Quantum Mechanics- I
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Lecture - 37
Perturbation Theory – II

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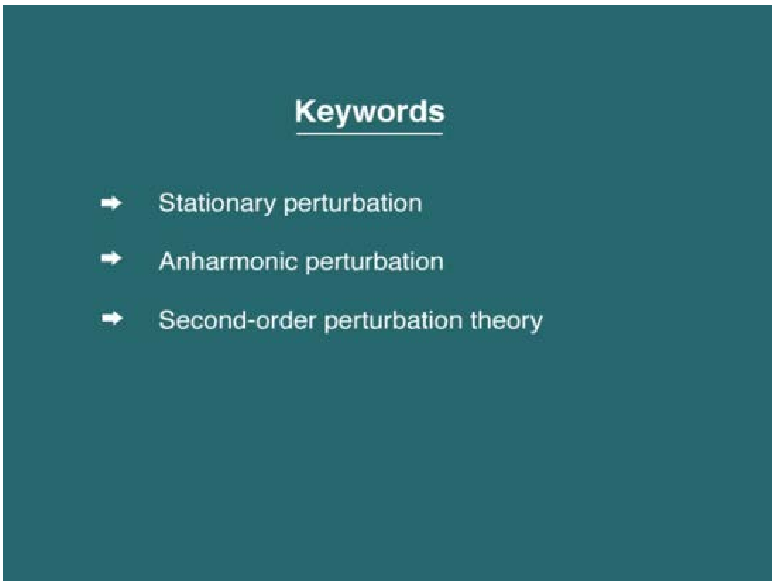

In the last lecture we established the framework of the Rayleigh Schrodinger perturbation theory in other words, stationary perturbation theory. The perturbing Hamiltonian was independent of time and just to get the notation strength.

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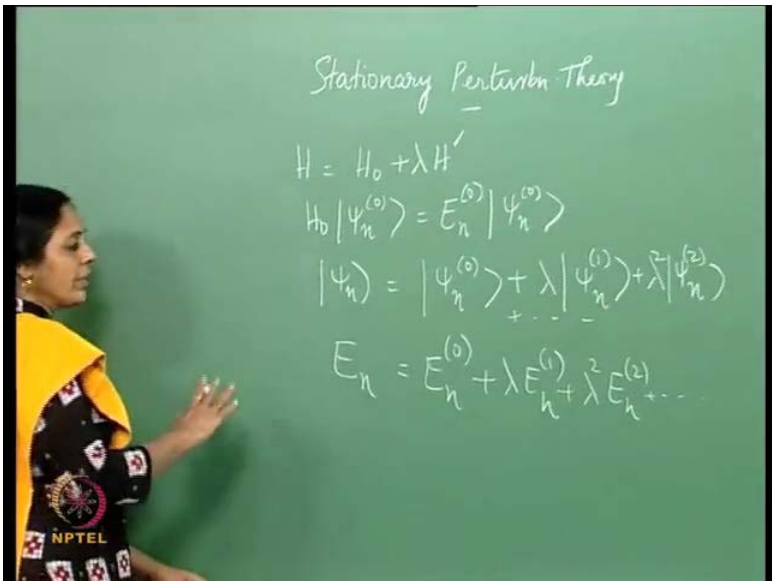

Let us look at some of the notation that we used yesterday. So, the Hamiltonian have the unperturbed part H naught and lambda H prime which was the perturbation and then of course, the original unperturbed Hamiltonian had a discrete set of Eigen states psi n 0 the corresponding Eigen values being given by E n 0.

Because of the perturbation both the energy and the wave functions change. However, the new wave functions could still be expanded in terms of the old basis set psi n 0 and the new wave functions could well be written as the old one plus the effect of the perturbation. So, to 1st order it would be lambda psi n 1 then lambda squared psi n 2 plus. Correspondingly, the new value of the energy would be the old unperturbed value plus to 1st order in lambda you had E n 1 then the contribution to 2nd order was E n 2 and so on.

So, this is what we had and we also established 2 interesting and important results namely: an expression for psi n 1 and an expression for E n 1. In fact we had an expression for E n s where s could be 1, 2, 3 anything.

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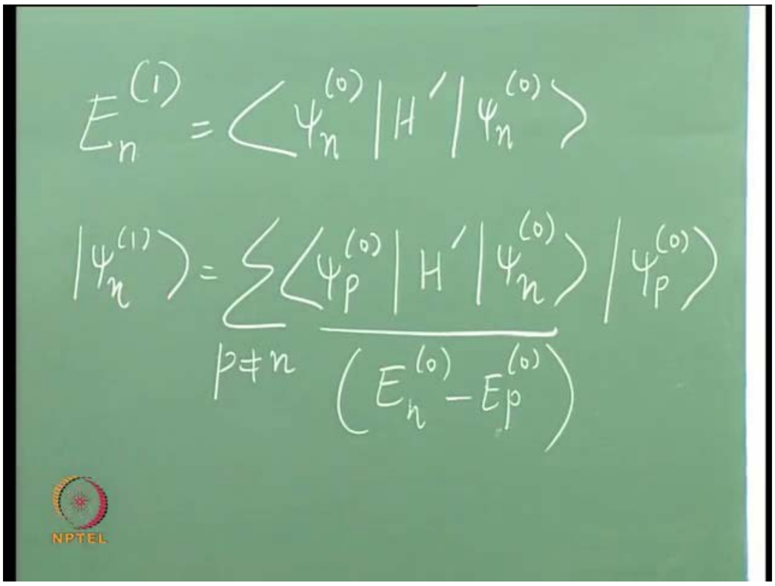

So, basically we had the result that E n 1 that is the energy because of the perturbation the extra energy contribution is simply the expectation value of H prime in the unperturbed basis psi n 0. Further, the 1st order wave function the contribution psi n 1 is summation over p not equal to n, psi p 0 H prime psi n 0 and of course, there is a state there psi p 0 divided by E n 0 minus E p 0. It is pretty clear that we are looking at the non degenerate case because if indeed there is a degeneracy there is going to be a problem here because if n is equal to p there is a problem in the denominator and the formalism has to be adapted suitably if we discuss degenerate perturbation theory.

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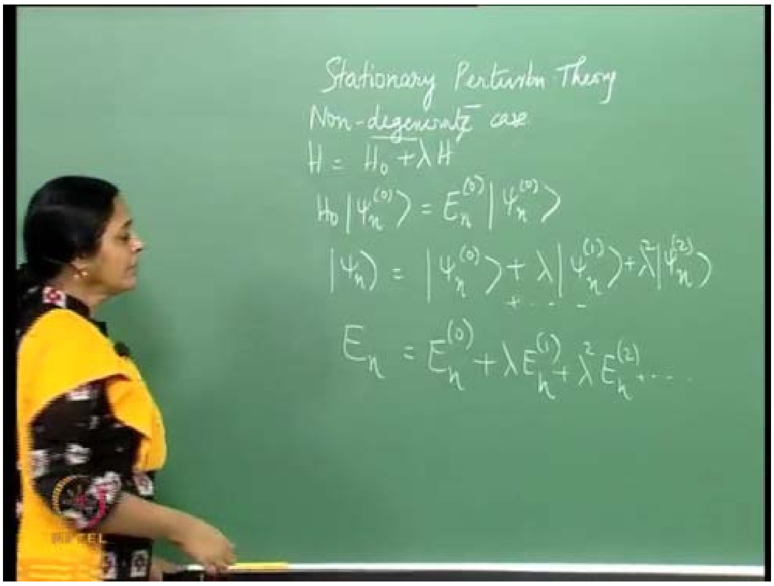

But right now we are looking at the non degenerate case. So, that is what we are doing. (Refer Slide Time: 02:43) We use this to find out the 1st order contribution E n 1 and ket psi n 1 in the case of the linear harmonic oscillator to which there was a perturbation added.

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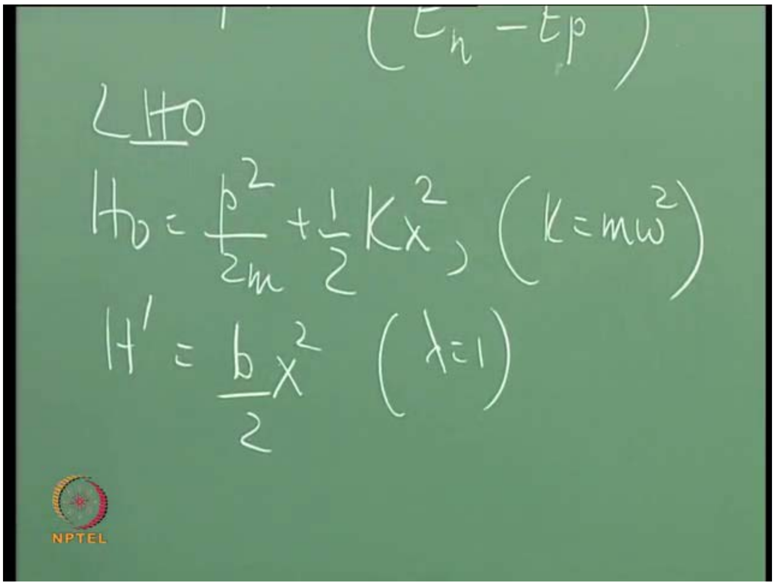

So, in the case of the linear harmonic oscillator example we had H naught which was p squared by 2 m plus half K x square so K is m omega square and H prime was simply b by 2 x squared. So, we need set lambda equals 1 and this was also of the form constant times x square and therefore, the harmonic nature was not described. So, this is the simplest example we can think of and today we look at something else we look at an anharmonic oscillator.

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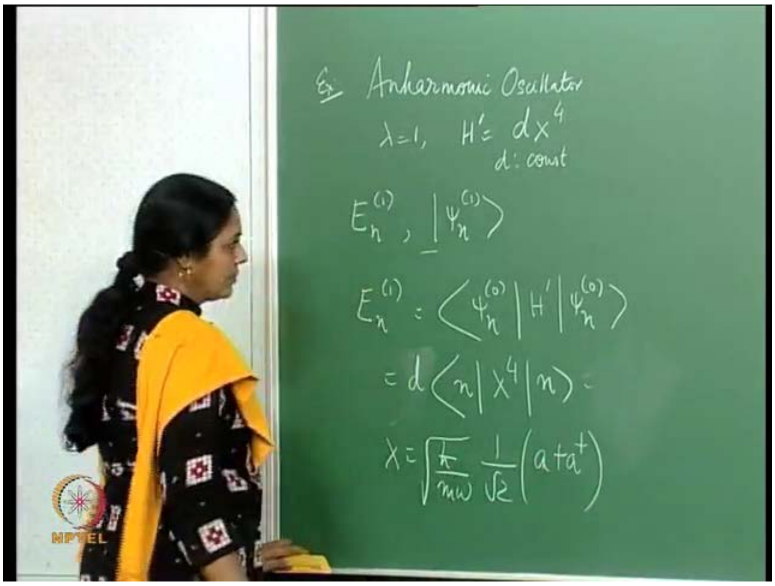

So, basically therefore, the perturbing term would not be quadratic in x so let us consider the case of the anharmonic oscillator is an example. So, again I set lambda equals 1 that is just for book keeping and let us say H prime is d x to the 4; d is a constant. So, what do I have here? I do not want to battle with an x cube term. If you just plotted potential v of x is equal to x cubed versus x you find that there is no lower bound. So I take a safe case I take h prime as d x to the 4. Now our aim is to find out what is E n 1 and psi n 1?. So, we just have to plug in values into that expression that we had. So, E n 1 is simply psi n 0 H prime psi n 0.

Since, we are discussing the oscillator fock basis. In my notation this is ket n and of course, there is a d x to the 4 ket n of course, you can do 1 of 2 things you can write the wave function the state in the position representation putting the Hermite polynomials do an integration and get hold of this expression. For the moment I would prefer to put in X in terms of a and a dagger the ladder operators. And then I just have recall that X is route of h cross by m omega 1 by root 2 a plus a dagger.

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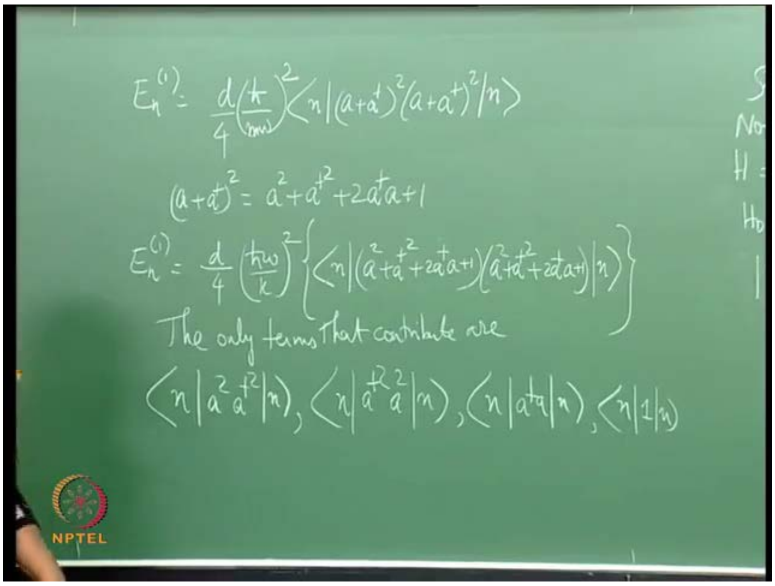

So, let us put that in here. So, E n 1 is d h cross by m omega whole squared because there is an x to the 4 and there is a 4 also out here. So, those are the overall constraints that I pick up and then I have the expectation value of a plus a dagger to the power of 4 so let me just write it in this fashion. So, this is the contribution. Of course, I know that a plus a dagger the whole squared can be written as a squared plus a dagger squared plus 2 a dagger a plus 1.

So I put that in there and I just have E n 1 is d by 4. I would like to write this as h cross omega by k the whole square because remember that m omega is just k by omega so that is what I have put on there. And then I have n a squared plus a dagger squared plus 2 a dagger a plus 1 times the same thing a squared plus a dagger squared plus 2 a dagger a plus 1 and a ket n out there. The point that I am trying to make is this: Out here a squared acting on n would lower it to the state n minus 2 and therefore, I need to have a term here I need to use only those operators here which will bring the state n minus 2 back to ket n, because finally I need to take the inner product of ket n with that state.

So, the only contributing terms because of the orthonormality of the states are n a squared a dagger squared ket n, n a dagger squared a squared ket n. Of course, n a dagger a ket n and then of course, just ket n 1 ket n. These are the only terms that can contribute because as you can see if the power of a dagger is different from the power of a there is going to be a mismatch and the inner product of ket n with this state it is going to be 0 .

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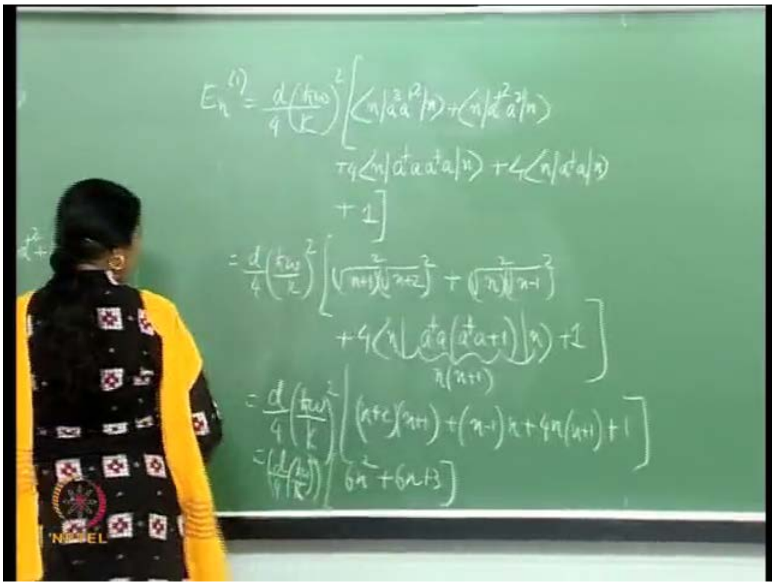

So, let us substitute that n and see what we get. So, E n 1 which is the 1st order contribution is d by 4 h cross omega by K the whole squared n a squared a dagger squared n plus n a dagger squared a squared n plus 4 expectation value of a dagger a a dagger a. Then, I also have a contribution from 2 a dagger a here and 1 there and similarly, from 2 a dagger a and 1 here the product.

Therefore, I have a 4 n a dagger a n and then of course, I have a 1 that was the last term there was a bra n, there was a ket n, there was a 1 out here. So, this is what I am going to have and this object a dagger squared on ket n gives me a root of n plus 1 times root of n plus 2 ket n plus 2. And a on ket n plus 2 gives me 1st an n plus 2 and then it gives me an n plus 1 so that is all that I get here. Similarly, from here I have root n root n minus 1 and when a dagger acts on ket n minus 2 it just increases it to n minus 1 and n.

So that is the contribution from the 2nd term. Now I would like to combine these 2 terms and write this as 4 n a dagger a times a dagger a plus 1 n plus 1. And this is clear, this is this is simply going to be n times n plus 1 and therefore, this object just becomes h cross omega by K the whole squared n plus 2 times n plus 1 that is from the 1st term and then an n minus 1 times n from this and then a 4 n times n plus 1 plus 1.

So, let us see this simplifies out. Apart from these overall constants I have an n squared here and an n squared there that is a 2 n squared plus a 4 n squared. So, I am just going to replace the n squared terms by 6 n squared and then that is a 2 n plus an n that is a 3 n minus an n here which is a 2 n, but then there is a 4 n there. So, that gives me a 6 n and as to the constants I have a 2 here and 1 there so that is a 3. So, this is what I have of course, I can make this look better and I can pull out a 3 and do things. So, essentially you can simplify this, but this is what you have h cross omega by k squared d by 4 6 n squared plus 6 n plus 3. So, this is the contribution from the anhormonic perturbation.

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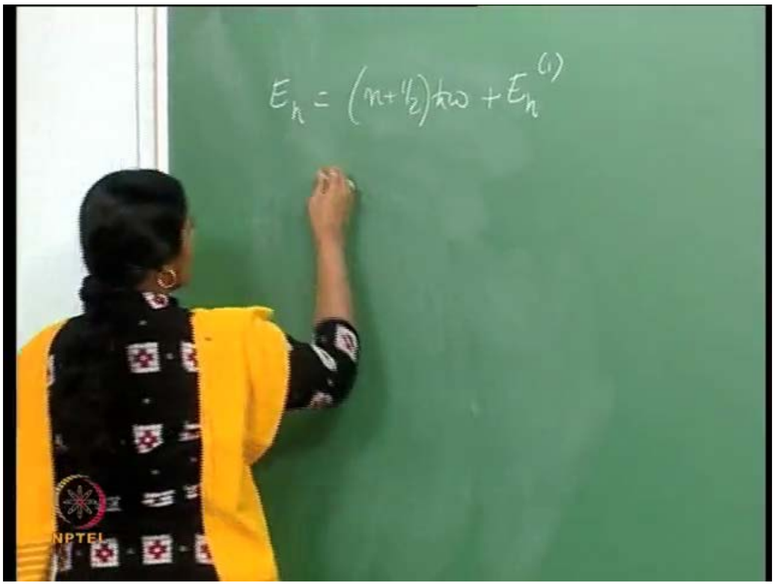

And therefore, in this case the total energy is simply going to be 1st order. In 1st order perturbation theory the energy is n plus half h cross omega which is E n 0 and then there is this extra contribution which we have just now figured out and that is E n 1. This is the case of the anhormonic oscillator where we are doing time independent 1st order perturbation theory.

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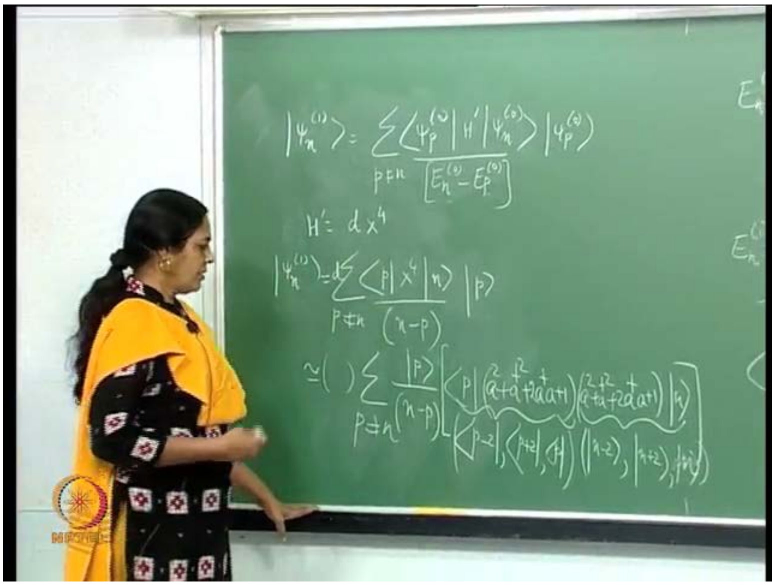

So, now let us look at the wave function itself. So psi n 1 in this case is summation over p not equal to n psi p 0 H prime psi n 0. That matrix element ket psi p 0 and the denominator have an E n 0 minus E p 0. This is what we showed as a general expression and now we need to substitute for H prime so that is the same as d x to the 4. So, that is the same as saying that psi n 1 is summation p not equal to n p x to the 4 n by E n 0 minus E p 0 and we know that that is just n minus p because this is an n plus half h cross omega and that is a p plus half h cross omega. So I just get an n minus p ket p

Once more I have to substitute for x to the 4. So, apart from constants I am not going to mention those here. I would essentially have the following: 1 by n minus p there is of course, a ket p and then I have p a squared plus a dagger squared plus a dagger a 2 a dagger a plus 1 times a squared plus a dagger squared plus 2 a dagger a plus 1 ket n. And this is what I need to simplify. Clearly there will be a Kronecker delta coming from this and that is going to change the value of p.

Now, if you look at this. This is going to contribute terms corresponding to ket n minus 2, ket n plus 2 and ket n. This object here bra p a squared plus a dagger squared plus 2 a dagger a plus 1 is merely the Hermitian conjugate of that except that I have replaced n with p and therefore, the contribution here gives me terms: p minus 2, ket p minus 2, ket p plus 2 and ket p that is what I get out of this. You have to look out for a situation where p is not equal to n and therefore, you cannot for instance have a contribution delta p n such a term will not contribute to this. Now, what would contribute would be delta p minus 2, n the Kronecker delta p minus 2, n delta p plus 2, n p, n minus 2 and p, n plus 2.

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So, essentially the contribution would be from the following. The 1st order contribution to the wave function would clearly have the summation and then there is a term which has delta p n plus 2. I am not putting down these things explicitly and then another which has delta p n minus 2 and then of course, delta p minus 2 with n plus 2 and a 4th term which is delta p plus 2 n minus 2. So, this is what I have and therefore, what are the states that contribute in this order? Again without putting in all the coefficients once I use the Kronecker delta and remove the summation. I will have a term which has n plus 4 another which has n minus 4 and then of course, n plus 2 and n minus 2. You could say psi n plus 4 psi n minus 4 psi n plus 2 and psi n minus 2, but I have just used this notation.

So, essentially the perturbation has done the following thing. The state which was originally ket n has now become to 1st order psi n 0 plus psi n 1. This was the original state and this is what I have to 1st order and this involves other states. It involves psi n plus 4, psi n minus 4, psi n plus 2 and psi n minus 2. The perturbation has done this. However, the system still continues to have a discrete spectrum. I am able to expand the perturbed wave function in terms of the original basis and then when I go to 2nd order there will be a different combination of states that will contribute in the 2nd order.

The 2nd order contribution we can calculate it using a similar program as I did in the 1st order, just a way bit messy perhaps, but we will attempt to do that. Now, that we have the contribution E n 1 and the wave function psi n 1 from the 1st order perturbation theory we have to use those as well as the zeroth order values E n 0 and ket psi n 0 feed that in to get the 2nd order expressions.

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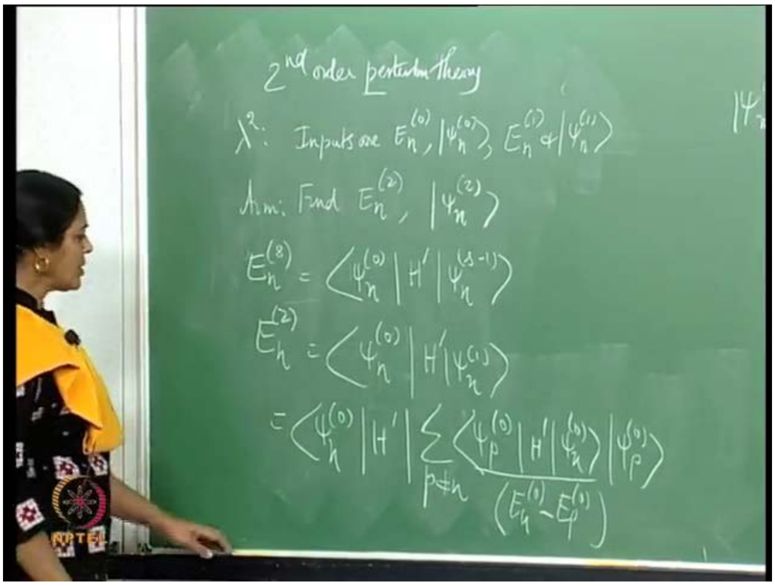

So, in 2nd order perturbation theory you want to look out for coefficients of lambda square. Inputs are E n 0, psi n 0, E n 1 and psi n 1 which we have computed from the 1st order calculation and the aim is to find the 2nd order contribution E n 2 and the corresponding perturbation contribution to the wave function that is psi n 2.

In order to get the expressions for E n 2, E n 2 is something we already know because we already have a general expression E n s is psi n 0 H prime psi n s minus 1. And indeed that is what helps because in order to find out the contribution to a certain order you need to know the wave function only to a lesser order. So, this anyway was the general expression for the s-th order contribution to the energy. But now we need to get an expression and therefore, in our particular case E n 2 is psi n 0 H prime psi n 1.

So, the input is psi n 1 in order to get E n 2. So, that is the same as psi n 0 H prime so psi n 1 itself came as a summation. It was a summation p not equal to n psi p 0 H prime psi n 0 times ket psi p 0 and there was a denominator E n 0 minus E p 0. So, this is E n 2.

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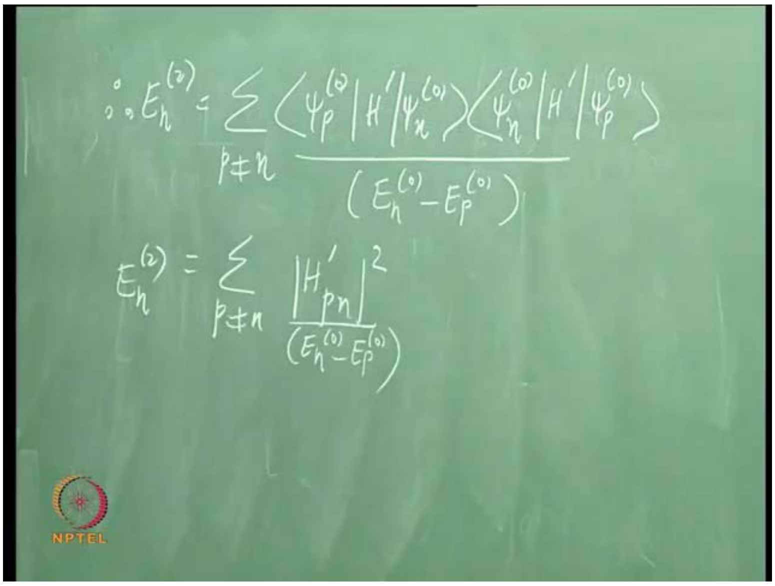

So, let us write this better so it tells me that E n 2 is summation p not equal to n. (Refer Slide Time: 22:57) I already have the matrix element psi p 0 H prime psi n 0. That was already here and I have another matrix element psi n 0 H prime psi p 0 and then I have this denominator E n 0 minus E p 0. And therefore, this can be written as summation p naught equal to n H prime p n H prime n p. So, I could well write this as h prime p n squared by E n 0 minus E p 0. So, this is clearly the expression for E n 2. But, now let us look at the wave function. How do we get an expression for ket psi n 2?

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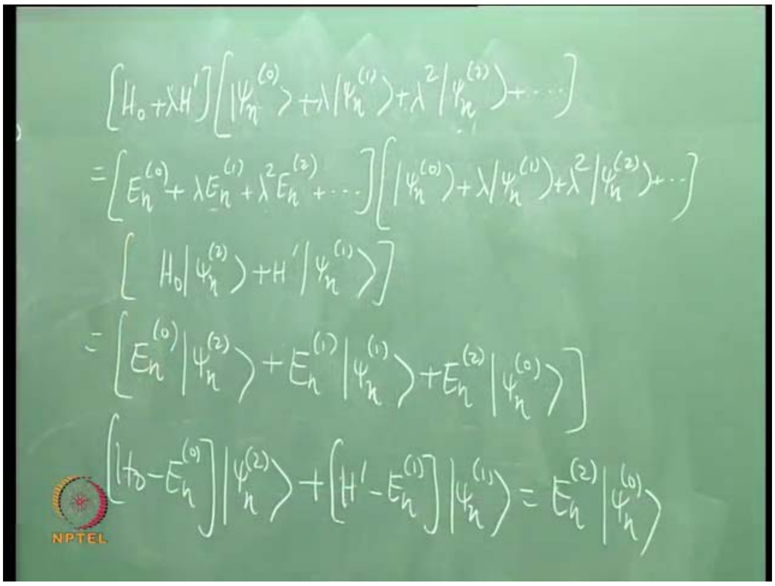

We repeat the algebra that we did yesterday. Start off with the Eigen value equation H naught plus lambda H prime acting on psi n 0 plus lambda psi n 1 plus lambda squared psi n 2 which is what we are ought to find plus so on is E n 0 plus lambda E n 1 plus lambda squared E n 2 and we have already got these values times psi n 0 plus lambda psi n 1. So, we write out the series like this. So, that is what you have. So, you need to look out for terms involving lambda squared that is what you mean by 2nd order perturbation. So, I get a contribution H naught psi n 2 from there plus lambda H prime lambda psi n 1 so plus H prime psi n 1 and that is all that I have from the left hand side of this equation. Now, this object is equal to look at this E n 0 psi n 2, there is a lambda E n 1 and a lambda psi n 1 there.

So, plus E n 1 psi n 1 and then of course, there is an E n 2 psi n 0. Now, it is clear how a general say n-th order perturbation theory or k-th order perturbation theory is going to be. It is going to involve states at this level it uses both H naught and H prime and it involves all states psi n k down to psi n 0 and similarly, it involves all the energy contributions up to E n k and wave functions up to psi n k. So, one can easily guess the general pattern and write that down, but for the moment we are interested in 2nd order perturbation theory.

So, what we can do is the following. Suppose, you choose k not equal to n and then you find out psi k 0 H naught psi n 2. Perhaps we can g roup the factors before that. Let me take the psi n 2s to 1 side so I have H naught minus E n 0 psi n 2 plus H prime minus E n 1 psi n 1 equals E n 2 psi n 0 makes things more convenient because now I will choose k naught equal to n and try to find various matrix elements.

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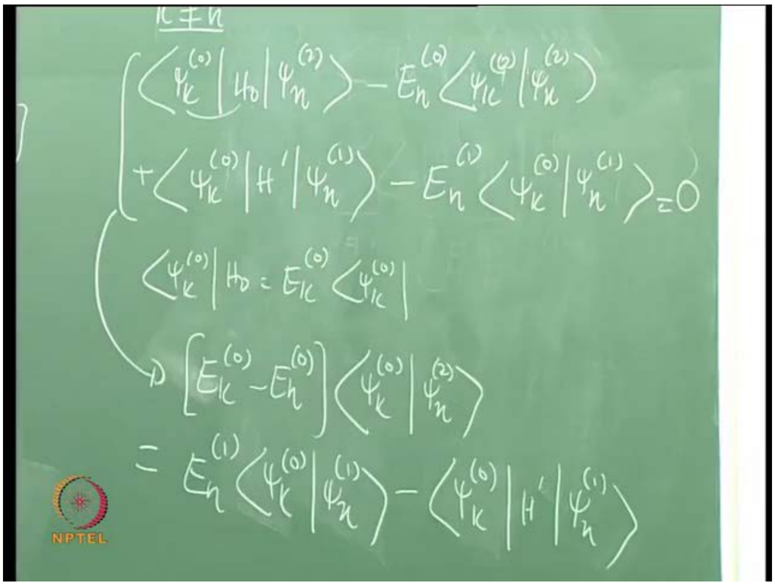

This is essentially the procedure that we followed even when we did 1st order perturbation theory except that we are going to repeat it here and therefore, I have choose k not equal to n and I have psi k 0 H naught psi n 2, That is the 1st term minus E n 0 psi k 0 psi n 2 this inner product so that is what I get from the 1st term. (Refer Slide Time: 27:13) Then from here I have plus psi k 0 H prime psi n 1 now. I will put in the expression for psi n 1 later when I simplify minus E n 1 that is a number psi k 0 psi n 1. Out here on the right hand side this is a number E n 2, but then I have the inner product psi k 0 psi n 0 and we have selected k not equal to n and therefore, this object is 0.

I have also use the fact that H naught psi k 0 is E k 0 psi k 0, because remember that the psi ks are the Eigen states of the unperturbed Hamiltonian psi k zeroes are the unperturbed Hamiltonians Eigen states. And then once I use that this expression simply becomes E k 0 minus E n 0 psi k 0 psi n 2. That is what I get from these 2 terms. That is equal to E n 1 psi k 0 psi n 1 minus psi k 0 H prime psi n 1. As I did yesterday I can simply bring down the E k 0 minus E n 0 to the denominator on the right hand side and that gives us the following.

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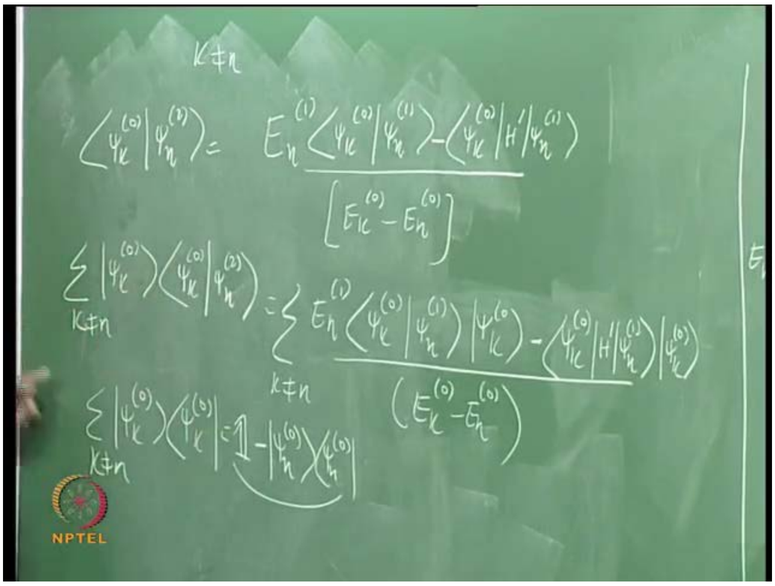

So I now have an expression for the overlap of psi k 0 with psi n 2 and that is just E n 1 psi k 0 psi n 1 that is the 1st term. Minus the matrix element psi k 0 H prime psi n 1 divided by E k 0 minus E n 0; remember that k is not equal to n. So, this is what I have. So, all we need to do is to do a summation over k naught equal to n psi k 0 with both the left hand side and the right hand side of that expression: E n 1 summation over k not equal to n psi k 0 psi k 0 that is the 1st term psi n 1 minus psi k 0 psi k 0.

So, I can write this better so I can just write this as E n 1 psi k 0 psi n 1 times psi k 0 that object that I have introduced there is my 1st term. Similarly, the 2nd term is psi k 0 H prime psi n 1 times psi k 0. So, this is what I have in the numerator and the denominator is an E k 0 minus E n 0. What do I have here? We know this and I merely emphasizing what I said in the last lecture. This is the completeness of states. But now you are choosing k not equal to n and therefore, this object is 1 minus psi n 0 psi n 0.

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If you substitute this out here for summation over k not equal to n psi k 0 psi k 0. The 1st term is simply psi n 2 so let us put that in that is because of the identity. The 2nd terms has the inner product of psi n 0 with psi n 2, and remember that psi n 2 is part of delta psi n. It is the 2nd order contribution to the perturbed wave function. And therefore, the formalism started off by saying that delta psi n has no contributions along the direction psi n 0 and therefore, that inner product is 0 and all I have here is psi n 2. This was precisely the manner in which we went about doing 1st order theory as well and therefore, on the left hand side I have psi n 2 ket psi n 2 for which I am trying to find an expression and I know the right hand side I have this object.

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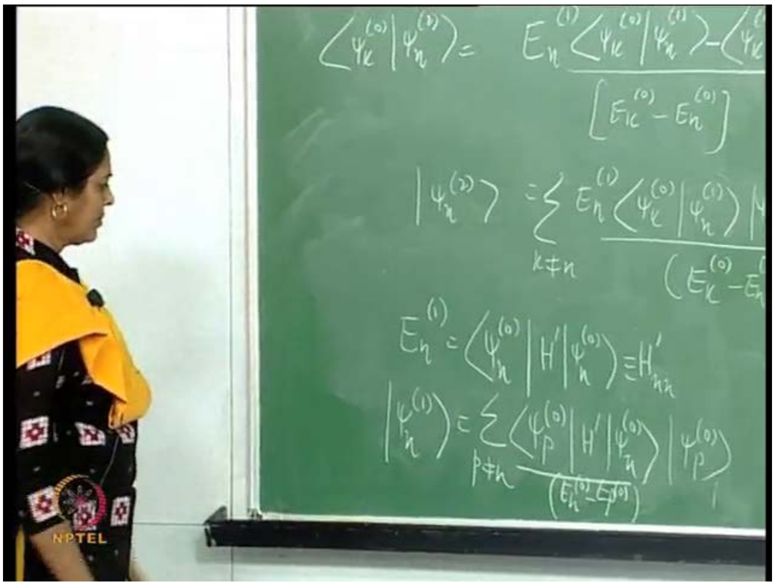

I have 2 terms here I should substitute for E n 1. E n 1 is simply the matrix element psi n 0 H prime psi n 0 and therefore, I would like to call this H prime n n the n n-th matrix element of H prime. Now, if I look at psi n 1 for that too I need to make a substitution. I recall that psi n 1 is summation p not equal to n, psi p 0 h prime psi n 0 times ket psi p 0 and then there was a denominator which was E n 0 minus E p 0. So, we have to put in as inputs this expression for E n 1. I can always call that H prime n n and then I have an H prime p n psi p 0 by E n 0 minus e p 0 which comes both here and there instead of psi n 1.

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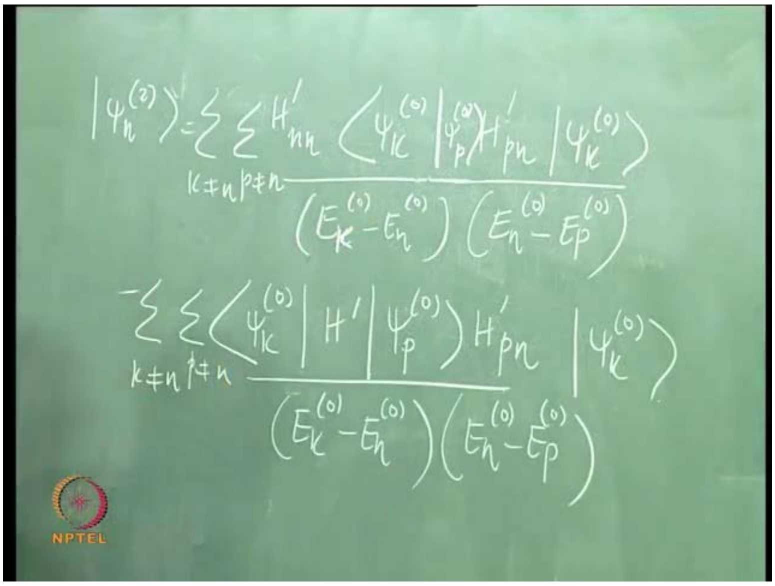

So, let us put that in and that should more or less complete the exercise. (Refer Slide Time: 38:14) The expression for psi n 2 which is the 2nd order contribution in the perturbation to the wave function is simply made up of 2 parts. The 1st one is summation k not equal to n H prime n n that comes from there. (Refer Slide Time: 34:07) There is an E k 0 minus E n 0 in the denominator which we will keep and then there was an inner product of psi k 0 with psi n 1 and for psi n 1 I have the following object. (Refer Slide Time: 38:14) I have h prime p n, but there is a summation p not equal to n.

So, let me write summation p not equal to n H prime p n which is a matrix element. And then of course, I have a psi p 0 out here which I put there, but that is not all I also have a psi k 0, that is my 1st term and then there is a 2nd term that comes with the negative sign. There was a summation k not equal to n any way. There is a psi k 0 H prime, but then I substitute for psi n 1 again. The fact that p is not equal to n and k is not equal to n does not prevent k from being equal to p and therefore, psi n 1 is H prime p n psi p 0.

I have a denominator E k 0 minus E n 0 which was always there, (Refer Slide Time: 34:07) but here I should have also introduced an E n 0 minus E p 0 when I expand it for psi n 1. So, here too there is an E n 0 minus E p 0 this was already there and this came because I wrote out an expression for psi n 1, but of course, the matter does not stop here remember that there is a ket psi k 0. So, this is what I have for psi n 2. Needless to say that this gives me a delta k p and therefore, one of the summations goes away such a thing does not happen in this term and I have to retain both the summations.

So, this is what I have finally, after using the Kronecker delta and getting rid of 1 summation. The 1st term is put out here and the 2nd term is what I have here. I have put that 1st and then put the 1st term in. The point is this that since n is not equal to p and n is not equal to k the problem of denominator that blows up do not arise. Clearly if we were dealing with degeneracies then something has to be done to take care of a situation where say E n 0 is equal to e p 0 if there is a degeneracy problem.

We will discuss the degeneracy situation later, but as it stands the message is that you do a perturbative expansion in the sense, you expand in powers of lambda. You could stop at 1st order, 2nd order, 3rd depending on how much successive terms contribute and you could decide whether the series can be truncated or not. Now, if you were working with problem where the higher order terms contribute significantly then clearly the perturbative approach is not going to help. Typically that is what happens most of the time when you deal with strong nuclear interactions, nuclear forces. On the other hand, perturbation is a very useful technique when we do problems involving electromagnetic interactions.

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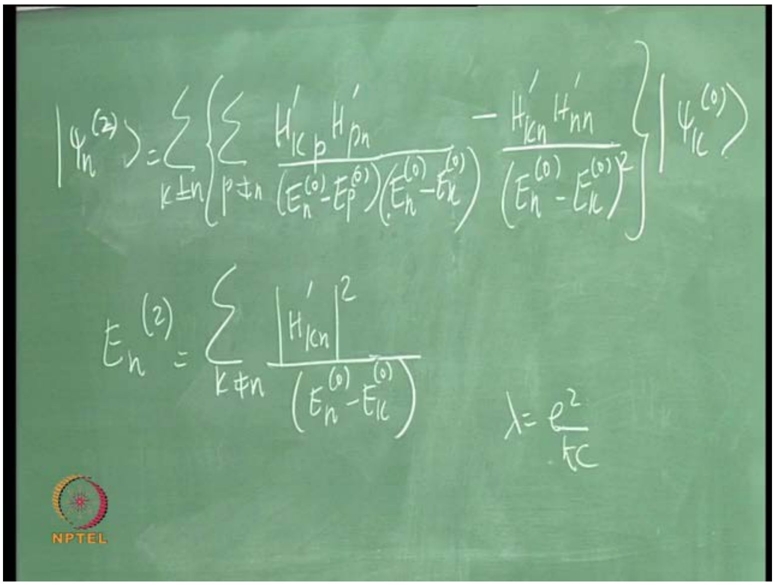

Because the electromagnetic coupling constant in terms of which do you perturbative expansion is given by e square by h cross C. So, your lambda in that case is e square by h cross c and that is small that is 1 by 197 and therefore, subsequent terms could in principle be smaller. Therefore, the only other wrinkle to this problem is the degenerate situation as I said and we will take that up a little later.

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