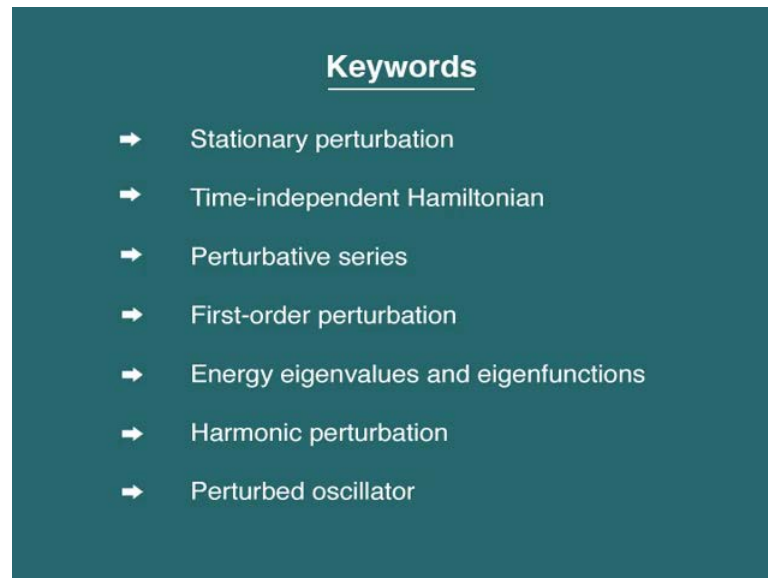


Quantum Mechanics-I
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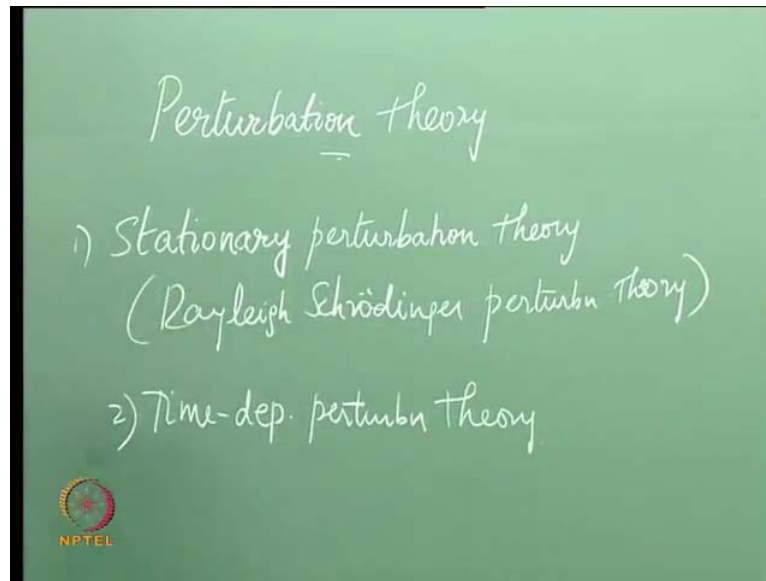
Lecture - 36
Perturbation Theory – I

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Over the last few lectures, we have looked at the dynamics of the state of a system. That means, that you subject the system to various potentials and then you look at the way the manner in which the wavefunction changes, when subject to those potentials. Several interesting things can happen. For instance, even in the case of a Harmonic oscillator potential, you know that an initial Gaussian, continues to be a Gaussian and merely oscillates, preserving its Gaussian form. So, this is the kind of statement that you could make, about a coherence state of light, which is moving in free space, because that too is modeled by Gaussian wavefunction. On the other hand, as you depart from coherence. You have seen, that the state of the system, for instance the one photon added state, does not preserve its shape or form as it moves.

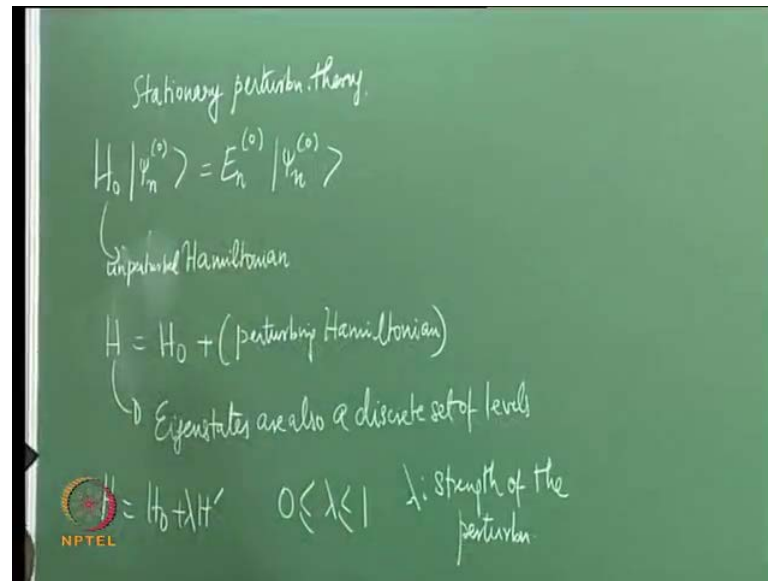
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Now we will look at a new class, a new variety of problems and these come under the title perturbation theory. In other words, you look at a system on which there is an external field or force, which acts as an external Hamiltonian in general. Another Hamiltonian, a perturbing Hamiltonian has to be added to the original Hamiltonian and therefore, the system is affected. Now, the external agent which acts on the physical system of concern could be a time dependent Hamiltonian or it could be guided by a time independent Hamiltonian.

So, depending on whether the external agent is modeled by a time dependent Hamiltonian or a time independent Hamiltonian, you will do stationary perturbation theory if it is time independent. So, stationary perturbation theory, also called the Rayleigh Schrodinger perturbation theory. Now, if you also have a time dependent Hamiltonian which models the external perturbation then, it is the time dependent perturbation theory.

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We will first be looking at stationary perturbation theory and the point here is this. Suppose, you started with the physical system whose Hamiltonian is given by H naught. This corresponds to the free system, which has not been subject to any external agent and suppose, the Eigenbasis are given by ψ_n 's. But, I will also put a superscript there, 0 to show that this is the unperturbed Eigenbasis and this is the Eigenvalue equation.

So, for instance, if you took a free Harmonic oscillator. H naught would be p squared by a linear Harmonic oscillator, H naught is the free Hamiltonian, by free I mean, unperturbed Hamiltonian. So, let us write unperturbed Hamiltonian and this in the case of the linear Harmonic oscillator would be p square by $2m$ plus half kx square, where k is $m\omega$ square. And these, would simply be the ket n 's or the Fock states of the oscillator and the E_n zeros, would be just n plus half h cross ω and this is the Eigenvalue equation, which you know and which you have solve for.

We have solved for this set of Eigenvalues and the Eigenfunctions using the Schrodinger formalism. We have solved for this and shown that these wave functions, that is in the position representation, they would be given by essentially the Hermite polynomials, apart from other factors. Now, once you apply an external perturbation, you have a new Hamiltonian and this Hamiltonian has an H naught plus a perturbing Hamiltonian.

When you say stationary perturbation theory, you mean the following thing. First of all we are dealing with discrete Eigenstates. So, here you have a set of discrete levels, ψ_1

0, ψ_2 , ψ_0 , because n can also take the value 0 in the case of Harmonic oscillator for instance. So, you have a discrete set of levels and there is this perturbing Hamiltonian which was some external field possibly which acted on the oscillator or on the given physical system at sometime. And then it has been removed so that the system now settles down and equilibrates to a new set of discrete levels, so this one's Eigenstate are also discrete, a discrete set of levels.

So, we are doing stationary perturbation theory in contrast to time dependent perturbation theory. Now, this perturbing Hamiltonian, I could just write it as some H' , but for the sake of book keeping, I would like to introduce a parameter λ here and λ can take values 0 to 1. Basically, if the perturbation is switched off, that is like saying that $\lambda = 0$ and you only have the unperturbed Hamiltonian. The system is not perturbed, $\lambda = 1$, the perturbation is comparable to H' . So, that is the way it is. λ can take any value from 0 to 1 and therefore, λ is the strength of the perturbation. So, I write the new Hamiltonian as $H + \lambda H'$.

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$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + |\Delta\psi_n\rangle$$

$$|\Delta\psi_n\rangle = \sum_{k \neq n} c_k |\psi_k^{(0)}\rangle$$

$$E_n = E_n^{(0)} + \Delta E_n$$

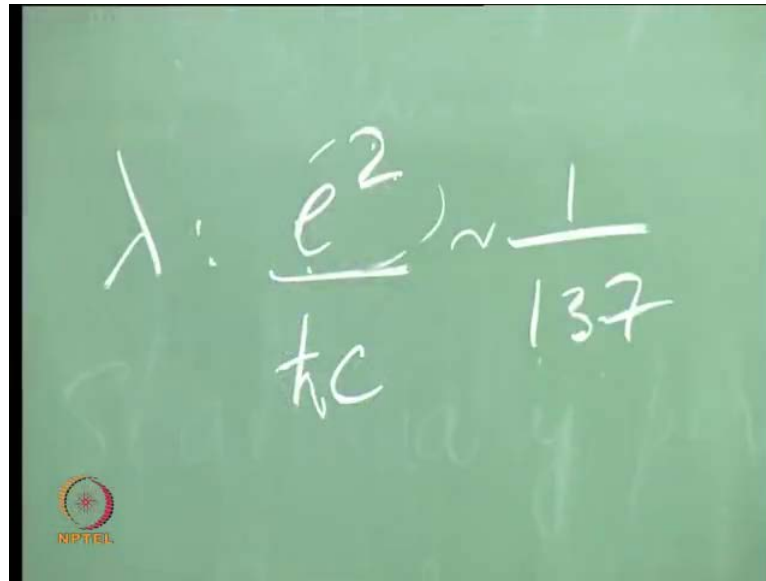
The very important feature here is the following. The Eigenstates of the new Hamiltonian let me refer to them as ψ_n and the new Eigenvalues as E_n . (Refer Slide Time: 03:37) The important thing is that the ψ_n 's are also expandable in terms of this basis set $\psi_n^{(0)}$. So, basically the perturbation changes $\psi_n^{(0)}$ by some quantity. I represent this in ket notation so ψ_n the n -th level, new state which is an Eigenstate of the full

Hamiltonian H is the old n -th level plus some $\delta \psi_n$. Now, this $\delta \psi_n$ can be expanded, in terms of the old basis. (Refer Slide Time: 03:37) So, the perturbation does not change the Hilbert space of the system per se in the sense, that I can retain the old basis set.

So, $\delta \psi_n$ can really be expanded in terms of the old basis set in this fashion, except that, I would assume that, the perturbation in this superposition does not have a non-zero coefficient corresponding to n . In other words, $\delta \psi_n$ does not have a contribution along the component ψ_n^0 , does not have a component along $\text{ket } \psi_n^0$. So, this is what I have for $\delta \psi_n$. Now, E_n itself correspondingly, will be the old energy Eigenvalue plus an addition δE_n because of the perturbation. Now, the aim of perturbation theory is to estimate δE_n and $\delta \psi_n$.

In other words, you want the new energy values and you also want the corresponding energy Eigenstates, by that I mean, the Eigenstates and the Eigenvalues of the full Hamiltonian H , which includes the free or the unperturbed Hamiltonian plus the perturbation (Refer Slide Time: 03:37). Now how do I go about doing this? The aim is to develop a perturbation series. In principle this is an infinite series and if it is possible to truncate the series somewhere, effectively if it is possible to make such an approximation. Then it is very good, because I do not have to work with an infinite series and perturbation is a very effective procedure. The perturbation series can be truncated and the series itself will be written in powers of this (Refer Slide Time: 03:37) strength λ .

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$$\lambda = \frac{e^2}{hc} \sim \frac{1}{137}$$

So, for instance if you are talking about electromagnetism, lambda is usually the parameter e^2 , where e is electric charge by h cross c and this is $1/137$ and therefore, if you made a series in powers of lambda. The 1st term lambda to the 1, that means the 1st order in the perturbation has $1/137$ multiplying things. The next order is $1/137$ squared and that is much smaller than $1/137$ and so on. So, you make an expansion in terms of the quantity whose powers, the strength of the perturbation itself is $1/137$ in some units.

And therefore, higher terms could possibly make lesser contribution and you can stop the series at some point, you can truncate the series and find out, what the wavefunction is. (Refer Slide Time: 08:23) ψ_n and the corresponding E_n to that order of approximation. On the other hand, it is possible that you will never be able to truncate the series. And then of course, perturbation theory itself is not particularly useful. So, we will see specific instances, where we can truncate the series and find out what the final wavefunction and the corresponding Eigenvalues are, to that approximation.

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$$\begin{aligned}
 H|\psi_n\rangle &= E_n|\psi_n\rangle \\
 [H_0 + \lambda H'] [|\psi_n^{(0)}\rangle + |\Delta\psi_n\rangle] &= [E_n^{(0)} + \Delta E_n] [|\psi_n^{(0)}\rangle + |\Delta\psi_n\rangle] \\
 \therefore H_0|\psi_n^{(0)}\rangle + \lambda H'|\psi_n^{(0)}\rangle + H_0|\Delta\psi_n\rangle + \lambda H'|\Delta\psi_n\rangle &= E_n^{(0)}|\psi_n^{(0)}\rangle + \Delta E_n|\psi_n^{(0)}\rangle + E_n^{(0)}|\Delta\psi_n\rangle + \Delta E_n|\Delta\psi_n\rangle
 \end{aligned}$$

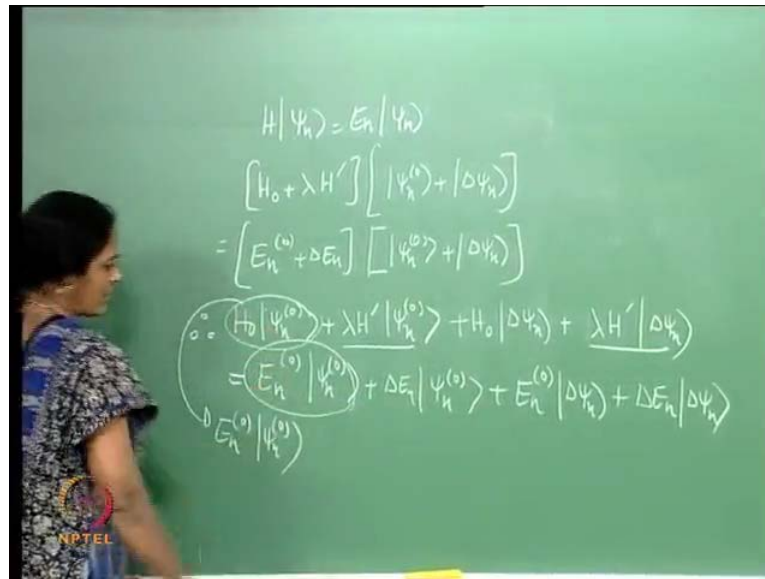
So, the 1st stage is to write $H \psi_n$ equal $E_n \psi_n$ as H naught plus λH prime ψ_n itself is ψ_n 0 plus $\Delta \psi_n$. This quantity is equal to E_n 0 plus $\Delta E_n \psi_n$ 0 plus $\Delta E_n \Delta \psi_n$. So, when I expand this: I have H naught ψ_n 0 plus λH prime ψ_n 0 plus H naught $\Delta \psi_n$ plus λH prime $\Delta \psi_n$ is E_n 0 ψ_n 0 plus $\Delta E_n \psi_n$ 0 plus E_n 0 $\Delta \psi_n$ plus $\Delta E_n \Delta \psi_n$. I merely expanded out things, in terms of H naught, H prime, ψ_n 0 $\Delta \psi_n$ and so on. But, I know that H naught ψ_n 0, I know that this quantity is E_n 0 ψ_n 0 and therefore, these two just cancel out and then what do I have?

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$$\begin{aligned}
 \lambda H'|\psi_n^{(0)}\rangle + H_0|\Delta\psi_n\rangle &= \Delta E_n|\psi_n^{(0)}\rangle + \Delta E_n|\Delta\psi_n\rangle \\
 \lambda H'|\psi_n^{(0)}\rangle + E_n^{(0)}|\Delta\psi_n\rangle &= \Delta E_n|\psi_n^{(0)}\rangle + \Delta E_n|\Delta\psi_n\rangle \\
 \langle\psi_n^{(0)}|\lambda H'|\psi_n^{(0)}\rangle + \langle\psi_n^{(0)}|E_n^{(0)}|\Delta\psi_n\rangle &= \Delta E_n \langle\psi_n^{(0)}|\psi_n^{(0)}\rangle + \Delta E_n \langle\psi_n^{(0)}|\Delta\psi_n\rangle \\
 = \Delta E_n \underbrace{\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle}_1 + E_n^{(0)} \underbrace{\langle\psi_n^{(0)}|\Delta\psi_n\rangle}_0 + \Delta E_n \underbrace{\langle\psi_n^{(0)}|\Delta\psi_n\rangle}_0 & \\
 \Delta E_n = \lambda \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle &
 \end{aligned}$$

I have $\lambda H' \psi_n^{(0)} + H_0 \delta \psi_n + \lambda H' \delta \psi_n$.

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So, I might as well just clubbed the two terms and write $\lambda H' \psi_n^{(0)} + H_0 \delta \psi_n$ and that is just $\psi_n^{(0)} + H_0 \delta \psi_n$. Notice that these two terms, just to care of each other, they balanced each other and therefore, I am left with $\delta E_n \psi_n^{(0)}$, out there plus $E_n^{(0)} \delta \psi_n + \delta E_n \delta \psi_n$. So, this is what I have. These two terms balanced out each other. (Refer Slide Time: 15:29)

I simply combined $\lambda H' \psi_n^{(0)} + H_0 \delta \psi_n$ and wrote that there as the 1st term. Then I had an $H_0 \delta \psi_n$ and on this side, I have a $\delta E_n \psi_n^{(0)}$ and $E_n^{(0)} \delta \psi_n$, plus a $\delta E_n \delta \psi_n$. My aim is to find δE_n . I need to find the extra amount and therefore, let me do this. So, I have $\lambda H'$ it is sandwiched between $\psi_n^{(0)}$ and $\psi_n^{(0)}$ that is my first term plus $\psi_n^{(0)} H_0 \delta \psi_n$. That is $\delta E_n \psi_n^{(0)}$ and that is 1, because we have chosen an orthonormal basis and therefore, this inner product is 1 plus $E_n^{(0)} \psi_n^{(0)} \delta \psi_n + \delta E_n \psi_n^{(0)} \delta \psi_n$.

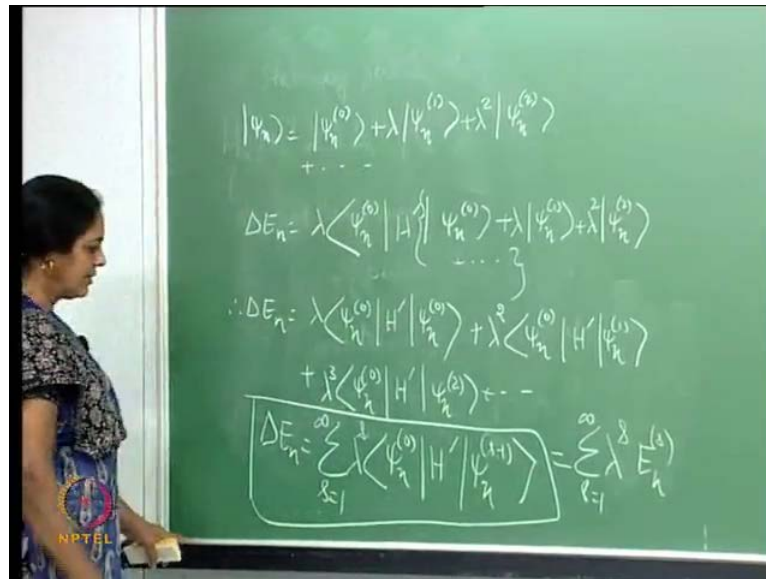
Notice the following: we said that $\delta \psi_n$, our assumption was that. (Refer Slide Time: 08:23) $\delta \psi_n$ is expanded in terms, is a superposition of the $\psi_k^{(0)}$, but not $\psi_n^{(0)}$ and therefore, this is 0. Those two terms drop out and therefore, I have δE_n equals this object $\psi_n^{(0)} \lambda H' \psi_n^{(0)} + \psi_n^{(0)} H_0 \delta \psi_n$. But, notice that $H_0 \psi_n^{(0)}$ is $E_n^{(0)} \psi_n^{(0)}$ and that term therefore drops out, because

ΔE_n does not have a contribution along $\psi_n^{(0)}$.

So, that term also drops out and therefore, I have a very simple relation like this. Let me pull the λ outside, $H' \psi_n$. So, this is ΔE_n . In other words, the effect of the perturbation is to shift the energy value which was originally $E_n^{(0)}$ by an amount ΔE_n , which is calculable and which is given in this manner. You merely have to find the following scalar quantity. You need to sandwich H' between ψ_n and $\psi_n^{(0)}$.

Notice that ψ_n is the full wavefunction, whereas $\psi_n^{(0)}$ was the unperturbed wavefunction and H' is the perturbing Hamiltonian, $\lambda H'$ is a perturbing Hamiltonian. So, here is a very simple way of estimating ΔE_n provided, I know what ψ_n is and as I said ψ_n has to be perturbatively estimated. In other words, you write ψ_n in the following manner as a series in powers of λ .

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So, ψ_n is $\psi_n^{(0)}$, if there is no perturbation, plus $\lambda \psi_n^{(1)}$. This is to 1st order in the perturbation plus $\lambda^2 \psi_n^{(2)}$; this is to 2nd order in the perturbation and so on. So, this is the manner in which ψ_n is expanded and you could estimate the wavefunction perhaps, by truncating the series here. That means to 1st order in the perturbation, or truncating the series here which means, you estimate ψ_n to 2nd order in the perturbation and so on.

So, now when you use that, you just have ΔE_n is $\lambda \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$. What I have

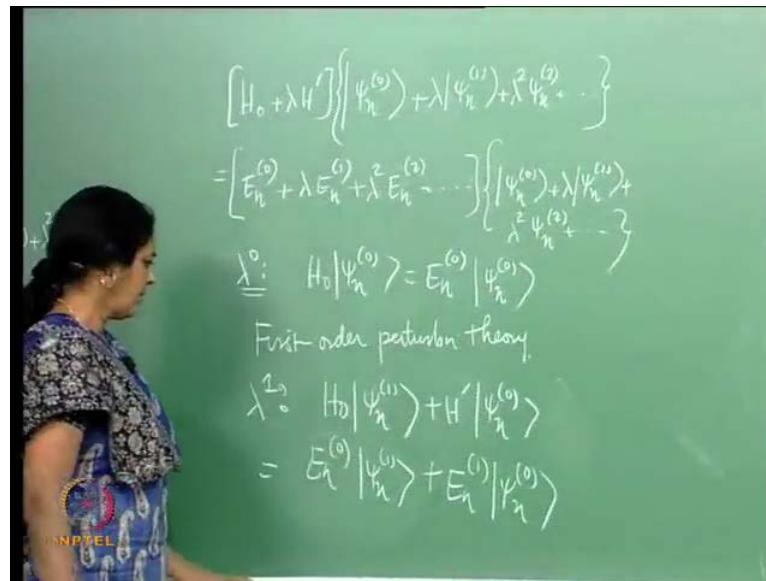
written here? (Refer Slide Time: 15:11) H' , which is merely the perturbing Hamiltonian, $\psi_n^{(0)}$ plus $\lambda \psi_n^{(1)}$ and so on that series. So, this is what I have. So, let us see what this gives us? Therefore, ΔE_n is $\lambda \psi_n^{(0)} H' \psi_n^{(0)}$. Suppose, you initially started with the state $\psi_n^{(0)}$, what is the probability amplitude that you land up in a final state $\psi_n^{(0)}$? So, that is what this gives you, plus $\lambda^2 \psi_n^{(0)} H' \psi_n^{(1)}$ plus $\lambda^3 \psi_n^{(0)} H' \psi_n^{(2)}$ and so on.

So, I can always write this in a compact form: ΔE_n is summation over s equals 1 to infinity, $\lambda^s \psi_n^{(0)}$ the unperturbed wavefunction, the perturbing Hamiltonian $\psi_n^{(s-1)}$. Now, this is a good thing for us to know because if you want to find ΔE_n to order λ , that means you set s equals 1. You merely need to know the wavefunction to a lower order $\psi_n^{(0)}$. If you wanted to estimate ΔE_n to the 2nd order, that is λ^2 times something. Then you need to know the wavefunction only to 1st order, because that is an $s-1$ out there.

So, basically if you know $\psi_n^{(0)}$ and $\psi_n^{(1)}$ you can estimate ΔE_n , to 2nd order in the perturbation. If you only know $\psi_n^{(0)}$, you can estimate ΔE_n to 1st order in the perturbation and so on. So, the wavefunction is something you need to know to a lower order, one order lower, in order to find out, the correction to the original energy to that order. So, that is a nice thing and therefore, I can well write this as summation s equals 1 to infinity, $\lambda^s E_n^{(s)}$, where $E_n^{(s)}$ is precisely this object.

So, you see ΔE_n is also expanded in powers of λ . You expanded ψ_n in powers of λ and the change ΔE_n also in powers of λ . So, the total energy will be $E_n^{(0)}$. So, that is to 1st order, to zeroth order in the perturbation you have $E_n^{(0)}$ plus ΔE_n , which is written in terms of the 1st order in λ times $E_n^{(1)}$ and so on. So that is what you have. Now you see we can feed all these things in and find out, what is a change in energy ΔE_n ? And what is the change in the wavefunction $\Delta \psi_n$?

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So, let us see how we go about this. So, go back to your equation and you have H naught plus lambda H prime $\psi_n^{(0)}$ plus delta $\psi_n^{(1)}$ plus lambda squared $\psi_n^{(2)}$ plus so on equals $E_n^{(0)}$, which was the unperturbed energy plus lambda $E_n^{(1)}$, from here, (Refer Slide Time: 19:55) plus lambda squared $E_n^{(2)}$ plus so on. So, I expand that also as a series in lambda times ψ_n . So, I can write that as $\psi_n^{(0)}$ plus lambda $\psi_n^{(1)}$ plus lambda squared $\psi_n^{(2)}$ plus so on.

Now, let us look at zeroth order that means, only look at terms which have no lambda dependents and equate them. For order 0 what do I have? I have H naught $\psi_n^{(0)}$ on that side, because every other terms contains lambda is $E_n^{(0)} \psi_n^{(0)}$. This is merely a statement that if you have the unperturbed system. Then it is guided by a Hamiltonian H naught and the basis states, the energy Eigenstates are $\psi_n^{(0)}$, the corresponding energy Eigenvalues are $E_n^{(0)}$, say discrete set of values.

Now, if you did 1st order perturbation theory, that means you compare coefficients, to order lambda to the 1 or lambda and equate them in this equation and what do I have? I have H naught $\psi_n^{(1)}$, from here plus H prime $\psi_n^{(0)}$ and that is all I can have here, because I need to just look at terms multiplying lambda and this comes with lambda squared, lambda cubed and so on beyond that. So, that the contribution is only from these two terms.

But on this side I have $E_n^{(0)}$. This is equal to $E_n^{(0)} \psi_n^{(0)}$. It cannot make a

contribution, because you are looking at powers of lambda so its $E_n^{(0)} \psi_n^{(1)}$, out here plus $E_n^{(1)} \psi_n^{(0)}$. So, the 1st order contribution $E_n^{(1)}$, but the wavefunction is $\psi_n^{(0)}$. So, this is what I have. I have this equation, if I work to order lambda that means 1st order perturbation theory. I can write this better, I can simply group terms and I can write.

(Refer Slide Time: 28:01)

The image shows a green chalkboard with handwritten mathematical equations. At the top left, there is a small '1.' and a lambda symbol. The main equation is:

$$[H_0 - E_n^{(0)}] \psi_n^{(1)} = [E_n^{(1)} - H'] \psi_n^{(0)}$$

Below this, there is a summation over $k \neq n$ of the left-hand side of the equation, which is then equated to the right-hand side. The derivation shows that the term $E_n^{(1)} \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$ is zero because $\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle = 0$ for $k \neq n$. This leaves the equation:

$$- \langle \psi_k^{(0)} | H' | \psi_n^{(0)} \rangle = - E_n^{(1)} \langle \psi_k^{(0)} | \psi_n^{(0)} \rangle$$

Since $\langle \psi_k^{(0)} | \psi_n^{(0)} \rangle = 0$ for $k \neq n$, the equation simplifies to:

$$E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$$

In the bottom left corner of the chalkboard, there is a small circular logo with the text 'NPTEL' below it.

So, this is 1st order perturbation theory. H naught minus $E_n^{(0)}$, $\psi_n^{(1)}$ equals $E_n^{(1)}$ minus H' $\psi_n^{(0)}$. So, we use lambda for book keeping purposes so you work to order lambda, lambda square lambda cubed, zeroth order in lambda which is the free case and so on. So, this is the equation that I have. My aim is to find out $E_n^{(1)}$ and I have a formula for that, because we have already said (Refer Slide Time: 19:55) that $E_n^{(1)}$ out here. Put s equals 1 so that is $\psi_n^{(0)} H' \psi_n^{(0)}$ that is $E_n^{(1)}$ so I know $E_n^{(1)}$. H' prime is given to me, that is the perturbing Hamiltonian, I know $\psi_n^{(0)}$ that is the old energy basis with which I began and my aim is to find out $\psi_n^{(1)}$.

So, there is a very simple way of doing this. So, let us choose k not equal to n and do the following: minus $E_n^{(0)} \psi_k^{(0)} \psi_n^{(1)}$ equals $E_n^{(1)} \psi_k^{(0)} \psi_n^{(0)}$ minus $\psi_k^{(0)} H'$ prime $\psi_n^{(0)}$. So, I have just used bra $\psi_k^{(0)}$ on this side. I know what this is. I know that H naught $\psi_k^{(0)}$ is $E_k^{(0)} \psi_k^{(0)}$ therefore, $E_k^{(0)} \psi_k^{(0)} \psi_n^{(1)}$ and they can have a non-zero overlap. Remember that $\psi_n^{(1)}$ is the wavefunction to 1st order in the perturbation. So, it is the 1st order contribution to $\Delta \psi_n$ and a very crucial input was that $\Delta \psi_n$

n did not have a contribution along ψ_n^0 and we have selected k not equal to n . So, $\Delta\psi_n$ when expanded in terms of the basis set, the ψ_k^0 's, it would have a component along ψ_k^0 in general, provided k is not equal to n and that is what I have used here. This is in general non-zero.

So, minus E_n^0 same thing out there ψ_k^0 , ψ_n^1 , this is 0, because we have chosen k not equal to n and since this is the Eigenbasis of the unperturbed Hamiltonian and they are mutually orthogonal. So, this term does not contribute, but I have equals minus ψ_k^0 , H' ψ_n^0 . So, you see once more what figures is nearly this matrix element of H' , between the unperturbed state ψ_n^0 and ψ_k^0 . In order to estimate things in the 1st order of the perturbation, I need to know only the wavefunction to zeroth order in the perturbation.

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$$\lambda H' |\psi_n\rangle + H_0 |\Delta\psi_n\rangle = \Delta E_n |\psi_n^{(0)}\rangle + E_n^{(0)} |\Delta\psi_n\rangle + \Delta E_n |\Delta\psi_n\rangle$$

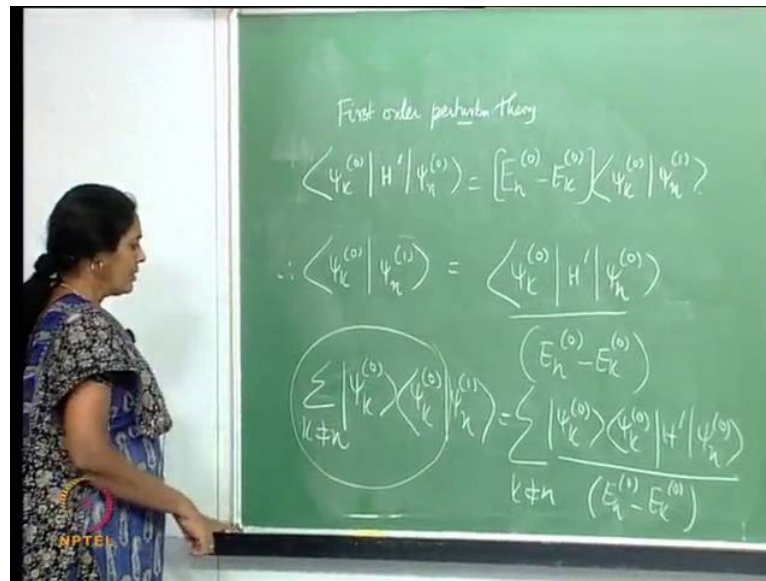
$$\langle \psi_n^{(0)} | \lambda H' |\psi_n\rangle + \langle \psi_n^{(0)} | H_0 |\Delta\psi_n\rangle = \Delta E_n \langle \psi_n^{(0)} | \psi_n^{(0)} \rangle + E_n^{(0)} \langle \psi_n^{(0)} | \Delta\psi_n \rangle + \Delta E_n \langle \psi_n^{(0)} | \Delta\psi_n \rangle$$

$$\Delta E_n = \lambda \langle \psi_n^{(0)} | H' | \psi_n \rangle$$

$$\Delta E_n = \sum_{s=1}^{\infty} \lambda^s E_n^{(s)} \text{ where } E_n^{(s)} = \langle \psi_n^{(0)} | H' | \psi_n^{(s-1)} \rangle$$

So, I need to put down ΔE_n . We have already shown that that is summation s is equal to 1, to infinity $\lambda^s E_n^s$ where E_n to any order is really this object, (Refer Slide Time: 19:55) $\langle \psi_n^0 | H' | \psi_n^{s-1} \rangle$. So, these are important things that we have already shown. So, that is the way it is. So, going back to this equation, (Refer Slide Time: 28:01) we are trying to estimate the wavefunction and the energy Eigenvalues to 1st order in the perturbation and we have an equation of this form and therefore, I can write.

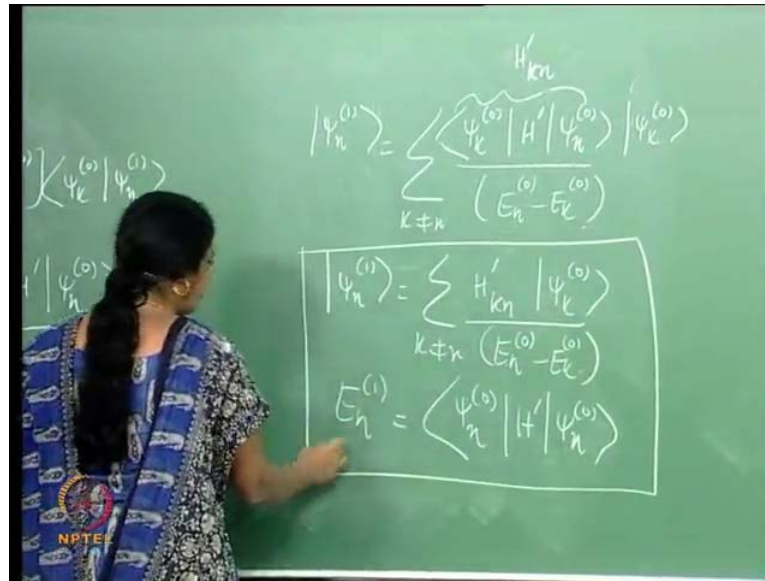
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So, 1st order perturbation so I have $\langle \psi_k^{(0)} | H' | \psi_n^{(0)} \rangle = [E_n^{(0)} - E_k^{(0)}] \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$ (Refer Slide Time: 28:01) times a non managing quantity in general, which is $\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$ inner product and this is what I have. So, I can well write it in the following fashion, remember I need to find out $\psi_n^{(1)}$, this is the quantity $\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$ that I need to estimate. So, take this matrix element and divide it by this number. The energy corresponding to the k-th level, the energy corresponding to the n-th level and n is not equal to k that is the way we have taken things.

So, if I want to estimate $\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$, all I have to do is to do a summation $k \neq n$, $\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle = \frac{\langle \psi_k^{(0)} | H' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}$. This object is summation $k \neq n$, $\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle = \frac{\sum_{k \neq n} \langle \psi_k^{(0)} | H' | \psi_n^{(0)} \rangle}{E_n^{(1)} - E_n^{(0)}}$. And this is very interesting, because since k is not equal to n and you are summing over the case, look at this part. This object should simply be equal to identity, if I had also put $k = n$.

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So, therefore, this reduces to identity minus the projector onto ket psi n, but because psi n 1 has no component along psi n 0, I have psi n 1 equal summation k not equal to n (Refer Slide Time: 33:03) and here unfortunately, I cannot simply do that summation, because there is an E k out here and this is a matrix element which I will call H prime n k n. But for the moment let me just write it down. Psi k 0, this is what I have, divided by E n 0 minus E k 0.

So, this summation extends all over and this is what I have. All I need to know is this matrix element which I will call H prime k n. It is the k n-th element of the matrix H prime. H prime is an operator and if you give a matrix representation, this is clearly the k n-th element of the matrix H prime and I need to know the unperturbed wave functions and I sum over all k's not equal to n and I know that this would not blow up, because n is not equal to k and this is the manner in which I find psi n 1.

So, I have psi n 1 is summation k not equal to n, H prime k n psi k 0 divided by E n 0 minus E k 0 and E n to 1st order is something that I know. (Refer Slide Time: 31:56) E n to 1st order is psi n 0, H prime psi n 0. So, you see this formalism turns out to be extremely useful, because to determine the energy values and the wavefunctions to 1st order, I only need to know the energy values and the wavefunctions to zeroth order.

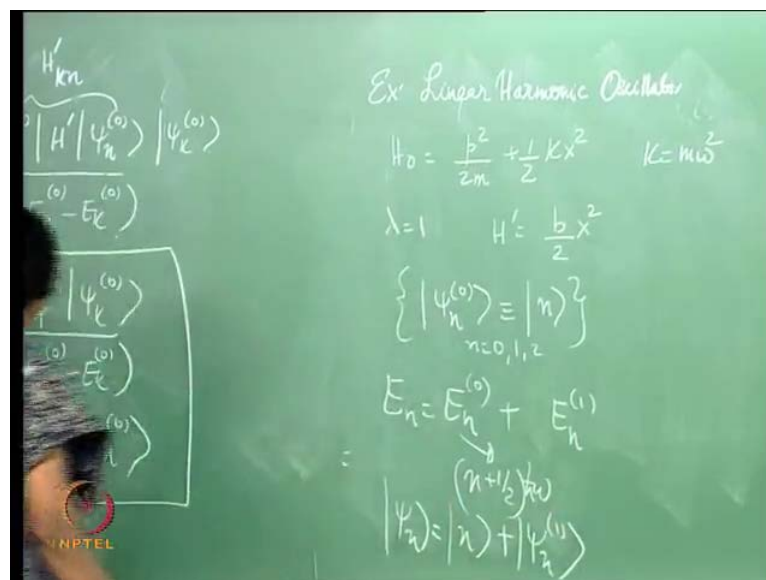
So, if I now compared, if I did 2nd order perturbation theory and I took that huge expression that we had earlier and I equate terms with coefficient lambda squared. Then I

will find that the aim would be to estimate ψ_n to 2nd order and E_n to 2nd order in that case. And all I would need would be the wavefunction to zeroth order and 1st order, which I would have estimated already, the zeroth order wavefunctions I know, they are the free Hamiltonian wave functions, Eigenstates and then the 1st order wavefunction which I would have gotten from here.

Similarly, I would need to know E_n 's, that entire set and the ψ_n 's. So, you see if I know the energy, zeroth order and 1st order and I know the wavefunction zeroth order and 1st order. I know the energy and the wavefunction to 2nd order and so on. So, I need to know these values to an order less than what I wish to determine and therefore, it becomes some kind of a recursion relation where I feed in the zeroth order values and get the 1st order values, feed in the 1st order values and get the 2nd order values and so on.

Now, these are the results that I get for the contribution to 1st order to the energy and to the wavefunction, because of the perturbation. So, let us use these formulae, let us try to illustrate this with a very simple example, the linear Harmonic oscillator, where I add a perturbation such that the Harmonic nature is still maintained.

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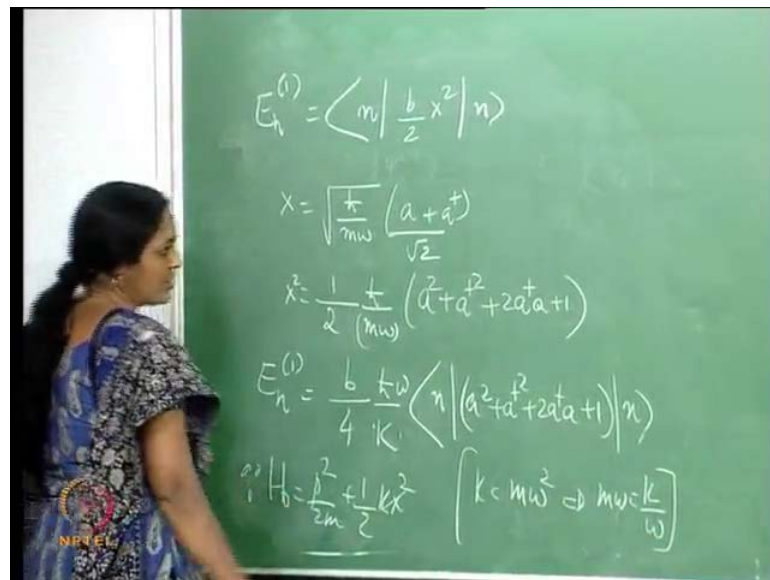


So, example, the linear Harmonic oscillator, it is the simplest example I can think of. So, you know that H naught is p squared by $2m$ plus half K x squared. So, K is m ω square and I give you an H prime. Let me set λ equals 1 then H prime is b by 2 X squared. So, since this is also quadratic in X , the Harmonic nature is going to be

maintained, there is no Anharmonicity in this problem. So, this is H prime, lambda was set is equal to 1. So, I wish to find out the new wavefunction. I know the old wavefunctions. I know that the set ψ_n^0 in my notation is simply ket n, n taking value: 0 1 2 3 etcetera. These are the Eigenstates over the free Hamiltonian, over the unperturbed Hamiltonian.

So, given that, (Refer Slide Time: 35:45) let me first estimate $E_n^{(1)}$, the 1st order contribution to the energy. Now to 1st order, the total energy will be E_n^0 which I know is n plus half \hbar cross omega plus lambda $E_n^{(1)}$, but I have set lambda equals 1 in this problem. So, this is going to be the contribution to energy to 1st order and similarly, ψ_n to 1st order would be ψ_n^0 which is simply ket n in my usual notation plus the contribution $\psi_n^{(1)}$, which I will calculate using this. (Refer Slide Time: 35:45) All I need is the matrix element of the perturbing Hamiltonian, the K n-th matrix element of the perturbing Hamiltonian. The Hamiltonian is given to me. So, I can well do this calculation. So, this is a very simple illustrative example to show the power perturbation theory.

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So, let us look at $E_n^{(1)}$ in our example. This is simply $\langle n | H' | n \rangle$ and since b is a constant I put that out and x squared has to be written and I will prefer to write it in terms of the ladder operators a and a^\dagger . You will recall that X is root of \hbar cross by m omega a plus a^\dagger by root 2. Let me remind you that this is what provides the length

scale in the problem. So, X^2 was a half \hbar cross by $m\omega a + a^\dagger$ the whole squared and if you keep the ordering right, this is what it is. And therefore, E_{n+1} is simply b by $4\hbar$ cross by $m\omega a^2 + a^\dagger^2 + 2a^\dagger a + 1$.

Now, since I had written my H naught as p^2 by $2m$ plus half Kx^2 . So, let us see K is really $m\omega^2$ and I seem to want $m\omega$ all the time. So, $m\omega$ is k by ω and therefore, I can write this as b by $4\hbar$ cross ω by K , because of this reason. So, let us see where this takes us. Look at this, a square is a lowering operator. So, when a square acts on n brings it down to 1st time it acts, a acts on n to take it down to $|n-1\rangle$ and then the a again, that makes it $|n-2\rangle$ and since they are orthogonal states, you do not get a contribution from this term which is the expectation value of a^2 in the state n .

Similarly, from a^\dagger^2 you do not get a contribution. However, you get a contribution from $a^\dagger a$ because you would recall that $|n\rangle$ is an Eigenstate of $a^\dagger a$ with Eigenvalue n .

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$$E_n^{(1)} = \frac{b \hbar \omega}{4K} (2n+1)$$

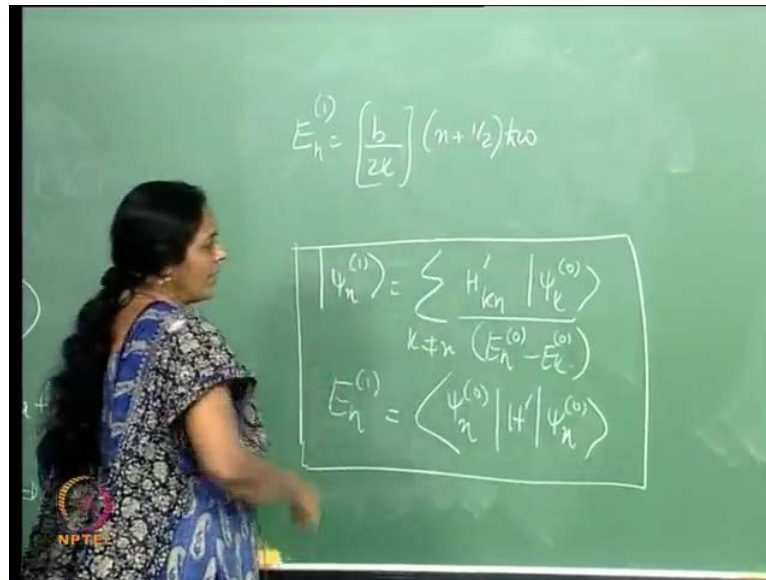
$$= \frac{b \hbar \omega}{2K} \left[n + \frac{1}{2} \right]$$

$$E_n = \left[\frac{b}{2K} + 1 \right] \left(n + \frac{1}{2} \right) \hbar \omega$$

And therefore, you have E_{n+1} is equal to b by $4K\hbar$ cross ω , (Refer Slide Time: 43:56) twice n from here plus 1 from there. So, this can be written as b by $2K\hbar$ cross ω $n + \frac{1}{2}$. So, this is what I have for E_{n+1} and therefore, E_n to 1st order is $E_n^{(0)}$ which is $n + \frac{1}{2} \hbar \omega$ plus $E_n^{(1)}$. So, it is simply b by $2K$ plus 1, $n + \frac{1}{2}$

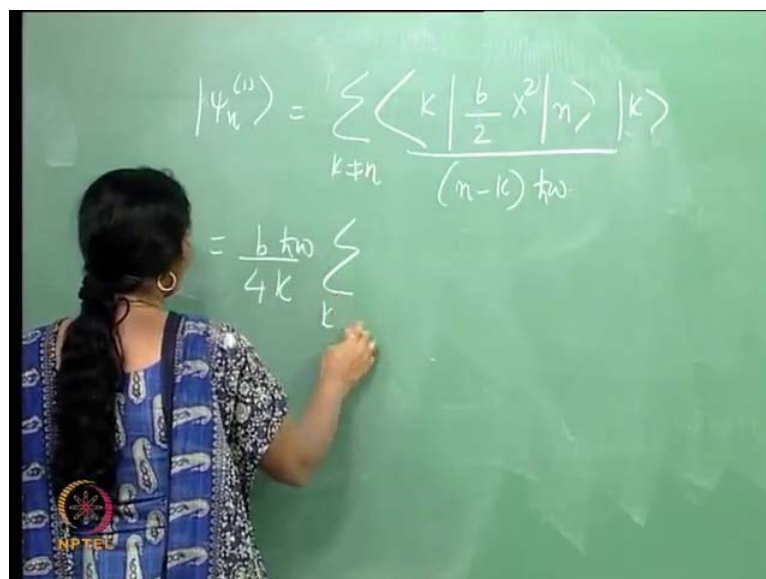
h cross omega. So, this is what I have. So, this is my value of energy inclusive of 1st order corrections, because of the perturbation. So, now let us go ahead and estimate (Refer Slide Time: 35:45) $\psi_n^{(1)}$, this involves H'_{kn} $\psi_k^{(0)}$ and let us find out that matrix element.

(Refer Slide Time: 46:27)



So, let me write this somewhere, for the Harmonic oscillator problem. I have found out E_n so let us just say $E_n^{(1)}$ is b by $2k$ times n plus half h cross ω . This is what I have. Now, as far as $\psi_n^{(1)}$ is concerned, I need to do the following thing.

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The wavefunction to 1st order in the perturbation is summation K not equal to n, I need the matrix element H'_{kn} , which is $\langle k | \frac{b}{2} X^2 | n \rangle$, which is $\frac{b}{4k}$. So, that is what I have there, (Refer Slide Time: 46:27) divided by $E_n^{(0)} - E_k^{(0)}$, recall that $E_n^{(0)}$ is $n + \frac{1}{2} \hbar \omega$ and $E_k^{(0)}$ is $k + \frac{1}{2} \hbar \omega$. So, you just have an $n - k$ and k is not equal to n , $\hbar \omega$. So, this object can well be written once more as $\frac{b}{4k \hbar \omega}$, summation, this K is not be confused with that k .

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$$\begin{aligned}
 |\psi_n^{(1)}\rangle &= \sum_{p \neq n} \frac{\langle p | \frac{b}{2} X^2 | n \rangle}{(n-p)\hbar\omega} |p\rangle \\
 &= \frac{b}{4k} \sum_{p \neq n} \frac{\langle p | a^2 + a^{\dagger 2} + 2a^{\dagger}a + 1 | n \rangle}{(n-p)} |p\rangle \\
 &= \frac{b}{4k} \left[\sum_{p \neq n} \frac{\sqrt{n}\sqrt{n-1} \delta_{p, n-2}}{(n-(n-2))} + \sum_{p \neq n} \frac{\sqrt{n+1}\sqrt{n+2} \delta_{p, n+2}}{(n-(n+2))} \right] |p\rangle
 \end{aligned}$$

This is K , which was $m \omega^2$. If you wish I am willing to write this, as p not equal to n in this fashion and therefore, we just have $\frac{b}{4k \hbar \omega}$. Summation over p not equal to n , this K is $m \omega^2$. And then you have $p a^2 + a^{\dagger 2} + 2 a^{\dagger} a + 1$ $n - p$ by $n - p$ $\hbar \omega$. So, the $\hbar \omega$ cancels out and I have a $\frac{b}{4k}$. Now, this is a nice thing to do because certain terms make a contribution; I have summation p not equal to n look at the 1st term. The 1st term brings out a $\sqrt{n} \langle n-1 |$, $\sqrt{n-1} \langle n-2 |$, $\delta_{p, n-2}$. The denominator is p is equal to $n - 2$ that is the 1st term.

The 2nd term gives me summation p not equal to n . The 2nd term gives me a dagger on \sqrt{n} , gives me $\sqrt{n+1} \langle n+1 |$, once more gives me $\sqrt{n+2} \langle n+2 |$. So, that is a $\delta_{p, n+2}$. The denominator is $n - n + 2$, that is the 2nd term. The 3rd term cannot make a contribution, because a dagger a on $\langle n |$ gives me $\langle n |$ and

this gives me a delta n p, but you have to sum over all p not equal to n. Similarly, the 4th term does not make a contribution and of course, I have ket p. So, this is what I have. Now, this is easy to simplify and all I get is the following. I can remove this summation and the delta sign and therefore, the p is to be replaced by n minus 2.

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$$|\psi_n^{(1)}\rangle = \frac{b}{8K} \sqrt{n} \sqrt{n-1} |n-2\rangle - \frac{b}{8K} \sqrt{n+1} \sqrt{n+2} |n+2\rangle$$

$$|\psi_n^{(0)}\rangle = \frac{b}{8K} \left[\sqrt{n} \sqrt{n-1} |n-2\rangle - \sqrt{n+1} \sqrt{n+2} |n+2\rangle \right]$$

So, I have psi n 1. This is the 1st order contribution to the wavefunction, is root n root n minus 1, the denominator is a 2, (Refer Slide Time: 48:46) of course, I have a b by 4 k. So, I have a b by 8 K and since p is replaced by n minus 2, I have ket n minus 2. That is the 1st term coming from here, (Refer Slide Time: 47:53) the 2nd term has a p replaced by n plus 2 and therefore, that gives me a minus 2. So, let me put a relative negative sign, minus b by 8 K again and I have a root of n plus 1, root of n plus 2 ket n plus 2. So, this is psi n 1. So, I have found out the contribution to energy and the contribution to the wavefunction in 1st order perturbation theory, if I were looking at a Harmonic oscillator with the Harmonic perturbation, in the sense that the perturbation is also a quadratic perturbation.

So, you see the contribution to 1st order does not come from psi n 0, it does not come from ket n. It comes from ket n minus 2 and it comes from ket n plus 2, which is consistent with the fact that our delta psi n did not have a component along psi n 0. So, this is what I have in 1st order perturbation. (Refer Slide Time: 46:27) So, here is the estimate of the energy and here is the estimate of the changed wavefunction and I have

just demonstrated 1st order perturbation theory to you. We will look at 2nd order perturbation theory and Harmonicity and so on in subsequent lectures.

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