Lecture 20 & 21

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1 Non-degenerate Perturbation theory

In this lecture we will begin our study of approximation methods. We will begin with "perturbation theory," which begins from an exactly solvable starting point and systematically computes corrections in a Taylor series like form. In particular we begin with a Hamiltonian of the form

$$H = H_0 + \lambda V \tag{1}$$

where H_0 is exactly solvable; we know all of its eigenstates $|n^{(0)}\rangle$ and eigenenergies $E_n^{(0)}$, such that $H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$. We have introduced a perturbation operator V, as well as a perturbation strength λ. One could absorb λ into V, or define V so that $\lambda = 1$, but it is convenient to retain λ as a free parameter while deriving the perturbation series as it is a convenient way to effectively count powers of V. Indeed, any physical quantity computed from (1) that has d powers of λ will necessarily have d powers of V.

We will compute $|n\rangle = |n(\lambda)\rangle$ and $E_n = E_n(\lambda)$ such that

$$H |n\rangle = E_n |n\rangle . \tag{2}$$

We assume that there is no degeneracy; there is a single state $|n\rangle$ with energy E_n. In the next lecture we will address the case of degeneracy. Note that since $H = H_0 + \lambda V$ is a function of λ, so are $|n\rangle$ and E, though we will often leave this dependence implicit. The computation of $|n\rangle$ and E will be done order-by-order in λ (and thus V). In particular we consider expanding

$$\begin{aligned} |n\rangle &= |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \lambda^3 |n^{(3)}\rangle + \cdots \\ E &= E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \lambda^3 E^{(3)} + \cdots \end{aligned} \tag{3}$$

so that $|n^{(d)}\rangle$ and $E^{(d)}$ are order d in V, but don't have λ dependence. We will systematically calculate these corrections order by order. We pause to comment that we do not include $1/n!$ factors that would enable us to associate $E^{(d)}$ with the n-th order derivative of E with respect to λ evaluated at $\lambda = 0$, as is typical in Taylor series. This is essentially a convention choice in how $E^{(d)}$ is defined and the choice we make here will be slightly more convenient for our purposes.

There is another subtlety that we will have to address which is gauge redundacies associated with $|n\rangle$ as a function of λ. As an example, for $V = 0$, where all corrections should be trivial, we could imagine the "perturbed" state $|n(\lambda)\rangle = e^{i\alpha(\lambda)} |n^{(0)}\rangle$; the exponential could then be expanded to generate a series with $|n^{(d)}\rangle \propto |n^{(0)}\rangle$. These corrections that are proportional to $|n^{(0)}\rangle$ do not change the state physically, they simply change its unphysical coefficient. In order to derive a canonical expression for $|n\rangle$ we will need to remove this gauge redundancy. To do this, we simply imagine deleting the part of $|n^{(d)}\rangle$ that lies along $|n^{(0)}\rangle$ and therefore impose

$$\langle n^{(0)} | n^{(d)} \rangle = 0, \qquad \text{for } d \geq 1. \tag{4}$$

That is, all corrections are required to change the unperturbed *state* rather than adjust its coefficient. We pause to comment that the set up we have outlined typically results in states that are not normalized, since

the leading order part $|n^{(0)}\rangle$ has a fixed coefficient of 1 in (3), but the state can always be renormalized after it is computed to the desired order.

We will begin by computing the first two orders in perturbation theory for the energy and the first order in the state. Later, we will discuss a systematic procedure to generate terms of arbitrary order. Consider the equation (2) keeping only terms up to linear order in λ

$$(H_0 + \lambda V)(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle) = (E_n^{(0)} + \lambda E_n^{(1)})(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle) \tag{5}$$

Equating the $O(\lambda)$ terms on both sides yields

$$H_0|n^{(1)}\rangle + V|n^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)}|n^{(0)}\rangle \tag{6}$$

Acting with $\langle n^{(0)}|$ on both sides and using $\langle n^{(0)}|n^{(1)}\rangle = 0$, yields

$$E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle \tag{7}$$

which amounts to just taking the expectation value of V in the unperturbed state. We note that this is the only correction that appears in perturbation theory if $[H_0, V] = 0$; indeed, in this case the perturbation may be simultaneously diagonalized with the Hamiltonian such that the unperturbed states $|n^{(0)}\rangle$ are exact. The vanishing of all higher-order corrections in this case will be a consistency check on the result as we will see. This statement is also true for a state $|n^{(0)}\rangle$ which is an eigenstate of V even if H_0 and V do not commute.

To obtain the first order correction to the eigenstates, we act with $\langle m^{(0)}|$ on Eq. 6 with $m \neq n$, to get

$$\langle m^{(0)}|n^{(1)}\rangle = \frac{\langle m^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \tag{8}$$

which leads to the full expression for $|n^{(1)}\rangle$:

$$|n^{(1)}\rangle = \sum_{m\neq n} \frac{|m^{(0)}\rangle\langle m^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \tag{9}$$

Note that, as anticipated, this correction vanishes if $[V, H_0] = 0$ which implies that its off-diagonal matrix elements vanish in the H_0 eigenbasis, i.e. $\langle m^{(0)}|V|n^{(0)}\rangle = 0$ for $m \neq n$.

To obtain the second order correction to the energy, we repeat the same steps leading to (7): first write the eigenvalue equation (2) keeping terms up to second order in λ, expand and equate the λ^2 terms, and act with $\langle n^{(0)}|$ on both sides. The resulting expression is

$$E_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle = \sum_{m\neq n} \frac{|\langle m^{(0)}|V|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}} \tag{10}$$

We see that this correction vanishes if $|n^{(0)}\rangle$ is an eigenbasis for V as anticipated. There are a few more remarks to make on this form of the second order energy correction.

1. The correction only depends on the difference between unperturbed energies.

2. Eigenvalues that are very far away from the one of interest have very little influence on perturbed state and thus very little influence on the second order energy correction.

3. The sign of the correction is such that eigenvalues are "repelled" with an equal and opposite "force." Indeed, the expression for $E_k^{(2)}$ has the same form but with the opposite sign, and the above expression is positive if $E_n^{(0)} > E_k^{(0)}$ and negative otherwise.

4. The second order correction and repulsion strength diverges as two eigenvalues approach each other. This indicates that our assumption of non-degeneracy above was not innocuous; as we approach degeneracy, the perturbation theory we have developed here degenerates. Said another way, the perturbation must be much smaller than the spacing between eigenvalues in order to trust the perturbation theory developed here.

The expression for the second order perturbation theory is rather complicated and requires the knowledge of all eigenstates and eigenenergies of the non-perturbed Hamiltonian. In many cases we can derive simple upper and lower bounds on the value of this term that provides a reasonable estimate for the value of this perturbative correction. Consider the correction to the ground state energy $n = 0$. The second order perturbative correction is given by

$$E_0^{(2)} = -|E_0^{(2)}|, \qquad |E_0^{(2)}| = \sum_{k\neq 0} \frac{|\langle k|V|0\rangle|^2}{\Delta_k}, \qquad \Delta_k = E_k - E_0 \tag{11}$$

Here, we are using the simplified notation where the superscript (0) is omitted. We can derive a simple lower bound on $|E_0^{(2)}|$ by taking the first term (or any small number of terms) of this expression leading to

$$|E_0^{(2)}| \geq \frac{|\langle 1|V|0\rangle|^2}{\Delta_{\min}} \tag{12}$$

We can also derive an upper bound using the observation

$$\Delta_k \geq \Delta_{\min} \tag{13}$$

We can simplify $|E_0^{(2)}|$ as

$$|E_0^{(2)}| \leq \frac{1}{\Delta_{\min}} \sum_{k\neq 0} |\langle k|V|0\rangle|^2 = \frac{1}{\Delta_{\min}} \left\{ \sum_k \langle 0|V|k\rangle\langle k|V|0\rangle - |\langle 0|V|0\rangle|^2 \right\} = \frac{\langle 0|V^2|0\rangle - |\langle 0|V|0\rangle|^2}{\Delta_{\min}} \tag{14}$$

Before discussing degenerate perturbation theory, it is instructive to discuss a more general derivation for the perturbative series that allows us to express the perturbative corrections to the eigenstates and eigenenergies at D-th order in terms of corrections at order $d < D$. To do this, we write writing $\Delta_n = E_n - E_n^{(0)}$ for the energy shift (not that this is different from Δ_k defined in Eq. 11)

$$(E_n^{(0)} - H_0)\,|n\rangle = (\lambda V - \Delta_n)\,|n\rangle\,. \tag{15}$$

This rewritten eigenequation will be the starting point for our expansion. The reason is that it relates the order D correction to $|n\rangle$ to orders $d < D$ on the right hand side, as both λV and Δ_n contain at least one power of λ.We begin by acting with $|n^{(0)}\rangle$ on the left. Since $H_0\,|n^{(0)}\rangle = E_n^{(0)}\,|n^{(0)}\rangle$ (likewise for the dual "bra" version because H_0 is Hermitian), the left hand side vanishes and we obtain

$$\langle n^{(0)}|\,(\lambda V - \Delta_n)\,|n\rangle = 0 \tag{16}$$

which says that $(\lambda V - \Delta_n)\,|n\rangle$ is orthogonal to $|n^{(0)}\rangle$

$$\Delta_n = \langle n^{(0)}|\,\lambda V\,|n\rangle \implies E^{(d)} = \langle n^{(0)}|\,V\,|n^{(d-1)}\rangle \tag{17}$$

so that we can compute the order d energy in terms of the order $d-1$ state.

Next, let us act with $\langle m^{(0)}|$ on Eq. 30 for $m \neq n$, we get

$$\langle m^{(0)}\,|n\rangle = \frac{1}{E_n^{(0)} - E_m^{(0)}}\,\langle m^{(0)}|\,(\lambda V - \Delta_n)\,|n\rangle \tag{18}$$

This leads to

$$|n\rangle = |n^{(0)}\rangle + \sum_{m\neq n} \frac{1}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle \langle m^{(0)}| (\lambda V - \Delta_n) |n\rangle . \tag{19}$$

Thus, starting from E and $|n\rangle$ up through order $d-1$, we can compute $E^{(d)}$ from (33) and then $|n^{(d)}\rangle$ from (19). It is easy to verify that these expressions reproduce the first and second order perturbative corrections we obtained earlier.

2 Degenerate Perturbation theory

Before jumping into non-degenerate perturbation theory, we will study a simple example. This simple example will allow us to practice applying non-degenerate perturbation theory, but it will also point us in the correct direction for developing degenerate perturbation theory.

The example is simply a two band Hamiltonian with

$$H_0 = \omega_0 + \omega\sigma_z, \qquad V = \varepsilon\sigma_x. \tag{20}$$

The unperturbed states are $|\pm\rangle = |\pm z\rangle$, and the first order energy correction vanishes:

$$E_\pm^{(1)} = \langle \pm| \varepsilon\sigma_x |\pm\rangle = 0. \tag{21}$$

The second order correction however is nonzero. Picking the negative state leads to

$$E_-^{(2)} = \frac{\langle +| V |-\rangle^2}{-\omega - (\omega)} = -\frac{\varepsilon^2}{2\omega}. \tag{22}$$

Let us compare to the exact solution. We will set $\lambda = 1$ for simplicity here since we already have ε to characterize the strength of the perturbation. Then the exact spectrum of $H = H_0 + \varepsilon V$ is

$$E_\pm = \omega_0 \pm \sqrt{\omega^2 + \varepsilon^2} \tag{23}$$

The above can be derived by brute force, analogy to a spin problem, or by squaring $H - \omega_0$ and obtaining $\omega^2 + \varepsilon^2$ and taking the square root, noting that there has to be a positive and negative branch since tr $(H - \omega_0) = 0$. In any case, for $\omega \gg \varepsilon$ we can expand the square root in small ε to obtain

$$E_\pm = E_\pm^{(0)} \pm \frac{\varepsilon^2}{2\omega} \tag{24}$$

which precisely matches the perturbation theory calculation.

However, in the degenerate limit $\omega \to 0$ we instead obtain

$$E_\pm = \omega_0 \pm \varepsilon \tag{25}$$

such that now there is a *first order* correction to the energies, despite the fact that the first order standard perturbation theory result (21) is zero. One way to view the origin of this issue is that, when there is degeneracy, there is no preferred basis for the eigenstates of H_0. If, instead, we choose the $|\pm x\rangle$ basis, for $\omega = 0$ the states would still be eigenstates of H_0 but we would recover the first order correction $\langle \pm x| V |\pm x\rangle = \pm\varepsilon$. These nonzero matrix elements in the $|\pm x\rangle$ basis can also manifest as off diagonal matrix elements in the $|\pm z\rangle$ basis, i.e.

$$\langle \pm z| V |\mp z\rangle = \varepsilon. \tag{26}$$

The conclusion is that, in degenerate perturbation theory, off-diagonal matrix elements of the perturbation within the degenerate subspace must be taken into account entirely.

Indeed, the problem must be solved essentially exactly within the degenerate subspace; there is no perturbative simplification to the energies (23) for generic ω, ε. But if the degenerate subspace is a small, isolated part of the entire spectrum of H_0, we don't want to solve the entire Hamiltonian H exactly. We should be able to perturbatively take into account the influence of remote energy levels on the degenerate subspace.

Our goal will then be to derive an effective Hamiltonian that only acts within a suitably perturbed degenerate subspace. The leading corrections to this effective Hamiltonian will be that of H_0 and the projected perturbation, and the subleading corrections will involve the influence of energy levels outside the degenerate subspace. This effective Hamiltonian can then be diagonalized afterwards.

We will begin by labeling eigenstates of the unperturbed degenerate eigenspace as $|n^{(0)}, l\rangle$, where n labels the degenerate eigenspace of interest and l labels the states within the eigenspace such that $H_0 |n^{(0)}, l\rangle = E^{(0)}_{n,l} |n^{(0)}, l\rangle$ where $E^{(0)}_{n,l}$ are not necessarily distinct for different l — we are allowing for degeneracy after all! We have, for simplicity, chosen a basis where H_0 acts diagonally, but this is not necessary and in general may not be the most natural basis. However, the basis of the degnerate subspace can also be changed after deriving the effective Hamiltonian. States that are outside the degenerate subspace we will continue to label as $|k^{(0)}\rangle$ with energes $E^{(0)}_k$; degeneracies amongst these states are unimportant for our purposes here, k simply indexes all of the states outside of the degenerate subspace of interest.

The effective Hamiltonian and perturbed degenerate states are defined by demanding that the action of H on $|n, l\rangle$ keeps the state within the degenerate subspace:

$$H |n, l\rangle = h_{n,ll'} |n, l'\rangle \tag{27}$$

Here h is a matrix in the l, l' indices that implicitly depends on λ because H does. We are using the repeated index summation convention, where the repeated l' above implies that the above equation should be interpreted with a sum over l'. We then expand

$$\begin{aligned} h_n &= h^{(0)}_n + \lambda h^{(1)}_n + \lambda^2 h^{(2)}_n + \cdots \\ |n, l\rangle &= |n^{(0)}, l\rangle + \lambda |n^{(1)}, l\rangle + \lambda^2 |n^{(2)}, l\rangle \cdots \end{aligned} \tag{28}$$

as before. Our gauge fixing condition is generalized to

$$\langle n^{(0)}, l | n^{(d)}, l'\rangle = 0, \qquad \text{for } d \geq 1. \tag{29}$$

so that every correction changes the makeup of the degenerate subspace, and doesn't have a part that rotates one basis state into another, for example. With this set up we can more or less directly generalize the non-degenerate perturbation theory to the degenerate case.

Expanding out the eigenequation (27), and writing $\Delta_{n,ll'} = h_{n,ll'} - E^{(0)}_n \delta_{ll'}$, we can manipulate the eigenequation as before to obtain

$$(E^{(0)}_{nl} - H_0) |n, l\rangle = (\lambda V \delta_{ll'} - \Delta_{nll'}) |n, l'\rangle . \tag{30}$$

We have introduced $\delta_{ll'}$ factors on the Hilbert space operators, like λV, that do not directly act on the l index of the state, in order to consistently have $|n, l'\rangle$ on the right hand side of the above equation and $|n, l\rangle$ on the left hand side. Acting with $\langle n^{(0)}, l''|$ from the left, the left hand side simplifies to

$$\langle n^{(0)}, l''| (E^{(0)}_{nl} - H_0) |n, l\rangle = (E^{(0)}_{nl} - E_{nl''}) \langle n^{(0)}, l'' | n, l\rangle = (E^{(0)}_{nl} - E_{nl''}) \delta_{l,l''} = 0 \tag{31}$$

where we used (29) in the second to final equality above. We then arive at

$$\langle n^{(0)}, l''| (\lambda V \delta_{ll'} - \Delta_{n,ll'}) |n, l'\rangle = 0 \tag{32}$$

which says that the state $(\lambda V \delta_{ll'} - \Delta_{n,ll'}) |n, l'\rangle$ is orthogonal to $|n^{(0)}, l''\rangle$ for all l''; that is, it is orthogonal to the unperturbed degenerate subspace. Again using $\langle n^{(0)}, l'' | n, l'\rangle = \delta_{l',l''}$, we have

$$\Delta_{nll'} = \langle n^{(0)}, l| \lambda V |n, l'\rangle \implies h^{(d)}_{l,l'} = \langle n^{(0)}, l| V |n^{(d-1)}, l'\rangle \tag{33}$$

so that we can compute the order d effective Hamiltonian in terms of the order $d-1$ states.

Next we act with $\langle k^{(0)}|$ on (30); i.e. we are acting with an eigenstate outside the degenerate subspace. We then obtain

$$\langle k^{(0)}|n,l\rangle = \frac{1}{E^{(0)}_{nl} - E^{(0)}_{k}} \langle k^{(0)}| \left(\lambda V \delta_{ll'} + \Delta_{n,ll'}\right) |n,l'\rangle \tag{34}$$

so that the basis expansion $|n,l\rangle = |n^{(0)},l\rangle + \sum_{k\neq n} \langle k^{(0)}|n,l\rangle\, |k^{(0)}\rangle$ yields

$$|n,l\rangle = |n^{(0)},l\rangle + \sum_{k\neq n} \frac{1}{E^{(0)}_{nl} - E^{(0)}_{k}} \langle k^{(0)}| \left(\lambda V \delta_{ll'} + \Delta_{n,ll'}\right) |n,l'\rangle\, |k^{(0)}\rangle\,. \tag{35}$$

The equations (33) and (35) again play the role of enabling us to calculate higher order terms in the expansion from lower order ones. Let us compute the first few corrections. The first order correction to the effective Hamiltonian is

$$h^{(1)}_{n,ll'} = \langle n^{(0)},l'|\, V\, |n^{(0)},l\rangle\,. \tag{36}$$

We see that the effective Hamiltonian takes into account the projection of V on the degenerate subspace entirely. For the two dimensional example above, this would represent no simplification at all, but if the degenerate subspace is small relative to the entire Hilbert space then (36) can be very helpful. Diagonalizing $h^{(1)}_{n,ll'}$ can range from easy to extremely difficult or impossible depending on the size and complexity of the degenerate space.

At higher order we arrive at corrections that change the makeup of the degenerate subspace through (35). At leading order, as before, we can replace $|n,l\rangle \to |n^{(0)},l\rangle$ on the right hand side so that the $\Delta_{n,ll'}$ term drops by orthogonality. We then obtain

$$|n^{(1)},l\rangle = \sum_{k\neq n} \frac{\langle k^{(0)}|\, V\, |n,l\rangle}{E^{(0)}_{nl} - E^{(0)}_{k}}\, |k^{(0)}\rangle\,, \tag{37}$$

and the associated second order correction to the effective Hamiltonian

$$h^{(2)}_{n,ll'} = \sum_{k} \frac{\langle n,l|\, V\, |k^{(0)}\rangle\, \langle k^{(0)}|\, V\, |n,l'\rangle}{E^{(0)}_{nl} - E^{(0)}_{k}}. \tag{38}$$

There is a nice way to think about (38); the perturbation kicks one out of the degenerate subspace, leading to the matrix element from $\langle k^{(0)}|\, V\, |n,l\rangle$ and then brings one back to the degenerate subspace, though not necessarily in the same state, leading to the matrix element $\langle n,l|\, V\, |k^{(0)}\rangle$. Because of the "intermediate" high energy state $|k^{(0)}\rangle$, this process is divided by $(E^{(0)}_{nl} - E^{(0)}_{k})^{-1}$ which suppresses the process if the intermediate state is very far away in energy.