HW 11 solution

P6.3 (a) $\psi_{gs}(x_1,x_2) = \psi_1(x_1)\psi_1(x_2)$

$$E_{gs} = 2E_1 = 2\cdot\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

, where $\psi_1(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right)$

$$\psi_{1st}(x_1,x_2) = \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2)\right)$$

$$E_{1st} = E_1 + E_2 = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 + \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\cdot 4$$

$$= 5\cdot\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

, where $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$

(b) For the ground state,

$$E'_{gs} = \langle\psi_{gs}|V(x_1,x_2)|\psi_{gs}\rangle$$

$$= \int_{x_1}\int_{x_2}\psi_1(x_1)\psi_1(x_2)\left[-aV_0\,\delta(x_1-x_2)\right]\psi_1(x_1)\psi_1(x_2)\,dx_1\,dx_2$$

$$= -aV_0\int_{x_1}\psi_1^2(x_1)\left[\int_{x_2}\psi_1^2(x_2)\,\delta(x_1-x_2)\,dx_2\right]dx_1$$

$$= -aV_0\int_{x_1}\psi_1^4(x_1)\,dx_1$$

$$= -aV_0\cdot\frac{4}{a^2}\int_0^a\sin^4\left(\frac{\pi}{a}x_1\right)dx_1$$

$$= -\frac{4V_0}{a}\cdot\frac{a}{\pi}\int_0^\pi\sin^4(x)\,dx$$

$$= -\frac{4V_0}{\pi}\cdot\frac{3\pi}{8} = \underline{-\frac{3}{2}V_0}$$

$$E^{1}_{1st} = \langle \psi_{1st} | V(x_1, x_2) | \psi_{1st} \rangle$$

$$= \frac{1}{2} \int_{x_1} \int_{x_2} \left(\psi_1^{x_1} \psi_2^{x_2} + \psi_2^{x_1} \psi_1^{x_2} \right) \left(-aV_0 \, \delta(x_1 - x_2) \right) \left(\psi_1^{x_1} \psi_2^{x_2} + \psi_2^{x_1} \psi_1^{x_2} \right) dx_1 \, dx_2$$

$$= -\frac{aV_0}{2} \int_{x_1} \left(\psi_1^{x_1} \psi_2^{x_1} + \psi_2^{x_1} \psi_1^{x_1} \right)^2 dx_1$$

$$= -2aV_0 \int_{x_1} \psi_1^2(x_1) \, \psi_2^2(x_1) \, dx_1$$

$$= -2aV_0 \cdot \frac{4}{a^2} \int_0^a \sin^2\left(\frac{\pi}{a} x_1\right) \sin^2\left(\frac{2\pi}{a} x_1\right) dx_1$$

$$= -\frac{8}{a} V_0 \cdot \frac{a}{\pi} \int_0^{\pi} \sin^2(x) \sin^2(2x) \, dx$$

$$= -\frac{8}{\pi} V_0 \cdot 4 \int_0^{\pi} \sin^2(x) \sin^2(x) \cos^2(x) \, dx$$

$$= -\frac{32}{\pi} V_0 \int_0^{\pi} \left[\sin^4 x - \sin^6 x \right] dx$$

$$= -\frac{32}{\pi} V_0 \left[\frac{3\pi}{8} - \frac{5\pi}{16} \right] = -2V_0$$

P6.4 (a) $H' = \alpha \delta(x - \frac{a}{2})$

$$\langle \psi_m^0 | H' | \psi_n^0 \rangle = \frac{2}{a} \int_0^a \sin\left(\frac{m\pi}{a} x\right) \alpha \delta\left(x - \frac{a}{2}\right) \cdot \sin\left(\frac{n\pi}{a} x\right) dx$$

$$= \frac{2\alpha}{a} \sin\left(\frac{m\pi}{2}\right) \sin\left(\frac{n\pi}{2}\right)$$

Thus

$$|H'_{mn}|^2 = \begin{cases} \frac{4\alpha^2}{a^2}, & \text{for } m \text{ and } n \text{ odd} \\ 0, & \text{for } m \text{ or } n \text{ even} \end{cases}$$

So no shift for even "n".
For odd "n",

$$E_n^2 = \sum_{\substack{m \neq n \\ m\,odd}} \frac{\frac{4\alpha^2}{a^2}}{\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \left[n^2 - m^2\right]}$$

$$= \frac{2m}{\cancel{\hbar^2}} \frac{\cancel{a^2}}{\pi^2} \frac{4\alpha^2}{\cancel{a^2}} \sum_{\substack{m \neq n \\ m\,odd}} \frac{1}{n^2 - m^2}$$

$$= \frac{8 m \alpha^2}{\hbar^2 \pi^2} \cdot \sum_{\substack{m \neq n \\ m\,odd}} \left(\frac{1}{m+n} - \frac{1}{m-n} \right) \cdot \frac{1}{2n}$$

for $n=1$

$$\sum \left(\frac{1}{m+1} - \frac{1}{m-1} \right) = \frac{1}{4} - \frac{1}{2}$$
$$+ \frac{1}{6} - \frac{1}{4}$$
$$+ \frac{1}{8} - \frac{1}{6}$$
$$\vdots \qquad = -\frac{1}{2}$$

for $n=3$

$$\sum \left(\frac{1}{m+3} - \frac{1}{m-3} \right) = \frac{1}{4} - \left(\frac{1}{-2} \right)$$
$$+ \frac{1}{8} - \frac{1}{2}$$
$$+ \frac{1}{10} - \frac{1}{4}$$
$$+ \frac{1}{12} - \frac{1}{6}$$
$$+ \frac{1}{14} - \frac{1}{8}$$
$$= -\frac{1}{6}$$

for $n=5$

$$\sum\left(\frac{1}{m+5}-\frac{1}{m-5}\right)=\frac{1}{6}-\left(-\frac{1}{4}\right)$$
$$+\frac{1}{8}-\left(-\frac{1}{2}\right)$$
$$+\frac{1}{12}-\frac{1}{2}$$
$$+\frac{1}{14}-\frac{1}{4}$$
$$+\frac{1}{16}-\frac{1}{6}$$
$$+\frac{1}{18}-\frac{1}{8}$$
$$+\frac{1}{28}-\frac{1}{10}$$
$$=-\frac{1}{10}$$

So we can see that

$$\sum_{\substack{m\pm n\\ \text{odd}}}\left(\frac{1}{m+n}-\frac{1}{m-n}\right)=-\frac{1}{2n}$$

Thus $$E_n^2=\frac{8m\alpha^2}{\hbar^2\pi^2}\cdot\left(\frac{1}{2n}\right)\left(-\frac{1}{2n}\right)$$
$$=-2m\left(\frac{\alpha}{\pi\hbar n}\right)^2$$

for odd n

For even n, $E_n^2=0$

(b) From Prob. 6.2. $H' = \epsilon \frac{1}{2} m\omega_0^2 x^2$

So $H'_{m0} = \epsilon \frac{1}{2} m\omega_0^2 \langle m | x^2 | 0 \rangle$

Because $x^2 = \frac{\hbar}{2m\omega_0}\left[a_+^2 + a_+a_- + a_-a_+ + a_-^2\right]$

and $\langle m | a_+^2 | 0 \rangle \underset{\substack{\uparrow \\ \text{Griffiths Eq 2.67}}}{=} \langle m | \sqrt{2!} \, | 2 \rangle$

$= \sqrt{2}\, \delta_{m2}$,

$\langle m | a_+a_- | 0 \rangle = 0$,

$\langle m | a_-a_+ | 0 \rangle = \langle m | a_- | 1 \rangle = \langle m | 0 \rangle = \delta_{m0}$,

, and $\langle m | a_-^2 | 0 \rangle = 0$.

Thus $H'_{m0} = \epsilon \cdot \frac{1}{2} m\omega_0^2 \cdot \frac{\hbar}{2m\omega_0}\left[\sqrt{2}\,\delta_{m2} + \delta_{m0}\right]$

$= \epsilon \frac{\hbar\omega_0}{4}\left[\sqrt{2}\,\delta_{m2} + \delta_{m0}\right]$

Thus $E_0^2 = \sum_{m \neq 0} \frac{|H'_{m0}|^2}{E_0^0 - E_m^0}$

$= \frac{|H'_{20}|^2}{E_0^0 - E_2^0} = \frac{\epsilon^2 \frac{(\hbar\omega_0)^2}{8}}{\frac{1}{2}\hbar\omega_0 - \frac{5}{2}\hbar\omega_0}$

$= \underbrace{-\frac{\epsilon^2}{16}\hbar\omega_0}$

This is the same as the 2nd order term in prob. 6.2(a) for $n = 0$.

Prob. 6.8. $H' = a^3 V_0\, \delta(x - \frac{a}{4})\, \delta(y - \frac{a}{2})\, \delta(z - \frac{3a}{4})$

The ground state has $(n_x, n_y, n_z) = (1, 1, 1)$

$$E'_{gs} = \langle \psi_{gs} | H' | \psi_{gs} \rangle$$

$$= a^3 V_0 \int_x \int_y \int_z \left(\frac{2}{a}\right)^3 \sin^2\left(\frac{\pi}{a} x\right) \sin^2\left(\frac{\pi}{a} y\right)$$

$$\cdot \sin^2\left(\frac{\pi}{a} z\right) \delta(x - \frac{a}{4})\, \delta(y - \frac{a}{2})\, \delta(z - \frac{3a}{4})\, dx\, dy\, dz$$

$$= 8 V_0 \sin^2\left(\frac{\pi}{4}\right) \sin^2\left(\frac{\pi}{2}\right) \sin^2\left(\frac{3\pi}{4}\right)$$

$$= 8 V_0 \cdot \frac{1}{2} \cdot 1 \cdot \frac{1}{2} = \underline{2 V_0}$$

For the triply degenerate first excited states

$\psi(2, 1, 1) \equiv \psi_a$

$\psi(1, 2, 1) \equiv \psi_b$, $\psi(1, 1, 2) \equiv \psi_c$

The 3×3 matrix representation of H' is

$$H' = \begin{pmatrix} H'_{aa} & H'_{ab} & H'_{ac} \\ H'_{ba} & H'_{bb} & H'_{bc} \\ H'_{ca} & H'_{cb} & H'_{cc} \end{pmatrix}$$

$$H'_{aa} = 8 V_0 \sin^2\left(\frac{\pi}{2}\right) \sin^2\left(\frac{\pi}{2}\right) \sin^2\left(\frac{3}{4}\pi\right)$$

$$= 4 V_0$$

$$H'_{bb} = 8 V_0 \sin^2\left(\frac{\pi}{4}\right) \cancelto{0}{\sin^2(\pi)} \sin^2\left(\frac{3}{4}\pi\right)$$

$$= 0$$

$$H'_{cc} = 8 V_0 \sin^2\left(\frac{\pi}{4}\right) \sin^2\left(\frac{\pi}{2}\right) \sin^2\left(\frac{3}{2}\pi\right)$$

$$= 4 V_0$$

$$H'_{ab} = 8V_0 \sin\left(\frac{2\pi}{a}\cdot\frac{a}{4}\right)\sin\left(\frac{\pi}{a}\cdot\frac{a}{4}\right)$$
$$\sin\left(\frac{\pi}{a}\cdot\frac{a}{2}\right)\sin\left(\frac{2\pi}{a}\cdot\frac{a}{2}\right)$$
$$\sin\left(\frac{\pi}{a}\cdot\frac{3}{4}a\right)\sin\left(\frac{\pi}{a}\cdot\frac{3}{4}a\right)$$
$$= 0$$

$$H'_{ac} = 8V_0 \sin\left(\frac{2\pi}{a}\cdot\frac{a}{4}\right)\sin\left(\frac{\pi}{a}\cdot\frac{a}{4}\right)$$
$$\sin\left(\frac{\pi}{a}\cdot\frac{a}{2}\right)\sin\left(\frac{\pi}{a}\cdot\frac{a}{2}\right)$$
$$\sin\left(\frac{\pi}{a}\cdot\frac{3}{4}a\right)\sin\left(\frac{2\pi}{a}\cdot\frac{3}{4}a\right)$$
$$= 8V_0 \cdot \frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}\,(-1)$$
$$= -4V_0$$

$$H'_{bc} = 8V_0 \sin\left(\frac{\pi}{a}\cdot\frac{a}{4}\right)\sin\left(\frac{\pi}{a}\cdot\frac{a}{4}\right)$$
$$\sin\left(\frac{2\pi}{a}\cdot\frac{a}{2}\right)\sin\left(\frac{\pi}{a}\cdot\frac{a}{2}\right)$$
$$\sin\left(\frac{\pi}{a}\cdot\frac{3}{4}a\right)\sin\left(\frac{2\pi}{a}\cdot\frac{3}{4}a\right)$$
$$= 0$$

$$H' = 4V_0\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

$$H'\psi = 4V_0\epsilon\psi, \qquad \ulcorner E = 4V_0\epsilon \lrcorner$$

$$\Rightarrow \begin{vmatrix} 1-\epsilon & 0 & -1 \\ 0 & -\epsilon & 0 \\ -1 & 0 & 1-\epsilon \end{vmatrix} = 0$$

$$\Rightarrow (1-\epsilon)\left(-\epsilon(1-\epsilon)\right) + \epsilon = 0$$

$$\Rightarrow -\epsilon(\epsilon-1)(\epsilon-1) + \epsilon = 0$$

$$\Rightarrow \epsilon\left[1 - \epsilon^2 + 2\epsilon - 1\right] = 0$$

$$\Rightarrow \epsilon^2(-\epsilon + 2) = 0 \Rightarrow \epsilon^2(\epsilon - 2) = 0$$

$$\Rightarrow \epsilon = 0, \quad \epsilon = 2$$

doubly degenerate

So the 1st order corrections are $\underline{0,\ 0,\ 8V_0}$

Prob. 6.9. $H = V_0 \begin{pmatrix} 1-\epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix}$

(a) For $\epsilon = 0$

$$H = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Eigenvalues and eigenvectors are

$E_1^0 = V_0 \Rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $E_2^0 = V_0 \Rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, $E_3^0 = 2V_0 \Rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

(b) $H\psi = V_0 \lambda \psi$, eigenvalues are λV_0

$$\begin{vmatrix} 1-\epsilon-\lambda & 0 & 0 \\ 0 & 1-\lambda & \epsilon \\ 0 & \epsilon & 2-\lambda \end{vmatrix} = 0$$

$$\Rightarrow (1-\epsilon-\lambda)\left((1-\lambda)(2-\lambda) - \epsilon^2\right) = 0$$

$$\Rightarrow (\lambda - 1 + \epsilon)(\lambda^2 - 3\lambda + 2 - \epsilon^2) = 0$$

$$\Rightarrow \lambda = 1-\epsilon, \quad \lambda = \frac{3 \pm \sqrt{9 - 4(2-\epsilon^2)}}{2}$$

$$= \frac{3 \pm \sqrt{1 + 4\epsilon^2}}{2}$$

$$\simeq \frac{3 \pm (1 + 2\epsilon^2)}{2}$$

$$= \begin{cases} 1 - \epsilon^2 \\ 2 + \epsilon^2 \end{cases}$$

Thus the eigenenergies are up to the second order in ϵ^2

$$(1-\epsilon)V_0, \quad V_0\frac{3-\sqrt{1+4\epsilon^2}}{2} \simeq (1-\epsilon^2)V_0$$

$$, \quad V_0\frac{3+\sqrt{1+4\epsilon^2}}{2} \simeq (2+\epsilon^2)V_0$$

(c) V_0 $(\equiv E_1^0 = E_2^0)$ is doubly degenerate and $2V_0$ $(\equiv E_3^0)$ is nondegenerate.

$$E_3^1 = \langle \psi_3 | H' | \psi_3 \rangle,$$

$$H' = \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$E_3^1 = \epsilon V_0 (0\ 0\ 1) \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= \epsilon V_0 (0\ 0\ 1) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \underline{0}$$

$$E_3^2 = \sum_{m \neq 3} \frac{|H'_{m3}|^2}{E_3^0 - E_m^0}$$

$$H'_{13} = \epsilon V_0 (1\ 0\ 0) \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= \epsilon V_0 (1\ 0\ 0) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

$$H'_{23} = \epsilon V_0 (0\ 1\ 0) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \epsilon V_0$$

Thus $$E_3^2 = \frac{|H'_{13}|^2}{2V_0 - V_0} + \frac{|H'_{23}|^2}{2V_0 - V_0} = \underline{\epsilon^2 V_0}$$

$$\therefore\ E_3 \simeq E_3^0 + E_3^1 + E_3^2 = \underline{2V_0 + \epsilon^2 V_0}$$

Up to the second order, this is the same as what we obtained in (b).

(d) In the subspace spanned by the two degenerate states,

$$H' = \epsilon V_0 \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}$$

So according to the degenerate perturbation theory, the first order correction is obtained simply by solving this smaller matrix in the subspace.

That is, $\quad H'\psi = \epsilon V_0 \lambda \psi$

$$\Rightarrow \begin{vmatrix} -1-\lambda & 0 \\ 0 & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda(\lambda+1) = 0$$

$$\Rightarrow \lambda = 0, -1$$

So the first order energy correction is

$$0 \quad \text{or} \quad -\epsilon V_0$$

In other words, up to the first order

$$E = \underbrace{\begin{cases} V_0 - \epsilon V_0 \\ V_0 \end{cases}}$$

From (b) we obtained $\quad E = \underbrace{\begin{cases} (1-\epsilon) V_0 \\ V_0 \end{cases}}$

up to the first order in ϵ.
So they are consistent.

Prob. 7.1. $V(x) = \alpha |x|$, $\psi(x) = A e^{-bx^2}$

From Eq. 7.3 of Griffiths, $A = \left(\frac{2b}{\pi}\right)^{1/4}$

$\langle H \rangle = \langle T \rangle + \langle V \rangle$

$\langle T \rangle = \frac{\hbar^2 b}{2m}$ from Eq. 7.5

$$\langle V \rangle = \alpha A^2 \int_{-\infty}^{\infty} |x| e^{-2bx^2} dx = 2\alpha A^2 \int_0^{\infty} x e^{-2bx^2} \cancel{dx}$$

$$= 2\alpha A^2 \left[\frac{-e^{-2bx^2}}{4b}\right]_0^{\infty} = \frac{\alpha A^2}{2b} = \frac{\alpha}{\sqrt{2b\pi}}$$

$$\Rightarrow \langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2b\pi}}$$

$$\frac{\partial \langle H \rangle}{\partial b} = 0 = \frac{\hbar^2}{2m} - \frac{1}{2}\frac{\alpha}{\sqrt{2\pi}} \cdot b^{-\frac{3}{2}}$$

$$\Rightarrow b_{min} = \left[\frac{\alpha}{\sqrt{2\pi}} \cdot \frac{m}{\hbar^2}\right]^{\frac{2}{3}}$$

Thus $E_{gs} \le \langle H \rangle_{min} = b_{min}\left(\frac{\hbar^2}{2m} + \frac{\alpha}{\sqrt{2\pi}} \cdot b_{min}^{-\frac{3}{2}}\right)$

$$= \left[\frac{\alpha m}{\sqrt{2\pi}\,\hbar^2}\right]^{\frac{2}{3}} \left(\frac{\hbar^2}{2m} + \frac{\hbar^2}{2m} \cdot 2\right)$$

$$= \underline{\frac{3\hbar^2}{2m}\left(\frac{\alpha m}{\sqrt{2\pi}\,\hbar^2}\right)^{\frac{2}{3}}}$$

(b) $V(x) = \alpha x^4$

$$\langle V \rangle = \alpha A^2 \int_{-\infty}^{\infty} x^4 e^{-2bx^2} dx$$

$$= 2\alpha A^2 \cdot \sqrt{\pi}\,\frac{4!}{2!} \cdot \left(\frac{1}{2} \cdot \frac{1}{\sqrt{2b}}\right)^5$$

$$= \alpha \cdot \cancel{\left(\frac{2b}{\pi}\right)^{\frac{1}{2}}} \cdot \cancel{24}^{\,3} \cancel{\sqrt{\pi}} \cdot \frac{1}{\cancel{32}_{\,16}} \cdot \frac{1}{\cancel{4}b^2} \cdot \frac{1}{\cancel{\sqrt{2b}}}$$

$$= \frac{3\alpha}{16 b^2}$$

$$\langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2} \Rightarrow \frac{\partial\langle H\rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{3\alpha}{8b^3} = 0$$

$$\Rightarrow b_{min}^3 = \frac{3\alpha}{8}\cdot\frac{2m}{\hbar^2} \Rightarrow b_{min} = \left(\frac{3\alpha m}{4\hbar^2}\right)^{\frac{1}{3}}$$

$$\therefore \langle H\rangle_{min} = b\left(\frac{\hbar^2}{2m} + \frac{3\alpha}{16} b^{-3}\right)$$

$$= \left(\frac{3\alpha m}{4\hbar^2}\right)^{\frac{1}{3}}\left(\frac{\hbar^2}{2m} + \frac{3\alpha}{16}\cdot\frac{4\hbar^2}{3\alpha m}\right)$$

$$= \left(\frac{3\alpha m}{4\hbar^2}\right)^{\frac{1}{3}}\cdot\frac{3\hbar^2}{4m} = \underline{\frac{3}{4}\left(\frac{3\alpha\hbar^4}{4m^2}\right)}$$