Week 8 Worksheet Solutions
(Nondegenerate) Peturbation Theory

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Exercise 1. Let $H = H^0 + H^1$ be a perturbed hamiltonian. Suppose we know

$$H^0 |n^0\rangle = E_n^0 |n^0\rangle ,$$

where the $|n^0\rangle$ are the unperturbed, orthonormal, nondegenerate eigenstates.

a) Expand the exact solutions for H, $|n\rangle$ and E_n, in perturbation expansions.

b) Write the Schrödinger equation for H in terms of the above expansions.

c) Study the first order part of the equation from (b), and derive the first order corrections to the energies. You should get

$$E_n^1 = \langle n^0|H^1|n^0\rangle .$$

d) Along the way to solving (c), you should have come up with the equation

$$H^0 |n^1\rangle + H^1 |n^0\rangle = E_n^1 |n^0\rangle + E_n^0 |n^1\rangle .$$

Using this equation, find the expansion of $|n^1\rangle$ in the eigenbasis of H^0.
Hints: In order to find the component of $|n^1\rangle$ which is parallel to $|n^0\rangle$, enforce normalization of $|n\rangle$ to first order, i.e. $|n^0\rangle + |n^1\rangle$ should have norm 1. It will be helpful to write $|n^1\rangle = |n_\parallel\rangle + |n_\perp\rangle$, where $\langle n^0|n_\perp\rangle = 0$; also, use the fact that—to first order—$e^{ia} = 1 + ia$.

e) Derive the second order corrections to the energies, E_n^2.

a) We write

$$|n\rangle = \sum_{k=0}^{\infty} \lambda^k |n^k\rangle$$

$$E_n = \sum_{k=0}^{\infty} \lambda^k E_n^k.$$

b) Recall that $H = H^0 + \lambda H^1$. Then we have

$$\begin{aligned} H\,|n\rangle &= E_n\,|n\rangle \\ (H^0 + \lambda H^1)\sum \lambda^k\,|n^k\rangle &= \sum \lambda^{k+j} E_n^k\,|n^j\rangle\,. \end{aligned}$$

c) The order λ part of the equation from (b) is

$$H^0\,|n^1\rangle + H^1\,|n^0\rangle = E_n^1\,|n^0\rangle + E_n^0\,|n^1\rangle\,.$$

Bracket this equation with $\langle n^0|$ to obtain

$$E_n^0\,\langle n^0|n^1\rangle + \langle n^0|H^1|n^0\rangle = E_n^1 + E_n^0\,\langle n^0|n^1\rangle\,,$$

from which we immediately obtain the desired result.

d) The idea is that we want to write $|n^1\rangle$ in the eigenbasis of H^0. So we want to write

$$|n^1\rangle = \sum c_m\,|m^0\rangle\,,$$

and we know that the coefficients c_m are given by

$$c_m = \langle m^0|n^1\rangle\,.$$

Thus, we want to bracket the equation from (d) with $\langle m^0|$ with m not necessarily equal to n, and try to write down an equation for c_m. Doing this bracket, we have

$$E_m^0\,\langle m^0|n^1\rangle + \langle m^0|H^1|n^0\rangle = E_n^1\delta_{nm} + E_n^0\,\langle m^0|n^1\rangle\,.$$

Now, notice that if $m = n$, the equation we obtained doesn't tell us anything. But, if $m \neq n$, we immediately have

$$c_m = \frac{\langle m^0|H^1|n^0\rangle}{E_n^0 - E_m^0}.$$

For the case $m = n$, we follow the hint. Normalization of $|n\rangle$ to first order gives

$$1 = \langle n^0|n^0\rangle + \langle n^0|n_\parallel^1\rangle + \langle n_\parallel^1|n^0\rangle\,,$$

where we note that terms like $\langle n^1|n^1\rangle$ are second order and can be ignored. Since $|n^0\rangle$ is also assumed normalized, we have

$$0 = 2\text{Re}\,[\langle n^0|n_\parallel^1\rangle],$$

so that we can set

$$|n_\parallel^1\rangle = i a\,|n^0\rangle\,,$$

with $a \in \mathbb{R}$. Thus,

$$\begin{aligned}|n\rangle =&(1+ia)\,|n^0\rangle + |n^1_\perp\rangle\\ =&e^{ia}\,|n^0\rangle + |n^1_\perp\rangle\,.\end{aligned}$$

Since we can absorb the phase into the definition of $|n^0\rangle$, we find

$$\begin{aligned}|n^1\rangle &= |n^1_\perp\rangle\\ &= \sum_{m\neq n} \frac{\langle m^0|H^1|n^0\rangle}{E^0_n - E^0_m}\,|m^0\rangle\,,\end{aligned}$$

i.e. we can set $c_n = 0$.

e) We write down the second order equation obtained from the result of (b):

$$H^0\,|n^2\rangle + H^1\,|n^1\rangle = E^2_n\,|n^0\rangle + E^1_n\,|n^1\rangle + E^0_n\,|n^2\rangle\,.$$

Then we bracket with $\langle n^0|$ to find

$$\langle n^0|H^1|n^1\rangle = E^2_n,$$

so

$$E^2_n = \sum_{m\neq n} \frac{|\,\langle m|H^1|n\rangle\,|^2}{E^0_n - E^0_m}.$$

Exercise 2. Suppose you want to calculate the expectation value of some observable A in the n^{th} energy eigenstate of a system perturbed by H^1,

$$\langle A\rangle = \langle n|A|n\rangle.$$

Suppose further that all eigenstates are nondegenerate.

a) Replace $|n\rangle$ by its perturbation expansion, and write down the formula for the first order correction to $\langle A\rangle$, $\langle A\rangle^1$.

b) Use the first order corrections to the states,

$$|n^1\rangle = \sum_{m\neq n} \frac{\langle m^0|\,H^1\,|n^0\rangle}{E^0_n - E^0_m}\,|m^0\rangle\,,$$

to rewrite $\langle A\rangle^1$ in terms of the unperturbed eigenstates.

c) If $A = H^1$, what does the result of (b) tell you? Explain why this is consistent with the result of Exercise 1(e),

$$E^2_n = \sum_{m\neq n} \frac{|\,\langle m|H^1|n\rangle\,|^2}{E^0_n - E^0_m}.$$

a) We write

$$|n\rangle = |n^0\rangle + \lambda\, |n^1\rangle + \lambda^2\, |n^2\rangle + \cdots .$$

Thus,

$$\langle A\rangle = \langle n^0|A|n^0\rangle + 2\text{Re}\, \langle n^0|A|n^1\rangle + \cdots ,$$

so $\langle A\rangle^1 = 2\text{Re}\, \langle n^0|A|n^1\rangle$.

b) Plugging in the expression for $|n^1\rangle$ given above, we get

$$\langle A\rangle^1 = 2\text{Re} \sum_{m\neq n} \frac{\langle m^0|H^1|n^0\rangle}{E_n^0 - E_m^0} \langle n^0|A|m^0\rangle.$$

c) If $A = H^1$, then we get that the first order correction to the expectation value of H^1 is given by

$$2\sum_{m\neq n} \frac{|H^1_{mn}|^2}{E_n^0 - E_m^0},$$

where $H^1_{mn} = \langle m|H^1|n\rangle$. On the other hand, the equation from 1(e) is

$$E_n^2 = \sum_{m\neq n} \frac{|H^1_{mn}|^2}{E_n^0 - E_m^0}.$$

So we have found

$$\langle H^1\rangle^1 = 2E_n^2.$$

On the other hand,

$$\begin{aligned}\langle H\rangle &= \langle H\rangle^0 + \langle H\rangle^1 + \langle H\rangle^2 \cdots \\ &= \langle H^0\rangle^0 + \langle H^1\rangle^0 + \langle H^0\rangle^1 + \langle H^1\rangle^1 + \langle H^0\rangle^2 + \cdots ,\end{aligned}$$

where the ellipsis denotes third and higher order terms. Thus, if we truncate to second order, we must have

$$E_n^2 = \langle H^1\rangle^1 + \langle H^0\rangle^2 ,$$

where $\langle H^0\rangle^2$ denotes the expectation value of H^0 with respect to the state $|n^2\rangle$, and we expect this expectation value to be exactly $-E_n^2$.