

PROFESSOR: Good morning. We're going to continue doing perturbation theory today. We've finished doing non-degenerate perturbation theory, and then turned to the degenerate perturbation theory as well.

We had computed already the first order corrections to the state, first order corrections to the energy, and second order correction to the energy. So here in these formulas that I've written are all the results we have so far. And a useful thing is to ask yourself whether you know what every symbol here means. This is the state which changes with the deformation of the original state n_0 of the Hamiltonian H_0 . We have the Hamiltonian H of λ , which was equal to H_0 plus $\lambda \delta H$.

And n_0 was an eigenstate of H_0 with energy E_{n_0} . And we found that as you turn on λ , λ becomes non-zero. The energies change. The eigenstate changes. And here is λ , first order in λ , second order in λ . We didn't compute the state to second order in λ .

Moreover, we have the symbol δH_{kn} that was defined to be the matrix element on the unperturbed eigenstate of the operator δH . Well, that's another symbol in here.

We are summing over all states in the spectrum, except for the state n here because the denominator here would give you a 0. And this would be problematic in general. So that was what we derived. And these are the formulas we have.

It's worth making a few remarks as to what we see from these formulas because they're a little complicated. And you may not have immediate intuition about it. So a few remarks.

And the first one-- in fact, both remarks that I'm going to make concern the behavior of the energy as represented by this formula. First remark is that if you were to look at the ground state energy of the system, the first two terms here, so for n equals 0, if we call the ground state by the label n equals 0 for this state n equals 0, these first two terms on the energy overestimate the ground state energy. They always give you more than what the true ground state energy is for any value of λ .

That is kind of plausible, given that you see here that for the ground state energy, when n is equal to 0, and it's the lowest energy state, these differences are all positive. All these states

have more energy. Therefore, this term is negative. And the next correction to order λ^2 tends to lower the energy of the ground state.

So the claim is that the first λ ground state energy overestimate the true ground state energy. And so how do we see that? So we consider E_0 , because we're doing $n = 0$. This is the ground state. We start labeling with $n = 0$ sometimes. λH_{00} . That is the order λ estimate for the ground state energy.

The first term can be viewed as the expectation value of the original Hamiltonian on the ground state. That is E_0 because this H_0 and 0 is E_{00} . So this is E_{00} . Plus λ .

I'm sorry here. I made a little mistake. That should be ΔH . ΔH_{00} plus λ , the expectation value of ΔH on the same state. So these two things together are nothing but the expectation value on the ground state of H_0 plus $\lambda \Delta H$.

That's kind of nice. Isn't it? That these two terms really are nothing else but the expectation value on the ground state of this thing that we called H of λ .

And now comes the variational principal that says that if you evaluate the Hamiltonian on an arbitrary state, the expectation value of the Hamiltonian in an arbitrary state, you get more energy than the ground state energy of the system. You always get more. And when you hit the ground state, you get the lowest value.

So look at that. This is the Hamiltonian. And this is the unperturbed ground state. This is not the real ground state. The real ground state is what we're trying to find.

So this is like saying, OK, you're evaluating the exact Hamiltonian on some arbitrary state. Therefore, this is greater than or equal to the true ground state energy that we would call E_0 plus λ . True ground state energy.

Which in that notation, indeed, is E_0 plus λ . So that's a nice result. And it matches with the idea that for the ground state the order λ^2 correction is minus λ^2 times the sum over k different from 0 $\frac{\Delta H_{k0}^2}{E_k - E_0}$.

And this thing, as we mentioned, the numerator is positive. The denominator is positive because this was the ground state. And this is a non-degenerate ground state. And k , therefore, has more energy here, E_k . So everything is positive. So this is negative.

So actually here, there is a generalization of this observation. And you can imagine that you have now a particular state, n here. Then you have all these states that are above and all these states that are below.

So let's look at the second order correction to the energy of the state E_n , the second order correction. The first order correction shifts. The energy is proportional to ΔH_{mn} . But the second order correction is minus λ^2 , the sum over k different from n . So let's split it. k greater than n . And we'll write the same thing H_{kn} squared over E_{k0} minus E_{n0} .

And then I want to write the other states, the states where k is less than n . But let me do one thing here. On those states, I'll switch the order of the sum. I'll put E_{n0} , the order of the sign in the denominator, E_{k0} , and change the sign here.

So these two changes of sign are correlated. I changed the sign in the denominator. And I changed the sign in front.

And now, we see the following. All these states that are above n , k is greater than n . This difference is positive. This is manifestly positive. This is negative. So these states are kind of pushing your state down. The fact of this states on top is a negative correction are pushing the states down.

On the other hand, the lower states, the states with k less than n , again, I've ordered now convenient. The other states k now have less energy. So this is positive. This is positive. This is positive. So these states over here are actually pushing that state up.

So the upper states are pushing it down. The lower states are pushing it up. This is usually referred to as level repulsion. The levels repel each other. The upper states don't want the state n to go close to them. The lower states don't want them to go close to them either. So it's a nice dynamic that helps you understand what's going on here.

Another point we want to make has to do with the validity of this expansion. So in general, when you have series expansions the issues of convergence are delicate. So we can get a lot of insight just by doing an example. So let me talk about the validity of the perturbation series. This is supposed to give us some insight.

One thing we've said is that we think ΔH is supposed to be smaller than $\hbar\omega$. Now, these are operators. So the statement that they're smaller has to be made more precise. What is the size of an operator?

And you could think, well, we could say the entries of the matrix elements should be much smaller. And that is true, but it's not enough. For that, let's consider an example.

So this will be a two by two matrix Hamiltonian, in which H of λ will be given by some H_0 plus λ \hat{v} , which will be $E_1 \ 0 \ 0 \ E_2$ plus λ . That \hat{v} matrix will be of the form v v^* . And must be her mission. So v is a number. v^* is the complex conjugate.

These are the two energies, because the Hamiltonian is known. Each time we talk about the Hamiltonian that is known, we write that there's a diagonal matrix. We're saying, yes, that is the matrix element of the Hamiltonian in the basis of eigenstates, which we know. So a known Hamiltonian you can represent by a diagonal matrix.

So here is our whole matrix H of λ . And you could say, all right, our perturbation theory, practically speaking, is these formulas that allow us to compute the eigenvalues of this matrices, which are of this matrix, which is the energies of the system of the eigenstate and compute the eigenstates. For H_0 , these are the eigenvalues. And the eigenstates are $1 \ 0$ and $0 \ 1$.

So perturbation theory is really, you can think in terms of Hamiltonians, but also you can think of it in terms of matrices. It's allowing you to find the eigenvalues and eigenvectors of this matrices.

So this is a two by two matrix with numbers. You know how to compute the eigenvalues. So I'll give you the answer. The eigenvalues E plus minus are E_1 plus $E_2/2$ plus minus E_1 minus $E_2/2$ times the square root of 1 plus λ squared absolute value of V^2 squared E_1 minus $E_2/2$ squared. Long formula.

That's it. Those are the exact things. If you wanted to see this as a result in perturbation theory, you would say, well, λ squared v squared or λ v is small. And I'm going to think of this term as small. And I'm going to expand the square root.

And if I expand this square root, I'm going to get all kinds of terms with different powers of λ . You can also see there that there's no energy correction linear in λ . Because when you expand 1 plus ϵ square root, it's roughly 1 plus ϵ over 2 plus dot, dot.

And therefore, when you span the square root, the first correction is going to be proportional to λ squared. And that actually conforms to that because the matrix elements of the

Hamiltonian delta H_{nn} along the diagonals for the perturbation are 0. So there is no order λ correction.

So what do you do here then? You must do this expansion. And here, I write the relevant series. f of z , if you define it, as $1 + z^2$ is equal $1 + z^2$ over $2 - z^4$ over $8 + z^6/6$. And it's not that simple after that. Minus $5/128z^8$ plus order z to the 10. So that's this perturbative series expansion that you would use here.

And how good is the convergence of this series? Well, it's OK. It's something that when you study complex analysis you see this function $1 + \sqrt{z^2}$ has branch cuts at i and at $-i$ in the complex plane, in the z complex plane. Those are the branch cuts. These are the places where this square root becomes 0. And you have to deal with them.

And the function is convergent only up to here. There is a radius of convergence. A radius of convergence is 1. You can try it with Mathematica or with the program and take 30 terms, 40 terms.

And you will see that as long as you take a point z here, it converges. You take a point a little bit out, it blows up the series. So it has a radius of convergence. That's not so bad. Radius of convergence is OK.

But basically, we need z to be small, which corresponds here to the statement that λv z small for a fast convergence corresponds to λv absolute value being smaller than $E_1 - E_0$ absolute value over 2. Roughly smaller.

And now, we see that the thing that matters for a perturbation series to be good is also that the perturbation be small compared with the energy differences. Not just it should be small, the perturbation. It should be small compared with the energy difference.

So if you have a Hamiltonian with a state of energy 100 and a state of energy 101, you might say, well, if I take a perturbation of size two or three, that's very small compared to the energies. But it's not been small compared to the difference of energies. And that can cause the perturbation expansion to go wrong.

So this gives you extra insight that, in fact, being a small perturbation not only means small compared to the energies, but also small compared with the energy differences. Something that you see here as well. Energy differences are controlling things. And if the energy

differences are-- if the perturbation is not small compared to energy differences, then these ratios can be rather large. And the perturbation terms are very large. And nothing is very simple.

So that's what I wanted to say about the convergence of a perturbation expansion. More rigorous statements can be made, but we're not going to try to make them here.