Week 7 Worksheet
(Nondegenerate) Peturbation Theory

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Exercise 1. Let $H(\lambda) = H^0 + \lambda H'$ be a perturbed hamiltonian. Suppose we know

$$H^0 \psi_n^0 = E_n^0 \psi_n^0,$$

where the ψ_n^0 are unperturbed, orthonormal, nondegenerate eigenfunctions.

a) Write the ψ_n and E_n as power series in λ.

b) Write the Schrödinger equation for $H(\lambda)$ in terms of the above power series.

c) Truncate the above equation to first order, and derive the first order corrections to the energies. You should get

$$E_n^1 = \left\langle \psi_n^0 \middle| H' \middle| \psi_n^0 \right\rangle.$$

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

$$H^0 \psi_n^1 + H' \psi_n^0 = E_n^1 \psi_n^0 + E_n^0 \psi_n^1.$$

Rewrite this as an inhomogeneous differential equation for ψ_n^1, and solve it via the power series method, thus obtaining the first order corrections to the wavefunctions.

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

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',

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

Suppose further that all eigenstates are nondegenerate.

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

b) Use the first order corrections to the wavefunctions,

$$\psi_n^1 = \sum_{m \neq n} \frac{\left\langle \psi_m^0 \middle| H' \middle| \psi_n^0 \right\rangle}{E_n^0 - E_m^0} \psi_m^0, \tag{1}$$

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

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

a) We write

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \cdots .$$

Thus,

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

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

b) Plugging in the expression for ψ_n^1 given above, we get

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

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 $H'_{mn} = \langle \psi_m^0 | H' | \psi_n^0 \rangle$.

This is consistent with Equation 1, since we are looking for the expectation value *in the n^{th} energy eigenstate*.