QM 15-030-710-003 Winter ****
Assignment 5: Perturbation Theory

The due date for this assignment is **.**
Reading assignment: Chapter VI.

1. For a particle in an infinitely deep potential well of width a $(0 < x < a)$, find the first-order corrections to the energy levels under the following perturbations:

   a)
   $$V(x) = \frac{V_0}{a}(a - |2x - a|)$$

   b)
   $$V(x) = \begin{Bmatrix} V_0,\ b < x < a - b \\ 0,\ 0 < x < b \text{ and } a - b < x < a \end{Bmatrix}$$

   Analyze the conditions of applicability of the perturbation theory.

   Solution

   $$\psi_n^{(0)} = \sqrt{\frac{2}{a}} \sin \frac{\pi (n+1) x}{a}$$
   $$E_n^{(0)} = \frac{\hbar^2 \pi^2 (n+1)^2}{2ma^2}$$

   a)
   $$E_n^{(1)} = V_{nn} = V_0 \left(\frac{1}{2} + \frac{1 + (-1)^n}{\pi^2 (n+1)^2} \right)$$

   b)
   $$E_n^{(1)} = V_{nn} = \frac{V_0}{a} \left(a - 2b + \frac{a}{\pi (n+1)} \sin \frac{2\pi (n+1) b}{a} \right)$$

   The condition of applicability of the perturbation theory is that $|V_{nm}| \ll \left| E_n^{(0)} - E_m^{(0)} \right|$, whereof

   $$V_0 \ll \frac{\hbar^2 \pi^2 (n+1)}{ma^2}$$

   meaning that for a sufficiently large n the shift of energy levels can be calculated with perturbation theory.

2. Show that for an arbitrary perturbation $V(x)$, the first order correction $E_n^{(1)}$ to the energy levels in the potential of Problem 1 does not depend on n for sufficiently large n. Analyze the conditions of applicability of the perturbation theory.

   Solution

   $$E_n^{(1)} = \int_0^a V(x) \frac{2}{a} \sin^2 \frac{\pi (n+1) x}{a} dx = \frac{1}{a} \int_0^a V(x) \left(1 - \cos \frac{2\pi (n+1) x}{a} \right) dx$$

   The second term in parentheses is quickly oscillating for $n \gg 1$ and the corresponding integral $\to 0$. Therefore,

   $$E_n^{(1)} \approx \frac{1}{a} \int_0^a V(x)\, dx$$

   The actual condition of applicability of the perturbation theory is that $n \gg a/l$, where l is the characteristic scale on which the variations of $V(x)$ are substantial.

3. A charged linear harmonic oscillator is placed in the uniform electric field $\mathcal{E}$ directed along the axis of oscillations. Treating the electric field as a perturbation, evaluate the energy level corrections to second order and compare your result with the exact solution.

   Solution

   Using the normalized WF of the harmonic oscillator, $a = \sqrt{\hbar/m\omega}$,

$$\psi_n^{(0)}(x) = \frac{\exp\left[-\frac{1}{2}(x/a)^2\right]}{\sqrt{2^n\sqrt{\pi}an!}} H_n\left(\frac{x}{a}\right)$$

   the recurrence relation for the Hermite polynomials,

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0$$

   and the orthogonality of eigenfunctions, find the matrix elements of x_{nm} (and, therefore, of $V_{nm} = -e\mathcal{E}x_{nm}$)

$$x_{mn} = \frac{a}{\sqrt{2}} \left\{ \begin{array}{l} \sqrt{n+1},\ m = n+1 \\ \sqrt{n},\ m = n-1 \\ 0,\ \text{otherwise} \end{array} \right\}$$

   Consequently,

$$\begin{aligned} E_n &= E_n^{(0)} + E_n^{(1)} + E_n^{(2)} = E_n^{(0)} + V_{nn} + \sum_{m\neq n} \frac{|V_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} \\ &= \hbar\omega\left(n + \frac{1}{2}\right) - \frac{e^2\mathcal{E}^2a^2(n+1)}{2\hbar\omega} + \frac{e^2\mathcal{E}^2a^2n}{2\hbar\omega} = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{e^2\mathcal{E}^2a^2}{2\hbar\omega} \end{aligned}$$

   Notice, that this coincides with the exact energy, meaning that all higher order corrections must be zero.

4. A plane rotator with the moment of inertia I and the dipolar moment $\mathbf{d}$ is placed in a uniform electric field $\vec{\mathcal{E}}_0$ (directed in the plane of rotation) which can be treated perturbatively. Find the polarizability of the rotator's ground state.

   Hint: $V = -d\mathcal{E}_0\cos\phi = -d\mathcal{E}_0\left[\exp(i\phi) + \exp(-i\phi)\right]/2$.

   Solution

   For an unperturbed rotator,

$$\begin{aligned} \psi_m^{(0)} &= \frac{1}{\sqrt{2\pi}}\exp(im\phi) \\ E_m^{(0)} &= \frac{\hbar^2 m2}{2I} \end{aligned}$$

   Using the expression for the perturbation in the Hint,

$$V_{nk} = \begin{array}{c} -d\mathcal{E}_0/2,\ n = k+1 \text{ or } n = k-1 \\ 0,\ \text{otherwise} \end{array}$$

   find

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} = E_0^{(2)} = -\frac{d^2\mathcal{E}_0^2 I}{\hbar^2}$$

5. At $t = -\infty$, a particle in the ground state of the potential of Problem 1 is a subject to a weak, time-dependent perturbation of the following form:

   a) $V(x,t) = -xF_0\exp\left(-t^2/\tau^2\right)$
   b)$V(x,t) = -xF_0\exp\left(-|t|/\tau\right)$
   c)$V(x,t) = -xF_0/\left(1 + t^2/\tau^2\right)$

Using perturbation theory to the first order, evaluate the probabilities of transitions to other eigenstates at $t \to \infty$.

Solution

Matrix elements of the perturbation $\widehat{V} = -xF_0 f(t)$ are

$$V_{n0}(t) = -\frac{2}{a}F_0 f(t)\int_0^a x\sin\frac{(n+1)\pi x}{a}\sin\frac{\pi x}{a}dx = \left\{\begin{matrix} 0,\ n\text{-even} \\ 8a(n+1)F_0 f(t)/\pi^2 n^2 (n+2)^2,\ n\text{-odd}\end{matrix}\right\}$$

Using $\omega_{n0} = \hbar\pi^2 n(n+2)/2ma^2$ and the values of the integrals

$$I_1 = \int_{-\infty}^{\infty}\exp\left(i\omega_{n0}t - t^2/\tau^2\right)dt = \sqrt{\pi}\tau\exp\left(-\omega_{n0}^2\tau^2/4\right)$$

$$I_2 = \int_{-\infty}^{\infty}\exp\left(i\omega_{n0}t - |t|/\tau\right)dt = 2\tau/\left(1+\omega_{n0}^2\tau^2\right)$$

$$I_3 = \int_{-\infty}^{\infty}\frac{\exp(i\omega_{n0}t)}{1+t^2/\tau^2}dt = \pi\tau\exp(-\omega_{n0}\tau)$$

find

$$w_{0\to n}^{(1)} = \left\{\begin{matrix} 0,\ n\text{-even} \\ 64a^2F_0^2I_k^2(n+1)^2/\pi^4 n^4(n+2)^4,\ n\text{-odd}\end{matrix}\right\}$$

where $k = 1, 2, 3$. The condition of applicability of perturbation theory is $ma^3F_0 \ll \hbar^2\pi^2$.

6. A plane rotator with the dipole moment **d** is placed in a spatially uniform variable electric field $\vec{\mathcal{E}}(t)$, $\mathcal{E}(t) = f(t)\mathcal{E}_0$. Before the field was turned on, the rotator had a definite value of the projection of the angular momentum m. Using the first-order perturbation theory, evaluate the probabilities of different values of the projection and energy at $t \to \infty$. Consider a particular case

$$f(t) = \left\{\begin{matrix} 0,\ t<0 \\ \exp(-t/\tau),\ t>0\end{matrix}\right\}$$

Solution

Matrix elements of the perturbation $\widehat{V} = -d\mathcal{E}(t)\cos\phi$ are

$$V_{mm'} = \left\{\begin{matrix} -d\mathcal{E}(t)/2,\ m' = m+1 \text{ and } m' = m-1 \\ 0,\ \text{otherwise}\end{matrix}\right\}$$

Consequently,

$$w_{m\to m'}^{(1)} = \frac{1}{\hbar^2}\left|\int_{-\infty}^{\infty}\exp\left(i\omega_{m'm}t\right)\mathcal{E}(t)\,dt\right|^2$$

$$\omega_{m'm} = \left\{\begin{matrix} (2m+1)\hbar/2I,\ m' = m+1 \\ -(2m-1)\hbar/2I,\ m' = m-1\end{matrix}\right\}$$

and for $f(t)$ above

$$w_{m\to m'}^{(1)} = \frac{d^2\mathcal{E}_0^2\tau^2}{4\hbar^2\left(1+\omega_{m'm}^2\tau^2\right)}$$

For the ground state, in particular

$$w_{0\to 1}^{(1)} = w_{0\to -1}^{(1)} = \frac{d^2\mathcal{E}_0^2\tau^2}{4\hbar^2(1+\omega_0^2\tau^2)}$$

$$\omega_0 = \frac{\hbar}{2I}$$

7. A charged linear harmonic oscillator is subject to a spatially uniform electric field $\mathcal{E}(t) \propto 1/\left(1+t^2/\tau^2\right)$. Before the field was turned on, the oscillator was in the n-th stationary state. The total impulse of the force is P_0 . In the first order of the perturbation theory, find the probabilities of excitation to other possible states. Analyze the limiting cases $\omega\tau \ll 1$ and $\omega\tau \gg 1$.

Solution

$\mathcal{E}(t) = \mathcal{E}_0/\left(1+t^2/\tau^2\right)$ where $\mathcal{E}_0$ is related to P_0 via

$$P_0 = e\int_{-\infty}^{\infty} \mathcal{E}(t)\,dt = e\mathcal{E}_0\pi\tau$$

Using ($a = \sqrt{\hbar/m\omega}$),

$$V_{kn} = -e\mathcal{E}(t)\,x_{nm} = -\frac{ea\mathcal{E}(t)}{\sqrt{2}}\left\{\begin{array}{l}\sqrt{n+1},\ k=n+1\\ \sqrt{n},\ k=n-1\\ 0,\ \text{otherwise}\end{array}\right\}$$

and

$$\begin{aligned} I &= \int_{-\infty}^{\infty} \mathcal{E}(t)\exp(i\omega t)\,dt = \int_{-\infty}^{\infty} \mathcal{E}(t)\exp(-i\omega t)\,dt \\ &= \pi\tau\mathcal{E}_0\exp(-\omega\tau) \end{aligned}$$

find

$$w^{(1)}_{n\to k} = \frac{e^2a^2\left|I\right|^2}{2\hbar^2}\left\{\begin{array}{c} n+1,\ k=n+1\\ n,\ k=n-1\end{array}\right\}$$

where $e^2\left|I\right|^2 = P_0^2\exp(-2\omega\tau)$.