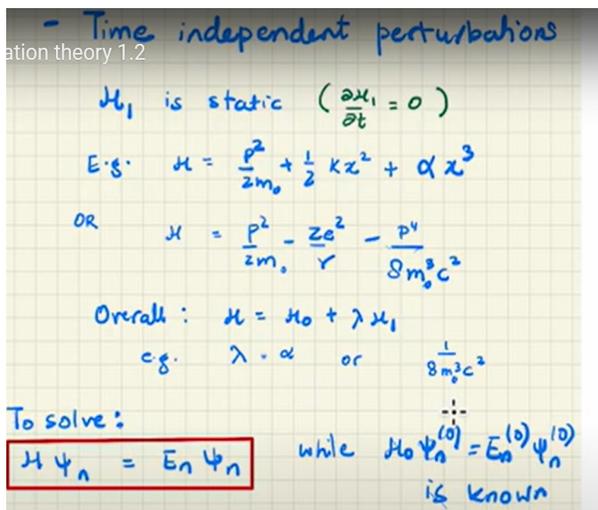


Foundation of Quantum Theory: Relativistic Approach
Change in atomic characteristics via field interactions
Perturbation theory 1.2
Prof. Kinjalk Lochan
Department of Physical Sciences
IISER Mohali

Lecture- 02

Okay, welcome all.

So, in the second lecture of this week, we are going to review aspects of time independent perturbation theory and we will see the development of the formulation of first order perturbation theory and what kind of corrections they lead to. We will also dwell with higher order corrections in the setting and we will do so by examples of couple of simply known systems like harmonic oscillators or hydrogen atoms. So this is the mandate for today's discussion and let us get going with the discussions of the perturbation theory. In the previous class, we have learnt that the time independent perturbation theory takes into account for a correct description of nature and it puts terms which are typically weaker than the strongest term which we consider in our standings.



Time Independent perturbations

$$\mathcal{H}_1 \text{ is static } \left(\frac{\partial \mathcal{H}_1}{\partial t} = 0 \right)$$

e.g.
$$H = \frac{p^2}{2m_e} + \frac{1}{2} kx^2 + \alpha x^3$$

or
$$H = \frac{p^2}{2m} - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} - \frac{p^4}{8m^3 c^2}$$

Overall
$$H = \hat{H}_0 + \lambda \hat{H}_1$$

e.g.
$$\lambda = \alpha \vee \frac{p^4}{8m^3 c^2}$$

To solve this

$$H \psi'_n = E_n \psi_n$$

While $H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$ is known

For example, if there is a harmonic oscillator whose Hamiltonian in the free case is given by the first

two terms $\frac{p^2}{2m_0} + \frac{1}{2} kx^2$

. Then as we discussed in the previous class we do not really know if there is a scope or not of additional higher order terms depending upon the shape of the potential if I try to move away from the minima we have seen that higher order terms can in principle be present for arbitrary potentials. Similarly there could be a scope for a higher order momentum dependency coming from the correct description of kinetic energy which is allowed in the special relativity.

All these examples we had discussed in the previous class and in this class we are going to develop formalism to how to handle these correction terms once we are certain that they are present. So for today's discussion we are focusing on time independent perturbation theory by that I mean there is no explicit dependence on time in the hamiltonian which is introduced into the free part. For example in the harmonic oscillator case when I allow for cubic order or quatric order correction terms that

$$\frac{p^4}{8m^3c^2}$$

Hamiltonian does not explicitly depend on time. These coefficients alpha or these coefficient for the fourth order momentum corrections. They are not supposed to contain any dependence on time explicitly so the whole Hamiltonian can depend on time implicitly through the position's dependence on the time but that is not a direct dependence that is the indirect dependence so therefore the partial derivatives are zero with respect to time total derivatives may not be zero because the total derivative will account for the change of the hamiltonian with respect to the position and then the positions change with respect to the time. So clear demarcation of a time independent. Hamiltonian would be its partial derivative with respect to time should be 0. So, overall as we have seen depending upon higher order correction terms in the potential or higher order correction terms in the kinetic term.

$$H \psi_n = E_n \psi_n$$
 while $H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$ is known

$$\Rightarrow (H_0 + \lambda H_1) (\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \dots)$$

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

To solve this

$$H \psi'_n = E_n \psi_n$$

While $H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$ is known

$$(H_0 + \lambda H_1) (\psi_n^{(0)} + \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \dots) = (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} \dots) (\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} \dots)$$

where $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle = 0 = \langle \psi_n^{(0)} | \psi_n^{(2)} \rangle$

We typically end up with a structure like whatever was our free theory by free theory I mean the system which we had exactly solved. For example harmonic oscillator this piece was the free theory for hydrogen atom hydrogen like atom this was the free theory now there is an extra term which is added to it which is λH_1 where λ is a parameter which tells you about the strength of the term which is coming about. This usually depends upon the parameters in the theory. For instance as we have seen in the arbitrarily shaped harmonic arbitrary shaped potentials minima if you remember the discussions in the previous class. The higher order terms dependent on the third derivative of the potential at the minima.

So the parameter α which I have written about in the present day slide, in today's slide, that α is virtually the third derivative of the potential at the minimum.

Similarly, for the fourth order momentum correction coming from the correct description of kinetic energy comes with a parameter 1 upon $8m^3c^2$. That is the mass of the particle times the speed of light and their various powers. So these are the parameters which tells us that certain new operators are coming along with a coupling parameter λ . For the first case, the operator part \mathcal{H}_1 is x^3 , while the coupling parameter part λ is α . While for the second part, the operator in the new Hamiltonian is p^4 ,

while the coupling parameter λ happens to be $-\frac{1}{8m^3c^2}$, the - sign is here as well.

So, in this way we are supposed to solve a problem of a renewed Hamiltonian a new information that we know has a right to exist. Previously we had solved for \mathcal{H}_0 alone now we know that the correct description does not contain \mathcal{H}_0 . Previously, we used to know the free theory's Hamiltonian. But there is a possibility of a new term which comes with some coupling parameter λ . So we will go ahead with a

general λ and in case by case basis we will see what λ happens and how much of the correction it leads to. So the idea at the hand is :

We need to solve the correct Hamiltonian, which is made up of two pieces, \mathcal{H}_0 and $\lambda \mathcal{H}_1$. And we want to know what are their eigen states. Previously, we used to know the free theory is Hamiltonian. By free theory, I mean I mean none of the correction terms were allowed. I knew the solutions of this.

For instance, I knew what are the eigenstates of ordinary harmonic oscillators and what are their eigenvalues. Similarly, I knew what is the correct energy eigenstates of ordinary hydrogen atom without the higher order correction and their eigenvalues. Now I know there are more terms than the usual terms which we have solved for. So, then I need to go back and solve this equation again and try to get a renewed information of what are the states which are correctly describing the physics of harmonic oscillator around arbitrary potential or correct description of kinetic energy in hydrogen atom or mixing of both. Even in harmonic oscillator, the p^2 term can be corrected by presence of quartic p^4 term coming from special energy.

All right. \mathcal{H}_0

So the idea is we will develop the game for \mathcal{H} , the total Hamiltonian being made from the free part and the perturbation part. And I know that once I have changed the Hamiltonian from being just \mathcal{H}_0 . The correct eigenstate can no longer be only $\psi_n^{(0)}$ was eigenstate of \mathcal{H}_0 . It can rarely so happen that it is also eigenstate of the full \mathcal{H} . Unless \mathcal{H}_0 and \mathcal{H}_1 commute, it is not going to be that case that $\psi_n^{(0)}$ is also an eigenstate of the \mathcal{H} as well. So the correct eigenstate $\psi_n^{(0)}$ should be different from $\psi_n^{(0)}$. So therefore there should be correction terms and we allow for corrections terms to be expandable in the parameter λ whatever is the coupling parameter. It could be first order in λ times some correction term + second order in λ which is λ^2 and correction term at the second order and so on. Similarly the energy eigenvalues I used to know for the free theory. In the correct description of the theory when I have added the extra term $E_n^{(0)}$ can no longer be the eigenvalue of the system. So therefore this has to be corrected as well. So therefore we would add extra terms with a power series expansion in λ . I have added a linear order terms in the \mathcal{H}_1 , this is the coupling parameter but I do not know if the effect of λ will only remain in the wave function at linear order or in the eigenfunction in the linear order. This I need to check and prove so in principle I am allowing for a power series expansion in the unknown things which are wave function and the energy eigenvalues so there I am not sure if the corrections are only order λ . They can be order λ^2 or higher orders as well. So therefore the picture is that we have to solve for a corrective expression or equation which is new Hamiltonian which is $\mathcal{H}_0 + \lambda \mathcal{H}_1$, times new eigenfunction which is previous eigenfunction + correction terms is equal to new eigenvalues which happens to be previous eigenfunction + correction term and the new eigenfunction again which we wrote down as previous eigenfunction + correction term. Now it is very important to note in this description we are assuming that these corrections terms $\psi_n^{(1)}$, $\psi_n^{(2)}$, they are already orthogonal to the previous eigenstates. Whatever we are adding to the previous eigenstates, those corrections are perpendicular or orthogonal to the previous eigenstates So, these are the correction terms. In vectorial description, if this vector was your eigenstate initially. Then there are some minute terms which are added in the perpendicular directions such that shifted vector becomes a correct eigen function. Now, why do we need to do that?

Why do we need to assume that the corrections terms are orthogonal to the previous eigen functions? This can be checked in the linear order perturbation theory as follows. So suppose we look at the first order correction term, which comes with single power of coupling parameter λ . So we are going to focus on the first order correction. Suppose $\psi_n^{(1)}$ is not orthogonal to $\psi_n^{(0)}$, that is the unperturbed eigenvalues, eigenvectors are not orthogonal to the newly corrections. So these new corrections can

also be projecting. They are not completely orthogonal to $\psi_n^{(0)}$. So, they could have some projections along $\psi_n^{(0)}$. Since this is just a wave function and a wave function can be decomposed in the basis of the eigen functions of a Hermitian observable which was Hamiltonian. So, I can write this wave functions into the superpositions of all the previous eigen functions. So, $\psi_n^{(0)}$, $\psi_n^{(0)}$ where l runs from 1 to ∞ . So in this decomposition, if $\psi_n^{(1)}$ is not orthogonal to $\psi_n^{(0)}$, there will be one term which will be along $\psi_n^{(0)}$. So this will be the term. Suppose it is allowed. I know under my perturbation theory, the correct description of eigenfunction goes from being only $\psi_n^{(0)}$ to $\psi_n^{(0)}$ + first order correction term. Up to first order, this is the correction.

If I want to include the second order term then there will be $\lambda^2 \psi_n^{(2)}$ as well but up to first order this $\psi_n^{(1)}$ tells me the correction to the wave function. So therefore this is $\psi_n^{(1)}$ up to first order. Now this $\psi_n^{(0)}$ up to first order can be collected as because this $\psi_n^{(1)}$ we have already decomposed in a series with terms not equal to n and one term which is equal to n . So what I will do I will just collect the coefficients of different eigen basis. So in this $\psi_n^{(1)}$ all the basis are being summed over and there is one term which is also $\psi_n^{(0)}$.

So therefore the renewed corrected eigenfunction will be the previously existing eigenfunction coming with coefficient 1 and λ times C_n which is here along the $\psi_n^{(0)}$ direction. So you can see that if $\psi_n^{(1)}$ has a projection along the $\psi_n^{(0)}$ direction it is going to feed to this 1 which is already existing and then the remaining term over here will come with a coefficient λ . So therefore the full wave function will become $1 + \lambda C_n$ along the $\psi_n^{(0)}$ direction and λ times C_n along all other basis vectors direction.

Handwritten derivation on grid paper:

$$|\psi_n^{(1)}\rangle = \sum_{l \neq n} C_n^l |\psi_l^{(0)}\rangle + C_n^n |\psi_n^{(0)}\rangle$$

$$|\psi_n^{(0)}\rangle \rightarrow |\psi_n^{(0)}\rangle + \lambda |\psi_n^{(1)}\rangle$$

$$|\psi_n\rangle = (1 + \lambda C_n^n) |\psi_n^{(0)}\rangle + \sum_{l \neq n} \lambda C_n^l |\psi_l^{(0)}\rangle$$

$$= (1 + \lambda C_n^n) \left[|\psi_n^{(0)}\rangle + \frac{\lambda}{1 + \lambda C_n^n} \sum_{l \neq n} C_n^l |\psi_l^{(0)}\rangle \right]$$

Normalized

$$|\psi_n\rangle = \frac{(1 + \lambda C_n^n) \left[|\psi_n^{(0)}\rangle + \frac{\lambda}{1 + \lambda C_n^n} \sum_{l \neq n} C_n^l |\psi_l^{(0)}\rangle \right]}{\sqrt{(1 + \lambda C_n^n)^2 + \frac{\lambda^2}{(1 + \lambda C_n^n)^2} \sum_{l \neq n} C_n^l^2}}$$

$$|\psi_n^{(1)}\rangle = \sum_{l \neq n} C_n^l |\psi_l^{(0)}\rangle + C_n^n |\psi_n^{(0)}\rangle$$

$$|\psi_n^{(1)}\rangle \Rightarrow |\psi_n^{(0)}\rangle + \lambda |\psi_n^{(1)}\rangle$$

$$|\psi_n\rangle = (1 + \lambda C_n^n) |\psi_n^{(0)}\rangle + \sum_{l \neq n} C_n^l \lambda |\psi_l^{(0)}\rangle = (1 + \lambda C_n^n) \left[|\psi_n^{(0)}\rangle + \frac{\lambda}{1 + \lambda C_n^n} \sum_{l \neq n} C_n^l |\psi_l^{(0)}\rangle \right]$$

Normalised

$$|\tilde{\psi}_n\rangle = (1 + \lambda C_n^n) \left[|\psi_n^{(0)}\rangle + \frac{\lambda}{1 + \lambda C_n^n} \sum_{l \neq n} C_n^l |\psi_n^{(l)}\rangle \right] / \sqrt{(1 + \lambda C_n^n)^2 + \frac{\lambda^2}{(1 + \lambda C_n^n)^2}}$$

Now, $1 + \lambda C_n^n$ can be pulled out as a common factor so that inside the bracket I would just be left with $\psi_n^{(0)} + \lambda$ divided by $1 + \lambda C_n^n$ the common factor which I have pulled out and the series which is over here. So the wave function, the corrected wave function up to linear order, corrected eigenfunction up to linear order is this. Now I want this to be normalized. That means I should calculate the

$\langle \psi_n^{(0)} | \psi_n^{(0)} \rangle$. If it is not equal to 1, I should divide the wave function by its magnitude which is this. So if I take this $\psi_n^{(0)}$ and compute the magnitude of this vector, I am going to get an answer which is this. $\sqrt{1 + \lambda C_{nn} + \lambda^2 (1 + C_{nn})}$ whole square.

So, just a second... I am probably I will get a $(C_n^1)^2$. . OK, alright.

Yes.

Now, this is the answer which is obtained after normalizing the state. So normalized corrected wave function should be this whole expression. But we knew that this expression cannot be trusted more than order λ because our story started with correction up to order λ if I want to include things up to order λ square or higher powers I should have started the story with higher powers of λ as well. So this expression which is over here has to be corrected only up to order λ so I should maintain things only up to order λ . Wherever I see a λ^2 I will throw that out because I had thrown λ^2 term from the beginning there was no λ^2 I had considered so better not to consider λ^2 anyway so wherever I will see a λ^2 I will throw that term away for example here is λ^2 I will just ignore it. Then the square root quantity in the denominator becomes a square root of a perfect square which will just yield you $1 + \lambda C_{nn}$. Now you see if you do this correction term carefully this $1 + \lambda C_{nn}$ which was outside as a common factor kills the denominator and you are left with this series inside where the summation now does not include 1 and does not include n and therefore again I would do the business of throwing order λ^2 terms away.

Here is one more term λ times this λ that will also be thrown out.

So I will be just maintaining this term and the first term λ multiplying the one and then this series.

So therefore the normalized wave function at the linear order is made up from $\psi_n^{(0)} + \lambda$ times the series where the series does not include the 'n' term.

So, therefore in the previous slide that is what the statement was if I want to write my corrected wave function up to linear order it would be the previous eigenfunction + a correction term which does not include projection along its previous direction.

So therefore, for normalized $\tilde{\psi}_n^{(0)}$ upto the order of λ , we only need to compute C_n^1 s, we only need to compute C_n^1 were were what?

C_n^1 the coefficients along the different basis vectors, which does not include the n. n is the eigenfunction for which we are trying to find the corrections. Ok? So that is another way of saying that the correction terms are orthogonal to $\psi_n^{(0)}$. Alright, so with this information we can proceed further and now I know that I have a perturbation equation which I can try to pick up terms order by order in λ . For example, if I go back to this slide and clean things up, so you see on the left hand side I have a $\mathcal{H}_0 + \lambda \mathcal{H}$ multiplying the power series expansion of the eigenfunction on the right hand side I have a power series expansion of energy eigenvalues multiplying the power series expansion of the eigenfunction. So when I open these terms I will get certain terms in various orders of λ , for example \mathcal{H}_0

acting on this $\psi_n^{(0)}$ will be free from any λ in the left hand side. On the right hand side similarly this $E_n^{(0)}$ multiplying this $\psi_n^{(0)}$ will also be free from any λ .

Now if I move forward to see how many terms are there with single λ , there is a possibility that this \mathcal{H}_0 acts on this part where one λ comes or this \mathcal{H}_1 acts on $\psi_n^{(0)}$. These are the two terms which will come at the linear order of λ . That is these terms will come with a λ multiplication. Similarly, if I want to compare what are the terms which will be arriving on the right hand side with a single power of λ , it may come again through two ways. First way will be this $E_n^{(0)}$ goes and hits this λ times $\psi_n^{(1)}$ or vice versa, this λ times $E_n^{(1)}$ here hits this $\psi_n^{(0)}$. So, this is how we will pluck up terms order by order and we will try to see what do we get at various orders. If I just collect the terms free of any λ , which is called order λ to the power 0. As we saw, only one term was there in the left-hand side, \mathcal{H}_0 acting on $\psi_n^{(0)}$. And the right-hand side, I had the eigenvalue, unperturbed eigenvalue, hitting the unperturbed eigen function. So, this is the unperturbed equation. Because perturbation comes with a λ , it is reasonable to expect that if no trace of λ is considered, then there should not be any change. Fair enough.

Order λ^0 : $\mathcal{H}_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$

Order λ^1 : $\mathcal{H}_0 \psi_n^{(1)} + \mathcal{H}_1 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^{(0)}$

$\langle \psi_n^{(0)} |$ projection gives

$\langle \psi_n^{(0)} | \mathcal{H}_1 | \psi_n^{(0)} \rangle = E_n^{(1)}$

$\langle \psi_l^{(0)} |$ projection with $l \neq n$

Order λ^0 : $\lambda = H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$

Order λ^1 : $H_0 \psi_n^{(1)} + H_1 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^{(0)}$

$\psi_n^{(0)}$ projection gives

$\langle \psi_n^{(0)} | \mathbf{H}_0 | \psi_n^{(0)} \rangle = E_n^{(0)}$

$\langle \psi_l^{(0)} |$ is a projection with $l \neq n$

$E_l^{(0)} \langle \psi_l^{(0)} | \psi_n^{(1)} \rangle + \langle \psi_l^{(0)} | \mathcal{H}_1 | \psi_n^{(0)} \rangle = E_n^{(0)} \langle \psi_l^{(0)} | \psi_n^{(1)} \rangle$

$\Rightarrow \langle \psi_l^{(0)} | \psi_n^{(1)} \rangle = \frac{\langle \psi_l^{(0)} | \mathcal{H}_1 | \psi_n^{(0)} \rangle}{(E_n^{(0)} - E_l^{(0)})}$

$E_l^{(0)} \langle \psi_l^{(0)} | \psi_n^{(1)} \rangle + \langle \psi_l^{(0)} | \mathbf{H}_0 | \psi_n^{(0)} \rangle = E_n^{(0)} \langle \psi_l^{(0)} | \psi_n^{(1)} \rangle$

$\langle \psi_l^{(0)} | \psi_n^{(1)} \rangle = \frac{\langle \psi_l^{(0)} | \mathbf{H}_0 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_l^{(0)}}$

Now if I want to see what happens at order λ to the power 1, that means what are the terms which are multiplying at the linear power of λ , I get two terms in the left hand side as we discussed, \mathcal{H}_0 hitting the $\psi_n^{(1)}$ or \mathcal{H}_1 hitting the $\psi_n^{(0)}$. On the right hand side again there are two terms, $E_n^{(0)}$ hitting the $\psi_n^{(1)}$ and $E_n^{(1)}$ hitting the $\psi_n^{(0)}$. Again to just remind you of this thing at the linear order of λ either this \mathcal{H}_0 can go

and hit this term and this $\lambda \mathcal{H}'$ can go and hit this term. Both these terms will contribute to order λ terms. Similarly, on the right hand side either this $E_n^{(0)}$ goes and hit this λ times $\psi_n^{(1)}$ or this λ times $E_n^{(1)}$ goes and hits the $\psi_n^{(0)}$.

So, these are the two possibilities in both left hand side and right hand side which we have listed down over here in the boxed equation. So, now this is a operator equation in which some operators are acting on the state. So, let me write as kets. So, these are kets and these are operators and while these are numbers, eigen functions correction. So, these are just numbers. So, since it is a vectorial equation. I can take the projection of the equation along any basis direction.

For example, I can hit the whole equation from $\psi_n^{(0)}$ bra from the left hand side. That means I will just take $\psi_n^{(0)}$ and throughout the equation, both the left hand side and the right hand side. When I hit the left hand side, the first term I get is $\psi_n^{(0)}$ hitting the \mathcal{H}_0 term and $\psi_n^{(1)}$. The first thing on the right hand side similarly I will get is $E_n^{(0)}$ which is a number it will just go across and then $\psi_n^{(0)}$ will go and hit the $\psi_n^{(1)}$. Now one interesting thing to see this that \mathcal{H}_0 is supposed to be a Hermitian operator therefore \mathcal{H}_0 hitting the $\psi_n^{(0)}$ from the left hand side will again gives me $E_n^{(0)}$ and the $\psi_n^{(0)}$ back. This is the eigenvalue equation for the Hamiltonian unperturbed Hamiltonian and that will get the $\psi_n^{(1)}$. So, left hand side, so the left hand side we had obtained $E_n^{(0)}$ times $\psi_n^{(0)}$ hitting the $\psi_n^{(1)}$ and the right hand side also the first term exactly give the same term which has been obtained from the left side. So, the first term on the left and the first term on the right after the projection along $\psi_n^{(0)}$ exactly cancel each other. So, this will be canceled with this which is the projection of this term along the $\psi_n^{(0)}$. And I will be left with the projection of the second term along the $\psi_n^{(0)}$ which is this in the left hand side and projection of the second term on the right hand side along the $\psi_n^{(0)}$ which here is $\langle \psi_n^{(0)} | \psi_n^{(0)} \rangle$. And since this is well normalized state $\psi_n^{(0)}$ it is well normalized state this is going to be 1. And therefore, we have written only $E_n^{(1)}$ on the right hand side.

So therefore, from this projection equation, we are just taking the projection along the $\psi_n^{(0)}$, we ended up getting an equation which tells us about $E_n^{(1)}$. The right hand side has $E_n^{(1)}$.

This is the first order correction in the energy eigenfunction. So energy eigen function, the first order correction has been obtained now. This first order correction will be obtainable if I compute the left hand side quantity. That is I take the perturbation Hamiltonian and do this computation, I will get to know what is the first order correction. That is the perturbation Hamiltonian is squeezed between the previous eigen functions. $\psi_n^{(0)}$ were the previous eigen functions, no longer they are eigen functions of the new Hamiltonian. Yet if I take the \mathcal{H}' and take its expectation along this $\psi_n^{(0)}$, then I will get the first order correction to the eigenvalue. Similarly, if I take the projection with respect to $\psi_l^{(0)}$ where l is different from n . I take this equation which is true for n and then I take the inner product with respect to $\psi_l^{(0)}$. Again in the left hand side, I will get the term which was H . This will come from taking the squeezing of \mathcal{H}_0 with $\psi_l^{(0)}$. \mathcal{H}_0 acting on $\psi_l^{(0)}$ will give me E_l^0 which is this and I will get the $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle$ and then on the right hand, the second term will be just the perturbation Hamiltonian \mathcal{H}' , $\psi_n^{(0)}$ was already there and then this gets squeezed with $\psi_l^{(0)}$.

So, therefore, I will get the second term on the left hand side is this: $\psi_l^{(0)}$, \mathcal{H}' in between and $\psi_n^{(0)}$. On

the right hand side, when I hit the right hand side with $\psi_l^{(0)}$, The first term, the $E_n^{(0)}$ is just a number, $\psi_l^{(0)}$ will go inside and hit the $\psi_n^{(1)}$. So, I will get $E_n^{(0)}$, $\psi_l^{(0)}$ hitting the $\psi_n^{(1)}$ because $E_n^{(0)}$ has come out as it was a complex number..real number. The second term $E_n^{(1)}$ is also a number, then therefore it will also come out and this $\psi_n^{(0)}$ will be hit upon from the left by $\psi_l^{(0)}$. So $\psi_l^{(0)}$, $\psi_n^{(0)}$ with $E_n^{(1)}$.

Now since again these are eigen functions of the unperturbed Hamiltonian which was Hermitian, they are supposed to be orthogonal.

So therefore if n is not equal to l which we have chosen, this will be 0 because they are orthogonal to each other. So the second term on the right does not contribute. I am left with only the first term which was $E_n^{(0)}$ coming with $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle$ this inner product and the left hand side had two terms $E_l^{(0)}$ with the $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle$ and then the same inner product which appears on the right hand side but with a different energy function here it right hand side it was $E_n^{(1)}$ and the perturbation Hamiltonian is squeezed between $\psi_n^{(0)}$ and $\psi_l^{(0)}$, two different unperturbed eigen functions.

In first order correction, it is squeezed between the same eigenfunction from left and right. When I take the projection with respect to $\psi_l^{(0)}$, the first term gets squeezed between two different eigen function, $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle$. So, what I can do, I can take this left hand side term and bring it on the right such that I will get $E_n^{(0)} - E_l^{(0)}$ as a common factor for this inner product. And therefore, this inner product, which is $\psi_l^{(0)}$, $\psi_n^{(1)}$ will be this much. Remember we had argued that $\psi_n^{(1)}$ is orthogonal to $\psi_n^{(0)}$. It does not have any projection along the $\psi_n^{(0)}$ zero direction. It does not have any projection along the $\psi_n^{(0)}$ zero direction. But it may have some projection along other basis direction when l is not equal to n. So, it has some non-zero projection along different directions when l is not equal to n. And those projections are obtained by the squeezing of the perturbation Hamiltonian between the two states n and l and their energy difference which comes in the denominator.

I hope this is clear to you.

We will do this with an example and try to find out what kind of corrections do come about in different systems. So, let us move on to some example. Just before going to the example, the inner product which we have obtained over here, the inner product between the first order correction along the different basis directions. That can be given a compact name. That is to say we have realized that $\psi_n^{(1)}$ can be decomposed along the unperturbed eigen states eigen functions. But for the fact it does not contain any projection along its own unperturbed direction. So I would have all the basis elements present apart from $\psi_n^{(0)}$. So, it is decomposable in this basis with one basis element missing which is $\psi_n^{(0)}$. And therefore, the projection which we have just obtained over here $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle$ is essentially these coefficients C_n^m .

Since $|\psi_n^{(1)}\rangle = \sum_{m \neq n} C_n^m |\psi_m^{(0)}\rangle$ *

$$\langle \psi_l^{(0)} | \psi_n^{(1)} \rangle = C_n^l = \frac{\langle \psi_l^{(0)} | H_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_l^{(0)}}$$

Since

$$|\psi_n^{(0)}\rangle = \sum_{m \neq n} C_n^m |\psi_m^{(0)}\rangle$$

$$\langle \psi_l^{(0)} | \psi_n^{(1)} \rangle = C_n^l =$$

$$\langle \psi_l^{(0)} | H_1 | \psi_n^{(0)} \rangle / E_n^{(0)} - E_l^{(0)}$$

Example: $H_0 = \frac{p^2}{2m} + \frac{1}{2} kx^2$
 $H_1 = \frac{p^4}{8m^3c^2}$:-

$$E_n^{(1)} = \langle \psi_n^{(0)} | \frac{p^4}{8m^3c^2} | \psi_n^{(0)} \rangle$$

Since $\hat{p} = \sqrt{\frac{\hbar}{2}} \frac{(\hat{a} - \hat{a}^\dagger)}{i\sqrt{m\omega}}$

$$= \frac{1}{8m^3c^2} \langle \psi_n^{(0)} | \left\{ \sqrt{\frac{\hbar}{2}} \frac{(\hat{a} - \hat{a}^\dagger)}{i\sqrt{m\omega}} \right\}^4 | \psi_n^{(0)} \rangle$$

$$C_n^1 = \frac{\langle \psi_n^{(0)} | \left(\sqrt{\frac{\hbar}{2}} \frac{(\hat{a} - \hat{a}^\dagger)}{i\sqrt{m\omega}} \right)^4 | \psi_n^{(0)} \rangle}{(n-l)\hbar\omega}$$

Example

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} kx^2$$

$$H_1 = \frac{p^4}{8m^3c^2}$$

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Since

$$\hat{p} = \sqrt{\frac{\hbar}{2}} \frac{(\hat{a} - \hat{a}^\dagger)}{i\sqrt{m\omega_0}}$$

$$= \frac{1}{8m^3c^2} \langle \psi_n^{(0)} | \sqrt{\frac{\hbar}{2}} \frac{(\hat{a} - \hat{a}^\dagger)}{i\sqrt{m\omega_0}}^4 | \psi_n^{(0)} \rangle$$

$$C_n^1 = \langle \psi_n^{(0)} | \sqrt{\frac{\hbar}{2}} \frac{(\hat{a} - \hat{a}^\dagger)}{i\sqrt{m\omega_0}}^4 | \psi_n^{(0)} \rangle / (n-l)\hbar\omega_0$$

So, if I compute $\langle \psi_l^{(0)} | \psi_n^{(1)} \rangle$ by assuming this definition of $\psi_n^{(1)}$, then you get to know that this projection is just giving you the coefficient C_n^m .

These coefficients are known now from the squeezing of the H_1 between n and l and their energy difference. For example n can be 1, l can be 2 then I will get the hamiltonian perturbation hamiltonians of diagonal element $(H_1)_{12}$ if n is 2, is 3, I will get the corresponding of diagonal matrix element 3 2 of the perturbation Hamiltonian. So, let us do one example to see this concept in more clarity.

So, we will take the Hamiltonian of a harmonic oscillator which is this and as we know we can insert a correction term coming from correct description of kinetic energy which is the fourth power of momentum which comes as a additional term.

Okay so therefore this is my perturbation hamiltonian and this the parameter what λ is $\frac{1}{8m^3c^2}$. So I'm just taking the definition of $\frac{1}{8m^3c^2}$ as inverse of $8m^3c^2$ as λ or I could define λ , fictitious λ here which will be put as one at the end of the day and then this whole thing will become the operator. So let us go along with this thing that a book-keeping parameter λ is inserted with which we will compare various powers of λ and then at the end of the day I will put λ to one okay so in that case as we have discussed. The first order correction $E_n^{(1)}$ is supposed to be the perturbation Hamiltonian expectation

with respect to unperturbed eigenstates So, this is my perturbation Hamiltonian $\frac{p^4}{8m^3c^2}$.

And if I want to know first order correction in the nth eigen function, what I will do?

I will take the Hamiltonian, perturbation Hamiltonian and obtain its expectation . So, let us do this thing in more detail. I know in harmonic oscillator, the operator p can be written in terms of the ladder operators a - a† divided by i up to some dimension full constants. This you can look up at any quantum mechanics book. Therefore, the fourth power of that is supposed to come up in the perturbation Hamiltonian. So, I will take the whole dimensionful perator p from here, take its fourth power and squeeze it between $\psi_n^{(0)}$ $\psi_n^{(0)}$ from left and right and that will give me the $E_n^{(1)}$. So this computation is supposed to give me $E_n^{(1)}$. Similarly if I want to know the projection C_n^l 's C_n^l 's is telling me the projection of the first order correction along the l-th unperturbed eigen basis. So C_n^l the subscript n is telling you about which eigen functions first order correction you are looking for I am looking for first order correction of nth eigenfunction and the upper index l tells you what is its projection along the unperturbed l-th basis.

So, similarly if I want to know C_n^l for this perturbation Hamiltonian, what I have to do?

I have to take this operator which is the fourth power of $\frac{p^4}{8m^3c^2}$ and squeeze it between $\psi_n^{(0)}$ from the right hand side and $\psi_n^{(1)}$ from the right left hand side and divide it by the energy difference of unperturbed system. Remember, C_n^l were the perturbation Hamiltonian squeezed with respect to $\psi_n^{(0)}$, $\psi_l^{(0)}$ from left and right and the denominator being obtained from the energy difference. In harmonic oscillator, energy difference is just $(n-1)\hbar\omega_0$ and the upstairs I have this fourth power squeezed between $\psi_n^{(0)}$ and $\psi_l^{(0)}$. Okay? Let us do it for the ground state.

Suppose I want to know with this higher order quartic momentum term what happens to the ground state, n is equal to 0. Previously I knew that the unperturbed harmonic oscillator's ground state energy

is just $\frac{1}{2}\hbar\omega_0$.

Now I want to know when I have added this kinetic term $\frac{p^4}{8m^3c^2}$, what happens to the ground state energy.

For the ground state $n=0$

$$\star E_0^{(1)} = \frac{\hbar^2}{2m^2\omega^2} \langle 0 | (\hat{a} - \hat{a}^\dagger)^4 | 0 \rangle$$

$$= \frac{\hbar^2}{2m^2\omega^2} \langle 0 | (\hat{a}^2 \hat{a}^{\dagger 2} + a a^\dagger a a^\dagger) | 0 \rangle$$

$$a | n \rangle = \sqrt{n} | n-1 \rangle$$

$$a^\dagger | n \rangle = \sqrt{n+1} | n+1 \rangle$$

$$\therefore a^{\dagger 2} | 0 \rangle = a^\dagger a^\dagger | 0 \rangle = \sqrt{2} | 2 \rangle$$

$$\langle 0 | a^2 = \langle 2 | \sqrt{2} \Rightarrow \langle 0 | a^2 a^{\dagger 2} | 0 \rangle = 2$$

$$\langle 0 | a a^\dagger a a^\dagger | 0 \rangle = 1$$

$$\therefore E_0^{(1)} = \frac{3\hbar^2}{2m^2\omega^2}$$

For the ground state $n=0$

$$\star E_n^{(0)} = \frac{\hbar^2}{2m^2\omega^2} \langle 0 | (\hat{a} - a^\dagger)^4 | 0 \rangle$$

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$$\langle 0 | a^2 = \langle 2 | \sqrt{2}$$

$$\langle 0 | a^2 a^{\dagger 2} | 0 \rangle = 2$$

$$\langle 0 | a a^\dagger a a^\dagger | 0 \rangle = 1$$

$$E_n^{(1)} = \frac{3\hbar^2}{2m^2\omega^2}$$

The first order correction to that energy is this quantity as we have listed down. I am going to compute this quantity with n is equal to 0. So, it would be a $-a^\dagger$ to the power 4 squeezed between n is equal to 0 from left and right. All the constants which were appearing here here, here have been combined to get

me $\frac{3\hbar^2}{2m^2\omega^2}$. You should verify this.

And ultimately, this is this computation I am supposed to find out. So, I have to open this quantity up and squeeze it between 0 and 0.

If you do this exercise, you will find out only this term survives. All other sums in the expansions vanish. And the rules of a and a^\dagger 's hitting any particular eigen states of Hamiltonian are also known for harmonic oscillator. Using these information, you can quickly prove that the first order correction is

this much, $\frac{3\hbar^2}{2m^2\omega^2}$. E_n^0 was supposed to be for ground state, so this is for n is equal to 0.

For ground state, it was known to be this is $\frac{1}{2}\hbar\omega_0$.

Once I have added first order perturbation, then this gets changed by $\frac{3\hbar^2}{2m^2\omega^2}$ and there will be second order term as well, third order term as well, but up to first order correction, this is the term. Similarly, if I want to know what is the first order correction to the ground state wave function, then I need to compute this C_0^1 . The perturbation Hamiltonian squeezed between 0 and the 1 from right and left and their energy differences which will be just -1 , $n-1$ for n is equal to 0 will just be -1 . So, therefore, now I have to compute a $-a^\dagger$ to the power 4 and squeeze it between 0 and 1 from the left and right. You can do this computation.

$$\begin{aligned}
 * C_0^1 &= \frac{\hbar^2}{2m\omega^2} \langle 1 | \underbrace{(a - a^\dagger)^4}_{(-1)\hbar\omega} | 0 \rangle \quad \left(+ \frac{3\hbar^2}{2m^2\omega^2} \right) \\
 C_0^1 &= -\frac{\hbar}{2m^2\omega^2} \langle 1 | \underbrace{(a - a^\dagger)^4}_{\vdots} | 0 \rangle \\
 &= -\frac{\hbar}{2m^2\omega^2} \langle 1 | (aa + a^\dagger a^\dagger - aa^\dagger - a^\dagger a) \\
 &\quad (aa + a^\dagger a^\dagger - aa^\dagger - a^\dagger a) | 0 \rangle \\
 &= -\frac{\hbar}{2m^2\omega^2} \langle 1 | \begin{bmatrix} aaaa + aa^\dagger a^\dagger - a^\dagger a^\dagger aa - a^\dagger a^\dagger a^\dagger a + \\ a^\dagger a^\dagger aa + a^\dagger a^\dagger a^\dagger a^\dagger - a^\dagger a^\dagger aa^\dagger - a^\dagger a^\dagger a^\dagger a - \\ aa^\dagger aa - aa^\dagger a^\dagger a^\dagger + aa^\dagger aa^\dagger + aa^\dagger a^\dagger a - \\ a^\dagger a^\dagger aaa - a^\dagger a^\dagger a^\dagger a^\dagger + a^\dagger a^\dagger aa^\dagger + a^\dagger a^\dagger a^\dagger a \end{bmatrix} | 0 \rangle
 \end{aligned}$$

$$* C_0^1 = \frac{\hbar^2}{2m^2\omega^2} \frac{1}{(-1)\hbar\omega} \langle 1 | (\hat{a} - a^\dagger)^4 | 0 \rangle$$

$$= \frac{-\hbar^2}{2m^2\omega^2} \langle 1 | (aa^\dagger + a^\dagger a^\dagger - aa^\dagger - a^\dagger a) (aa + a^\dagger a^\dagger - aa^\dagger - a^\dagger a) | 0 \rangle$$

$$\frac{-\hbar^2}{2m^2\omega^2} \langle 1 | \begin{pmatrix} aaaa & +aaa^\dagger a^\dagger & -aaaa^\dagger & aaa^\dagger a & + \\ a^\dagger a^\dagger aa & +a^\dagger a^\dagger a^\dagger a^\dagger & -a^\dagger a^\dagger aa^\dagger & -a^\dagger a^\dagger a^\dagger a & - \\ aa^\dagger aa & -aa^\dagger a^\dagger a^\dagger & +aa^\dagger aa^\dagger & +aa^\dagger a^\dagger a & - \\ a^\dagger aaa & -a^\dagger aa^\dagger a^\dagger & +a^\dagger aaa^\dagger & a^\dagger aa^\dagger a & . \end{pmatrix} | 1 \rangle$$

You can open up a - a[†] to the power 4. Ultimately, you will get a whole lot of terms. But this computation will be very simple once you have expanded it out. You will realize that none of these terms survive under the squeezing of 0 and 1 from the left and right. So therefore, when none of the terms survive, the overall correction is 0. That means C₀¹ is 0. That does not tell me that there is no correction. It just tells me that it has no projection along the first eigenfunction as well. But it may have some projection along the second eigenfunction C₀². So then again I have to do the same thing. I have to take, squeeze the operator between 0 and 2 divided by their energy difference. Overall I will get this coefficient and this time I will after this expansion just like whatever we have done over here. If I put it between 0 and 1, 0 and 2 this time, this time I will get that there is a non-zero contribution which will survive. So this will not be 0 unlike C₀¹. So C₀² is not 0. So, this is your exercise to do this computation cleanly and find out what is this box. This is the non-zero number which will survive. So, therefore, the new eigenfunction ψ_n⁽⁰⁾ ground state, new ground state is the previous ground state + C₀¹ times 1. It so happens that C₀¹ is zero. Therefore, no projection along the first eigenfunction first excited state, but second excited state comes as a correction in the correction term.

Similarly, you can prove that after that C₀³ is also 0, the next term which will survive will be C₀⁴. So, all these terms will appear at the order λ. As we discussed λ would be put to 1 at the end. So, once I have put in λ is equal to 1, the correct description of the wave function up to order λ, this is the corrected ground state. So, let me stop over here for today and for this discussion, then we move on to discuss higher order corrections and the second order correction to the system.