Problem set #2

5.1

$$\hat{V} = bx$$

a) $E_n^{(1)} = \langle n|x|n\rangle = 0$

since $\hat{x} = \sqrt{\dfrac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\hat{a}^{+} + \sqrt{n}\,\hat{a}\right)$

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

$$E_n^{(2)} = \sum_{n'\neq n} \frac{|V_{n'n}|^2}{E_n^{(0)} - E_{n'}^{(0)}} = \frac{\hbar b^2}{2m\omega}\left(\frac{n+1}{-\hbar\omega} + \frac{n}{\hbar\omega}\right) = \frac{-b^2}{2m\omega^2}$$

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) - \frac{b^2}{2m\omega^2}$$

b) $$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2 + bx = \underbrace{\frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x+\frac{b}{m\omega^2}\right)^2}_{\text{unperturbed } \hat{H}_0 \text{ with shifted origin } x \to x + b/m\omega^2} - \frac{b^2}{2m\omega^2}$$

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) - \frac{b^2}{2m\omega^2}$$

5.3

Unperturbed basis $\quad \psi_{nm}(x,y) = \frac{2}{L} \sin\frac{\pi n x}{L} \sin\frac{\pi m y}{L}$

Ground state : $E_{11} = \frac{\pi^2\hbar^2}{mL^2}$ — non-degenerate

First excited state : $E_{12} = E_{21} = \frac{5\pi^2\hbar^2}{2mL^2}$

$$E_{11}^{(1)} = \langle 11|\hat{V}|11\rangle = \lambda \langle 1|x|1\rangle \langle 1|y|1\rangle = \lambda \langle 1|x|1\rangle^2$$

$$\langle 1|x|1\rangle = \frac{2}{L}\int_0^L x \sin^2\frac{\pi x}{L}\, dx = \frac{2L}{\pi^2}\int_0^\pi t \sin^2 t\, dt = \frac{2L}{\pi^2}\cdot\frac{\pi^2}{4} = \frac{L}{2}$$

$$E_{11}^{(1)} = \lambda\, L^2/4$$

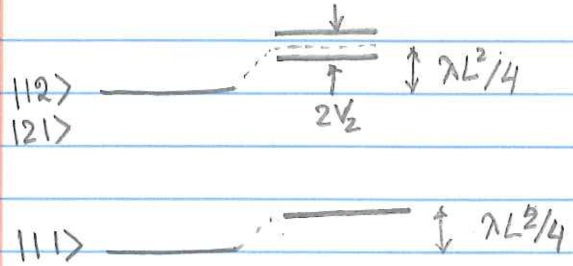
For the first excited state

$$\langle 21|V|21\rangle = \langle 12|V|12\rangle = \lambda \langle 1|x|1\rangle\langle 2|x|2\rangle = \lambda\frac{L^2}{4} = V_1$$

$$\langle 21|V|12\rangle = \lambda\langle 2|x|1\rangle\langle 1|y|2\rangle = \lambda\,|\langle 1|x|2\rangle|^2 = \frac{256}{81\pi^2}\lambda L^2 = V_2$$

$$\hat{V} = \begin{pmatrix} V_1 & V_2 \\ V_2 & V_1 \end{pmatrix} \Rightarrow \det\begin{vmatrix} V_1 - \Delta E & V_2 \\ V_2 & V_1 - \Delta E \end{vmatrix} = 0$$

$$(V_1 - \Delta E)^2 - V_2^2 \Rightarrow \Delta E_\pm = V_1 \pm \Delta V_2 = \frac{\lambda L^2}{4}\left(1 \pm \frac{1024}{81\pi^4}\right)$$



Eigen vectors

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(|12\rangle \pm |21\rangle\right)$$

5.11

a) $$\det\begin{vmatrix} E_1^{(0)}-E & \lambda\Delta \\ \lambda\Delta & E_2^{(0)}-E \end{vmatrix} = 0$$

solving quadratic equation

$$E_\pm = \frac{E_1^{(0)}+E_2^{(0)}}{2} \pm \sqrt{\frac{(E_1^{(0)}-E_2^{(0)})^2}{4} + \lambda^2\Delta^2}$$

If $\Delta E^{(0)} \equiv (E_1^{(0)} - E_2^{(0)})$; and

$\psi = \alpha\varphi_1^{(0)} + \beta\varphi_2^{(0)}$

$$\frac{1}{2}\left(\Delta E^{(0)} \mp \sqrt{(\Delta E^{(0)})^2 + 4\lambda^2\Delta^2}\right) \cdot \alpha + \lambda\Delta\cdot\beta = 0$$

To simplify the notation

$$\frac{\Delta E^{(0)}}{\sqrt{(\Delta E^{(0)})^2+4\lambda^2\Delta^2}} = \cos t \, ; \quad \frac{2\lambda\Delta}{\sqrt{(\Delta E^{(0)})^2+4\lambda^2\Delta^2}} = \sin t$$

$$(\cos t \mp 1)\alpha + \sin t\cdot\beta = 0 \quad \Rightarrow \alpha = -\frac{\sin t}{\cos t \mp 1}\beta$$

$$\beta^2\left(1 + \frac{\sin^2 t}{(\cos t\mp 1)^2}\right) = 2\beta^2\frac{1}{1\mp\cos t} = 1$$

$$\beta = \sqrt{\frac{1\mp\cos t}{2}} \Rightarrow \begin{matrix}\beta_- = \cos t/2 \\ \beta_+ = \sin t/2\end{matrix}$$

$$\alpha_- = -\frac{\sin t}{\sqrt{2(1+\cos t)}} = -\frac{2\cos t/2\,\sin t/2}{2\cos t/2} = -\sin t/2$$

$$\alpha_+ = \frac{\sin t}{\sqrt{2(1-\cos t)}} = \cos t/2$$

So two eigenstates are

E_+: $\psi_+ = \cos t/2\ \varphi_1^{(0)} + \sin t/2\ \varphi_2^{(0)}$

E_-: $\psi_- = -\sin t/2\ \varphi_1^{(0)} + \cos t/2\ \varphi_2^{(0)}$

b) $|\lambda\Delta| \ll |E_1^{(0)} - E_2^{(0)}|$

$$E_\pm \approx \frac{E_1^{(0)} + E_2^{(0)}}{2} \pm \left(\frac{E_1^{(0)} - E_2^{(0)}}{2} + \frac{\lambda^2\Delta^2}{E_1^{(0)} - E_2^{(0)}} \right)$$

$$E_+ \approx E_1^{(0)} + \frac{\lambda^2\Delta^2}{E_1^{(0)} - E_2^{(0)}} \qquad \Psi_+ \simeq \varphi_1^{(0)} + \frac{\lambda\Delta}{\Delta E^{(0)}} \varphi_2^{(0)}$$

$$E_- \approx E_2^{(0)} - \frac{\lambda^2\Delta^2}{E_1^{(0)} - E_2^{(0)}} \qquad \Psi_- \approx -\frac{\lambda\Delta}{\Delta E^{(0)}} \varphi_1^{(0)} + \varphi_2^{(0)}$$

Perturbation theory

$$\varphi_1' \simeq \varphi_1^{(0)} + \varphi_2^{(0)} \frac{V_{21}}{E_1^{(0)} - E_2^{(0)}} = \varphi_1^{(0)} + \frac{\lambda\Delta}{E_1^{(0)} - E_2^{(0)}} \varphi_2^{(0)}$$

$$E_1' \simeq E_1^{(0)} + \frac{|V_{21}|^2}{E_1^{(0)} - E_2^{(0)}} = E_1^{(0)} + \frac{\lambda^2\Delta^2}{E_1^{(0)} - E_2^{(0)}}$$

$$\varphi_2' \simeq \varphi_2^{(0)} + \varphi_1^{(0)} \frac{V_{12}}{E_2^{(0)} - E_1^{(0)}} = \varphi_2^{(0)} - \varphi_1^{(0)} \frac{\lambda\Delta}{E_1^{(0)} - E_2^{(0)}}$$

$$E_2 \simeq E_2^{(0)} + \frac{|V_{12}|^2}{E_2^{(0)} - E_1^{(0)}} = E_2^{(0)} - \frac{\lambda^2\Delta^2}{E_1^{(0)} - E_2^{(0)}}$$

c) $|\lambda\Delta| \gg |E_1^{(0)} - E_2^{(0)}|$

$$E_\pm \approx \frac{E_1^{(0)} + E_2^{(0)}}{2} \pm |\lambda\Delta| \qquad t \approx \frac{\pi}{2} \quad \cos t/2 = \sin t/2 \approx \frac{1}{\sqrt{2}}$$

$$\Psi_\pm = \frac{1}{\sqrt{2}} \left(\varphi_1^{(0)} \pm \varphi_2^{(0)} \right)$$

From perturbation theory for a two-fold degenerate system we get exactly the same!

A1

$$|n^{(2)}\rangle = \sum_{k,k'\neq n} \frac{\langle k'^{(0)}|\hat{V}|k^{(0)}\rangle\langle k^{(0)}|\hat{V}|n^{(0)}\rangle}{(E_k^{(0)}-E_{k'}^{(0)})(E_n^{(0)}-E_k^{(0)})}\,|k'^{(0)}\rangle -$$

$$-\sum_{k\neq n} \frac{\langle n^{(0)}|\hat{V}|n^{(0)}\rangle\langle k^{(0)}|\hat{V}|k^{(0)}\rangle}{(E_k^{(0)}-E_n^{(0)})^2}\,|k^{(0)}\rangle$$

$$-\frac{1}{2}\sum_{k\neq n} \frac{|\langle k|\hat{V}|n\rangle|^2}{(E_k^{(0)}-E_n^{(0)})^2}\cdot|n^{(0)}\rangle$$

A2

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 x^2}{2} + \alpha x^3 + \beta x^4$$

Using $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}^+ + \hat{a})$, one can calculate

$$\langle n-3|x^3|n\rangle = \langle n|x^3|n-3\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} \sqrt{n(n-1)(n-2)}$$

$$\langle n-1|x^3|n\rangle = \langle n|x^3|n-1\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} 3n^{3/2}$$

and all other matrix elements vanish

Thus, there is no first-order correction $\Delta E^{(1)}$ for the αx^3 term, and the second-order correction is

$$\Delta E^{(2)} = -\frac{15}{4}\frac{\alpha^2}{\hbar\omega}\left(\frac{\hbar}{m\omega}\right)^3 \left(n^2 + n + \frac{11}{30}\right)$$

Similarly $\langle n|x^4|n\rangle = \left(\frac{\hbar}{m\omega}\right)^2 \frac{3}{4}(2n^2 + 2n + 1)$, thus this term gives non-zero first-order correction

$$\Delta E^{(1)} = \frac{3}{4}\beta\left(\frac{\hbar}{m\omega}\right)^2 (2n^2 + 2n + 1)$$

A3

$$\hat{V} = -qx\mathcal{E}$$

$$\Delta E^{(1)} = \langle 1|\hat{V}|1\rangle = \frac{1}{a}\int_{-a}^{a} x\cos^2\frac{\pi x}{2a}\,dx = 0$$

$$\Delta E^{(2)} = \sum_{n=2}^{\infty}\frac{|\langle 1|\hat{V}|n\rangle|^2}{E_1 - E_n} = -\frac{8ma^2}{\pi^2\hbar^2}\sum_{n=2}^{\infty}\frac{|\langle 1|\hat{V}|n\rangle|^2}{(n^2-1)}$$

$$\underset{\uparrow\,\text{odd}}{\langle 1|\hat{V}|n\rangle} = \frac{q\mathcal{E}}{a}\int_{-a}^{a} x\cos\frac{\pi x}{2a}\cos\frac{\pi n x}{2a}\,dx = 0$$

$$\underset{\uparrow\,\text{even}}{\langle 1|\hat{V}|n\rangle} = \frac{q\mathcal{E}}{a}\int_{-a}^{a} x\cos\frac{\pi x}{2a}\sin\frac{\pi n x}{2a}\,dx = -\frac{8na}{\pi^2(n^2-1)^2}\,q\mathcal{E}$$

$$\Delta E^{(2)} = -\frac{8ma^2}{\pi^2\hbar^2}\left(\frac{8a}{\pi^2}\right)^2(q\mathcal{E})^2\sum_{\substack{k=1\\ n=2k}}^{\infty}\frac{(2k)^2}{(4k^2-1)^5} =$$

96
96

$$= \frac{8192}{\pi^6}\,m\left(\frac{q\mathcal{E}a^2}{\hbar}\right)^2\sum_{k=1}^{\infty}\frac{k^2}{(4k^2-1)^5}$$