} |\psi_n\rangle$$

In most of the times, we so we have for the simplistic part of the system and then we argue that more complicated parts are subdominant. So, whatever we could obtain is good enough information. However, if you want to be more precise in our understanding, we should consider all the terms in the Hamiltonian which are present. And in the time independent perturbation theory, ultimately tells me about the time independent version that is the eigenstates which do not evolve in time. How accurately do I know the eigenstates, the true eigenstate? So, I in a fully developed Hamiltonian where all the potential terms are present, all the kinetic terms which come from correct description of relativity come through. The true eigenstate is made up from the piece which we solved at the non-relativistic setting with a simplified potential. And then order by order, we started including effects of other terms which could be present in the Hamiltonian. And the result of that for each such perturbation Hamiltonian, the eigenfunctions get corrected in a power series of the expansion parameter λ . So we could see a couple of examples where we updated our knowledge of the true eigenstate by expanding things in λ . And similarly, for energy eigenvalues as well, it will no longer be only the free theories that is unperturbed Hamiltonian eigenvalue. It would also get corrected with the parameter with which the perturbation comes about. And it will be a power series in that as well. So that is what we have learnt. However, in all of this effectively it is just telling us about the correct description of the system, but it does not tell about the dynamics in the system. In the sense suppose I get a correct description of the eigenfunctions or eigenvalue up to whatever order of λ we wish. Let us say we go up to λ to the power 10 then I would have a $\psi_n^{(0)} + \lambda\psi_n^{(1)}$ up to going λ to the power 10 times $\psi_n^{(0)}$ and similarly for energy eigenvalue so then I say okay all other higher orders are very very minute so my description of energy eigenfunction and energy eigenvalue is good enough for me.

No experimental resolution is able to tell me anything beyond this 10th power of perturbation parameter. And then I want to know if I describe my initial state as a good enough description by this power field expansion up to 10th power, then how does it evolve in time? So then I know what are the correct true eigenfunctions up to order λ to the power 10 or 100 or whatever you have or in principle up to infinity as well. You truly know what is the correct eigenfunction not only approximately. Then at time t is equal to 0 if I give my state it will be just a superposition of all the possible eigen states of the Hamiltonian which would be given like this. Remember these ψ_n are the correct eigenfunctions. The eigenfunctions coming on the left hand side which is the true eigenfunction of the full Hamiltonian. Then if in this state at time t is equal to 0, if I ask what is the probability that the state would be found in the n th true eigenfunction, then the Born rule tells me it would be just the projection of the state along the $\psi_n^{(0)}$ basis and mod square of that. So therefore, it would be $|c_n|^2$ at time t is equal to 0. The description is asking for a component along the n -th direction, which is c_n . And therefore, the probability of the system to be found in the n th eigenfunction of the correct Hamiltonian, the full

Hamiltonian, would be $|c_n|^2$. Now, if I ask, what is the probability that after while t is equal to capital T , what would be the probability of the same thing? What would be the likelihood the state will still be found in the eigenbasis ψ_n then I will first time evolve it and time evolve with $e^{\frac{-i E_n T}{\hbar}}$ and since these ψ_n 's are eigenfunction of the full Hamiltonian this operation will just give me a phase $e^{\frac{-i E_n T}{\hbar}}$ will come here because $e^{\frac{-i H T}{\hbar}}$ acting on ψ_n will just give me back $e^{\frac{-i E_n T}{\hbar}}$ and the state ψ_n back. So this is what happens after time evolution so this will be a new state after time T . Then I ask the question what is the probability that the state would be found after time T along the eigenbasis ψ_n will be the answer again projection of the time evolved state along the ψ_n basis and mod square of that. So, this time it will give me if I take the projection along the ψ_n . I will get this number this complex number and mod square of this will again be $|c_n|^2$ because this being a total phase will go out of the computation and I will get $P_n(T) = P_n(0)$ that means the probability still remains the same along the n -th eigen direction so there was there is no dynamics in this sense this is time independent theory therefore it does not bring any change, that is to say if I initially give you a state which is c_n 's are zero for all other n 's for all n not equal to let us say 1, apart from ground state all the states are not occupied that is there is no projection along that that means system is in the ground state and therefore if I time evolve it will develop some phases but still it will remain in the ground state there is no probability that it will start in the ground state and go to the excited state. This is not allowed. This is not allowed in time independent perturbation theory. No transition is allowed. Similarly, if I started from excited state, the time independent perturbation theory is unable to bring me down. Okay, so there is no probability that the system will come down by itself. Time independent perturbation theory does not allow that. But we see this happening in nature. Atoms get excited and atoms get de-excited as well. So, evidently this is not a phenomena dictated by time independent perturbation theory. Because we see dynamics and a dynamics has to come through not from correct knowledge of Hamiltonian, but something which breaks this time independence. So, that takes us in the domain of time independent perturbation, time dependent perturbation theory rather. So, therefore any dynamics which is effectively the change in the probability along the state along any direction comes if the states were eigenstate of a one Hamiltonian at the beginning of process and the evolution happens with a different Hamiltonian. So, this became a total phase over here which did not matter at the end because of the fact that the states here are eigenstate of the Hamiltonian H here. So, if I started with a decomposition where this were eigenstate of some initial Hamiltonian, but as the time evolves, the Hamiltonian also changes, then no longer the new Hamiltonian after time t will take this as eigenfunctions, because it was eigenfunction of the Hamiltonian at time t is equal to 0. At some different time Hamiltonian has itself changed. So their eigenstates will also change. So this will no longer be eigenstates of that new Hamiltonian. And therefore this phase kind of thing would not come about. So therefore the dynamics will only come if the Hamiltonians change in time. That is to say you have to insert a correction piece to the Hamiltonian which changes in time. So all the processes of dynamics which we see in the atomic physics, molecular physics or physics in general where electrons in an atom goes up, comes down, sends photon, absorbs a photon. All these things are the discussion under time dependent Hamiltonian. This cannot happen in time independent Hamiltonian because Hamiltonian does not change in time. Probabilities do not change in time.

Okay.



$$\mathcal{H}_0 \rightarrow \mathcal{H}_0 + \mathcal{H}'(t)$$

Then

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n(t)/\hbar} |n\rangle \rightarrow \sum_n c_n(t) e^{-iE_n(t)/\hbar} |n\rangle$$

Previously without perturbation

$$\mathcal{H}_0 \psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\text{Now } (\mathcal{H}_0 + \mathcal{H}') \psi = i\hbar \frac{\partial \psi}{\partial t}$$

So therefore, If I do this, that I initially try to write down the time dependent description of the state after a while. If theory was time independent, I know it will just pick up a phase. This would be in time independent picture. Now, once a time dependency is brought about, this expression will be corrected into not only the phase, but the magnitude of the projection will also change. c_n s are supposed to develop a time dependent character on their magnitude as well apart from phase, if the Hamiltonian has a time dependency. So if Hamiltonian has no time dependency, the c_n s become a constant. If Hamiltonian becomes a time dependent thing, the c_n s will also change along time. So not only phases will change, their magnitude will also change. And then we ask that if this is the possibility, so this is what we are assuming will happen, that probability should change. So only phase should not come, the magnitude also should change because in mod squares, this will survive. And this should better be a function of time. It cannot be independent of time if we are talking about dynamics. We need to change the probabilities of being found in this eigenstate or that eigenstate. So therefore we are looking for a true description of the time evolved eigenstate like this. And this better satisfy the time dependent Schrodinger equation. Previously we were solving for time independent Schrodinger equation because we were dealing with time independent theory. Time dependent Schrodinger equation will be the Hamiltonian of the system acting on the wave function evolves it in time like this. Effectively this is the time dependent Schrodinger equation. Now I have known that my new description is the true Hamiltonian is \mathcal{H}_0 plus some time dependent function $H(t)$ or \mathcal{H}' . This should be equal to the

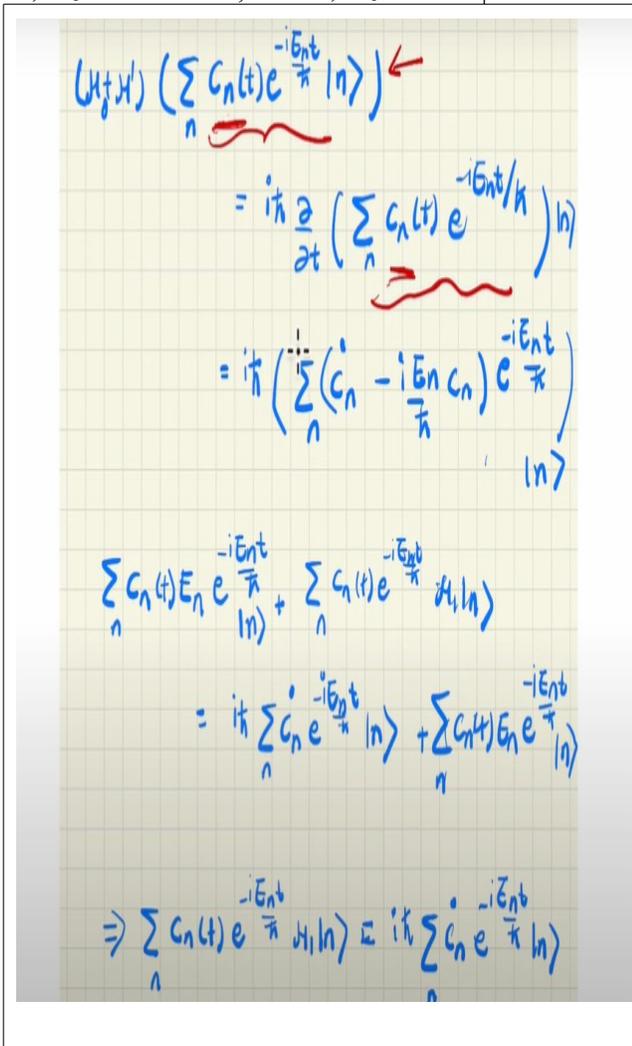
$$i\hbar \frac{\partial \psi}{\partial t} .$$

This is the time dependent equation which we will try to solve. Again in this set of notes which we discussed that the time dependent wave function after a while will be given like this where c_n 's are

supposed to carry the information of dynamics that means the Hamiltonian which depends on time. So therefore I will feed this ψ_n in the left hand side as well as on the right hand side. Remember left hand side and right hand side both there were ψ 's coming. These ψ 's are to be written as the proposal in which the magnitude of the projection coefficient also changes in time. Ok? So let us do this operation and try to see what do we get out of it. So right hand side I would just take the time derivative.

So first the time derivative will try to go inside the summation and try to look wherever time dependence is coming about. The time dependency is there in the coefficient c_n and the time dependency is in the exponential, this. $|n\rangle$'s are supposed to be time independent. So, the total derivative will hit the c_n 's, will hit the exponentials but is not hit the eigenstates $|n\rangle$. Ok, so ultimately I am going to get this. First derivative c_n , the derivative action hits the c_n and the exponential will just go for the ride, which is outside here. And in the second case the exponential is hit upon by the derivative and the c_n 's just go for the ride, which are here. So ultimately the total derivative of the wavefunction on the right hand side give me an expression like this. Ok? Fine.

Now, secondly if I look for the left hand side, left hand side was made up from two pieces H_0 and H_1 or H' , H_l let us call it, not H' , H_l . These $|n\rangle$'s were the eigenstates of the Hamiltonian at time $t=0$.



Handwritten derivation on grid paper:

$$(H_0 + H_1) \left(\sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle \right)$$

$$= i\hbar \frac{\partial}{\partial t} \left(\sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle \right)$$

$$= i\hbar \left(\sum_n (\dot{c}_n - \frac{iE_n}{\hbar} c_n) e^{-iE_n t/\hbar} |n\rangle \right)$$

$$\sum_n c_n(t) E_n e^{-iE_n t/\hbar} |n\rangle + \sum_n c_n(t) e^{-iE_n t/\hbar} H_1 |n\rangle$$

$$= i\hbar \sum_n \dot{c}_n e^{-iE_n t/\hbar} |n\rangle + \sum_n c_n(t) E_n e^{-iE_n t/\hbar} |n\rangle$$

$$\Rightarrow \sum_n c_n(t) e^{-iE_n t/\hbar} H_1 |n\rangle = i\hbar \sum_n \dot{c}_n e^{-iE_n t/\hbar} |n\rangle$$

$$(H_0 + H_1) \left(\sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle \right) =$$

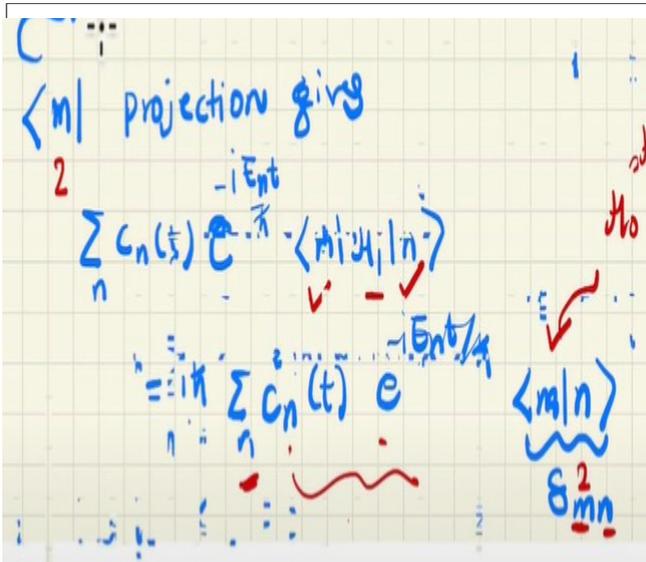
$$i\hbar \frac{\partial}{\partial t} \left(\sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle \right) = i\hbar \left(\sum_n (\dot{c}_n - \frac{iE_n}{\hbar} c_n) e^{-iE_n t/\hbar} |n\rangle \right)$$

$$\left(\sum_n c_n(t) E_n e^{-iE_n t/\hbar} |n\rangle + \sum_n c_n(t) e^{-iE_n t/\hbar} H_1 |n\rangle \right) =$$

$$i\hbar \sum_n \dot{c}_n e^{-iE_n t/\hbar} |n\rangle + \sum_n c_n(t) E_n e^{-iE_n t/\hbar} |n\rangle$$

→

$$\sum_n c_n(t) e^{-iE_n t/\hbar} H_1 |n\rangle = i\hbar \sum_n \dot{c}_n e^{-iE_n t/\hbar} |n\rangle$$



$\langle m |$ projection gives

$$\sum_n c_n(t) e^{-iE_n t/\hbar} \langle m | \psi(t) \rangle =$$

$$i\hbar \sum_n c_n(t) e^{-iE_n t/\hbar} \langle m | n \rangle = \delta_{mn}$$

At time t is equal to 0, if I assume that this ψ is 0 that means I start my time dependency at time t is equal to 0 and some function comes at time t is equal to 0 and changes it. So, therefore at time t is equal to 0 these functions n are eigenfunctions of the Hamiltonian \mathcal{H}_0 . So, \mathcal{H}_0 acting on n will give me E_n . So left hand side, first this term goes, goes across these complex numbers and hits the state and gives me n times the state back. Fine.

However, these n 's are not supposed to be the eigenfunctions of \mathcal{H} . So \mathcal{H} will also go across these complex numbers, hit the n , but this time it will not be able to give you eigenvalue times the wave function back. That was true only for \mathcal{H}_0 because n 's were eigenfunctions of \mathcal{H}_0 .

So I am left with this expression where this is set of complex numbers multiplied with n then set of complex number and an operator let us call it operator acting on the state n and the right hand side I have set of complex number with n and another set of complex number with n . So now you see that this term, second term over here is exactly cancel the first term in the left. Just like in the time independent perturbation theory, we were seeing that some terms on the left and some terms on the right get cancelled out, which is the unperturbed pictures. Previous times, those were terms which were cancelling were things which were independent of λ . Similarly here these are the things which are getting cancelled out which are independent of the dynamics, meaning at time t is equal to 0 if Hamiltonian did not change at all then this statement would have remained true. So these two cancel out. The remaining terms are one term in the left hand side which is the perturbation Hamiltonian \mathcal{H}' , which is a function of our time by the way which is hitting the state n and then summation over all such n . And right hand side \dot{c}_n 's which have appeared are getting multiplied with exponential phase and this eigenstate n . Like before, like in the time independent perturbation theory, I would want to project this equation along a specific eigenfunction. So, what I do, I take m -th eigenfunction and take inner product of the whole equation. I take m and bring it from the left to the whole equation, both sides. So, in the left hand side, this state m will go across the complex number c_n and exponential, these are complex numbers and will go and hit, squeeze the \mathcal{H} between right hand side n and left hand side m which I have brought about. Similarly on the right hand side if I take this m , m will go across all the complex

number and will hit this n , m and n inner product will appear on the right hand side. But these are eigenfunctions of Hamiltonian \mathcal{H}_0 and \mathcal{H}_0 is supposed to be Hermitian. So therefore they are orthogonal, m and n are orthogonal. So I will get this δ_{mn} out of it. So you see right hand side I have a summation with some c_n and some exponential and a Kronecker δ_{mn} . So n can take a value 0, 1, 2, 3, 4, 5 whatever you will but all of those terms will be 0 unless one term n achieves the same value as m . Suppose m were 2 then here it will survive as δ_{2n} that means n will only this series will only survive for n is equal to 2. Similarly, if I multiply from the left 3, this series will only survive for n is equal to 3 and so on. So, ultimately only one term will survive from this, which will be true for n is equal to m , all other terms are 0. So, therefore, I have just written the right hand side here, one term has survived when n is equal to m , which is this equation $i\hbar \dot{c}_m$. The $i\hbar$ here only one term which survives which is \dot{c}_m which is here and then exponential with n is equal to m this is the this is the thing which will survive in the right hand side which now have just flipped the right and left hand side among themselves what was previously the left hand side the whole summation is there and this m \mathcal{H}_1 , and squeezing there so no here I do not know whether I am going to get a δ_{mn} or not I do not know that. So therefore I will leave the series as it is. So you see I have equation $i\hbar \dot{c}_m$ is appearing over here. I can take this $i\hbar$ into the right hand side and it will become $\frac{1}{i\hbar}$, $\frac{1}{i\hbar}$ can be written as a $-i\hbar$. So $\frac{1}{i\hbar}$ is also equal to $-i\hbar$. So this is $\frac{-i}{\hbar}$. Then this summation. In this there are all terms present n is equal to 1, 2, 3, 4 up to infinity actually minus infinity to infinity you can say. In one of these n will become equal to m . So, let us separate that out. In all this summation there is one term when n is equal to m then this will be that term and then the series will proceed with all the terms which are n different from m . So, I have just broken the series in one piece and remaining all the terms.

dependent perturbation theory 1.1

$$\dot{c}_m = -\frac{i}{\hbar} \left(c_m \langle m | \mathcal{H}_1(t) | m \rangle + \sum_{n \neq m} c_n \langle m | \mathcal{H}_1(t) | n \rangle e^{-i(E_n - E_m)t/\hbar} \right)$$

* clearly $c_m = 0$ if $\mathcal{H}_1 = 0$

We can iteratively feed the values

- If at the beginning of perturbations some $c_2 = 1$ and $c_1 = c_3 = c_4 = \dots = 0$

Then

$$\dot{c}_1 = -\frac{i}{\hbar} \left(\langle 1 | \mathcal{H}_1(t) | 2 \rangle e^{-i(E_2 - E_1)t/\hbar} \right)$$

$$\dot{c}_2 = -\frac{i}{\hbar} \langle 2 | \mathcal{H}_1(t) | 2 \rangle$$

$$\dot{c}_3 = -\frac{i}{\hbar} \langle 3 | \mathcal{H}_1(t) | 2 \rangle e^{-i(E_2 - E_3)t/\hbar}$$

$$\langle m | \mathcal{H}_1 | n \rangle$$

$$\dot{c}_m = \left(\frac{-i}{\hbar} c_m \langle m | \mathcal{H}_1(t) | m \rangle + \sum_{n \neq m} c_n \langle m | \mathcal{H}_1(t) | n \rangle e^{-i(E_n - E_m) \frac{t}{\hbar}} \right)$$

★ Clearly $\dot{c}_m = 0$ if $\mathcal{H}_1 = 0$

We can iteratively feed the values

- If at the beginning of perturbations some $c_2 = 1$ and $c_1 = c_3 = c_4 \dots = 0$

$$\text{Then } \dot{c}_1 = \frac{-i}{\hbar} \left(\langle 1 | \mathcal{H}_1(t) | 2 \rangle e^{-i(E_2 - E_1) \frac{t}{\hbar}} \right)$$

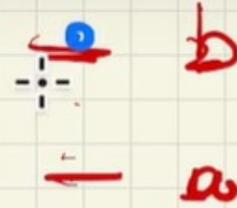
$$\dot{c}_2 = \frac{-i}{\hbar} \langle 2 | \mathcal{H}_1(t) | 2 \rangle$$

$$\dot{c}_3 = \frac{-i}{\hbar} \left(\langle 3 | \mathcal{H}_1(t) | 2 \rangle e^{-i(E_2 - E_3) \frac{t}{\hbar}} \right)$$

Example: A two level system

$$H_0 |a\rangle = E_a |a\rangle$$

$$H_0 |b\rangle = E_b |b\rangle$$



is perturbed by

$$H_1 = \begin{pmatrix} 0 & V \\ V^* & 0 \end{pmatrix} \cos \omega t$$

from initial configuration $c_b(0) = 1$

$$c_a(0) = 0$$

$$\dot{c}_a = -\frac{i}{\hbar} \left[c_a(0) \langle a | H_1 | a \rangle + c_b(0) \langle a | H_1 | b \rangle e^{-i(E_b - E_a)t/\hbar} \right]$$

$$= -\frac{i}{\hbar} [V \cos \omega t] e^{-i\Delta E t/\hbar}$$

$$\dot{c}_b = -\frac{i}{\hbar} \left[c_b(0) \langle b | H_1 | b \rangle + c_a(0) \langle b | H_1 | a \rangle e^{i(E_b - E_a)t/\hbar} \right]$$

And then I take this exponential on the left hand side, bring it on the right hand side such that it will become $e^{\frac{-iE_m t}{\hbar}}$. This side it was minus, when I bring it to the right hand side it will become plus. So

for all the terms $(E_n - E_m)$ will appear in the exponential. So I have added $e^{\frac{iE_m t}{\hbar}}$. Together they become $(E_n - E_m)t$ upon \hbar . Only for n is equal to m this exponential's argument becomes 0 and becomes 1. So the n is equal to m term will not come with any exponential. All other terms will come with the energy difference between n and m . Okay, so you see, obviously there are two things which we can see from here. If there is no time dependence in the theory, that means no perturbation depends on time or \mathcal{H} , is not present, $\mathcal{H}(t)$ is not present or $\mathcal{H}(t)$ is 0, then both these terms become 0 and the left hand side which is just \dot{c}_m will become 0. That means if time dependency is switched off, the magnitude of the projection does not change in time. That is what which was expected. However, we want to know if Hamiltonian, a time dependent Hamiltonian is indeed present, then what happens? So, then we can try to look for the solution in a perturbative iterative order. It will become more clear if I just take a specific case and try to know what is the answer. So you see I am trying to get the rate of change of m -th projection coefficient c_m . It depends upon what it was c_m and it depends upon what other c_m s were as well. So rate of change in the magnitude of the projection along one particular direction depends on

the coefficients along all direction. It depends on itself as well, but it does depend on other coefficients c_n as well. So it is a coupled equation. c_m will depend on c_n and c_n will depend on c_m . That means let us take a particular case where only two of the terms are there. Hamiltonian which has only two eigenstates, 1 and 2. So then \dot{c}_1 will depend on c_1 and c_2 and \dot{c}_2 will depend again on c_2 and c_1 . So therefore, Time derivative of one depends on both of them and time derivative of other also depends on both of them. So, therefore, it will become a coupled differential equation. Let us look at a particular example in which I am looking for a case where the system was in the ground state initially. So, c_2 or excited state in the first excited state to begin with. So, suppose a Hamiltonian which has many eigenstates. See this is one. This is 2, this is 3, this is 4 and so on. I am assuming at the beginning of the process the system was in the first excited state which was c_2 . So that means c_2 was 1 and all other c 's were 0. c_1 was 0, c_3 was 0, c_4 was 0 and all other c 's were 0. That is system was in the first excited state at the beginning of time. What will happen as the time evolves? c_1 will no longer will remain 0, c_2 will no longer remain 1 and c_3, c_4 will no longer remain 0 because of the time dependent Hamiltonians presence. So, let us look at what will be the coupled equation. So, if I want to know what is \dot{c}_1 , I will put m is equal to 1. Then if I put m is equal to 1, I will get \dot{c}_1 in the left hand side would be equal to $\frac{-i}{\hbar}$. Then the first term is c_1 and the squeezing of the Hamiltonian between 1 and 1. So this squeezing of the Hamiltonian between 1 and 1 will come with a coefficient c_1 . However at time t is equal to 0, c_1 is 0. So that term will drop off. Then the second term will come which will be c_2 . So second term will come from here, this series, n is being summed over. So, n is equal to 2, $c_2, \langle 1 | \mathcal{H}' | 2 \rangle$ and then the exponential with energy difference. So, I will get this term. The third term will be n is equal to 3, c_3 times $\langle 1 | \mathcal{H}' | 3 \rangle$ and this exponential energy difference, but c_3 happens to be 0 as well. Similarly, c_4 happens to be 0. So, all other terms will go away. Only one term in this whole series will survive, which is m is equal to 1 and n is equal to 2. So, effectively only one term from this expansion in this series survives, which is this. Similarly, if I look for $\dot{c}_2, \dot{c}_3, \dots$, m is equal to 2 will be put everywhere. And then I have to vary for different, different n 's. So, for example, n is equal to 1. I will get a c_1 . Here it will be 2 from the left. n has to become 1. And in the second part, n can take all the values, but not n is equal to 2. So it can take n is equal to 1. So I have a c_1 , then $\langle 2 | \mathcal{H}' | 1 \rangle$ with acting upon state 1. However, c_1 is supposed to be 0. So this will be dropped off. All the terms in this series will drop off for n is equal to 2, for m is equal to 2 and only this term, the first term survive which is c_2 , sorry I should have c_2 and the perturbation Hamiltonian \mathcal{H}' , squeezed between 2 and 2. c_2 happens to be 1 to start with, so it will come with like this. Similarly you can work out that \dot{c}_3 only one term will survive which will be $\langle 3 | \mathcal{H}' | 2 \rangle$ acting on 2 and the energy gap between 2 and 3. So these will be the set of coupled equations which will be true at time t is equal to 0. So at time t is equal to 0 the coefficients have taken these values all c 's are 0 but for c_2 is equal to 1, but their time derivative had taken this value at initial time. So, you see this c_2 is starting at value 1 with this rate of change, c_1 is starting from 0 with this rate of change, c_3 is starting from 0 with this rate of change. So, therefore after a while they will no longer be remaining at their same value because they have non-zero rate of change with respect to time. So, let us do this exercise just once more for a two level system as we discussed, only c_1 and c_2 are there, c_1 and c_2 , state 1 and state 2 or call it a and b . So, therefore these are the eigenstates of the unperturbed Hamiltonian with eigenvalue E_a and E_b .

Example: A two level system

$$\mathcal{H}_0 | a \rangle = E_a | a \rangle$$

$$\mathcal{H}_0 | b \rangle = E_b | b \rangle$$

is perturbed by

$$\begin{pmatrix} 0 & V \\ V^* & 0 \end{pmatrix} \cos \omega t$$

From initial configuration of $c_b(0) = 1, c_a(0) = 0$

$$\dot{c}_a = \frac{-i}{\hbar} \left[c_a(0) \langle a | \mathcal{H} | a \rangle + c_b(0) \langle a | \mathcal{H} | b \rangle e^{\frac{-i(E_b - E_a)t}{\hbar}} \right]$$

$$= \frac{-i}{\hbar} [V \cos \omega t] e^{-\frac{\Delta E t}{\hbar}}$$

$$\dot{c}_b = \frac{-i}{\hbar} [c_b(0) \langle b | \mathcal{H} | b \rangle + c_a(0) \langle a | \mathcal{H} | a \rangle e^{\frac{-i(E_b - E_a)t}{\hbar}}]$$

Handwritten derivation showing the integral for $c_a(t)$:

$$\Rightarrow c_a(t) - c_a(0) = -\frac{i}{\hbar} V \int_0^t \cos \omega t' e^{-\frac{i \Delta E t'}{\hbar}} dt'$$

$$c_a(t) = \frac{-i}{2\hbar} V \int_0^t (e^{i(\omega - \frac{\Delta E}{\hbar})t'} + e^{-i(\omega + \frac{\Delta E}{\hbar})t'}) dt'$$

$$c_a(t) - c_a(0) = \frac{-i}{\hbar} V \int_0^t \cos \omega t' e^{-\frac{i \Delta E t'}{\hbar}} dt'$$

$$c_a(t) = \frac{-i}{2\hbar} V \int_0^t (e^{i(\omega - \frac{\Delta E}{\hbar})t'} + e^{-i(\omega + \frac{\Delta E}{\hbar})t'}) dt'$$

$$= \frac{-i \hbar V}{2} \left[\frac{e^{i(\omega - \frac{\Delta E}{\hbar})t} - 1}{i(\omega - \frac{\Delta E}{\hbar})} - \frac{e^{-i(\omega + \frac{\Delta E}{\hbar})t} - 1}{i(\omega + \frac{\Delta E}{\hbar})} \right]$$

Defining $\frac{\Delta E}{\hbar} = \Omega$ and using the fact that

$$\frac{e^{ix} - 1}{ix} = e^{i\frac{x}{2}} \frac{(e^{i\frac{x}{2}} - e^{-i\frac{x}{2}})}{2i\frac{x}{2}}$$

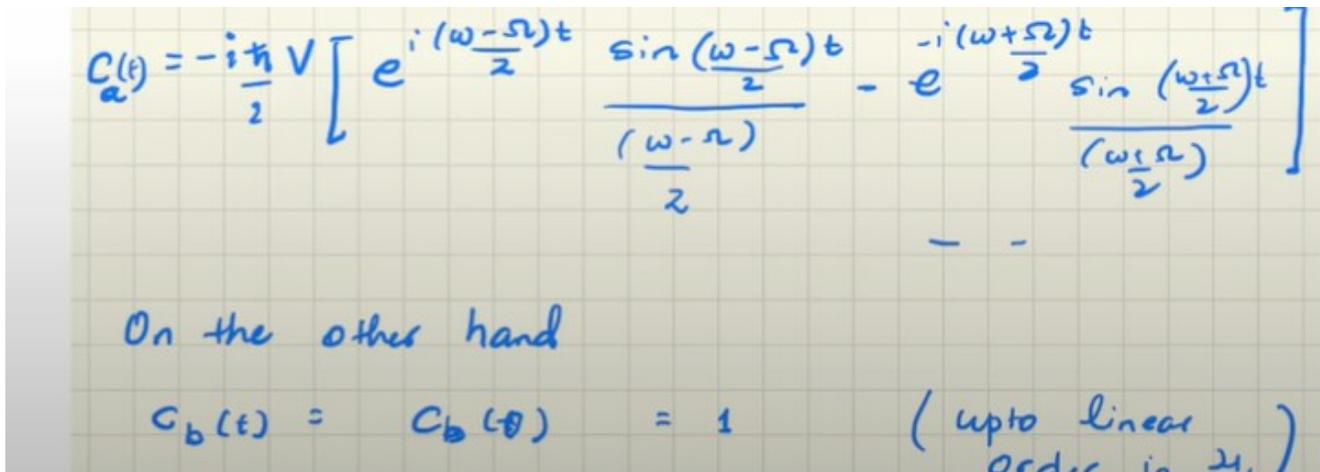
$$= e^{i\frac{x}{2}} \frac{\sin \frac{x}{2}}{\frac{x}{2}}$$

$$= -i \hbar \frac{V}{2} \left[\frac{e^{i(\omega - \frac{\Delta E}{\hbar})t} - 1}{i(\omega - \frac{\Delta E}{\hbar})} - \frac{e^{-i(\omega + \frac{\Delta E}{\hbar})t} - 1}{i(\omega + \frac{\Delta E}{\hbar})} \right]$$

Defining $\frac{\Delta E}{\hbar} = \Omega$ and using the fact that $\frac{e^{ix} - 1}{ix} = \frac{e^{ix/2}(e^{ix/2} - e^{-ix/2})}{2ix} = \frac{e^{ix/2} \sin x/2}{x/2}$

$$c_a(t) = -i\hbar \frac{V}{2} \left[e^{i(\omega - \Omega)t/2} \frac{\sin(\omega - \Omega)t/2}{(\omega - \Omega)/2} - e^{i(\omega + \Omega)t/2} \frac{\sin(\omega + \Omega)t/2}{(\omega + \Omega)/2} \right]$$

On the other hand $\dot{c}_b(t) = c_b(0) = 1$
(upto linear order of \mathcal{H}_1)



So \mathcal{H}_0 acting on $|a\rangle$ gives me $|a\rangle$ back with eigenvalue E_a . \mathcal{H}_0 acting on $|b\rangle$ gives me $|b\rangle$ back with eigenvalue E_b . And then I insert a time dependent perturbation \mathcal{H}_1 , which has this matrix structure in the basis $|a\rangle, |b\rangle$. So in the basis $|a\rangle, |b\rangle$, $\langle a|, \langle b|$. This is the structure that Hamiltonian perturbation, Hamiltonian in this system has this matrix appearance. Its diagonal terms are 0, its off diagonal terms are non-zero and they are complex conjugate of each other because it has to be Hermitian thing. Time dependency is here, $\cos \omega t$ is multiplied to everything. And then I start the same thing that I am starting from an excited state discussion where atom is in higher state and then I want to know whether it will come down to the ground state or not.

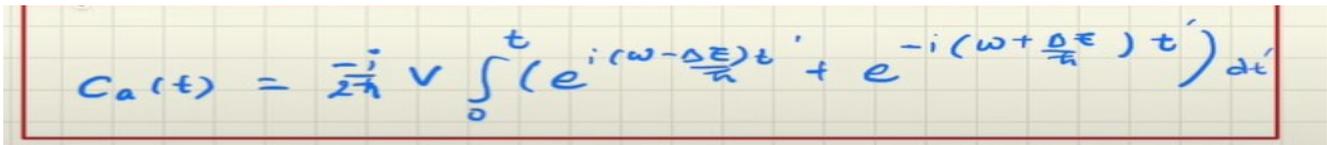
That means is to say I start with c_b at time $t = 0$ is 1 and c_a at time $t = 0$ is 0. The state has system has a probability of 1 of being found in eigenstate $|b\rangle$ and probability of being found in the eigenstate $|a\rangle$. Now we want to know after some while, after some time whether these probabilities remain 1 or 0, 1 and 0 or become something else. So, again we will look for the time dependent equation, differential equation for their coefficients. \dot{c}_a is supposed to be $c_a(0)$ and the perturbation squeezed between $\langle a|, |a\rangle$, this is the first term. This is the first term over here. Let me just clean it up. This is the first term in this equation. This term, the Hamiltonian squeeze between the m -th eigendirection, eigenfunction. So \mathcal{H}_1 squeezed between $\langle a|$ and $|a\rangle$ and the second term is c_b with the perturbation Hamiltonian squeezed between m and n which is $|a\rangle$ and $|b\rangle$ and the exponential with their energy difference. So \dot{c}_a will be $c_a(0)$ times the diagonal element of \mathcal{H}_1 here which is 0. So this term will go out to 0. Then $c_b(0)$ times the off diagonal element this one times this exponential. So, $c_b(0)$ was supposed to be 1, off diagonal element was supposed to be $V \cos \omega t$ and the exponential energy gap is $e^{-i(E_b - E_a)t/\hbar}$. So, $E_b - E_a$. I am going to call it ΔE . So, this is ΔE upon t upon ΔE times t upon \hbar . Similarly, if I write down

the equation for \dot{c}_b the first term will be the Hamiltonian squeezed between $|b\rangle$ and $|b\rangle$, then $c_b(0)$ multiplying that plus $c_a(0)$ Hamiltonian squeezed between $|a\rangle$ and $|b\rangle$, this time the second off diagonal element and this exponential energy difference. So, you see there is a sign difference here, here it is $E_m - E_n$ should appear and here it $E_n - E_m$ should appear. So, second state minus first state, here also second state minus first state. So, in this case if I look at this $c_b(0)$ was supposed to be 1, however the diagonal element of the \mathcal{H} , the second diagonal element between $|b\rangle$, $|b\rangle$ is 0. So, therefore the this term is 0 and the second term which is the off diagonal element second off diagonal element V^* and the energy eigenvalue difference in the exponential. But this comes with $c_a(0)$. So, $c_a(0)$ is supposed to be 0. So, therefore \dot{c}_b right hand side both the terms are 0 therefore \dot{c}_b is 0. It tells me that it \dot{c}_b does not change in time. This is slightly worrisome for us because we wanted things to change. We do not want system to remain in the same case.

So what is happening ? \dot{c}_a has become non zero. That means it will no longer remain at value 0. \dot{c}_b has taken a value zero. That means it will no longer change in time.

So it will happen that it will remain at one and this will remain not zero. So how to interpret that? First let us see what does it mean. So, I do not have to worry about c_b , c_b remains to value 1 from this equation. But the first coefficient c_a that does not remain to value 0.

So I just integrate this equation.



$$c_a(t) = \frac{i}{2\hbar} V \int_0^t (e^{i(\omega - \frac{\Delta E}{\hbar})t'} + e^{-i(\omega + \frac{\Delta E}{\hbar})t'}) dt'$$

I take this equation integrate over time from 0 to some future time t . Then the left hand side, this will be just the difference of c_a at time t is equal to 0 minus time, time t is equal to some time t minus time t is equal to 0. So, left hand side will be the difference between $c_a(t)$ and $c_a(0)$. Right hand side of this equation will be the integration of right hand side between 0 to t . So, V is a function which is independent of time remember we had declared the Hamiltonian the perturbation Hamiltonian is this in which all the time dependency is in the \cos function this V and V^* are not supposed to be function of

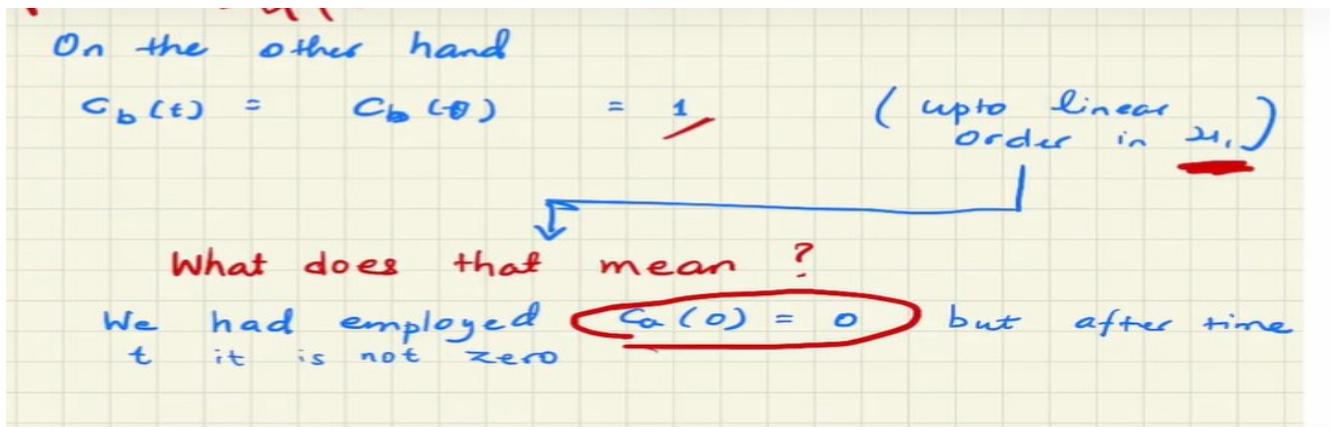
time so that will come out of the integration inside I will be left with $\cos \omega t$ and $e^{\frac{-i\Delta E t}{\hbar}}$ here. Now one can do this integration fairly straightforward in a fairly straightforward manner, that is to write down $\cos \omega t = \frac{e^{i\omega t} + e^{-i\omega t}}{2}$. If I write it like this, this integration will become sum of two terms, one

with first exponential combining with the exponential here and then the second exponential in of the \cos combining with this exponential here. I will get these two terms with a extra 2 coming from the denominator of \cos . the expression which I wanted, what is the value of $c_a(t)$ at a time away from 0. This boxed equation tells me that $c_a(t)$ will no longer remain 0, it will become non-zero if this integral is non-zero. So, one can compute this integral, this is again a straight forward exercise, exponential integrations are very simple to do. You will get from first integration the first terms integration we will

get this which is e to the power the exponential back with the coefficient of time in the exponent in the denominator and its limit at t minus limit at t is equal to 0. And similarly for the second term I will get this term. So, you see that the $c_a(t)$ has become non zero, it has taken this value. One can further simplify by calling this $\frac{\Delta E}{\hbar}$ as some frequency Ω , this is the frequency gap between the two level system. And then using the fact that this object over here or over here, they have a structure like $(e^{ix} - 1)/ix$.

Here the x happens to be $\omega - \Omega$ and here the x happens to be $\omega + \Omega$. But both of them have the similar structure and this $(e^{ix} - 1)/ix$ can simply be converted into $e^{ix/2}$ and then $sinc$ function of x by 2. $sinc$ meaning $sinc$ is $\sin x/x$. In this case, I am getting $\sin x/2$, $(\sin x/2)/(x/2)$. So that means this term can be written as a $sinc$ function and this term can also be written as a $sinc$ function with $e^{ix/2}$ multiplying individual $sinc$ s. So in this case, x was $\omega - \Omega$.

So therefore, this will become $e^{i(\omega - \Omega)t/2}$ and then the $sinc$ function which will be this here. And similarly for the second term, I will get another $sinc$ function which is over here. So, you see $c_a(t)$ has become non-zero, $c_b(t)$ still remains to 1. So, what is happening? If one probability of being found in that state is 1, why the probability of the system being found in eigenstate $|a\rangle$ is non-zero, because total probability cannot be greater than 1. So, the resolution is that if I take $|c_a|^2$, then you see this whole thing will get mod squared and therefore, I will get an answer which is V^2 , $\hbar^2 \frac{V^2}{4}$ and then the box which is inside that mod square, but you see it is quadratic in the V . It is answer quadratic in V . However, when I tried to compute $c_b(t)$, $c_b(t)$ was trying to get me an answer. This was supposed to be V^* . It so happened that it was zero. That's why c_b was \dot{c}_b was supposed to be zero. So \dot{c}_b is zero at time $t=0$ only. That means if I go slightly away then \dot{c}_b at a time slightly away would depend upon c_b at time t times the diagonal $\langle b | \mathcal{H} | b \rangle + c_a(t)$ with $e^{\frac{-i\Delta E t}{\hbar}}$ and off diagonal element of $\langle b | \mathcal{H} | a \rangle$. So $c_a(t)$ will not become 0.



$c_a(0)$ was 0. c_a at time t is equal to 0 was 0, but c_a at any arbitrary time is not 0. So \dot{c}_b will become non-zero at a future time. At time t is equal to 0, it starts with value c_b is equal to 0 and \dot{c}_b is equal to 1, c_b is equal to 1 and \dot{c}_b is equal to 0. At a future time, I have seen that \dot{c}_b will not be equal to 0. Therefore, c_b will be different from 1 by a tiny amount and that tiny amount is order V^2 . Whatever this loses, c_a has to

gain. c_a is gaining at the order of V , $|c_a|^2$ is gaining at the order of V^2 . So therefore, in the linear order of \mathcal{H}_s , this $c_b(t)$ is 0. But if I want to be higher order in \mathcal{H}_s , that means I go to future and future time, c_a will no longer remain 0 and therefore c_b will no longer remain 1. So therefore, I have to, I just in this expression when I did, when I wrote down these quantities where I claimed, when I claimed that \dot{c}_a is this thing and \dot{c}_b is zero, this is truly true at t is equal to zero.

At a future time I have to supply what is the the values of c_a and c_b at future times. That means at time t is equal to 0, it remains 0. But if I go for t is equal to some small t' , then this will become t' here and t' here. And I know from the integration that at a future time, c_a no longer remains 0. Therefore, this term will no longer remain 0. And \dot{c}_b will turn alive. So, c_a starts building from 0 upwards. It will become larger and larger. No longer it will remain 0 and c_b will start becoming different from 1. So, initially it was like this after a time t it will have some lesser probability of being found in excited state. So, this was c_b is equal to 1 and c_a is equal to 0, after a time t Both of them will have non-zero probability. It would be higher. It would be something 1 minus some $|V|^2$ times some integration which we had done. And this will be $|V|^2$ times that integration. So, you see it will become slightly less than 1 and this will become slightly over 0. So, therefore, under this perturbation theory approach, time dependent Hamiltonian approach, effectively the off diagonal term and the diagonal term both decide undergoing the integration that we have to integrate this quantity, how much the rate of change would be. In the two level case and in this particular example, we had taken a particular Hamiltonian whose diagonals were 0. This was my construction and off diagonals were this. Therefore, only off diagonal terms decide what would be the rate of change of c_a and c_b both. They will all be proportional to V . Remember V is the off diagonal term. So off diagonal terms of this Hamiltonian decides what is the rate of the growth of the coefficient of c_a and what is the rate of the decay of the coefficient c_b . So ultimately the Hamiltonian along with the temporal part, temporal part was $\cos \omega t$ which we wrote temporal part of the Hamiltonian was $\cos \omega t$ which we wrote as two exponentials $e^{i \omega t}$ and $e^{-i \omega t}$ therefore this integration came. But suppose it was not $\cos \omega t$ but some other function then that function would get multiplied with the exponential of energy gap upon \hbar times t' and that integration one has to do. That is to say an exercise which you can try that instead of the $\cos \omega t$, suppose it was a $\sin \omega t$ here. So, let me write down as a proposal exercise for you. If it was $\sin \omega t$ here, then I will get different answer. Still it will be, \sin can also be written as 2 exponential with a minus here and divided by 2 i . So, an extra i will come about. So you can do this exercise for $\sin \omega t$ dependency, $\cos \omega t$ dependency or any other dependency in the perturbation Hamiltonian and you have to just compute the integration $c_a(t)$ which is here or here rather and $c_b(t)$ will be obtainable at a future time while feeding the value of $c_a(t)$ here. We will see in more detail in the next discussion session if I try doing that what kind of structure appears. But you can see the structure c_a starts building up from its initial value via this integration. Once it has built up to some value $c_a(t)$ it will go and start disturbing this evolution of \dot{c}_b here it will appear. Okay, and you see here it was this integration when I was writing for \dot{c}_a , c_b was appearing here, which was the surviving integral. So, here it was a c_b . So, we had assumed it is 1, but at a future time it will no longer be 1, it will be different from 1. How much different from 1?

This integration will tell us. So, ultimately you see a coupled equations structure is coming about that $c_a(t)$ depends, its time derivative depends on c_b and c_b 's time derivative depends on c_a . So, they are mutually affecting each other. In the next class, we will discuss about this and put things in more clear perspective to see how these coupled equations work. So, let us stop here for today.