PHYS 661 - Quantum Mechanics II

Modern Quantum Mechanics by *J. J. Sakurai*
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Homework 2

Problem 1 - N-state All-to-All System
Consider an N-state system with a perturbation

$$V = \begin{pmatrix} v & v & \dots & v \\ v & v & & \\ \vdots & & \ddots & \\ v & & & v \end{pmatrix}, \qquad v \in \mathbb{R}$$

where $\langle n^{(0)} | V | m^{(0)} \rangle = v$ for all n, m. Let us for simplicity assume that the unperturbed Hamiltonian is just zero, $H_0 = 0$, i.e. $E_n^{(0)} = 0$ for all $n = 1, 2, \dots, N$. In this case we can use Brillouin-Wigner (BW) perturbation theory.

(a) Before doing perturbation theory, find the eigenvalues of V and their degeneracies exactly.

(b) By using BW perturbation theory, evaluate the correction to the energy E of a state up to and including third-order corrections in v. You should get an equation for E of the form $E = a_0 + a_1 v + a_2 \frac{v^2}{E} + a_3 \frac{v^3}{E^2}$. (No need to try to solve that equation.)

(c) Going beyond 3rd order, the equation for the perturbed energy E will be of the form $E = a_0 + \sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k$. Find the general nth order coefficient a_n. Using your result, sum up the series $\sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k$. Solve the resulting equation for E.

Solution. (a) The perturbation V of the system can be written as

$$V = \begin{pmatrix} v & v & \dots & v \\ v & v & & \\ \vdots & & \ddots & \\ v & & & v \end{pmatrix} = v \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & & \\ \vdots & & \ddots & \\ 1 & & & 1 \end{pmatrix},$$

where the matrix of ones on the right clearly has rank 1 since it has only 1 linearly independent column, making the eigenvalues N with multiplicity 1, and 0 with multiplicity $N-1$.

Similarly, the eigenvalues of V are $\lambda = 0$ that is $(N-1)$-fold degenerate and $\lambda = vN$ that is unique.

(b) The general correction to the energy E of a state using Brillouin-Wigner is given by

$$E_n = E_n^{(0)} + \lambda \sum_{p=0}^{\infty} \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^p \middle| n^{(0)} \right\rangle.$$

We are asked to find the correction to the energy up to and including the third-order correction in v, which means we will stop evaluating the sum at $p = 2$. Recall the form of the projector

$$\phi_n = \sum_{k \neq n} \left| k^{(0)} \right\rangle \left\langle k^{(0)} \right|,$$

and that $\langle n^{(0)} | V | m^{(0)} \rangle = v$ for all n, m.

- **Ground State**: We are given that $H_0 = E_n^{(0)} = 0$.

- **First-Order**: For $p = 0$, we have that
$$\left\langle n^{(0)} \middle| V \middle| n^{(0)} \right\rangle = v.$$
- **Second-Order**: For $p = 1$, we have that
$$\begin{aligned}\left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right) \middle| n^{(0)} \right\rangle &= \frac{\lambda}{E_n} \left\langle n^{(0)} \middle| V \phi_n V \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda}{E_n} \sum_{k \neq n} \left\langle n^{(0)} \middle| V \middle| k^{(0)} \right\rangle \left\langle k^{(0)} \middle| V \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda}{E_n} \sum_{k \neq n} v^2 \\ &= \frac{\lambda}{E_n} (N-) v^2.\end{aligned}$$
- **Third-Order**: For $p = 2$, we have that
$$\begin{aligned}\left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^2 \middle| n^{(0)} \right\rangle &= \frac{\lambda^2}{E_n^2} \left\langle n^{(0)} \middle| V \phi_n V \phi_n V \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda^2}{E_n^2} \sum_{k \neq n} \left\langle n^{(0)} \middle| V \middle| k^{(0)} \right\rangle \left\langle k^{(0)} \middle| V \phi_n V \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda^2}{E_n^2} \sum_{k, k' \neq n} \left\langle n^{(0)} \middle| V \middle| k^{(0)} \right\rangle \left\langle k^{(0)} \middle| V \middle| k'^{(0)} \right\rangle \left\langle k'^{(0)} \middle| V \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda^2}{E_n^2} \sum_{k, k' \neq n} v^3 \\ &= \frac{\lambda^2}{E_n^2} (N-1)^2 v^3.\end{aligned}$$

Thus, after replacing, we get
$$\begin{aligned}E_n &= E_n^{(0)} + \lambda \sum_{p=0}^{2} \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^p \middle| n^{(0)} \right\rangle \\ &= E_n^{(0)} + \lambda \left\langle n^{(0)} \middle| V \middle| n^{(0)} \right\rangle + \lambda \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right) \middle| n^{(0)} \right\rangle + \lambda \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^2 \middle| n^{(0)} \right\rangle \\ &= 0 + \lambda v + \frac{\lambda}{E_n} (N-1) v^2 + \frac{\lambda^2}{E_n^2} (N-1)^2 v^3.\end{aligned}$$

(c) The nth-order correction to the energy is
$$\begin{aligned}E_n^{(n)} &= \lambda \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^{n-1} \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda^n}{E_n^{n-1}} \left\langle n^{(0)} \middle| V \left(\phi_n V \right)^{n-1} \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda^n}{E_n^{n-1}} \sum_{k_1, k_2, \ldots, k_{n-1} \neq n} \left\langle n^{(0)} \middle| V \middle| k_1^{(0)} \right\rangle \left\langle k_1^{(0)} \middle| V \middle| k_2^{(0)} \right\rangle \cdots \left\langle k_{n-1}^{(0)} \middle| V \middle| n^{(0)} \right\rangle \\ &= \frac{\lambda^n}{E_n^{n-1}} \sum_{k_1, k_2, \ldots, k_{n-1} \neq n} v^n \\ &= \frac{\lambda^n}{E_n^{n-1}} (N-1)^{n-1} v^n,\end{aligned}$$

which means that the nth-order coefficient $a_n = (N-1)^{n-1}\lambda^n$.

The sum of the series is

$$\begin{aligned}
\sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k &= \sum_{k=0}^{\infty} (N-1)^k \lambda^{k+1} v \left(\frac{v}{E}\right)^k \\
&= \sum_{k=0}^{\infty} \lambda v \left(\frac{(N-1)\lambda v}{E}\right)^k \\
&= \frac{\lambda v}{1 - \frac{(N-1)\lambda v}{E}} \\
&= \frac{\lambda v E}{E - (N-1)\lambda v} \\
&= \frac{vE}{E - (N-1)v}.
\end{aligned}$$

where we set $\lambda = 1$ in the last line.

The series for the energy is then

$$\begin{aligned}
E &= a_0 + \sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k \\
&= 0 + \frac{vE}{E - (N-1)v} \\
&= 0 + \frac{vE}{E - (N-1)v} \\
\implies E(E - (N-1)v) &= vE \\
E &= (N-1)v + v \\
E &= Nv,
\end{aligned}$$

as expected from part (a).

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Problem 2 - 1D δ-potential Well Under Electric Field
Consider a 1D potential well $U(x) = -\alpha\delta(x)$. The ground state of this system is a bound level with wave function $\psi_0(x) = \sqrt{\kappa}e^{-\kappa|x|}$ and energy $E_0^{(0)} = -\frac{\hbar^2\kappa^2}{2m}$, where $\kappa = \frac{m\alpha}{\hbar^2}$. The excited state wave functions are $\psi_{+,k}(x) = \frac{1}{\sqrt{\pi}}\cos\left(k|x| + \frac{\varphi_k}{2}\right)$ and $\psi_{-,k} = \frac{1}{\sqrt{\pi}}\sin(kx)$, both with energy $E_k^{(0)} = \frac{\hbar^2k^2}{2m}$. (The subscript $\pm$ denotes spatial parity eigenvalues.) Consider a perturbation $V = bx$ acting on the ground state. Calculate the first and second order energy shifts to the ground state energy. In the case of continuous spectrum the 2nd order correction to the ground state energy is

$$E^{(2)} = \sum_{\sigma=\pm}\int_0^\infty \frac{1}{E_0^{(0)} - E_k^{(0)}} |\langle\sigma, k|V|0\rangle|^2 \,\mathrm{d}k.$$

Hint: $\int_0^\infty xe^{-\kappa x}\sin(kx)\,\mathrm{d}x = \frac{2\kappa k}{(\kappa^2+k^2)^2}$.

Solution. The energy shift to the ground state is given by

$$\Delta_n = \lambda V_{nn} + \lambda^2 \sum_{k\neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}} + \cdots,$$

where

$$V_{nk} \equiv \left\langle n^{(0)}\middle|V\middle|k^{(0)}\right\rangle.$$

Consider $\lambda = 1$. We have

$$\begin{aligned}\Delta_n &= E_n - E_n^{(0)}\\ &= E_0^{(0)} + E^{(1)} + E^{(2)}\\ &= -\frac{\hbar\kappa^2}{2m} + \lambda\left\langle n^{(0)}\middle|V\middle|n^{(0)}\right\rangle + \lambda^2\sum_{\sigma=\pm}\int_0^\infty \frac{|\langle\sigma|V|0\rangle|^2}{E_0^{(0)} - E_k^{(0)}}\,\mathrm{d}k.\end{aligned}$$

The first-order energy shift of the ground state energy is given by

$$\begin{aligned}\left\langle n^{(0)}\middle|V\middle|n^{(0)}\right\rangle &= \langle\psi_0|V|\psi_0\rangle\\ &= \int_{-\infty}^\infty \psi_0^*(x)V\psi_0(x)\,\mathrm{d}x\\ &= \int_{-\infty}^\infty \left(\sqrt{\kappa}e^{-\kappa|x|}\right)(bx)\left(\sqrt{\kappa}e^{-\kappa|x|}\right)\mathrm{d}x\\ &= \kappa b\int_{-\infty}^\infty xe^{-2\kappa|x|}\,\mathrm{d}x\\ &= 2\kappa b\int_0^\infty xe^{-2\kappa x}\,\mathrm{d}x\\ &= 2\kappa b\left(\frac{1}{4\kappa^2}\right)\\ &= \frac{b}{2\kappa}.\end{aligned}$$

The second-order energy shift of the ground state energy is given by

$$\sum_{\sigma=\pm}\int_0^\infty \frac{|\langle\sigma|V|0\rangle|^2}{E_0^{(0)} - E_k^{(0)}}\,\mathrm{d}k = \int_0^\infty \frac{|\langle +|V|0\rangle|^2 + |\langle -|V|0\rangle|^2}{E_0^{(0)} - E_k^{(0)}}\,\mathrm{d}k.$$

- Solving for the first term, we have

$$
\begin{aligned}
|\langle + | V | 0 \rangle|^2 &= \left| \int_{-\infty}^{\infty} \psi_{+,k}^*(x) V \psi_0(x) \, \mathrm{d}x \right|^2 \\
&= \left| \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{\pi}} \cos\left(k|x| + \frac{\varphi_k}{2} \right) \right) (bx) \left(\sqrt{\kappa} e^{-\kappa|x|} \right) \mathrm{d}x \right|^2 \\
&= \frac{b}{\pi\kappa} \left| \int_{-\infty}^{\infty} x \cos\left(k|x| + \frac{\varphi_k}{2} \right) e^{-\kappa|x|} \, \mathrm{d}x \right|^2 \\
&= 0,
\end{aligned}
$$

since the integrand is an odd function.

- Solving for the second term, we have

$$
\begin{aligned}
|\langle - | V | 0 \rangle|^2 &= \left| \int_{-\infty}^{\infty} \psi_{-,k}^*(x) V \psi_0(x) \, \mathrm{d}x \right|^2 \\
&= \left| \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{\pi}} \sin(kx) \right) (bx) \left(\sqrt{\kappa} e^{-\kappa|x|} \right) \mathrm{d}x \right|^2 \\
&= \frac{b^2\kappa}{\pi} \left| \int_{-\infty}^{\infty} x \sin(kx) \, e^{-\kappa|x|} \, \mathrm{d}x \right|^2 \\
&= \frac{4b^2\kappa}{\pi} \left| \int_{0}^{\infty} x \sin(kx) \, e^{-\kappa x} \, \mathrm{d}x \right|^2 \\
&= \frac{4b^2\kappa}{\pi} \left| \frac{2\kappa k}{(\kappa^2 + k^2)^2} \right|^2 \\
&= \frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4}.
\end{aligned}
$$

Replacing these values in the second-order energy shift, we get

$$
\begin{aligned}
\sum_{\sigma=\pm} \int_0^{\infty} \frac{|\langle \sigma | V | 0 \rangle|^2}{E_0^{(0)} - E_k^{(0)}} \, \mathrm{d}k &= \int_0^{\infty} \frac{1}{E_0^{(0)} - E_k^{(0)}} \left(0 + \frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4} \right) \mathrm{d}k \\
&= \int_0^{\infty} \frac{1}{-\frac{\hbar^2\kappa^2}{2m} - \frac{\hbar^2 k^2}{2m}} \left(\frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4} \right) \mathrm{d}k \\
&= -\int_0^{\infty} \frac{2m}{\hbar^2(\kappa^2 + k^2)} \frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4} \, \mathrm{d}k \\
&= -\int_0^{\infty} \frac{32 b^2 m \kappa^2 k^2}{\hbar^2 \pi (\kappa^2 + k^2)^5} \, \mathrm{d}k \\
&= -\frac{32 b^2 m \kappa^2}{\hbar^2 \pi} \left(\frac{5\pi}{256\kappa^7} \right) \\
&= -\frac{5 b^2 m}{8\hbar^2 \kappa^5}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\Delta_n &= E_0^{(0)} + E^{(1)} + E^{(2)} \\
&= -\frac{\hbar\kappa^2}{2m} + \frac{b}{2\kappa} - \frac{5b^2 m}{8\hbar^2\kappa^5} \\
&= \frac{4\hbar^2\kappa^4(b - \hbar\kappa^3) - 5b^2 m}{8\hbar^2\kappa^5}.
\end{aligned}
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