

PHYS 517: Quantum Mechanics II

Homework #6

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1. (**Sakurai 5.1**) A simple harmonic oscillator (in one dimension) is subjected to perturbation

$$\lambda H_1 = bx,$$

where b is a real constant. You may assume without proof that

$$\langle u_{n'} | x | u_n \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n+1} \delta_{n',n+1} + \sqrt{n} \delta_{n',n-1})$$

- (a) Calculate the energy shift of the ground state to lowest nonvanishing order.

Solution:

The the energy shift in unperturbed r^{th} state ket $|n^r\rangle$ is given by

$$\Delta_n = b \langle n^0 | V | n^z 0 \rangle + b^2 \sum_{r \neq n} \frac{|\langle n^0 | V | n^r \rangle|^2}{E_n^0 - E_r^0} + \dots$$

The first order correction for ground state term is

$$b \langle n^0 | V | n^0 \rangle = b \langle 0 | x | 0 \rangle = b \sqrt{\frac{\hbar}{2m\omega}} (\delta_{0,1} + \delta_{0,-1}) = 0$$

Matrix element $\langle n | x | n' \rangle$ clearly vanishes for when n and n' differ by any other quantity than one, 1. The infinite sum gives only single non vanishing term when $|n^r\rangle = |1\rangle$ in that case

$$b^2 \sum_{r \neq n} \frac{|\langle n^0 | V | n^r \rangle|^2}{E_n^0 - E_r^0} = b^2 \frac{|\langle 0 | x | 1 \rangle|^2}{\frac{1}{2}\hbar\omega - \frac{3}{2}\hbar\omega} = b^2 \frac{\left| \sqrt{\frac{\hbar}{2m\omega}} \right|^2}{-\hbar\omega} = -\frac{b^2}{2m\omega^2}$$

This is the first nonvanishing term in the energy correction. □

- (b) Solve this problem exactly and compare with your result in (1a).

Solution:

The total hamiltonian after pertubation becomes

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + bx$$

We can rearrange the terms by completing square for the last two terms to get

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 \left(x + \frac{b}{m\omega^2} \right)^2 - \frac{b^2}{2m\omega^2}$$

This is again a Hamiltonian for a simple harmonic oscillator. The added quantity with x doesnot change the behaviour of the oscillator as it is just coordinate translation, the last term is a constant

energy term. This will give energy eigenvalues exactly as we had before with with an added constant of

$$-\frac{b^2}{2m\omega^2}$$

This is exactly what was found in (1a). □

2. (**Sakurai 5.2**) In nondegenerate time-independent perturbation theory, what is the probability of finding in a perturbed energy eigenstate ($|k\rangle$) the corresponding unperturbed eigenstate ($|k^{(0)}\rangle$)? Solve this upto terms of order g^2

Solution:

The probability of perturbed state to be found in the unperturbed state can be calculated by the normalization constant that normalizes the unperturbed state ket. Let us suppose that Z_n normalizes the perturbed state ket

$$|n\rangle_N = \sqrt{Z_n} |n\rangle$$

where $|n\rangle$ is the perturbed state ket and $|n\rangle_N$ is the normalized ket. This can be found by the relation

$${}_N \langle n|n\rangle_N = Z_n \langle n|n\rangle = 1$$

Using the expansion of perturbed kets we get

$$\begin{aligned} \Rightarrow \frac{1}{Z_n} = \langle n|n\rangle &= (\langle n^0| + \lambda \langle n^1| + \lambda^2 \langle n^2| + \dots) \times (|n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \dots) \\ &= 1 + \lambda^2 \langle n^1|n^1\rangle + \mathcal{O}(\lambda^3) \\ &= 1 + \lambda^2 \sum_{k \neq n} \frac{|\langle k|V|n\rangle|^2}{(E_n^0 - E_k^0)^2} + \mathcal{O}(\lambda^3) \end{aligned}$$

So the probability is given by Z_n which is just the inverse of above quantity using the binomial expansion we get

$$Z_n = \left[1 + \lambda^2 \sum_{k \neq n} \frac{|\langle k|V|n\rangle|^2}{(E_n^0 - E_k^0)^2} + \mathcal{O}(\lambda^3) \right]^{-1} = 1 - \lambda^2 \sum_{k \neq n} \frac{|\langle k|V|n\rangle|^2}{(E_n^0 - E_k^0)^2} + \mathcal{O}(\lambda^3)$$

This expression gives the probability of finding the perturbed ket in the original unperturbed state ket. □

3. Consider a one dimensional infinite square well potential

$$H_0 = \frac{p^2}{2m} + U(x)$$

where

$$U(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

Now consider a perturbation by placing a delta function at the center of the well

$$V(x) = \frac{\hbar^2}{mL} \delta\left(x - \frac{L}{2}\right)$$

- (a) What is the unperturbed energy levels and wavefunctions?

Solution:

The schrodingers equation is

$$H |\psi\rangle = E |\psi\rangle$$

Let the wave function of the system be $\psi(x) = \langle x|\psi\rangle$. Also the hamiltonian can be written with operator p as $p^2 = (i\hbar\nabla)^2 \equiv -\hbar^2 \frac{d^2}{dx^2}$ so the schrodingers equation becomes

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n(x) = E_n \psi_n(x)$$

This is a well known second order differential equation whose solution are well known to be

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

These are the required wavefunction and energy levels for the unperturbed system. □

- (b) What is the first order correction to the energy shift?

Solution:

The first order correction in energy shift is given by

$$\begin{aligned} \langle \psi_1 | V | \psi_1 \rangle &= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) \delta\left(x - \frac{L}{2}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) dx \\ &= \frac{2}{L} \sin^2\left(\frac{\pi}{2}\right) = \frac{2}{L} \end{aligned}$$

So the first order energy correction is $2/L$. □

- (c) What is the first order correction to the ground state wavefunction?

Solution:

The correction for wave function is given by the expression

$$|n\rangle = |n^0\rangle + \lambda \sum_{k \neq n} |k^0\rangle \frac{\langle n | V | k \rangle}{E_n^0 - E_k^0} + \mathcal{O}(\lambda^2)$$

For ground state $n = 1$ so the correction becomes

$$\langle 1 | V | k \rangle = \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) \delta\left(x - \frac{L}{2}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{k\pi}{L}x\right) dx = \frac{2}{L} \sin\left(\frac{k\pi}{2}\right)$$

The Energy difference with the ground state are

$$E_1 - E_k = \frac{\pi^2\hbar^2}{2mL^2} (1^2 - k^2)$$

So the perturbed ground state wave function becomes

$$|1\rangle = \psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) + \sum_{k \neq 1} \sqrt{\frac{2}{L}} \sin\left(\frac{k\pi}{L}x\right) \left(\frac{4Lm}{\pi^2\hbar^2}\right) \frac{\sin\left(\frac{k\pi}{2}\right)}{1 - k^2}$$

This is the required perturbed eigenstate for the ground state of the potential. □

- (d) What is the second order correction to the energy shift specially for the ground state?

Solution:

The second order shift in energy is given by

$$\sum_{r \neq n} \frac{|\langle n^0 | V | n^r \rangle|^2}{E_n^0 - E_r^0}$$

For the state wavefunctions we have

$$\langle n|V|r\rangle = \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \delta\left(x - \frac{L}{2}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{r\pi}{L}x\right) dx = \frac{2}{L} \sin\left(\frac{n\pi}{2}\right) \sin\left(\frac{r\pi}{2}\right)$$

The Energy differences are

$$E_n - E_r = \frac{\pi^2 \hbar^2}{2mL^2} (n^2 - r^2)$$

Substituting this back we get

$$\Delta_n = \frac{4Lm}{\pi^2 \hbar^2} \sum_{n \neq r}^{\infty} \frac{\sin\left(\frac{n\pi}{2}\right) \sin\left(\frac{r\pi}{2}\right)}{n^2 - r^2}$$

For ground state $n = 1$ so the energy correction for ground state becomes

$$\Delta_1 = \frac{4Lm}{\pi^2 \hbar^2} \sum_{r \neq 1}^{\infty} \frac{\sin\left(\frac{r\pi}{2}\right)}{1 - r^2}$$

These are the required energy corrections. □

4. Calculate the ground state wave function for Simple Harmonic Oscillator with the perturbation $V = \frac{1}{2}\varepsilon m\omega^2 x^2$.

Solution:

The ground state wave function without the perturbation for simple harmonic oscillator is

$$\langle x|0\rangle = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \exp\left[-\frac{m\omega x^2}{2\hbar}\right]$$

The perturbation scales the frequency by a factor of $\sqrt{1 + \varepsilon}$ substituting this in the frequency of unperturbed state we get

$$\langle x|0\rangle = \sqrt[4]{\frac{m\sqrt{(1 + \varepsilon)}\omega}{\pi\hbar}} \exp\left[-\frac{m\sqrt{(1 + \varepsilon)}\omega x^2}{2\hbar}\right]$$

Since the perturbation factor $\varepsilon \ll 1$ we can use the binomial expansion as

$$(1 + \varepsilon)^{1/8} \approx 1 + \frac{\varepsilon}{8} \quad (1 + \varepsilon)^{1/2} \approx 1 + \frac{\varepsilon}{2}$$

Using these we get

$$\begin{aligned} \langle x|0\rangle &= \sqrt[4]{\frac{m\omega}{\pi\hbar}} \left(1 + \frac{\varepsilon}{8}\right) \exp\left[-\frac{m\omega x^2}{2\hbar} \left(1 + \frac{\varepsilon}{2}\right)\right] \\ &\approx \sqrt[4]{\frac{m\omega}{\pi\hbar}} \exp\left[-\frac{m\omega x^2}{2\hbar}\right] + \varepsilon \left[\frac{1}{8} - \frac{m\omega x^2}{4\hbar}\right] \sqrt[4]{\frac{m\omega}{\pi\hbar}} \exp\left[-\frac{m\omega x^2}{2\hbar}\right] \end{aligned}$$

This is the required perturbed energy eigenstate. □