# 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

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

c) The order $\lambda$ part of the equation from (b) is

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

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

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

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

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

so that we can set

$$\left| n_{\parallel}^1 \right\rangle = i a \left| n^0 \right\rangle ,$$

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

$$\begin{aligned} \left| n \right\rangle =& (1 + i a) \left| n^0 \right\rangle + \left| n_{\perp}^1 \right\rangle \\ =& e^{ia} \left| n^0 \right\rangle + \left| n_{\perp}^1 \right\rangle . \end{aligned}$$

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

$$\left| n^1 \right\rangle = \left| n_{\perp}^1 \right\rangle ,$$

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

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

$$H^0 |n^2\rangle + H^1 |n^1\rangle = E_n^2 |n^0\rangle + E_n^1 |n^1\rangle + E_n^0 |n^2\rangle .$$

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

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

so

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

**Exercise 2.** Suppose you want to calculate the expectation value of some observable $A$ in the $n^{\text{th}}$ 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,

$$|n^1\rangle = \sum_{m\neq n} \frac{\langle m^0|\, H^1\, |n^0\rangle}{E_n^0 - E_m^0} |m^0\rangle ,$$

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),

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

a) We write

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

Thus,

$$\langle A\rangle = \langle n|A|n\rangle + 2\mathrm{Re}\,\langle n|A|n\rangle + \cdots ,$$

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

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

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

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

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

where $H'_{mn} = \langle m | H' | n \rangle$. This is consistent with the equation from 1(d), since we are looking for the expectation value *in the* $n^{\text{th}}$ *energy eigenstate*.