Week 4 Worksheet Solutions
(Nondegenerate) Peturbation Theory

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Exercise 1. 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,

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

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 second order corrections to the energy,

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

a) We write

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

Thus,

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

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

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

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

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 second order energy correction 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 $-E_n^2$.