Graduate Quantum Mechanics II - Problem Set 7 - Solution

Problem 1)

This is a somewhat simpleminded test that the time-independent Perturbation Expansion doesn’t produce any nonsense if applied to a (very) simple problem: Assume you know the complete set of eigenfunctions $|\phi_n\rangle$ of some Hamiltonian $H_0$ with $H_0|\phi_n\rangle = E_n |\phi_n\rangle$ (no degeneracy). Now assume we introduce as a “perturbation” an additional term to the Hamiltonian, which is simply a constant potential: $H_p = V_p$ (real constant).

1) Calculate the new energies of the system to first order perturbation theory. Explain your results in comparison with what you would expect.

Solution:

In first order perturbation theory, $E_n' = E_n + \langle \phi_n | H_p | \phi_n \rangle = E_n + V_p \langle \phi_n | \phi_n \rangle = E_n + V_p$. This is indeed what one would expect – the addition of the constant term to the potential simply raises all energy eigenvalues by the same amount.

2) Calculate the “perturbed” wave function to first order. Evaluate your result. Again, comment on the result in light of what one would expect.

Solution:

$|\phi_n'\rangle = |\phi_n\rangle + \sum_{m \neq n} \frac{\langle \phi_m | H_p | \phi_n \rangle}{E_n - E_m} |\phi_m\rangle = |\phi_n\rangle + \sum_{m \neq n} \frac{V_p \langle \phi_m | \phi_n \rangle}{E_n - E_m} |\phi_m\rangle = |\phi_n\rangle + 0$, i.e. the wave function is unchanged. This makes sense since an energy offset by a constant has no observable consequences and therefore the eigenstates should remain the same.

3) What is the 2nd order correction to the energies?

Solution:

For the same reason, the answer is that the 2nd order correction is zero. In fact, the 1st order answer is the only change needed to all orders of perturbation theory.

Problem 2)

Consider the Harmonic Oscillator in one dimension. The Hamiltonian is given by $H_0 = \frac{P^2}{2m} + \frac{m\omega^2}{2} X^2$ with eigenfunctions $|\phi_n\rangle$ and eigenvalues $E_n = (n + \frac{1}{2})\hbar\omega$. Now we introduce a “perturbing” additional potential of the form $H_p = \lambda X^2$, $H = H_0 + H_p$.

Let’s calculate the new ground state wave function $|\psi_0'\rangle$ and the ground state energy $E_0'$, $H|\psi_0'\rangle = E_0'|\psi_0'\rangle$ of the system, in three different ways:
1) Write down the exact solution of the full Hamiltonian, using your knowledge of the Harmonic Oscillator and its ground state eigenfunction (without any complicated calculations). Expand the new ground state energy up to 2nd order in \( \lambda \) and the new ground state wave function up to 1st order in \( \lambda \) (meaning, write both of them as a Taylor series around \( \lambda = 0 \) up to 2nd power in \( \lambda \) for \( E_0' \) and up to 1st power in \( \lambda \) for \( \psi_0' \)).

Solution:

The new Hamiltonian is
\[
H = H_0 + H_p = \frac{P^2}{2m} + \left( \frac{m\omega^2}{2} + \lambda \right) X^2 = \frac{P^2}{2m} + \frac{m\omega'^2}{2} X^2 \text{ with } \omega'^2 = \omega^2 + \frac{2\lambda}{m}.
\]
The ground state solution is the usual HO ground state with the new frequency:
\[
H|\psi_0\rangle = \frac{1}{2} \hbar \omega'|\psi_0\rangle \text{ with } \psi_0'(x) = \left( \frac{m\omega'}{\hbar \pi} \right)^{1/4} e^{-m\omega' x^2/2\hbar}. \]
The new ground state energy can be written in powers of the (small) parameter \( \lambda \) as follows:
\[
E_0' = \frac{1}{2} \hbar \omega' = \frac{1}{2} \hbar \sqrt{\omega^2 + \frac{2\lambda}{m}} = \frac{1}{2} \hbar \omega \sqrt{1 + \frac{2\lambda}{m\omega^2}} = \frac{1}{2} \hbar \omega \left( 1 + \frac{1}{2} \frac{2\lambda}{m\omega^2} - \frac{1}{8} \left( \frac{2\lambda}{m\omega^2} \right)^2 \ldots \right) = E_0 + \frac{\lambda \hbar}{2m\omega} - \frac{\lambda^2 \hbar}{4m^2\omega^3}.
\]

For the Taylor expansion of the new wave function I get
\[
\psi_0'(x) = \left( \frac{m\omega'}{\hbar \pi} \right)^{1/4} e^{-m\omega' x^2/2\hbar} = \left( \frac{m\omega}{\hbar \pi} \right)^{1/4} e^{-m\omega x^2/2\hbar} + \frac{d\psi_0'(x)}{d\omega'} \frac{d\omega'}{d\lambda} \lambda + \ldots =
\psi_0(x) + \left( \frac{m}{\hbar \pi} \right)^{1/4} \frac{1}{4} \omega^{-3/4} e^{-m\omega x^2/2\hbar} - \frac{m}{2\hbar} \left( \frac{m\omega}{\hbar \pi} \right)^{1/4} e^{-m\omega x^2/2\hbar} \frac{\lambda}{m\omega} = \psi_0(x) + \left( \frac{m\omega}{\hbar \pi} \right)^{1/4} \left[ - \frac{\lambda x^2}{4m\omega^2} \frac{1}{2\hbar \omega} \right] e^{-m\omega x^2/2\hbar}.
\]

2) Use the variational method to find the new ground state of the full Hamiltonian. Choose as your “trial wave function” a Gaussian with arbitrary width and follow the usual recipe to find the optimal width, the corresponding wave function and the energy of the ground state. Comment on your result (compare with 1).

Solution:

We use as our trial wave function \( \phi(x) = \left( \frac{2\alpha}{\pi} \right)^{1/4} e^{-\alpha x^2} \) which is properly normalized. The expectation value of the full Hamiltonian is then
Therefore the only element in the sum that is not zero is that for $m = 2$:

$$\langle E \rangle = \left\langle \phi \right| \frac{\hbar^2}{2m} + \left( \frac{m\omega^2}{2} + \lambda \right) X^2 \left| \phi \right\rangle = \int_{-\infty}^{\infty} dx \phi^*(x) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2} + \left( \frac{m\omega^2}{2} + \lambda \right) x^2 \phi(x) \right] =
$$

$$\left( \frac{2\alpha}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx e^{-\alpha x^2} \left[ \frac{\hbar^2}{2m} \frac{\partial}{\partial x} + \left( \frac{m\omega^2}{2} + \lambda \right) e^{-\alpha x^2} \right] = \left( \frac{2\alpha}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx e^{-2\alpha x^2} \left[ \frac{\hbar^2}{2m} \left( 2\alpha - 4\alpha^2 x^2 \right) + \left( \frac{m\omega^2}{2} + \lambda \right) \right]
$$

$$= \frac{\hbar^2 \alpha}{m} + \left( \frac{2\alpha}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx e^{-2\alpha x^2} \left[ \frac{m\omega^2}{2} + \lambda - \frac{2\hbar^2 \alpha^2}{m} \right] = \frac{\hbar^2 \alpha}{m} + \left( \frac{m\omega^2}{2} + \lambda - \frac{2\hbar^2 \alpha^2}{m} \right) \frac{1}{4\alpha} = \frac{\hbar^2 \alpha}{m} \left( \frac{m\omega^2}{2} + \lambda \right) \frac{1}{4\alpha}
$$

We need to find the value of $\alpha$ which makes this expression a minimum. Taking the derivative with respect to $\alpha$ yields $0 = \frac{\hbar^2}{2m} - \left( \frac{m\omega^2}{2} + \lambda \right) \frac{1}{4\alpha^2} \Rightarrow 4\alpha^2 = \left( \frac{m^2\omega^2}{\hbar^2} + \frac{2m\lambda}{\hbar^2} \right)$ or

$$\alpha = \frac{m}{2\hbar} \sqrt{\omega^2 + \frac{2\lambda}{m}} = \frac{m\omega'}{2\hbar}$$

which is the same result we found before. In particular, the wave function assumes the correct shape and normalization with this choice of $\alpha$, and the ground state energy becomes $E_0 \Rightarrow \frac{\hbar^2 \alpha}{2m} + \left( \frac{m\omega^2}{2} + \lambda \right) \frac{1}{4\alpha} = \frac{\hbar \omega'}{4} + \frac{m}{2} \omega^2 \frac{\hbar}{2m\omega} = \frac{\hbar \omega'}{2}$

q.e.d.

3) Find the perturbed wave function up to first order and the new energy up to second order perturbation theory. Make sure you evaluate any expressions involving expansions in terms of HO eigenstates as far as you can to get the most simple (and directly interpretable) result. Compare with 1) – do you get the same answer?

**Hint:** You can find useful information in Lecture Note 16 from last semester.

**Solution:**

We first find the perturbed wave function:

$$|\psi_0\rangle = |\psi_0\rangle + \sum_{m>0} \frac{\langle \psi_m | H | \psi_0 \rangle}{E_0 - E_m} |\psi_m\rangle = |\psi_0\rangle + \sum_{m>0} \frac{\langle \psi_m | X^2 | \psi_0 \rangle}{E_0 - E_m} |\psi_m\rangle \, .$$

From PHYS621 we remember that $X = \sqrt{\frac{\hbar}{m\omega}} \hat{X}$ and $\hat{X} = \frac{1}{\sqrt{2}} (a + a^\dagger)$ so we can write

$$\langle \psi_m | X^2 | \psi_0 \rangle = \frac{\hbar}{2m\omega} \langle \psi_m | (a + a^\dagger)^2 | \psi_0 \rangle \, .$$

We note that $a |\psi_0\rangle = 0$ and

$$a^\dagger |\psi_0\rangle = |\psi_i\rangle \Rightarrow (a + a^\dagger)^2 |\psi_0\rangle = (a + a^\dagger) |\psi_i\rangle = |\psi_0\rangle + \sqrt{2} |\psi_z\rangle \Rightarrow X^2 |\psi_0\rangle = \frac{\hbar}{2m\omega} (|\psi_0\rangle + \sqrt{2} |\psi_z\rangle)$$

Therefore the only element in the sum that is not zero is that for $m = 2$:
\[
\sum_{m=0}^{\infty} \lambda \frac{\langle \psi_m | \mathcal{X}^2 | \psi_0 \rangle}{E_0 - E_m} = \frac{\sqrt{2} \hbar \lambda}{2m \omega} \frac{1}{\sqrt{\frac{1}{2} \hbar \omega - \frac{1}{2} \hbar \omega}} |\psi_2 \rangle = - \frac{\lambda \sqrt{2}}{4m \omega^2} |\psi_2 \rangle .
\]

Putting it all together we find

\[
|\psi_0 \rangle = |\psi_0 \rangle - \frac{\lambda \sqrt{2}}{4m \omega^2} |\psi_2 \rangle \Rightarrow \psi_0 (x) = \psi_0 (x) - \frac{\lambda \sqrt{2}}{4m \omega^2} \left( \frac{m \omega}{\hbar \pi} \right)^{1/4} \sqrt{\frac{1}{8}} H_2 \left( \sqrt{\frac{m \omega}{\hbar}} x \right) e^{-m \omega^2 \hbar / 2h}
\]

\[
\psi_0 (x) + \left( \frac{m \omega}{\hbar \pi} \right)^{1/4} \left[ - \frac{\lambda}{8m \omega^2} \left( \frac{4m \omega}{\hbar} x^2 - 2 \right) \right] e^{-m \omega^2 \hbar / 2h} = \psi_0 (x) + \left( \frac{m \omega}{\hbar \pi} \right)^{1/4} \left[ - \frac{\lambda}{2 \hbar \omega} x^2 + \frac{\lambda}{4m \omega^2} \right] e^{-m \omega^2 \hbar / 2h}
\]

which is exactly what we found in our Taylor expansion under part 1.

For the energy, we can use our results above (both to evaluate \( \langle \psi_0 | \mathcal{X}^2 | \psi_0 \rangle \) and for the numerator of the 2nd order term) to get

\[
E_0' = E_0 + \lambda \langle \psi_0 | \mathcal{X}^2 | \psi_0 \rangle + \sum_{m=0}^{\infty} \lambda^2 \frac{\langle \psi_m | \mathcal{X}^2 | \psi_0 \rangle^2}{E_0 - E_m} =
\]

\[
E_0 + \frac{\hbar}{2m \omega} + \left( \frac{\sqrt{2} \hbar \lambda}{2m \omega} \right)^2 \frac{1}{\sqrt{\frac{1}{2} \hbar \omega - \frac{1}{2} \hbar \omega}} = E_0 + \frac{\hbar \lambda}{2m \omega} - \frac{\hbar^2 \lambda^2}{2m^2 \omega^2} \frac{1}{2 \hbar \omega} = E_0 + \frac{\hbar \lambda}{2m \omega} - \frac{\hbar^2 \lambda^2}{4m^2 \omega^3}
\]

again in full agreement with part 1.