

MITOCW | L2.3 Degenerate Perturbation theory: Example and setup

PROFESSOR: OK, degenerate perturbation theory. OK, we've done nicely our non-degenerate case. So we'll get degenerate done in a very clear way, I think.

One more blackboard. So the first thing I want to say about degenerate perturbation theories, when it fails and why it fails and what goes wrong. So degenerate perturbation theory.

Trivial example to begin with, why not, h of λ , again, is equal to h_0 plus $\lambda \delta h$. And for h_0 , we'll take original Hamiltonian with energies 1 and 1, and for δh , I'll take an off-diagonal Hamiltonian, a Pauli matrix, and that's our δh .

And then we say OK, blindly, not worry about this degeneracy, and use the formulas that we have for non-degenerate states. And we would say well, for the first state and the second state what do we have? E , I'll call them 1 and 2, not 0 and 1. So let's call them 1 of λ will be equal to the first value, 1, plus, if the formula is right, δh times λ , 1, 1. The matrix element of the perturbation in the 1, 1 state.

Similarly, E_2 , the other eigenvalue, should be 1, there's the second eigenvalue, plus $\lambda \delta h_{2,2}$. That's what the formula would say. But this is completely incorrect. Why? Because $\delta h_{1,1}$ is the 1, 1 element of δh , and it's 0. And the 2, 2 element of δh is also 0, and therefore this says 1 and 1, that the eigenvalues haven't changed.

On the other hand, we know that the matrix, the total matrix, which is 1λ , $\lambda 1$ has eigenvectors, $1/\sqrt{2}$, $1/\sqrt{2}$, and $1/\sqrt{2}$, $1/\sqrt{2}$ minus 1, with eigenvalues-- this is our eigenvectors and eigenvalues-- $1 + \lambda$ and $1 - \lambda$.

So the eigenvalues of the matrix are $1 + \lambda$ and $1 - \lambda$. And this formula, to first order in λ , gave us nothing. It failed badly. It's a disaster. So you can say, well, what happened? And maybe a clue is on the fact of the eigenvectors. These are the eigenvectors of the total matrix. These are in fact, also the eigenvectors of the perturbation.

On the other hand, when we said OK, this is the first state, the first eigenvector, we thought of it as 1, 0 on the Hamiltonian, on that eigenvector gave you the energy 1. The second energy corresponds to the eigenvector 0, 1. That's what we usually use for our matrices.

So here is the strange thing that seems to have happened. For the original Hamiltonian, [INAUDIBLE] we had this eigenvector and this eigenvector, and then suddenly you turn on the perturbation and λ can be 10^{-1000} , and already the eigenvectors jump and become this one. They go from this one to that one. You just add a perturbation that you even cannot measure, and the eigenvectors change. That's crazy.

The explanation is this thing that we usually, sometimes forget to say in a mathematically precise way. These are not the eigenvectors of the original matrix. Since the original matrix is degenerate, this is one possible choice of eigenvectors. Any linear combination of them is an eigenvector. So this space of eigenvectors of this matrix is the span of these things.

So there was no reason to say, oh, these were the eigenvectors before, and now they've changed. They're this. No. Before, you don't know what are the eigenvectors. They're ambiguous. There's no way to decide who they are. This, this, or any linear combination. Remember, when you have a degenerate eigenstate, any superposition of them is a degenerate eigenstate.

So the explanation is that, in some sense, these eigenvectors of the perturbed Hamiltonian is one of the possible choices of a basis of eigenvectors for the original space, and what the perturbation does is break the degeneracy. All those equivalent eigenvectors suddenly are not all equivalent. There are some preferred ones.

So the fact is that the formulas are not working right, and we have to do this again. So here is what we're going to do. We're going to set this up for a systematic analysis to get this right. So systematic analysis.

So again, we say H_0 is known and it will have an $E_1, 0$, an $E_2, 0$, like that, until you encounter an $E_n, 0$ that happens to be equal to the next one, $E_{n+1}, 0$, and happens to be equal to the next one, all the way to an $E_{n+N-1}, 0$, which is then smaller than the next one, which is E_{n+N} and then again.

So I'm saying in funny ways the fact that, yes, you had some states and suddenly you hit a collection of N energy eigenvalues that are identical. They're all equal to E_n . All n states have energy E_n . So it is as if you have this matrix H_0 and there are all kinds of numbers. And then there's a whole block where all the entries of size n by n where all the entries are the same. So $n, n+1, n+2$, up to $N-1$ is n entries, and they all have the same energy.

And the corresponding eigenstates are going to be called n -- we're going to use the label n for all of them, even though the energies are all the same. So there's just an E_n energy. So we have N states, so there will be an n_1 , an n_2 , up to an n_N . All those states are going to form an orthonormal basis for a space that we're going to call v_n .

So the space spanned by this state, we're going to go v_n , with the n reminding you it has to do with the n states, states with energy described by the label n . So this is the degenerate subspace. This is the space of all those states that have energy E_n . So I'll state that here.

So it's quite important to get our notation right here. Otherwise we don't understand what's going on. So h_0 , n_0k , they all have energy E_n , n_0k . And this is for k equals 1 up to N . Now OK, this is your degenerate subspace. These are all the states. And we now want to know what happens to this space, to all these states, when the energy turns on.

This is not just a theoretical construct. When you start asking what happens to the first excited states in the hydrogen atom, you already have four states there, l equals 1, l equals 0 states, n equals 2. And you have degenerate states and immediately you're stuck in this situation.

So I will also use the notation that the total space, a curly h , is the sum of v_n plus a \hat{v} . This is called the direct sum. At this point it just doesn't matter too much. These are linearly independent subspaces, v_n and \hat{v} , and basically you think as \hat{v} as all the other states. Yes, there were these degenerate subspace and all the other states of our \hat{v} . So \hat{v} is the span of all other states. And we'll call them p_0 , or what letter? Yeah, p_0 , with p equals some numbers.

So this is a good notation. It allows you to distinguish. The degenerate states use 2 labels. Maybe you only needed 1 label, but you will get confused with the notation if you just use 1 label. So if that's the case, degenerate state, but by putting the n here you now know that you're talking about degenerate states. When you have a single label you're talking about the other states in the space. So it's very good when your notation makes it easy to think and recognize the equations that you have.

And \hat{v} in this, are orthogonal spaces. \hat{v} is perpendicular to v_n . The inner product of any state outside of degenerate space, with a state in the general space, is 0.

OK. Very good. So let's now do the important thing. I can do it here, I think. I'll do it here. So what do we want to do? What is the question here? The question is the following. We have a

state n_0^k . We have N of those states, and we want to figure out what they become as you turn on the perturbation. So using the old notation, we'll say they become this.

And what is that going to be? It is going to be n_0^k , the original state, what it was, plus order λ , the first correction, so n_1 for this k state, plus dot dot dot. For the energies, we have E_n^0 . That was the energy of every state in the degenerate subspace. Now it's going to become $E_n \lambda$. But if I say $E_n \lambda$ I'm already making a mistake, because I'm looking at the fixed k . And a fixed k means we chose one of these states, and any single one of the states, the energy can grow in a different way.

So I should call this E_{nk} , because we're talking about this state, will be equal to E_n^0 -- yes, they all have the same first zeroth order energy. But then E_{nk1} plus $\lambda^2 E_{nk2}$ and so on. So this is the fate of the k th state. And the degeneracy will be broken to first order if these E_{nk} 's become different numbers, because if they become different numbers in λ they're going to start splitting the states.

Remember this picture we had last time of several states at one point? If the order λ corrections are different, the states split. The degeneracy is resolved. And we can calculate things more easily. If it's not resolved to first order, it's harder. It will be all of next lecture to figure out what happens in that case.

We discussed last time that the n_1 correction didn't have any component along the n_0 vector. We could always arrange that to happen. Here, we can arrange something similar to happen. So we will still assume, and we can check that's always possible, that v_{np} , the corrections to the state k at order p for p equals 1, 2, 3, because it's not 0, are orthogonal to n_0^k .

So this state doesn't have any component along n_0^k , and this state doesn't have any component along the original one. It's always possible to do that, just like we did it in the non-degenerate case. Moreover, this is something I want you to notice. We're saying that the state n_1 doesn't have any component along the state n_0 for a given k , but the state n_1 can have components along n_0 for a different k . So while they've n th order or a p th order correction doesn't have component along this, it can have component for an l here, where l is different from k .

So it means that n_{pk} still can have a component in v_n . Remember, v_n is this whole thing. So if you're doing the k th one, well, n_{1k} doesn't have a component along that one, but it may have a component along all the others. So it may still have a component, that correction, in v_n . In

fact, that's what will make the problem a little hard to do, but it's a good thing to try to figure out this thing.

So what is the equation we want to solve? The usual equation, $\langle n | H(\lambda) | n \rangle$ is equal to $E_n(\lambda)$. So we produce the general state that's its energy for the full Hamiltonian. That's our Schrodinger equation. So what do we have to do? We have to do exactly what we did before, plug in that series, separate the terms with various lambdas, and see what we get.

So here is what we get. To order lambda to the 0, you get $\langle n | H_0 | n \rangle = E_n^0$. And that equation, as it was the case for the non-degenerate case-- sorry for the redundancy-- it's trivially satisfied. We've stated that those are the energies in the top equation on that blackboard. So this equation we don't need to worry about. That's not too difficult.

$\langle n | H_1 | n \rangle = \langle n | H_1 | n \rangle + \sum_{k \neq n} \frac{\langle n | H_1 | k \rangle \langle k | H_0 | n \rangle}{E_n^0 - E_k^0}$

Last equation. I'm starting to get lazy to write them out, but we must. $\langle n | H_2 | n \rangle = \langle n | H_2 | n \rangle + \sum_{k \neq n} \frac{\langle n | H_2 | k \rangle \langle k | H_0 | n \rangle}{E_n^0 - E_k^0} + \sum_{k \neq n} \frac{\langle n | H_1 | k \rangle \langle k | H_1 | n \rangle}{E_n^0 - E_k^0} + \sum_{k \neq n} \frac{\langle n | H_1 | k \rangle \langle k | H_1 | n \rangle}{E_n^0 - E_k^0}$. OK and these equations are equations for k fixed, but every term in the equation has the same k, but k then can run from 1 up to n. So three equations times n times, there we go.

OK, these are our equations this time. And we need to understand them. In fact, we need to solve them. What we've gained experience with the non-degenerate case is going to come very useful here, although some things are not going to be exactly the same. We're going to try to find the energy corrections here, but calculating the state $|n\rangle$ is going to be a little harder.

We won't finish today-- we won't have much time left-- but what's going to happen is that you can calculate the state $|n\rangle$, the part in the space V_n . But the part in the degenerate subspace, where I said that $|n\rangle$ still can have a component in the degenerate subspace, cannot be calculated from this equation. So even when we're finished doing this first equation, you're going to find this equation, you still have not calculated all of the states $|n\rangle$. You're going to have to go through the second equation to find the missing part of the state $|n\rangle$. So it's going to be pretty interesting.