6.14 Hitta den lägsta ordningens korrektion till energinivåerna hos den endimensionella harmoniska oscillatorn.

Eq. (6.53):

$$E_r^1 = -\frac{1}{2mc^2}\langle (E-V)^2\rangle = -\frac{1}{2mc^2}[E^2 - 2E\langle V\rangle + \langle V^2\rangle]$$

där, för den harmoniska oscillatorn, vi har

$$E = (n+\tfrac{1}{2})\hbar\omega, \quad V = \tfrac{1}{2}m\omega^2 x^2 .$$

Men (från uppgift 2.12) $\langle x^2\rangle = (n+\frac{1}{2})\frac{\hbar}{m\omega}$ och således

$$E_r^1 = -\frac{1}{2mc^2}\left[(n+\tfrac{1}{2})^2\hbar^2\omega^2 - (n+\tfrac{1}{2})^2\hbar^2\omega^2 + \tfrac{1}{4}m^2\omega^4\langle x^4\rangle\right] = -\frac{m\omega^4}{8c^2}\langle x^4\rangle$$

Vidare

$$x^4 = \frac{\hbar^2}{4m^2\omega^2}(a_+^2 + a_+a_- + a_-a_+ + a_-^2)(a_+^2 + a_+a_- + a_-a_+ + a_-^2)$$

och

$$\langle x^4\rangle = \frac{\hbar^2}{4m^2\omega^2}\langle n| a_+^2a_-^2 + a_+a_-a_-a_+ + a_+a_-a_+a_- + a_-a_+a_+a_- + a_-a_+a_-a_+ + a_-^2a_+^2 |n\rangle = \frac{\hbar^2}{4m^2\omega^2}(n(n-1) + (n+1)n + n^2 + n(n+1) + (n+1)^2 + (n+1)(n+2)$$

$$= \frac{\hbar^2}{4m^2\omega^2}(n^2 - n + n^2 + n + n^2 + n^2 + n + n^2 + 2n + 1 + n^2 + 3n + 2) =$$

$$= \frac{\hbar^2}{4m^2\omega^2}(6n^2 + 6n + 3)$$

$$\Rightarrow E_r^1 = -\frac{m\omega^4}{8c^2}\cdot\frac{\hbar^2}{4m^2\omega^2}\cdot 3(2n^2 + 2n + 1) = -\frac{3}{32}\left(\frac{\hbar^2\omega^2}{mc^2}\right)(2n^2 + 2n + 1)$$

6.16 Vi ska beräkna kommutatorer

a) $[\bar{L}\cdot\bar{S}, L_x] = [L_x S_x + L_y S_y + L_z S_z, L_x] = S_x[L_x, L_x] + S_y[L_y, L_x]$
$+ S_z[L_z, L_x] = S_y(-i\hbar L_z) + S_z(i\hbar L_y) = i\hbar(L_y S_z - L_z S_y) = i\hbar(\bar{L}\times\bar{S})_x$

Samma gäller för L_y och L_z och alltså

$$[\bar{L}\cdot\bar{S}, \bar{L}] = i\hbar(\bar{L}\times\bar{S})$$

b) Kommutatorn $[\bar{L}\cdot\bar{S}, \bar{S}]$ beräknas enl. samma princip med $\bar{S}\longleftrightarrow\bar{L}$

$$[\bar{L}\cdot\bar{S}, \bar{S}] = i\hbar(\bar{S}\times\bar{L})$$

c) $[\bar{L}\cdot\bar{S}, \bar{J}] = [\bar{L}\cdot\bar{S}, \bar{L}+\bar{S}] = [\bar{L}\cdot\bar{S}, \bar{L}] + [\bar{L}\cdot\bar{S}, \bar{S}] = i\hbar(\bar{L}\times\bar{S} + \bar{S}\times\bar{L})$
$= i\hbar(\bar{L}\times\bar{S} - \bar{L}\times\bar{S}) = 0$

d) L^2 kommuterar med alla komponenter av $\bar{L}$ och $\bar{S}$. Således
$[\bar{L}\cdot\bar{S}, L^2] = 0$

e) Pss. $[\bar{L}\cdot\bar{S}, \bar{S}^2] = 0$

f) $[\bar{L}\cdot\bar{S}, J^2] = [\bar{L}\cdot\bar{S}, \bar{S}^2 + 2\bar{L}\cdot\bar{S} + \bar{L}^2] = [\bar{L}\cdot\bar{S}, \bar{S}^2] + 2[\bar{L}\cdot\bar{S}, \bar{L}\cdot\bar{S}] + [\bar{L}\cdot\bar{S}, \bar{L}^2]$
$= 0$

6.17 Härled

$$E^1_{fs} = \frac{(E_n)^2}{2mc^2}\left(3 - \frac{4n}{j+1/2}\right)$$

från

$$E^1_r = -\frac{(E_n)^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$$

och

$$E^1_{so} = \frac{(E_n)^2}{mc^2}\left[\frac{n[j(j+1) - l(l+1) - 3/4]}{l(l+1/2)(l+1)}\right]$$

$j = l + \frac{1}{2}$

$$\Rightarrow E^1_r = -\frac{(E_n)^2}{2mc^2}\left[\frac{4n}{j} - 3\right]$$

$$E^1_{so} = \frac{(E_n)^2}{mc^2}\left[\frac{n(j(j+1) - (j-\frac{1}{2})(j+\frac{1}{2}) - \frac{3}{4}}{(j-\frac{1}{2})j(j+\frac{1}{2})}\right] =$$

$$= \frac{(E_n)^2 n}{mc^2}\left[\frac{j^2 + j - j^2 + \frac{1}{4} - \frac{3}{4}}{j(j-\frac{1}{2})(j+\frac{1}{2})}\right] = \frac{(E_n)^2 n}{mc^2}\left[\frac{j-\frac{1}{2}}{j(j-\frac{1}{2})(j+\frac{1}{2})}\right] = \frac{(E_n)^2}{mc^2}\frac{n}{j(j+\frac{1}{2})}$$

$$E^1_{fs} = E^1_r + E^1_{so} = \frac{(E_n)^2}{2mc^2}\left[-\frac{4n}{j} + 3 + \frac{2n}{j(j+\frac{1}{2})}\right] = \frac{(E_n)^2}{2mc^2}\left[3 + 2n\frac{1-2j-1}{j(j+\frac{1}{2})}\right] =$$

$$= \frac{(E_n)^3}{2mc^2}\left[3 - \frac{4n}{j+\frac{1}{2}}\right]$$

$\square$

6.21 Vi har åtta tillstånd med $n=2$.

$n=2,\ l=0\ (j=\frac{1}{2}),\ l=1\ (j=\frac{1}{2},\frac{3}{2})$

$$\left.\begin{array}{l}|1\rangle = |2\,0\,\tfrac{1}{2}\,\tfrac{1}{2}\rangle \\ |2\rangle = |2\,0\,\tfrac{1}{2}\,-\tfrac{1}{2}\rangle\end{array}\right\} \quad g_J = \{\text{Landé g-faktor}\} = 1 + \frac{j(j+1)-l(l+1)+\frac{3}{4}}{2j(j+1)} = 2$$

$$\left.\begin{array}{l}|3\rangle = |2\,1\,\tfrac{1}{2}\,\tfrac{1}{2}\rangle \\ |4\rangle = |2\,1\,\tfrac{1}{2}\,-\tfrac{1}{2}\rangle\end{array}\right\} \quad g_j = 1 + \frac{\frac{3}{4}-2+\frac{3}{4}}{\frac{3}{2}} = \frac{2}{3}$$

Väteatomens energinivåer med finstruktur inräknad

$$E_{nj} = -\frac{13.6\,\text{eV}}{n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right]$$

I de fyra fallen ovan har vi

$$E_{nj} = -3.4\,\text{eV}\left[1 + \frac{\alpha^2}{4}\left(\frac{2}{1} - \frac{3}{4}\right)\right] = -3.4\,\text{eV}\left[1 + \frac{5}{16}\alpha^2\right]$$

$$\left.\begin{array}{l}|5\rangle = |2\,1\,\tfrac{3}{2}\,\tfrac{3}{2}\rangle \\ |6\rangle = |2\,1\,\tfrac{3}{2}\,\tfrac{1}{2}\rangle \\ |7\rangle = |2\,1\,\tfrac{3}{2}\,-\tfrac{1}{2}\rangle \\ |8\rangle = |2\,1\,\tfrac{3}{2}\,-\tfrac{3}{2}\rangle\end{array}\right\} \quad g_J = 1 + \frac{\frac{15}{4}-2+\frac{3}{4}}{2\cdot\frac{15}{4}} = 1 + \frac{\cancel{10}^{\,2}}{\cancel{4}_{\,2}}\cdot\frac{\cancel{2}}{\cancel{15}_{\,3}} = \frac{4}{3}$$

$$\text{Här}\quad E_{nj} = -3.4\,\text{eV}\left[1 + \frac{\alpha^2}{4}\cdot\left[\frac{2}{2} - \frac{3}{4}\right]\right] = -3.4\,\text{eV}\left[1 + \frac{\alpha^2}{16}\right]$$

Zeemankorrektionen ges av $E'_Z = \mu_B g_J B_{ext} m_j$

där μ_B är Bohrmagnetonen och B_{ext} är det externa magnetfältet.
Således

$E_1 = -3.4\,\text{eV}(1 + \frac{5}{16}\alpha^2) + \mu_B B_{ext}$

$E_2 = -3.4\,\text{eV}(1 + \frac{5}{16}\alpha^2) - \mu_B B_{ext}$

$E_3 = -3.4\,\text{eV}(1 + \frac{5}{16}\alpha^2) + \frac{1}{3}\mu_B B_{ext}$

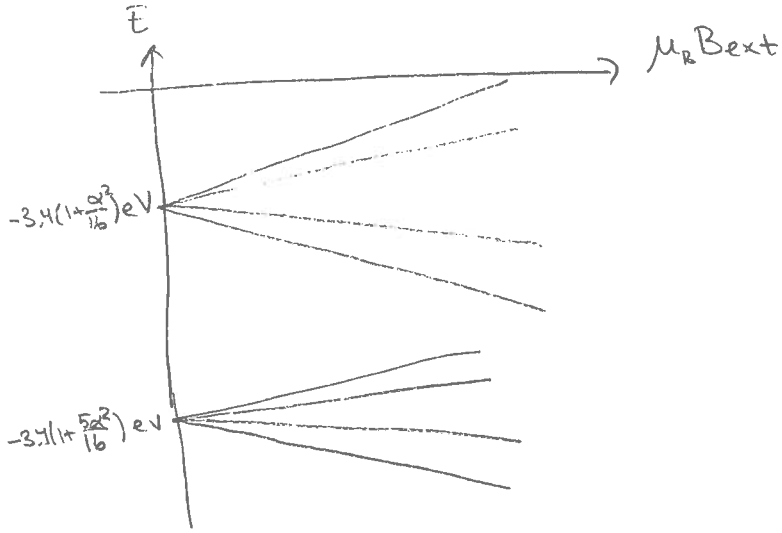
$E_4 = -3.4\,\text{eV}(1 + \frac{5}{16}\alpha^2) - \frac{1}{3}\mu_B B_{ext}$

$E_5 = -3.4\,\text{eV}(1 + \frac{1}{16}\alpha^2) + 2\mu_B B_{ext}$

$E_6 = -3.4\,\text{eV}(1 + \frac{1}{16}\alpha^2) + \frac{2}{3}\mu_B B_{ext}$

$E_7 = -3.4\,\text{eV}(1 + \frac{1}{16}\alpha^2) - \frac{2}{3}\mu_B B_{ext}$

$E_8 = -3.4\,\text{eV}(1 + \frac{1}{16}\alpha^2) - 2\mu_B B_{ext}$


E
$\mu_B B_{ext}$
$-3{,}4(1+\frac{\alpha^2}{16})$ eV
$-3{,}4(1+\frac{5\alpha^2}{16})$ eV

6.32 Hamiltonfunktion $H(\lambda)$, λ någon parameter. Låt $E_n(\lambda)$ och $\psi_n(\lambda)$ vara egenvärdena och egenfunktionerna till $H(\lambda)$. Då

$$\frac{\partial E_n}{\partial \lambda} = \left\langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \right\rangle \quad \text{(Feynman-Hellmanns sats)}$$

a) Vi börjar från

$$E_n' = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

Således måste störningen H' bestämmas.

$$H' = H(\lambda_0 + d\lambda) - H(\lambda_0) = \frac{\partial H}{\partial \lambda} d\lambda \quad \text{(derivatan evalueras i } \lambda_0\text{)}$$

Förändringen i energi ges av

$$dE_n = E_n' = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \langle \psi_n | \frac{\partial H}{\partial \lambda} | \psi_n \rangle d\lambda$$

$$\Rightarrow \frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial H}{\partial \lambda} | \psi_n \rangle$$

b) Tillämpa formeln på den harmoniska oscillatorn, $E_n = (n+\frac{1}{2})\hbar\omega$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

i) $\lambda = \omega$

$$\frac{\partial E_n}{\partial \omega} = (n+\tfrac{1}{2})\hbar, \quad \frac{\partial H}{\partial \omega} = m\omega x^2 \Rightarrow (n+\tfrac{1}{2})\hbar = \langle n | m\omega x^2 | n \rangle$$

Men $V = \frac{1}{2}m\omega^2 x^2$ och således är

$$\langle V \rangle = \frac{1}{2}\omega \langle n | m\omega x^2 | n \rangle = \frac{1}{2}(n+\tfrac{1}{2})\hbar\omega$$

$$\Rightarrow \boxed{\langle V \rangle = \frac{1}{2}(n+\tfrac{1}{2})\hbar\omega}$$

ii) $\lambda = \hbar$

$$\frac{\partial E_n}{\partial \hbar} = (n+\tfrac{1}{2})\omega, \quad \frac{\partial H}{\partial \hbar} = -\frac{\hbar}{m}\frac{d^2}{dx^2} = \frac{2}{\hbar}\left(-\frac{\hbar^2}{m}\frac{d^2}{dx^2}\right) = \frac{2}{\hbar}T$$

$$\Rightarrow (n+\tfrac{1}{2})\omega = \frac{2}{\hbar}\langle n | T | n \rangle = \frac{2}{\hbar}\langle T \rangle$$

$$\Rightarrow \boxed{\langle T \rangle = \frac{1}{2}(n+\tfrac{1}{2})\hbar\omega}$$

(iii) $\lambda = m$

$$\frac{\partial E_n}{\partial m} = 0 \quad \frac{\partial H}{\partial m} = \frac{\hbar^2}{2m^2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\omega^2 x^2 = \frac{-1}{m}\langle T\rangle + \frac{1}{m}\langle V\rangle$$

$$\Rightarrow \langle V\rangle = \langle T\rangle$$

6.36 Stark effekt:

$$H_S' = eE_{ext}z = eE_{ext}r\cos\theta$$

störning till Bohr-hamiltonianen.

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{r}$$

a) Grundtillståndet

$$|1\,0\,0\rangle = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}$$

$$E_S' = \langle 1\,0\,0|H'|1\,0\,0\rangle = eE_{ext}\frac{1}{\sqrt{\pi a^3}}\int r\cos\theta\, e^{-2r/a}r^2\sin\theta dr\,d\theta\,d\phi$$

$$= 2eE_{ext}\sqrt{\frac{\pi}{a^3}}\int_0^\infty r^3e^{-2r/a}dr\,\underbrace{\left[\frac{1}{2}\sin^2\theta\right]_0^\pi}_{=0} = 0$$

b) Det första exciterade tillståndet är fyrfaldigt degenererat. Bestäm första ordningens korrektioner till energin. Till hur många nivåer delas E_2 upp?

$$|1\rangle = \frac{1}{\sqrt{2\pi a}}\cdot\frac{1}{2a}\left(1-\frac{r}{2a}\right)e^{-r/2a}$$

$$|2\rangle = \frac{-1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta e^{i\phi}$$

$$|3\rangle = \frac{1}{\sqrt{2\pi a}}\frac{1}{4a^2}re^{-r/2a}\cos\theta$$

$$|4\rangle = \frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta e^{-i\phi}$$

Bestäm vilka som är nollskilda genom att titta på vinkeldelarna

$$\langle 1|H_S'|1\rangle \propto \int_0^\pi \cos\theta\sin\theta d\theta = 0$$

$$\langle 1|H_S'|2\rangle \propto \int_0^\pi \cos\theta\sin^2\theta d\theta = 0$$ (notera att detta är $\langle 2|H'|1\rangle^*$)

$$\langle 1|H_S'|3\rangle \propto \int_0^\pi \cos^2\theta\sin\theta d\theta \neq 0$$

$$\langle 1|H_S'|4\rangle \propto \int_0^\pi \cos\theta\sin^2\theta\, d\theta = 0$$

$$\langle 2|H_S'|2\rangle \propto \int_0^\pi \sin^3\theta\cos\theta\, d\theta = 0$$

$$\langle 2|H_S'|3\rangle \propto \int_0^{2\pi} e^{-i\phi}\, d\phi = 0$$

$$\langle 2|H_S'|4\rangle = \int_0^{2\pi} e^{i\phi}d\phi = 0$$

$$\langle 3|H_S'|3\rangle = \int_0^\pi \cos^3\theta\sin\theta\, d\theta = 0$$

$$\langle 3|H_s'|4\rangle \propto \int_0^{2\pi} e^{-i\phi}\,d\phi$$

$$\langle 4|H'|4\rangle \propto \int_0^{\pi} \sin^3\theta\cos\theta\,d\theta$$

Bara ett element som måste beräknas

$$\langle 1|H_s'|3\rangle = eE_{ext}\frac{1}{\sqrt{2\pi a}}\frac{1}{2a}\frac{1}{\sqrt{2\pi a}}\frac{1}{4a^2}\int\left(1-\frac{r}{2a}\right)e^{-r/2a}\,r e^{-r/2a}\cos\theta(r\cos\theta)r^2\sin\theta\,dr\,d\theta$$

$$= \frac{eE_{ext}}{2\pi a 8a^3}(2\pi)\underbrace{\left[\int_0^{\pi}\cos^2\theta\sin\theta\,d\theta\right]}_{\left[-\frac{1}{3}\cos^3\theta\right]_0^{\pi}=\frac{2}{3}}\int_0^{\infty}\left(1-\frac{r}{2a}\right)r^4 e^{-r/a}\,dr$$

$$= \frac{eE_{ext}}{8a^4}\frac{2}{3}\left(\int_0^{\infty} r^4 e^{-r/a}dr - \frac{1}{2a}\int_0^{\infty} r^5 e^{-r/a}\,dr\right) = \frac{eE_{ext}}{12a^4}\left(4!\,a^5 - \frac{1}{2a}5!\,a^6\right) =$$

$$= \frac{eE_{ext}a}{12}(24-60) = -3eE_{ext}a = \langle 3|H_s'|1\rangle^* \text{ (men den är reell)}$$

Störningsmatrisen blir

$$W = -3eE_{ext}a\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Bestäm egenvärdena (för att kunna bestämma splittringen)

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

$$= (-\lambda)^4 - (-\lambda)^2 = \lambda^2(\lambda^2-1) = 0 \qquad \lambda_{1,2} = 0,\ \lambda_{3,4} = \pm 1$$

Således är de störda energierna $E_2, E_2, E_2 + 3eE_{ext}a, E_2 - 3eE_{ext}a$.