HW1 : Solution.

HW Solutions

Albers.

Chapter 7

Approximation Methods for Bound States

Problem 7.1 State Vectors in Second Order
The states can be computed from

$$|\psi_n\rangle = |\psi_n^o\rangle + \sum_{m\neq n} \frac{|\psi_m^o\rangle\langle\psi_m^o|\, \Delta_n - H' \,|\psi_n\rangle}{E_m^o - E_n^o} \tag{7.9}$$

while from Equations (7.5) and (7.21), the level shift is

$$\Delta_n = \langle\psi_n^o|\, H' \,|\psi_n\rangle \tag{S7.1}$$

Expand:

$$\Delta_n = \Delta_n^1 + \Delta_n^2 + \cdots \tag{S7.2a}$$

$$|\psi_n\rangle = |\psi_o\rangle + |\psi_1\rangle + |\psi_2\rangle + \cdots \tag{S7.2b}$$

write equation (7.9) as

$$|\psi_n\rangle = |\psi_n^o\rangle + \sum_{m\neq n} \frac{|\psi_m^o\rangle\langle\psi_m^o|}{E_m^o - E_n^o} \left(\Delta_n^1 + \Delta_n^2 + \cdots - H'\right)\left(|\psi_o\rangle + |\psi_1\rangle + |\psi_2\rangle + \cdots\right) \tag{S7.3}$$

and collect terms order by order.
Through first order

$$|\psi_n^o\rangle = |\psi_n^o\rangle - \sum_{m\neq n} \frac{H'_{mn}|\psi_m^o\rangle}{E_n^o - E_m^o} \tag{S7.4}$$

and through second order

$$\Delta_n = H'_{nn} + \sum_{m\neq n} \frac{|H'_{mn}|^2}{E_m^o - E_n^o} \tag{S7.5}$$

The second-order term in the expansion of the state vector is

$$|\psi_n^2\rangle = \sum_{m\neq n} \frac{|\psi_m^o\rangle}{E_m^o - E_n^o}\langle\psi_m^o|\, \Delta_n^2 \,|\psi_n^o\rangle + \sum_{m\neq n} \frac{|\psi_m^o\rangle}{E_m^o - E_n^o}\langle\psi_m^o|\, \Delta_n^1 - H' \,|\psi_n^1\rangle \tag{S7.6}$$

or

$$|\psi_n^2\rangle = -\sum_{\substack{m\neq n\\ k\neq n}} |\psi_m^o\rangle \frac{H'_{nn}H'_{kn}}{(E_m^o - E_n^o)(E_k^o - E_n^o)}\langle\psi_m^o|\,\psi_k^o\rangle + \sum_{\substack{m\neq n\\ k\neq n}} |\psi_m^o\rangle \frac{H'_{kn}}{(E_m^o - E_n^o)(E_k^o - E_n^o)}\langle\psi_m^o|\,H'\,|\psi_k^o\rangle$$

$$= \boxed{-\sum_{m\neq n} |\psi_m^o\rangle \frac{H'_{nn}H'_{kn}}{(E_m^o - E_n^o)^2} + \sum_{\substack{m\neq n\\ k\neq n}} |\psi_m^o\rangle \frac{H'_{mk}H'_{kn}}{(E_m^o - E_n^o)(E_k^o - E_n^o)}}$$

Problem 7.2 Oscillator with Cubic Perturbation
The unperturbed energies are $\omega(n+\frac{1}{2})$. The perturbation is

$$\begin{aligned} H' &= -\beta x^3 = -\beta(2m\omega)^{-\frac{3}{2}}(a+a^\dagger)^3 \\ &= -\beta(2m\omega)^{-\frac{3}{2}}\left(a^{\dagger 3} + 3a^{\dagger 2}a + 3a^\dagger a^2 + a^3 + 3a + 3a^\dagger\right) \end{aligned}$$

The perturbation H' connects states whose levels differ by 1 or 3; it has no diagonal elements, so ther
first-order energy shift.
The matrix elements needed are

$$\begin{aligned} \langle 1|\,H'\,|0\rangle &= -\beta(2m\omega)^{-\frac{3}{2}}\langle 1|\,3a^\dagger\,|0\rangle = -3\beta(2m\omega)^{-\frac{3}{2}} \\ \langle 3|\,H'\,|0\rangle &= -\beta(2m\omega)^{-\frac{3}{2}}\langle 3|\,a^{\dagger 3}\,|0\rangle = -\sqrt{6}\beta(2m\omega)^{-\frac{3}{2}} \\ \langle 2|\,H'\,|1\rangle &= -\beta(2m\omega)^{-\frac{3}{2}}\langle 2|\,3a^{\dagger 2}a + 3a^\dagger\,|1\rangle = -6\sqrt{2}\beta(2m\omega)^{-\frac{3}{2}} \\ \langle 4|\,H'\,|1\rangle &= -\beta(2m\omega)^{-\frac{3}{2}}\langle 4|\,a^{\dagger 3}\,|1\rangle = -\sqrt{24}\beta(2m\omega)^{-\frac{3}{2}} \end{aligned}$$

The second-order shift of the ground state is

$$\Delta_o = -\frac{1}{\omega}|\langle 1|\,H'\,|0\rangle|^2 - \frac{1}{3\omega}|\langle 3|\,H'\,|0\rangle|^2 = \boxed{-\frac{1}{\omega}\beta^2\frac{1}{(2m\omega)^3}(9+2) = -11\frac{1}{\omega}\beta^2\frac{1}{(2m\omega)^3}} \quad (\text{)$$

The second-order shift of the first excited state is state is

$$\begin{aligned} \Delta_1 &= \frac{1}{\omega}|\langle 0|\,H'\,|1\rangle|^2 - \frac{1}{\omega}|\langle 2|\,H'\,|1\rangle|^2 - \frac{1}{3\omega}|\langle 4|\,H'\,|1\rangle|^2 \\ &= \boxed{\frac{1}{\omega}\beta^2\frac{1}{(2m\omega)^3}(9-72-8) = -71\frac{1}{\omega}\beta^2\frac{1}{(2m\omega)^3}} \end{aligned} \quad (\text{)$$

Problem 7.3 Harmonic Oscillator Perturbation Problem
The second-order shift of the n-th energy level is

$$\Delta_n^2 = -\sum_{m\neq n}\frac{|H'_{mn}|^2}{E_m^o - E_n^o} \quad (\text{S}$$

Now

$$H'_{mn} = \frac{\lambda}{2}\langle\psi_m^o|\,x^2\,|\psi_m^o\rangle = \frac{\hbar\lambda}{4m\omega}\langle\psi_m^o|\,(a^2 + a^{\dagger 2} + 2a^\dagger a + 1)\,|\psi_n^o\rangle \quad (\text{S}$$

The last two terms contribute only when $m = n$. The remaining terms connect $|\psi_n^o\rangle$ to $|\psi_{n\pm 2}^o\rangle$ only. T

$$H'_{n+2,n} = \frac{\hbar\lambda}{4m\omega}\langle\psi_{n+2}^o|\,a^{\dagger 2}\,|\psi_n^o\rangle = \frac{\hbar\lambda}{4m\omega}\sqrt{(n+1)(n+2)} \quad (\text{S}$$

while

$$H'_{n-2,n} = \frac{\hbar\lambda}{4m\omega}\langle\psi^o_{n-2}|\, a^2\,|\psi^o_n\rangle = \frac{\hbar\lambda}{4m\omega}\sqrt{n(n-1)} \qquad \text{(S7.15)}$$

Of course $H'_{n-2,n}$ is automatically zero when $n = 0$ or $n = 1$. Thus

$$\Delta^2_n = -\left[\frac{|H'_{n+2,n}|^2}{2\hbar\omega} + \frac{|H'_{n-2,n}|^2}{-2\hbar\omega}\right] = \frac{1}{2\hbar\omega}\frac{\hbar^2\lambda^2}{16m^2\omega^2}\left[n(n-1) - (n+1)(n+2)\right]$$
$$= \frac{1}{2\hbar\omega}\frac{\hbar^2\lambda^2}{16m^2\omega^2}[-4n-2] = \boxed{-\left(n+\frac{1}{2}\right)\frac{\hbar\lambda^2}{8m^2\omega^3}} \qquad \text{(S7.16)}$$

The exact eigenvalues are

$$E_n = (n+\frac{1}{2})\hbar\omega\left[1+\frac{\lambda}{m\omega^2}\right]^{\frac{1}{2}} = (n+\frac{1}{2})\hbar\omega\left[1+\frac{1}{2}\frac{\lambda}{m\omega^2} - \frac{1}{8}\left(\frac{\lambda}{m\omega^2}\right)^2 + \cdots\right] \qquad \text{(S7.17)}$$

in agreement with the second order perturbation computation.

√ Problem 7.4 Infinite Well with Delta Function Revisited

The unperturbed energies are

$$E_n = \frac{n^2\pi^2}{8ma^2} \qquad \text{(S7.18)}$$

The first order shifts are

$$\Delta_n = H'_{nn} = \beta E_o a\psi_n(0)^2 \qquad \text{(S7.19)}$$

For even n the wave functions are odd, so there is no shift. For odd n,

$$\Delta_n = \beta E_o a\frac{1}{a} = \beta E_o \qquad \text{(S7.20)}$$

independent of n.

The off-diagonal matrix elements are also

$$H'_{mn} = \beta E_o \qquad \text{(S7.21)}$$

provided both n and m are odd, and zero otherwise. So there is a shift of the odd levels only, given by

$$\boxed{\Delta^{(2)}_n = -\beta^2 E_o^2\frac{1}{E_o}\sum_{\substack{m\neq n\\ m\text{ odd}}}^{\infty}\frac{1}{m^2-n^2} = -\frac{\beta^2 E_o}{4n^2}} \qquad \text{(S7.22)}$$

in agreement with equation (S3.44). The sum can be calculated as follows:

$$\sum_{m\neq n, m\text{ odd}}^{\infty}\frac{1}{m^2-n^2} = -\frac{1}{2n}\sum_{\substack{m\neq n\\ m\text{ odd}}}^{\infty}\left[\frac{1}{m+n} - \frac{1}{m-n}\right] = -\frac{1}{2n}\left[\sum_{\substack{m=1\\ m\text{ odd}}}^{\infty}\frac{1}{m+n} - \sum_{\substack{m=2n+1\\ m\text{ odd}}}^{\infty}\frac{1}{m-n} - \frac{1}{2n}\right]$$
$$= -\frac{1}{2n}\left[\sum_{\substack{k=n+1\\ k\text{ even}}}^{\infty}\frac{1}{k} - \sum_{\substack{k=n+1\\ k\text{ even}}}^{\infty}\frac{1}{k} - \frac{1}{2n}\right] = \frac{1}{4n^2} \qquad \text{(S7.23)}$$

Problem 7.5 A Two-State System
The full Hamiltonian is

$$H = \begin{pmatrix} E_o + \epsilon_1 & -A \\ -A & E_o + \epsilon_2 \end{pmatrix} \tag{S7.24}$$

The exact eigenvalues are solutions to the characteristic equation:

$$(E_o + \epsilon_1 - \lambda)(E_o + \epsilon_2 - \lambda) - A^2 = 0 \tag{S7.25}$$

or

$$\lambda = E_o + \frac{\epsilon_1 + \epsilon_2}{2} \pm \frac{1}{2}\sqrt{(\epsilon_1 - \epsilon_2)^2 + 4A^2} \tag{S7.26}$$

When $\epsilon_i \ll |A|$, the unperturbed eigenstates are

$$|\psi_\pm\rangle = \frac{|\psi_1\rangle \pm |\psi_2\rangle}{\sqrt{2}} \tag{S7.27}$$

with eigenvalues $E_o \mp A$. The nonvanishing elements of the perturbation are $\langle\psi_i|\, H'\, |\psi_i\rangle = \epsilon_i$. The first-order effect is

$$\langle\psi_\pm|\, H'\, |\psi_\pm\rangle = \frac{\epsilon_1 + \epsilon_2}{2} \tag{S7.28}$$

To this order the energies are

$$E = E_o \pm A + \frac{\epsilon_1 + \epsilon_2}{2} \tag{S7.29}$$

When $|A| \ll \epsilon_i$, take the original states as the unperturbed states. The "unperturbed" eigenvalues are $E_o + \epsilon_i$. The first-order perturbation is zero. The second order energy shifts are

$$\Delta_1^{(2)} = |H'_{12}|^2 \frac{1}{E_1^{(o)} - E_2^{(o)}} = \frac{A^2}{\epsilon_1 - \epsilon_2} \tag{S7.30}$$

and

$$\Delta_2^{(2)} = -\Delta_1^{(2)} \tag{S7.31}$$

which is also what you get by expanding the exact formula through second order in A.

Problem 7.6 External Electric Quadrupole Field
Part a) Since $\mathbf{E} = -\nabla V(r)$,

$$\boxed{H' = eG(x^2 - y^2)} \tag{S7.32}$$

Part b) Define as usual

$$r^{\pm 1} = \mp \frac{x \pm iy}{\sqrt{2}} \tag{S7.33}$$

H' is the sum of two components of a rank-two spherical tensor: $H' = Q_2^2 + Q_2^{-2}$ where

$$Q_2^{\pm 2} = eGr^{\pm}r^{\pm} \tag{S7.34}$$

The other components, $Q_2^{\pm 1}$ and Q_2^0, can be obtained by commuting $Q^{\pm 2}$ with the components of $\mathbf{J}$ as in section 5.2.2, but you do not need them here.

It follows that $\langle 3,2,m'|\, H'\, |3,2,m\rangle$ vanishes unless $m' - m = \pm 2$. So do not bother to work out any others. In particular, from the first selection rule (Section 5.2.4)

$$\langle 3,2,m+2|\, H'\, |3,2,m\rangle = \langle 3,2,m+2|\, Q_2^2\, |3,2,m\rangle \tag{S7.35}$$

$$\langle 3,2,m-2|\, H'\, |3,2,m\rangle = \langle 3,2,m+2|\, Q_2^{-2}\, |3,2,m\rangle \tag{S7.36}$$