Homework #3 solutions

5.12

Non-degenerate PT

$$\Delta E_1^{(2)} = \sum_{n=3} \frac{|V_{1n}|^2}{E_1 - E_n} = -\frac{V_{13}^2}{E_2 - E_1} = -\frac{a^2}{E_2 - E_1}$$

$$\Delta E_2^{(2)} = -\frac{b^2}{E_2 - E_1}$$

$$\Delta E_3^{(2)} = \frac{a^2 + b^2}{E_2 - E_1}$$

same expression for the proper degenerate PT must be ok!

Now, diagonalize the matrix

$$\det\begin{pmatrix} E_1 - \lambda & 0 & a \\ 0 & E_1 - \lambda & b \\ a^* & b^* & E_2 - \lambda \end{pmatrix} = 0$$

$$(E_1 - \lambda)^2 (E_2 - \lambda) - |b|^2 (E_1 - \lambda) - |a|^2 (E_1 - \lambda) = 0$$

$$\lambda_0 = E_1$$

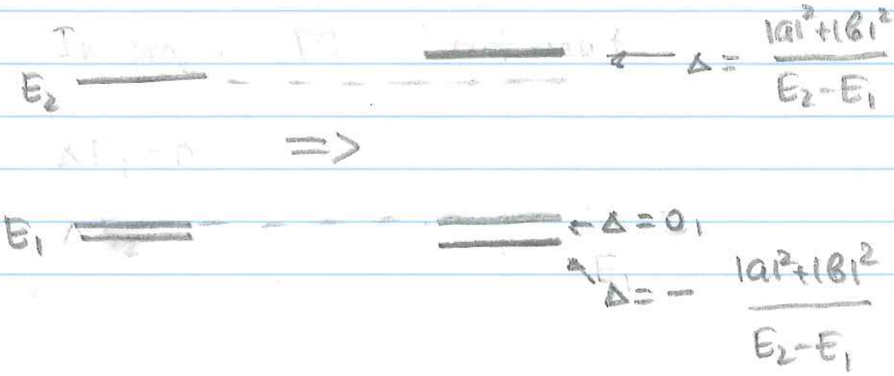
$$\lambda^2 - (E_1 + E_2)\lambda + E_1 E_2 - |b|^2 - |a|^2 = 0$$

$$\lambda_{1,2} = \frac{E_1 + E_2}{2} \pm \sqrt{\frac{(E_2 - E_1)^2}{4} + |b|^2 + |a|^2} \approx$$

$$\approx \frac{E_1 + E_2}{2} \pm \frac{E_2 - E_1}{2} \pm \frac{(|a|^2 + |b|^2)}{E_2 - E_1}$$

$$\lambda_2 = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

$$\lambda_1 = E_1 - \frac{|a|^2 + |b|^2}{E_2 - E_1}$$



coinside with the "naive" calculation above

5.13

$2S_{1/2}$ ———— $\updownarrow \delta$
$2P_{1/2}$ ————

$$\begin{array}{cccccc} \text{state:} & s & s & p & p \\ m_j: & 1/2 & -1/2 & 1/2 & -1/2 \end{array}$$

$$\hat{H}_0 = \begin{pmatrix} \delta & 0 & 0 & 0 \\ 0 & \delta & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$\vec{E} = E\,\vec{e}_z$

Selection rules: $\Delta m = 0$, $\Delta l = \pm 1$

non-zero elements:

$\langle s, m=\pm\frac{1}{2} | -eEz | p, m=\pm\frac{1}{2} \rangle =$

$= (-eE)\ \langle 2s | r | 2p \rangle \times \{ \text{angular part} \}$

$$\psi_{nlm} = R_{nl}(r)\, \mathcal{Y}_l^{j=l\pm 1/2, m}$$

$$\mathcal{Y}_l^{j=l\pm 1/2, m} = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \pm\sqrt{l\pm m+\frac{1}{2}}\ Y_l^{m-1/2} \\ \sqrt{l\mp m+\frac{1}{2}}\ Y_l^{m+1/2} \end{pmatrix}$$

$$\psi_{2s\,1/2} = \begin{pmatrix} Y_0^0 \\ 0 \end{pmatrix} \qquad \psi_{2s\,-1/2} = \begin{pmatrix} 0 \\ Y_0^0 \end{pmatrix}$$

$$\psi_{2p\,1/2} = \frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{2}\,Y_1^0 \\ Y_1^1 \end{pmatrix} \qquad \psi_{2p\,-1/2} = \frac{1}{\sqrt{3}} \begin{pmatrix} Y_1^{-1} \\ -\sqrt{2}\,Y_1^0 \end{pmatrix}$$

Obviously, the non-zero elements are b/w states $2s\ m=1/2 \Leftrightarrow 2p\ m=1/2$ or b/w $2s\ m=-1/2 \Leftrightarrow 2p\ m=-1/2$ → two identical independent systems, can separate

$$\hat{H}_0 = \begin{pmatrix} \delta & 0 \\ 0 & 0 \end{pmatrix} \begin{array}{l} s, m=\pm 1/2 \\ p, m=\pm 1/2 \end{array} \qquad \hat{V} = \begin{pmatrix} 0 & V_0 \\ V_0 & 0 \end{pmatrix}$$

$$V_0 = \langle 2s\ m=1/2 | -e\mathcal{E}z | 2p\ m=1/2 \rangle = 3e\mathcal{E}a_0$$

Exact solution

$$\det\begin{pmatrix} \delta-\lambda & V_0 \\ V_0 & -\lambda \end{pmatrix} = 0$$

$$-\lambda(\delta-\lambda) - V_0^2 = 0$$

$$\lambda^2 - \delta\lambda - V_0^2 = 0$$

$$\lambda_{1,2} = \frac{\delta}{2} \pm \sqrt{\frac{\delta^2}{4} + V_0^2}$$

For $\delta \gg V_0$

$$\lambda_{1,2} \simeq \frac{\delta}{2} \pm \frac{\delta}{2} \pm \frac{V_0^2}{\delta}$$

$\lambda_1 \simeq \delta + V_0^2/\delta$

$\lambda_2 \simeq -V_0^2/\delta$

quadratic effect

For $\delta \ll V_0$

$\lambda_{1,2} \simeq \pm V_0 + \delta/2$ linear effect

5-18

$$\hat{V} = \frac{e^2A^2}{2mc^2} = \frac{e^2B^2}{8mc^2}(x^2+y^2)$$

Since $x^2+y^2 = r^2 - z^2$, $\hat{V}$ is diagonal in our standard basis

$$\langle n\ell m|\hat{V}|n\ell m\rangle = \frac{e^2B^2}{8mc^2}\langle n\ell m|x^2+y^2|n\ell m\rangle =$$

$$= \frac{e^2B^2}{4mc^2}\langle x^2\rangle = \frac{e^2B^2}{12mc^2}\langle r^2\rangle$$

$$\langle r^2\rangle = \frac{1}{\pi a_0^3}4\pi\int r^2 e^{-2r/a_0} r^2 dr = \left(\frac{a_0}{2}\right)^5 \frac{1}{\pi a_0^3}\cdot 4\pi\overbrace{\int x^4 e^{-x} dx}^{4! = 24} =$$

$$\langle r^3\rangle = \frac{24}{8}a_0^2 = 3a_0^2$$

$$\Delta E = \frac{e^2B^2}{12mc^2}\cdot 3a_0^2 = \frac{a_0^2 e^2}{4mc^2}a_0^2 = -\frac{1}{2}\chi B^2$$

$$\chi = -\frac{a_0^2 e^2}{2mc^2}$$

A1. Selection rules are still $\Delta l = \pm 1$, $\Delta m_\ell = 0$, $\Delta m_s = 0$

Closest s-state $2S_{1/2}$

States with $m_j = \pm 3/2$ are not coupled (their $m_\ell = \pm 1$)

Thus, it is only possible to couple $|m_j = \pm 1/2\rangle$ states.

$$|m_j = 1/2\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{2}\, Y_1^0 \\ Y_1^1 \end{pmatrix} \qquad |m_j = -1/2\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} Y_1^{-1} \\ \sqrt{2}\, Y_1^0 \end{pmatrix}$$

Since $\Delta m_S = 0$ $2P|m_j = 1/2\rangle$ couples only to $2S|m_s = 1/2\rangle$ state, and $2P|m_j = -1/2\rangle$ couples to $2S|m_s - 1/2\rangle$ state; no mixing b/w these pairs.

Thus, the shift for each of $|m_j = \pm 1/2\rangle$ levels is exactly the same

$$\Delta E = \frac{|\langle 2S\, m_s = 1/2 | V | 2P\, m_j = 1/2\rangle|^2}{E_{2p} - E_{2s}} = \frac{9e^2 \mathcal{E}^2 a_0^2}{\Delta_{FS}}$$

$2P_{3/2}$ ——— $\Longrightarrow$ ═══ $m_j = \pm 1/2$

$\Delta E = \dfrac{9e^2 \mathcal{E}^2 a_0^2}{\Delta_{FS}}$

$m_j = \pm 3/2$

A2. Charge density $\rho = \frac{3|e|}{4\pi R^3}$

$$V_R = \begin{cases} -e^2/r & r>R \quad \text{(same as point charge)} \\ -\frac{e^2}{R}\left[\frac{3}{2} - \frac{1}{2}\frac{r^2}{R^2}\right] & r<R \end{cases}$$

Thus $\delta V = \begin{cases} 0 & r>R \\ e^2\left(\frac{1}{r} + \frac{1}{2}\frac{r^2}{R^3} - \frac{3}{2R}\right) & r<R \end{cases}$

Don't need to worry about l, m degeneracy!

a) $\Delta E_{1S} = \langle 100|\delta V|100\rangle = \frac{1}{4\pi a_0^3}\int_0^R d^3\vec{r}\, e^{-2r/a_0}\,\delta V =$

$$= \frac{e^2}{a_0^3}\int_0^R \left(\frac{1}{r} + \frac{1}{2}\frac{r^2}{R^3} - \frac{3}{2R}\right)e^{-2r/a_0}\, r^2 dr =$$

$$= \frac{e^2}{a_0^3}\left[\left(\frac{a_0}{2}\right)^2\int_0^{2R/a_0} x e^{-x}dx + \frac{1}{2}\left(\frac{a_0}{2}\right)^5\frac{1}{R^3}\int_0^{2R/a} x^4 e^{-x}dx - \frac{3}{2R}\left(\frac{a_0}{2}\right)^3\int_0^{2R/a} x^2 e^{-x}dx\right]$$

$$R/a_0 = \alpha \ll 1$$

$$\Delta E_{1S} = \frac{e^2}{a_0}\left[\frac{1}{4}\int_0^{\alpha} x e^{-x}dx + \frac{1}{64}\frac{1}{\alpha^3}\int_0^{\alpha} x^4 e^{-x}dx - \frac{3}{16}\frac{1}{\alpha}\int_0^{\alpha} x^2 e^{-x}dx\right]$$

$$\int_0^{2\alpha} x e^{-x}dx = (1 - e^{-2\alpha}(1+2\alpha))$$

$$\int_0^{\alpha} x^4 e^{-x}dx = 24(1 - e^{-2\alpha}(1+2\alpha+2\alpha^2 + \frac{4\alpha^3}{3} + \frac{2}{3}\alpha^4))$$

$$\int_0^{\alpha} x^2 e^{-x}dx = 2(1 - e^{-2\alpha}(1+2\alpha+2\alpha^2))$$

$$\Delta E_{1S} = \frac{e^2}{a_0}\left[\left(\frac{1}{4} + \frac{3}{8\alpha^3} - \frac{3}{8}\frac{1}{\alpha}\right) - e^{-2\alpha}\left(\frac{1}{4} + \frac{\alpha}{2} + \frac{3}{8\alpha^3} + \frac{3}{4\alpha^2} + \frac{3}{4\alpha} + \frac{1}{2} + \frac{\alpha}{4} - \frac{3}{8\alpha} - \frac{3}{4} - \frac{3\alpha}{4}\right)\right.$$

$$\Delta E_{1S} = \frac{e^2}{8\alpha^3 a_0}\underbrace{\left[(2\alpha^3 - 3\alpha^2 + 3) - e^{-2\alpha}(3 + 6\alpha - 3\alpha^2)\right]}_{\text{first non-vanishing term} \sim \alpha^5}$$

$$\Delta E_{1s} = -\frac{2e^2}{5a_0}\alpha^2$$

b) Following similar steps for

$$2s: |200\rangle = \frac{1}{\sqrt{32a_0^3}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$$

$$2p: |210\rangle = \frac{1}{\sqrt{32a_0^3}}\left(\frac{r}{a_0}\right)e^{-r/2a_0}$$

obtain

$$\Delta E_{2s} = \frac{e^2}{20a_0}\alpha^2$$

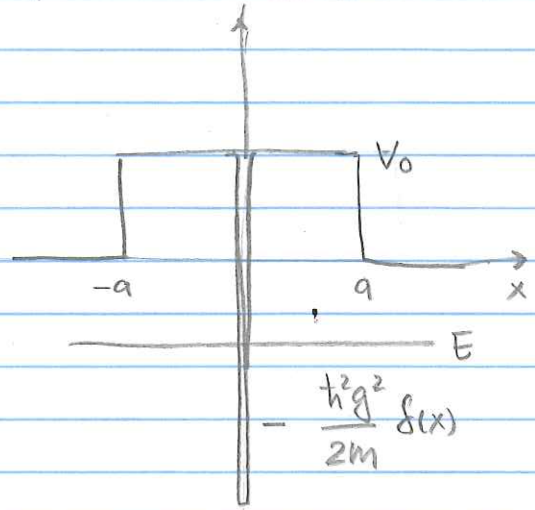
$$\Delta E_{2p} = -\frac{e^2}{480a_0}\alpha^4 \leftarrow$$ effect is strongly suppressed for p state

c) $$\left|\frac{\Delta E_{1s}}{E_{1s}}\right| \sim \frac{2e^2/5a_0\,\alpha^2}{e^2/2a_0} = \frac{4}{5}\alpha^2 \sim \left(\frac{10^{-15}\,m}{10^{-10}\,m}\right)^2 \sim 10^{-10}$$

$$\left|\frac{\Delta E_{2s}}{E_{2s}}\right| \sim \frac{1/20\;e^2/a_0\,\alpha^2}{1/8\;e^2/a_0} = \frac{2}{5}\alpha^2 \sim 5\cdot10^{-11}$$

$$\left|\frac{\Delta E_{2p}}{E_{2p}}\right| \sim \frac{\frac{1}{480}\;e^2/a_0\,\alpha^4}{1/8\;e^2/a_0} = \frac{1}{60}\alpha^4 \sim 5\cdot10^{-22}$$

Q1: Potential



Ground-state wavefunction is symmetric

$$\psi(x) = \begin{cases} A e^{-k_0|x|} & |x|<a \\ B e^{-k|x|} + C e^{k|x|} & 0<|x|<a \end{cases}$$

$k_0 = \sqrt{\frac{2m|E|}{\hbar^2}}$ $\quad k = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

$\psi(x)$ is continuous everywhere

$\frac{d\psi}{dx}$ has a discontinuity at $x=0$

$$A e^{-k_0 a} = B e^{-ka} + C e^{ka} \quad (1)$$

$$-k_0 A e^{-k_0 a} = -k B e^{-ka} + k C e^{ka} \quad (2)$$

$$-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\Big|_{x=+0} - \frac{d\psi}{dx}\Big|_{x=-0}\right] = \frac{\hbar^2 g^2}{2m}\psi(0)$$

$$-2k(-B+C) = g^2(B+C)$$

$$2k(B-C) = g^2(B+C)$$

$$(2k-g^2)B = (2k+g^2)C$$

$$\frac{B}{C} = \frac{2k+g^2}{2k-g^2}$$

Dividing (2) by (1) we get

$$\frac{k(-Be^{-ka}+Ce^{ka})}{Be^{-ka}+Ce^{ka}} = -k_0$$

$$-kBe^{-ka} + kCe^{ka} = -k_0 Be^{-ka} - k_0 Ce^{ka}$$

$$(k-k_0)Be^{-ka} = (k+k_0)Ce^{ka}$$

$$\frac{B}{C} = \frac{k+k_0}{k-k_0}\, e^{2ka}$$

Equation for calculating the bound state energy

$$\left(\frac{k+k_0}{k-k_0}\right)e^{2ka} = \frac{2k+g^2}{2k-g^2} \quad \text{or} \quad \left(\frac{k-k_0}{k+k_0}\right)e^{-2ka} = \frac{2k-g^2}{2k+g^2} \quad (3)$$

if $V_0 = 0$ $k = k_0$, the left part $= 0$

and thus $2k_0 - g^2 = 0$

$$\sqrt{\frac{2m|E_0|}{\hbar^2}} = \frac{g^2}{2}$$

$$E_0 = -\frac{\hbar^2 g^4}{8m}$$

Now, for $V_0 \geq 0$ $k - k_0 \geq 0$, thus we must have $2k - g^2 \geq 0$ for the equation (3) to have a solution

$$\sqrt{\frac{2m(V_0 + |E|)}{\hbar^2}} \geq \frac{g^2}{2}$$

$$V_0 + |E| = V_0 - E \geq \frac{\hbar^2 g^4}{8m} = -E_0$$

and $\underline{E \leq V_0 + E_0}$

Thus, the higher is the potential step, the shallower the energy level is.