Problem Set #4, Due: Wednesday February 15 by 11:00am

PHY 362K - Quantum Mechanics II, UT Austin, Spring 2017
(Dated: February 10, 2017)

I. PERTURBED HARMONIC OSCILLATOR

Consider a perturbed Harmonic oscillator with Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{1}$$

where the "bare" Hamiltonian is:

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{2}$$

and we perturb with a linear potential:

$$\hat{V} = g\hat{x} \tag{3}$$

where g is a constant.

1. Perturbatively compute the energy levels of $\hat{H}$ to second order in V and the energy eigenstates to first order in V.

   Solution: The first order correction to the energy levels is given by

   $$E_n^1 = \langle n^0|\hat{V}|n^0\rangle = g\langle n^0|\hat{x}|n^0\rangle$$

   We can write $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$, making this substitution and recalling that $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, we find:

   $$\begin{aligned} E_n^1 &= g\sqrt{\frac{\hbar}{2m\omega}}\left(\langle n^0|\hat{a}|n^0\rangle + \langle n^0|\hat{a}^\dagger|n^0\rangle\right) \\ &= g\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\langle n^0|(n-1)^0\rangle + \sqrt{n+1}\langle n^0|(n-1)^0\rangle\right) \end{aligned}$$

   but the states $|n^0\rangle$ are orthogonal, so this expression reduces to

   $$\boxed{E_n^1 = 0} \tag{4}$$

   The second order correction to the energy levels is given by

   $$E_n^2 = \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{|\langle m^0|\hat{V}|n^0\rangle|^2}{E_n^0 - E_m^0} = g^2 \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{|\langle m^0|\hat{x}|n^0\rangle|^2}{E_n^0 - E_m^0}$$

   writing $\hat{x}$ in terms of the creation and annihilation operators, this becomes

   $$E_n^2 = g^2\frac{\hbar}{2m\omega} \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{|\langle m^0|\hat{a} + \hat{a}^\dagger|n^0\rangle|^2}{E_n^0 - E_m^0}$$

but we know that the ground state energies of the unperturbed harmonic oscillator are $E_n^0 = \hbar\omega(n+1/2)$, so we can write

$$\begin{aligned}
E_n^2 &= g^2 \frac{\hbar}{2m\omega} \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{|\langle m^0|\hat{a}|n^0\rangle + \langle m^0|\hat{a}^\dagger|n^0\rangle|^2}{\hbar\omega(n+1/2) - \hbar\omega(m+1/2)} \\
&= \frac{g^2}{2m\omega^2} \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{|\sqrt{n}\langle m^0|(n-1)^0\rangle + \sqrt{n+1}\langle m^0|(n+1)^0\rangle|^2}{n-m} \\
&= \frac{g^2}{2m\omega^2} \left(\frac{|\sqrt{n}|^2}{n-(n-1)} + \frac{|\sqrt{n+1}|^2}{n-(n+1)} \right)
\end{aligned}$$

where the last line follows from the orthogonality of the energy eigenstates of the unperturbed Hamiltonian, $|n^0\rangle$. Simplifying, we find

$$\boxed{E_n^2 = -\frac{g^2}{2m\omega^2}} \tag{5}$$

The first order correction to the energy eigenstates is given by

$$\begin{aligned}
|n^1\rangle &= \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{\langle m^0|\hat{V}|n^0\rangle}{E_n^0 - E_m^0}|m^0\rangle = g\sqrt{\frac{\hbar}{2m\omega}} \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{\langle m^0|\hat{a}+\hat{a}^\dagger|n^0\rangle}{\hbar\omega(n+1/2) - \hbar\omega(m+1/2)}|m^0\rangle \\
&= \frac{g}{\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}} \sum_{\substack{m=0 \\ m\neq n}}^{\infty} \frac{\sqrt{n}\langle m^0|(n-1)^0\rangle + \sqrt{n+1}\langle m^0|(n+1)^0\rangle}{n-m}|m^0\rangle \\
&= \frac{g}{\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}} \left[\frac{\sqrt{n}}{n-(n-1)}|(n-1)^0\rangle + \frac{\sqrt{n+1}}{n-(n+1)}|(n+1)^0\rangle \right]
\end{aligned}$$

where the last line follows from the orthogonality of the energy eigenstates of the unperturbed Hamiltonian. Simplifying, we find

$$\boxed{|n^1\rangle = \frac{g}{\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}} \left[\sqrt{n}|(n-1)^0\rangle - \sqrt{n+1}|(n+1)^0\rangle\right]} \tag{6}$$

2. What is the condition on g for this perturbative approximation to be accurate?

   Solution:

3. Why does the first order correction to energy vanish? (Hint: consider the symmetries of the $\frac{1}{2}m\omega^2\hat{x}^2$ potential). Similarly, can you explain the presence/absence of even/odd n terms in the first order correction to the energy eigenstates?

   Solution: Let $\hat{P}$ be the parity operator, which is a unitary operator that maps $\hat{x}$ to $-\hat{x}$ and $\hat{p}$ to $-\hat{p}$. Note that since all occurrences of $\hat{x}$ and $\hat{p}$ in $\hat{H}_0$ are raised to an even power, $\hat{H}_0$ is unaffected by the parity operator, which is to say that $\hat{P}^\dagger\hat{H}_0\hat{P} = \hat{H}_0$. However, since $\hat{V} = g\hat{x}$, $\hat{V}$ switches signs under the parity operator, which is to say that $\hat{P}^\dagger V\hat{P} = -\hat{V}$. Now, note that since $\hat{P}$ is unitary,

$$\hat{P}^\dagger\hat{H}_0\hat{P} = \hat{H}_0 \implies \hat{H}_0\hat{P} = \hat{P}\hat{H}_0$$

which is to say that $\hat{H}_0$ and $\hat{P}$ commute. Therefore $\hat{H}_0$ and $\hat{P}$ have simultaneous eigenstates. Therefore $\hat{P}|n^0\rangle = \lambda|n^0\rangle \implies |n^0\rangle = \frac{\hat{P}|n^0\rangle}{\lambda}$. So we can write

$$E_n^1 = \langle n^0|\hat{V}|n^0\rangle = \frac{\langle n^0|\hat{P}^\dagger\hat{V}\hat{P}|n^0\rangle}{\lambda^*\lambda} = \frac{\langle n^0|(-\hat{V})|n^0\rangle}{\lambda^*\lambda}$$

but $\hat{P}$ is unitary, so $|\lambda|^2 = 1$, therefore

$$E_n^1 = -\langle n^0|\hat{V}|n^0\rangle = -E_n^1 \implies E_n^1 = 0$$

So the fact that H_0 is symmetric under parity while the perturbation $\hat{V}$ is antisymmetric forces the first order correction to the energy to vanish.

4. This problem can also be exactly solved (without much effort – try changing variables to re-write it as a different harmonic oscillator Hamiltonian). What are the exact energies? How does this compare to the perturbative approximation for small g? (Hint: you might also use this to check your answer to the previous parts.)

II. HIGHER ORDERS IN PERTURBATION THEORY AND WAVE-FUNCTION RENORMALIZATION

Consider a generic Hamiltonian:

$$\hat{H} = \hat{H}_0 + \lambda\hat{V} \tag{7}$$

As in class, we will treat $\lambda\hat{V}$ as a perturbation and expand the full eigenstates, $|n\rangle$, and eigenenergies, ε_n of $\hat{H}$ in a power series in λ:

$$|n\rangle = \sqrt{Z_n}\left(\sum_{k=0}^{\infty}\lambda^k|n^k\rangle\right)$$
$$\varepsilon_n = \sum_{k=0}^{\infty}\lambda^k\varepsilon_n^k \tag{8}$$

where $|n^0\rangle$ are the eigenstates of the unperturbed Hamiltonian, $\hat{H}_0$: $\hat{H}_0|n^0\rangle = \varepsilon_n^0|n^0\rangle$You may assume that: $\varepsilon_n^0 \neq \varepsilon_m^0$ for all $m \neq n$ (i.e. there are no degeneracies).

In class we worked out expressions for $|n^1\rangle$ and $\varepsilon_n^{1,2}$.

1. Wave-function (re)normalization: The normalization constant Z_n dropped out of the eigenvalue equation for $\hat{H}$. However, properly normalizing $|n\rangle$ becomes important if we want to compute, say, the expectation value $\langle n|\hat{O}|n\rangle$ of other observables, $\hat{O}$. Note that since $Z_n = |\langle n_0|n\rangle|^2$, we can physically interpret this quantity as the probability that a particle in the exact $\hat{H}$-eigenstate $|n\rangle$ is measured in the the unperturbed eigenstate $|n^0\rangle$.
   (a) Find Z_n up to second order in λ so that $|n\rangle$ is properly normalized ($\langle n|n\rangle = 1$). At what order in λ does the first non-zero correction to $Z_n^0 = 1$ appear?
   (b) Show, to this order, that $Z_n = \dfrac{\partial\varepsilon_n}{\partial\varepsilon_n^0}$ (Note: though you will demonstrate this up to second order in λ, this relationship actually holds to all orders!).
2. Next Higher order terms: Compute the expression for the second order correction to the energy eigenstates, $|n^2\rangle$, and third order correction to the energies, ε_n^3 in terms of the unperturbed eigenstates and energies of $\hat{H}_0$.

III. DEGENERATE PERTURBATION THEORY EXAMPLE – TWO SPINS-1/2

Consider two spins-1/2, with spin-operators $\hat{\mathbf{S}}_{1,2} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}$, where $\sigma^{x,y,z}$ are Pauli operators, and Hamiltonian:

$$H = J\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 + g\hat{S}_1^x \left(\frac{1}{\hbar}\hat{S}_2^z + \frac{1}{2}\right) \tag{9}$$

Suppose that, $J, g > 0$, and $g \ll J$, and compute the energy-eigenstates to first order in g, and the energies to second order in g (be sure to properly take care of any degeneracies).

Hint: to solve for the unperturbed eigenstates with $g = 0$, you can use that $\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 = \frac{1}{2}\left[\left(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2\right)^2 - \hat{\mathbf{S}}_1^2 - \hat{\mathbf{S}}_2^2\right]$, and the properties of adding angular momentum that you learned last semester.