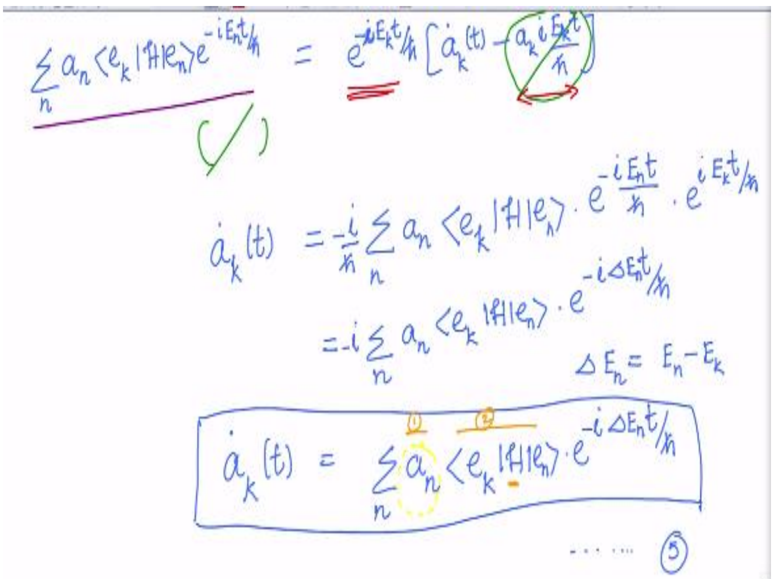
Optical Spectroscopy and Microscopy
Prof. Balaji Jayaprakash
Centre for Neuroscience
Indian Institute of Science – Bangalore

Lecture – 11
Fundamentals of Optical Measurement and Instrumentation

Hello and welcome to the lecture series on optical spectroscopy and microscopy. So far in this lecture series, what we have seen is that how to describe the interaction of the light with the matter with the idea that if we can actually quantitatively develop a framework of understanding the way or describing how the light interacts with the matter and that might probably provide us with a fundamental understanding of how this whole process happens and then it might help us in understanding the complex processes or other processes that might happen as a consequence of this basic interaction.

In that direction, what we have done is we have looked into the time-dependent perturbation theory and in our formalism, how we use the Dirac's quantum mechanics formalism of eigenkets and bras and we use those properties to obtain an expression for the expansion coefficients ak, to be more precise we were actually writing down an expression for ak dot in the last lecture, alright. So now show you how we can proceed forward and get an expression for ek itself and what it means and how does it relate to the practical situation okay.

(Refer Slide Time: 02:17)

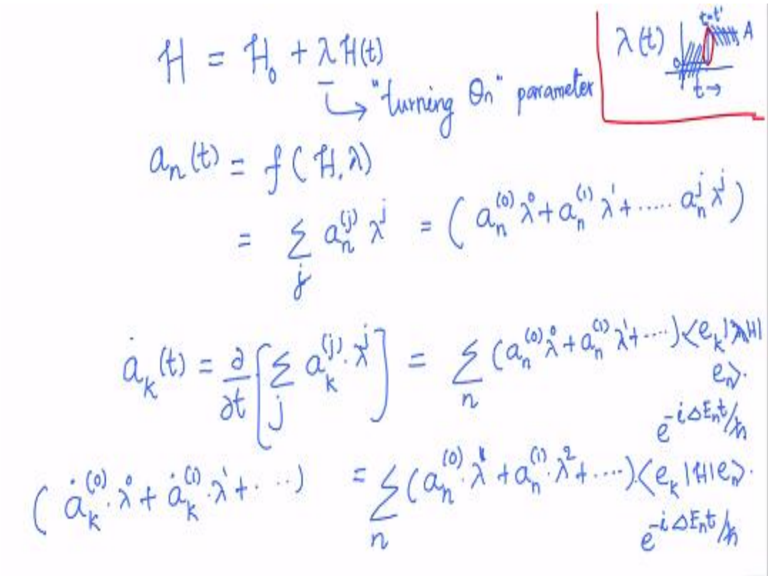


So now the equation that we had in the last lecture was this, ak dot of t = summation of an ek Hamiltonian en e to the power -i delta Ent over H cross right. So that is the expression that we had. So until now, we have not made any approximations. We have made some assertions, we made some assumptions, but we never made any approximations until here. So if you could evaluate these terms and write down these terms, then the solution that we get for the derivative of ak is very exact.

So you could get this solution and integrate it, integrate it over time 0 to t, then get an expression for ak itself and that would be a true description or exact description of the system as a function of time after you let the system interact with the light. Now while it can be very exact and wonderful to write down this expression, practically it may not be of that greater use if you do not make a few further progress to relate it to an experimentally observed quantities, right.

So in order to do that, we have to make some approximations from now on because it is little too cumbersome to deal with this expression as such **so** and it is convenient to make that approximation, it makes more sense as you see in real life that those kind of approximations really hold good. So what are those approximations?

(Refer Slide Time: 04:17)



Number one we realize the Hamiltonian that we have written right, the time-dependent perturbation Hamiltonian we have wrote it as the sum of the unperturbed Hamiltonian plus the perturbation itself. Now here, I am going to introduce a small change here that is I am going to say it is not just H but at term lambda times H okay, where H is the perturbation and it is of course a function of t. So when you do this, the lambda is called as typically turning on parameter.

Simply what it means is that as the value of lambda changes from 0 to 1, it equates it to you letting the system interact with the light, I mean, or with any perturbation for that matter, right. So when lambda = 0, there is no perturbation because this whole term goes to 0 and when lambda becomes equal to 1, the perturbation is fully on right. In some ways, its like a switch that you flip to turn the perturbation, if you like. It is not exact but I am just going to kind of a little bit of a stretch here.

What you can think of is that lambda in turn is also a function of time, but you know in a very specific way. The way being that it is 0 until a point t = 0 okay, I mean some t = t prime okay. This is the time axis until t = t prime, it is actually 0 alright. At t = t prime, you are turning on this lambda from that point onwards right at t = t prime, from that point onwards you have a value of some amplitude A which is greater than 0, so I was going to write it as 1, but you can think of that as some amplitude A to be general.

See that the problem, I am just going to tell you the problem of just generally writing lambda as a function of t is that you will later realize that the whole point of me trying to do this lambda business is to be able to expand my coefficients ans, right. I know this an is a function of t and of course it is changing as a function of t only because of this perturbation being applied right, otherwise these ans are corresponding to the expansion coefficients of the basis eigenkets which are basically eigenkets of the H0 itself.

So, it depends on which of ens that are occurring that will be there. So, it is just like once and 0, whether the system is in a state en or not, so that settle right that it does not change with respect to time. These ans then represent the initial states of the system per se. So in that case, this ans definitely are a function of the perturbation Hamiltonian H. Now if I say I am going to write it as lambda times H, I actually would like to write it as H and as a function of lambda.

Once I say this, then what it allows me to do is that I would be able to write it as I mean if I write it as this, it is clearly as a function of H and in fact I can write it as a function of H and lambda, so I can then do a power series expansion for an in terms of lambda. Now if I were to do that, then it would be something similar to an. So if I am going to write it as a power series expansion, I will write it as for j terms, I mean j going from 0 to infinity an of j, j in the parentheses here represents the coefficient, the jth coefficient of lambda to the power j okay.

Or in other words I would actually like to write it as, I will write down few terms. What we are actually saying is an j lambda to the power 0 which is equal to 1 + an1 lambda to the power 1, in general you can write as an to the power j lambda to the power j okay. Now the important point here is for this to be operational, you will realize that if the lambda has a dependence on time, it becomes very problematic alright, so that is the problem.

I mean it is very easy to say it like that, but what the thing we realize is that if you do this, then this expansion you have to understand, it is not definitely exact, it is very much of a stretch, but you have to see that this expansion were to be valid in this region and that region alone because there the lambda is not changing as a function of time, it is as well could be lambda equal to some C constant, right, that is exactly what is happening here and it is not valid in any small interval here.

This where it is suddenly getting turned on, but it is customary to introduce this lambda, you will see it becomes a very convenient mathematically as less it allows us to make progress to equate these ans to or the coefficients to an exponentially observable parameters. So we will proceed forward with that. If you are not very comfortable, it is not, I mean I would not insist that we need to make this assumption or make this as a reality, but this just make you feel any comfortable, then you can think of this scenario.

Otherwise to imagine this as a switch that turns on and off the perturbation. In that scenario, everything holds good. Now, I have written down a power series expansion of the coefficients an of t in terms of lambda the turning on parameter, the powers of the lambda the turning on parameter. So now what we can do is that I can put this back into the equation number 5. Our equation number 5 is for ak dot of t. So there, we are basically saying the n = k.

So we can write it as ak dot of t is given by dou by dou t of summation j ak j times lambda j which is equal to this ans here we have to replace it again. So this ans and if you have to do that with the power series expansion, so summation over n, I am going to use this term here which is the power series, an was 0 times lambda to the power 0 + an of 1 lambda to the power 1 and so on times this term right, now the next term, this is the first term we finished alright.

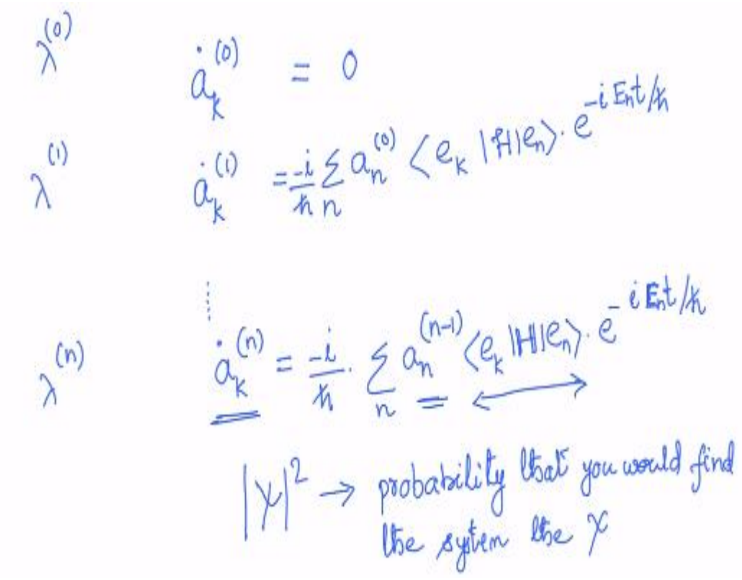
Now the second term we are writing down, this everything remains the same, but the second term, the Hamiltonian here that Hamiltonian here had to be replaced by lambda times H right. So we have to do that. So the way we do that is ek lambda the perturbation Hamiltonian en alright times e to the power – i delta EnT by H cross right. Now we see that we have 2 polynomials here right, polynomial on the left hand side and then the polynomial on the right hand side and what we are going to do is that if you equate this, we have 2 polynomials.

One on the left hand side and one on the right hand side. Now what we can do is that we can equate the coefficients of the same powers of lambda right. So let me expand this in terms of this, so that you can see what I am actually referring to. So if you were to write down this in like term by term basis, then it can be written as ak dot right, see this is why it is important to have the lambda as independent of time right. So I can actually write it as ak of dot the zeroth order times lambda to the power 0 which is 1 and ak1 lambda 1 and so forth equals this whole term.

However, what you see is that this lambda is not being an operator it is a scalar can come out of this whole integral in which case what you will see is that that lambda gets multiplied here okay. So it is as if that each of these terms are multiplied by lambda as a result what we have is summation over n, see this summation is over the different eigenkets, different energy eigenkets right. So we have that intact still and what we have is an of 0, however now what we have is lambda to the power 0 times lambda which is actually 0 + 1 is 1.

So every term or every lambda term gets a boost of +1 okay and you can write it as ek perturbation Hamiltonian en times e to the power minus -i delta EnT over H cross. So now if you are thinking about, if you watch it carefully you have 2 polynomials right. Then the coefficients of this polynomial say ak dot and so forth, the coefficients of this polynomial should be equal for its powers which means first thing we realize is that ak0 that the zeroth order for the first one.

(Refer Slide Time: 18:57)



Let us write down the first one. So equating lambda to the power 0 coefficients, on the left hand side we have ak dot right, on the right hand side we do not have any term with lambda to the power 0 which means the coefficient is actually 0 and the first order term for this we can go back and look at it that is this would be having coefficient drawn from this. So what we have is an summation over n an of 0 alright that is this and lambda goes away because we are equating the coefficients times ek H en this whole term ek the perturbation Hamiltonian en e to the power –iEnT by h cross.

I hope I have not missed any terms, so ek H en e to the power minus so that is exactly the same term that we have written here. So like that we can go ahead and write down, so this is for lambda to the power 1. We can equate in general to lambda power n as ak somewhere here we have actually missed an i h cross term when we have canceled out here. So this would be actually ak of t -i by h cross alright. So that would carry on till here h cross -i by h cross, so the same thing here, I forgot this term so -i by h cross so that would come in here too.

So -i over h cross, then we need to put that I mean we did not quite account for that. So -i over h cross, so equals –i over h cross times summation over n an the n–1 th order term ek Hamiltonian d to the power –iEnT by h cross, alright. So what do we have here? So what we have is that we can write down a general expression for the coefficient ak okay except if we want to write down this coefficient ak to an nth order, we need to know the coefficient, we need to be able to write down the coefficient to the n-1 order.

If you know this, then you would be able to write down the coefficients for the nth order or in other words we have a recursive, then if you want to know you have to go one step at a time back or one step at a time forward to keep getting this coefficient to a higher and higher order of accuracy, right because remember these ak0, ak1 are coming from this polynomial right, the polynomial that we did here okay, and so in this we have the ak n0 ak n to the power if the first order, in general ak n to the power jth order and this basically means that you are writing the an in terms to various different accuracies.

If you do not calculate these or in general if you were to restrict your an writing down till some nth term, then that is your accuracy. You could progressively increase your accuracy by going more and more in this direction or taking advantage of the fact that if you look at the real expression, it could be converging and then you can terminate it at reasonable limits of that is of use for all practical purposes. So that is the goal here right.

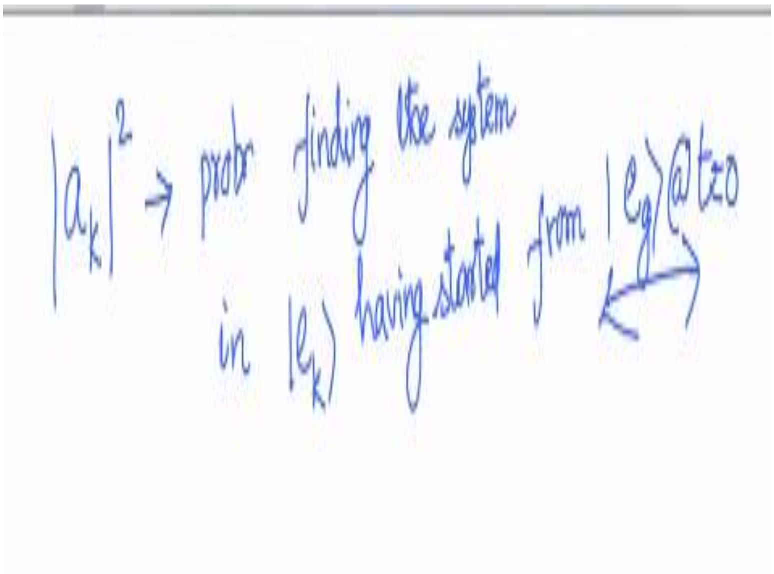
We could actually now write down an expression for the ak to nth order of its accuracy in terms of ek and en where ens in general are the eigenkets of the unperturbed Hamiltonian and the perturbation Hamiltonian itself right. So you have let us say n different eigenkets, what you are actually having is you are forming a matrix of k by n and then this actually is a matrix element right, the ek H en and if you write down this, we call it as a matrix element. Then we would know the ak fn, that is fantastic.

So, now can we actually take it forward and make some related to laboratory measurement and then make some observations of what we will see, what property would have we missed if we did not go through this exercise, how do we do this? The first one we realize is that while aks, this ak dot basically dou by dou t of ak are very convenient to write down the chi itself okay, but what we actually are interested is you can relate it to the measurable things, observable physical quantities is the fact that that what Born said that if you have a vector chi or vector psi representing a state of a system.

Now what is the physical meaning of such vector. There are various different interpretation around, but the one that most of the people would agree on is called the Born’s interpretation where he said that, thanks to Max Born, if you have a state vector sign represented by ket like this, then the modulus square of this okay modulus square of not this, it could actually if you have a state vector psi and what Born said is you could take the modulus square and that modulus square would tell you the probability that you would find the system in the state corresponding to chi.

So now this the chi here are the wave functions, so what it means is that how do we extract this modulus square from these akn's.

(Refer Slide Time: 29:33)



In order to do that what we are going to do is that, you can think of, I mean we have done that already right, to get the meaning out of this probability what we are actually after is you realize the modulus square of these aks alright and this I am going to state and we will in the next class say how I am stating that and we also see how we can actually calculate. The modulus square represents the probability of finding the system in state ek having started from state eg at t = 0.

So this will be coming from an initial condition, but I am going to just state this basically what we will see is that if we calculate the modulus ek square right, modulus square of the ek the coefficient, then that will be equivalent to the probability of e finding the system in the state ek having the system started from eg the ground state okay. We will see in the next class how do we obtain this ek coefficients or the modulus ek square.

Also the reason why ek square is really the probability and how is this statement, the ek square, equating the ek square to the probability comes directly from Born's interpretation of chi square a being the probability of you being able to find the system in a state kind, okay. Thank you and see you in the next class.