Notes for Quantum Mechanics

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Lecture 31
Perturbation theory (non-degenerate, time independent)

Note for class: I fixed my wrong signs. Check your notes.

You may have noticed, that often when we solve problems - we solve them for small values of something. This is a time honored way of figuring out approximate solutions - it is called perturbation theory. As you know the solutions to the Schroedinger equation are most often difficult (if not imposible) to find. Try solving the SHO problem but add and extra potential term ax^4 to the potential. Real problems usually are not simple. If you remember even the pendulum has pieces of the potential that go like ax^4 (actually its $a\theta^4$) – the nice thing though is that these corrections to the standard x^2 potential are small. This will often be true (though not always. Non-perturbative systems are a big thing these days in physics - but we wont try to solve anything like that - they are hard!).

The standard problem has a Hamiltonian $\hat{H}_0$ which we can solve exactly, e.g. for the SHO its $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$

Added to this is some sort of small perturbation $\hat{H}'$ which in the case on an anharmonic oscillator like a pendulum is $a\,\hat{x}^4$. So for our example the final Hamiltonian is $\hat{H}=\hat{H}_0+\hat{H}' = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 + a\,\hat{x}^4$.

There is always a question of how "small" is "small". This takes some judgement.Its a problem - we'll talk about it in class.

What do we know? We will assume we know the solutions to the unperturbed Hamiltonian $\hat{H}_0$ that is we know

$$\hat{H}_0\,|n\rangle^{(0)} = E_n{}^{(0)}|n\rangle^{(0)} \tag{1}$$

- note how I indicate that the energies and states are of the unperturbed hamiltonian with a $\square^{(0)}$ which means the "zeroth" order answer. $\square^{(1)}$ will mean a first order correction. What order means will be made clear in a moment

$$\text{We want to find solutions to } \hat{H}\,|n\rangle = E_n|n\rangle \tag{2}$$

Now for bookkeeping purposes we will write $\hat{H}=\hat{H}_0+\lambda\hat{H}'$

The λ's will keep track of the small stuff for us. At the end we can dial λ to 1, or to look at the limit of no perturbation we can let λ=0. The power of λ is the "order" or the correction.

So we are looking for solutions to

$$(\hat{H}_0+\lambda\hat{H}')\,|n\rangle = E_n|n\rangle \tag{3}$$

We can use λ to write

$$|n\rangle = |n\rangle^{(0)} + \lambda\, |n\rangle^{(1)} + \lambda^2 |n\rangle^{(2)} + ... \quad (4)$$

$$E_n = E_n^{(0)} + \lambda \mathrm{E}_n^{(1)} + \lambda^2\, E_n^{(2)} + ... \quad (5)$$

Now of course we will have to figure out $|n\rangle^{(1)}$, $|n\rangle^{(2)}$....$E_n^{(1)}$, $E_n^{(2)}$... and it may seem to be just adding a lot of new stuff to figure out, but we have the λ's which tell us how small the term is, and we will throw away stuff which comes with too many powers of λ (in practice - more than 2 is too many). Remember $E_n^{(1)}$ and $|n\rangle^{(1)}$ are much smaller than $E_n^{(0)}$ and $|n\rangle^{(0)}$; $E_n^{(2)}$ and $|n\rangle^{(2)}$ are much smaller than $E_n^{(1)}$ and $|n\rangle^{(1)}$ etc; That is why the λ's keep track of how small stuff is. We will see that it helps.

So just plug in eqn (4) and (5) into eqn (3)

$$(\hat{H}_0 + \lambda \hat{H}')\,(|n\rangle^{(0)} + \lambda\, |n\rangle^{(1)} + \lambda^2\, |n\rangle^{(2)} + ...) = (E_n^{(0)} + \lambda \mathrm{E}_n^{(1)} + \lambda^2\, E_n^{(2)} + ..)(|n\rangle^{(0)} + \lambda\, |n\rangle^{(1)} + \lambda^2\, |n\rangle^{(2)} + .)$$

Lets just keep the first order corrections i.e. terms that have more than 1 λ in front of it, and assume that the rest are so small we won't worry about it. Someone else might worry about it later.

$$(\hat{H}_0 + \lambda \hat{H}')\,(|n\rangle^{(0)} + \lambda\, |n\rangle^{(1)}) = (E_n^{(0)} + \lambda \mathrm{E}_n^{(1)})(|n\rangle^{(0)} + \lambda\, |n\rangle^{(1)})$$

$$\hat{H}_0 |n\rangle^{(0)} + \lambda\, \hat{H}_0\, |n\rangle^{(1)} + \lambda\, \hat{H}'\, |n\rangle^{(0)} + \lambda^2\, \hat{H}'\, |n\rangle^{(1)} = E_n^{(0)} |n\rangle^{(0)} + \lambda \mathrm{E}_n^{(0)}\, |n\rangle^{(1)} + \lambda \mathrm{E}_n^{(1)} |n\rangle^{(0)} + \lambda^2\, E_n^{(1)}\, |n\rangle^{(1)}$$

Now we dropped all terms with a λ^2 before so we will do that again

$$\hat{H}_0 |n\rangle^{(0)} + \lambda\, \hat{H}_0\, |n\rangle^{(1)} + \lambda\, \hat{H}'\, |n\rangle^{(0)} = E_n^{(0)} |n\rangle^{(0)} + \lambda \mathrm{E}_n^{(0)}\, |n\rangle^{(1)} + \lambda \mathrm{E}_n^{(1)} |n\rangle^{(0)}$$

$$\hat{H}_0 |n\rangle^{(0)} - E_n^{(0)}\, |n\rangle^{(0)} + \lambda\, (\hat{H}_0\, |n\rangle^{(1)} + \hat{H}'\, |n\rangle^{(0)} - E_n^{(0)}\, |n\rangle^{(1)} - E_n^{(1)} |n\rangle^{(0)}) = 0$$

where I have now grouped together the powers of λ. Now λ can be anything between 0 and 1 so each of the terms in front of each power of λ must be 0. We get two eqns.

$$\hat{H}_0 |n\rangle^{(0)} = E_n^{(0)}\, |n\rangle^{(0)} \quad (6)$$

$$(\hat{H}_0 - E_n^{(0)})\, |n\rangle^{(1)} == (E_n^{(1)} - \hat{H}')|n\rangle^{(0)} \quad (7)$$

Now there is something interesting about eqns 6 and 7, and indeed all the other higher order eqns, i.e if you save all terms like λ^3 or λ^4 etc.

You can take $|n\rangle^{(1)}$ and add a constant times $|n\rangle^{(0)}$ and it will still be a solution - so there is a degree of freedom that we are free to do something with. We will get rid of it by choosing a constraint eqn that will make life easy for us

$\langle n^{(1)}\, |n\rangle^{(0)} = 0$ i.e. that the first order correction to the wave function in perpendicular to it. (8)

Eqn (6) is just the same eqn as (1) and tells us what we knew before, that for the 0th order hamiltonian, the original unperturbed states and energies are the solution. Now remember the $|n\rangle^{(0)}$'s are eigenfunctions of $\hat{H}_0$ and form orthogonal eigenfuctions which span the entire space. Hence we can write

$|n\rangle^{(1)} = \sum_m c_{\mathrm{nm}} |m\rangle^{(0)}$ i..e. we have expanded $|n\rangle^{(1)}$ in terms of the $|m\rangle^{(0)}$ (9)

Now lets put (9) into (7)

$$(\hat{H}_0 - E_n^{(0)}) \sum_m c_{\mathrm{nm}}\, |m\rangle^{(0)} = (E_n^{(1)} - \hat{H}')|n\rangle^{(0)}$$

$$\sum_m c_{\mathrm{nm}}\, (E_m^{(0)} - E_n^{(0)}) |m\rangle^{(0)} = E_n^{(1)} |n\rangle^{(0)} - \hat{H}'\, |n\rangle^{(0)}$$

Now operate from the left with $\langle k^{(0)} |$

$c_{\mathrm{nk}}\ (E_k{}^{(0)}\text{-}E_n{}^{(0)}) = E_n{}^{(1)}\ \delta_{\mathrm{kn}} - \langle k^{(0)} |\ \hat{H}'\ |n\rangle^{(0)}$

We will use a standard convention and set $\langle k^{(0)} |\ \hat{H}'\ |n\rangle^{(0)} = \hat{H}_{\mathrm{kn}}'$

$$c_{\mathrm{nk}}\ (E_k{}^{(0)}\text{-}E_n{}^{(0)}) = E_n{}^{(1)}\ \delta_{\mathrm{kn}} - \hat{H}_{\mathrm{kn}}' \qquad (10)$$

Now first set n=k to get

$E_n{}^{(1)} = \hat{H}_{\mathrm{nn}}'$ that is the first order correction to the energy is just the perturbation sandwiched between the zeroth order wave function.

For n≠k we get

$c_{\mathrm{nk}} = \frac{\hat{H}_{\mathrm{kn}}'}{E_n{}^{(0)} - E_k{}^{(0)}}$ plugging this into (8) we get

$|n\rangle^{(1)} = \sum_{m;\, m\neq n} \frac{\hat{H}_{\mathrm{mn}}'}{E_n{}^{(0)} - E_m{}^{(0)}} |m\rangle^{(0)}$

Now you might be wondering about the c_{nn} term which using eqn 10 gives *a* funny answer.

:Let look at (9) again and operate to the left with $\langle n^{(0)}|$.

$\langle n^{(0)} |\ |n\rangle^{(1)} = c_{\mathrm{nn}}$ but from (8) we get that this term is zero.

Now just for your information here is the second order correction to the energy

$E_n{}^{(2)} = \sum_{m;\, m\neq n} \frac{|\hat{H}_{\mathrm{nm}}'|^2}{E_n{}^{(0)} - E_m{}^{(0)}}$

So finally to summarize we get for the first order corrections, in terns of the pertubation and the zeroth order wave functions we set λ=1 and get

$(\hat{H}_0 + \hat{H}')\ |n\rangle = E_n |\mathrm{n}\rangle$

$|n\rangle = |n\rangle^{(0)} + |n\rangle^{(1)} + |n\rangle^{(2)} + \ldots.$

$E_n = E_n{}^{(0)} + E_n{}^{(1)} + E_n{}^{(2)} + \ldots.$

$$E_n{}^{(1)} = \hat{H}_{\mathrm{nn}}' \qquad (11)$$

$$|n\rangle^{(1)} = \sum_{m;\, m\neq n} \frac{\hat{H}_{\mathrm{mn}}'}{E_n{}^{(0)} - E_m{}^{(0)}} |m\rangle^{(0)} \qquad (12)$$