Homework 5 solution

7.24 Find the energies under a weak field Zeeman effect on the eight n=2 states $|2, l, j, m_j\rangle$. The total energies are the fine structure energies plus the energies due to the external field,

$$E_n = -\frac{13.6eV}{n^2}\left[1 - \frac{\alpha^2}{4n^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)\right] + \mu_B g_j B_{ext} m_j$$

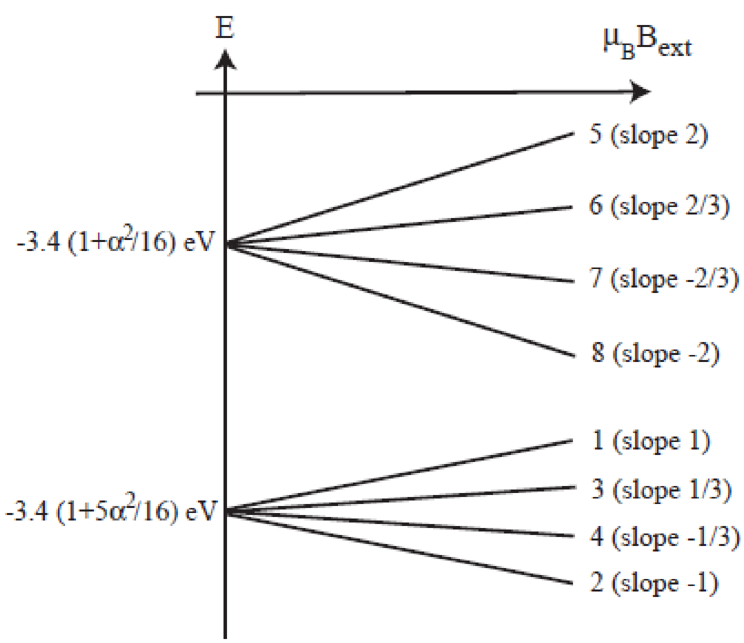
For $n = 2$, j can be equal to either 1/2 or 3/2 so when the external field is zero there are two possible energies for these states (as shown figure at end). The lande g-factor times m_j determines the slope

The lande g-factors for the states labeled 1 thru 8 are the

$$\left.\begin{aligned} |1\rangle &= |2\;0\;\tfrac{1}{2}\;\tfrac{1}{2}\rangle \\ |2\rangle &= |2\;0\;\tfrac{1}{2}\;-\tfrac{1}{2}\rangle \end{aligned}\right\} g_J = \left[1 + \frac{(1/2)(3/2) + (3/4)}{2(1/2)(3/2)}\right] = 1 + \frac{3/2}{3/2} = 2.$$

$$\left.\begin{aligned} |3\rangle &= |2\;1\;\tfrac{1}{2}\;\tfrac{1}{2}\rangle \\ |4\rangle &= |2\;1\;\tfrac{1}{2}\;-\tfrac{1}{2}\rangle \end{aligned}\right\} g_J = \left[1 + \frac{(1/2)(3/2) - (1)(2) + (3/4)}{2(1/2)(3/2)}\right] = 1 + \frac{-1/2}{3/2} = 2/3.$$

$$\left.\begin{aligned} |5\rangle &= |2\;1\;\tfrac{3}{2}\;\tfrac{3}{2}\rangle \\ |6\rangle &= |2\;1\;\tfrac{3}{2}\;\tfrac{1}{2}\rangle \\ |7\rangle &= |2\;1\;\tfrac{3}{2}\;-\tfrac{1}{2}\rangle \\ |8\rangle &= |2\;1\;\tfrac{3}{2}\;-\tfrac{3}{2}\rangle \end{aligned}\right\} g_J = \left[1 + \frac{(3/2)(5/2) - (1)(2) + (3/4)}{2(3/2)(5/2)}\right] = 1 + \frac{5/2}{15/2} = 4/3.$$



7.44 Using Kramer's relation

$$\frac{s+1}{n^2}\left\langle r^s\right\rangle-(2s+1)a\left\langle r^{s-1}\right\rangle+\frac{s}{4}\left[(2l+1)^2-s^2\right]a^2\left\langle r^{s-2}\right\rangle=0$$

to evaluate expectations. For $s=0$

$$\frac{1}{n^2}\langle 1\rangle-a\left\langle\frac{1}{r}\right\rangle+0=0\Rightarrow\boxed{\left\langle\frac{1}{r}\right\rangle=\frac{1}{n^2a}.}$$

For $s=1$

$$\frac{2}{n^2}\langle r\rangle-3a\langle 1\rangle+\frac{1}{4}\left[(2l+1)^2-1\right]a^2\left\langle\frac{1}{r}\right\rangle=0\Rightarrow\frac{2}{n^2}\langle r\rangle=3a-l(l+1)a^2\frac{1}{n^2a}=\frac{a}{n^2}\left[3n^2-l(l+1)\right].$$

$$\boxed{\langle r\rangle=\frac{a}{2}\left[3n^2-l(l+1)\right].}$$

For $s=2$

$$\frac{3}{n^2}\langle r^2\rangle-5a\langle r\rangle+\frac{1}{2}\left[(2l+1)^2-4\right]a^2=0\Rightarrow\frac{3}{n^2}\langle r^2\rangle=5a\frac{a}{2}\left[3n^2-l(l+1)\right]-\frac{a^2}{2}\left[(2l+1)^2-4\right]$$

$$\begin{aligned}\frac{3}{n^2}\langle r^2\rangle&=\frac{a^2}{2}\left[15n^2-5l(l+1)-4l(l+1)-1+4\right]=\frac{a^2}{2}\left[15n^2-9l(l+1)+3\right]\\&=\frac{3a^2}{2}\left[5n^2-3l(l+1)+1\right];\quad\boxed{\langle r^2\rangle=\frac{n^2a^2}{2}\left[5n^2-3l(l+1)+1\right].}\end{aligned}$$

For $s=3$

$$\frac{4}{n^2}\langle r^3\rangle-7a\langle r^2\rangle+\frac{3}{4}\left[(2l+1)^2-9\right]a^2\langle r\rangle=0\Longrightarrow$$

$$\begin{aligned}\frac{4}{n^2}\langle r^3\rangle&=7a\frac{n^2a^2}{2}\left[5n^2-3l(l+1)+1\right]-\frac{3}{4}\left[4l(l+1)-8\right]a^2\frac{a}{2}\left[3n^2-l(l+1)\right]\\&=\frac{a^3}{2}\left\{35n^4-21l(l+1)n^2+7n^2-\left[3l(l+1)-6\right]\left[3n^2-l(l+1)\right]\right\}\\&=\frac{a^3}{2}\left[35n^4-21l(l+1)n^2+7n^2-9l(l+1)n^2+3l^2(l+1)^2+18n^2-6l(l+1)\right]\\&=\frac{a^3}{2}\left[35n^4+25n^2-30l(l+1)n^2+3l^2(l+1)^2-6l(l+1)\right].\end{aligned}$$

$$\boxed{\langle r^3\rangle=\frac{n^2a^3}{8}\left[35n^4+25n^2-30l(l+1)n^2+3l^2(l+1)^2-6l(l+1)\right].}$$

For $s = -1$

$$0 + a\left\langle \frac{1}{r^2} \right\rangle - \frac{1}{4}\left[(2l+1)^2 - 1\right] a^2 \left\langle \frac{1}{r^3} \right\rangle = 0 \Rightarrow \boxed{\left\langle \frac{1}{r^2} \right\rangle = al(l+1)\left\langle \frac{1}{r^3} \right\rangle.}$$

But if we know $\langle \frac{1}{r^2} \rangle = \frac{1}{(l+1/2)n^3a^2}$

$$al(l+1)\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{(l+1/2)n^3a^2} \Rightarrow \boxed{\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{l(l+1/2)(l+1)n^3a^3}.}$$

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

a) Show that the ground state is not affected by the perturbation to first order,

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

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

$$\int_0^\pi \cos\theta\sin\theta\,d\theta = \left.\frac{\sin^2\theta}{2}\right|_0^\pi = 0. \quad \text{So} \quad E_s^1 = 0.$$

b) For the degenerate states,

$$\begin{aligned}
|1\rangle = \psi_{2\,0\,0} = &\ \frac{1}{\sqrt{2\pi a}}\frac{1}{2a}\left(1-\frac{r}{2a}\right)e^{-r/2a}\\
|2\rangle = \psi_{2\,1\,1} = &\ -\frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta e^{i\phi}\\
|3\rangle = \psi_{2\,1\,0} = &\ \frac{1}{\sqrt{2\pi a}}\frac{1}{4a^2}re^{-r/2a}\cos\theta\\
|4\rangle = \psi_{2\,1\,-1} = &\ \frac{1}{\sqrt{\pi a}}\frac{1}{8a^2}re^{-r/2a}\sin\theta e^{-i\phi}
\end{aligned}$$

Many of the matrix elements are zero!

$$\begin{aligned}
\langle 1|H_s'|1\rangle &= \{\ldots\}\int_0^\pi \cos\theta\sin\theta\,d\theta = 0\\
\langle 2|H_s'|2\rangle &= \{\ldots\}\int_0^\pi \sin^2\theta\cos\theta\sin\theta\,d\theta = 0\\
\langle 3|H_s'|3\rangle &= \{\ldots\}\int_0^\pi \cos^2\theta\cos\theta\sin\theta\,d\theta = 0\\
\langle 4|H_s'|4\rangle &= \{\ldots\}\int_0^\pi \sin^2\theta\cos\theta\sin\theta\,d\theta = 0\\
\langle 1|H_s'|2\rangle &= \{\ldots\}\int_0^{2\pi} e^{i\phi}\,d\phi = 0\\
\langle 1|H_s'|4\rangle &= \{\ldots\}\int_0^{2\pi} e^{-i\phi}\,d\phi = 0\\
\langle 2|H_s'|3\rangle &= \{\ldots\}\int_0^{2\pi} e^{-i\phi}\,d\phi = 0\\
\langle 2|H_s'|4\rangle &= \{\ldots\}\int_0^{2\pi} e^{-2i\phi}\,d\phi = 0\\
\langle 3|H_s'|4\rangle &= \{\ldots\}\int_0^{2\pi} e^{-i\phi}\,d\phi = 0
\end{aligned}$$

Only one needs to be evaluated!

$$
\begin{aligned}
\langle 1|H_s'|3\rangle &= eE_{\text{ext}}\frac{1}{\sqrt{2\pi a}}\frac{1}{2a}\frac{1}{\sqrt{2\pi a}}\frac{1}{4a^2}\int\left(1-\frac{r}{2a}\right)e^{-r/2a}re^{-r/2a}\cos\theta(r\cos\theta)r^2\sin\theta\,dr\,d\theta\,d\phi \\
&= \frac{eE_{\text{ext}}}{2\pi a8a^3}(2\pi)\left[\int_0^{\pi}\cos^2\theta\sin\theta\,d\theta\right]\int_0^{\infty}\left(1-\frac{r}{2a}\right)e^{-r/a}r^4\,dr \\
&= \frac{eE_{\text{ext}}}{8a^4}\frac{2}{3}\left\{\int_0^{\infty}r^4e^{-r/a}\,dr-\frac{1}{2a}\int_0^{\infty}r^5e^{-r/a}\,dr\right\} = \frac{eE_{\text{ext}}}{12a^4}\left(4!a^5-\frac{1}{2a}5!a^6\right) \\
&= \frac{eE_{\text{ext}}}{12a^4}24a^5\left(1-\frac{5}{2}\right) = eaE_{\text{ext}}(-3) = -3aeE_{\text{ext}}.
\end{aligned}
$$

$$
\mathsf{W} = -3aeE_{\text{ext}}\begin{pmatrix}0&0&1&0\\0&0&0&0\\1&0&0&0\\0&0&0&0\end{pmatrix}.
$$

We need the eigenvalues of this matrix. The characteristic equation is:

$$
\begin{vmatrix}-\lambda&0&1&0\\0&-\lambda&0&0\\1&0&-\lambda&0\\0&0&0&-\lambda\end{vmatrix} = -\lambda\begin{vmatrix}-\lambda&0&0\\0&-\lambda&0\\0&0&-\lambda\end{vmatrix}+\begin{vmatrix}0&-\lambda&0\\1&0&0\\0&0&-\lambda\end{vmatrix} = -\lambda(-\lambda)^3+(-\lambda^2) = \lambda^2(\lambda^2-1) = 0.
$$

The eigenvalues are 0, 0, 1, and −1, so the perturbed energies are

$$
\boxed{E_2,\ E_2,\ E_2+3aeE_{\text{ext}},\ E_2-3aeE_{\text{ext}}.\quad \text{Three levels.}}
$$

(c) The eigenvectors with eigenvalue 0 are $|2\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$ and $|4\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$; the eigenvectors with eigenvalues ±1 are $|\pm\rangle \equiv \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\\pm1\\0\end{pmatrix}$. So the "good" states are $\boxed{\psi_{211},\ \psi_{21-1},\ \frac{1}{\sqrt{2}}(\psi_{200}+\psi_{210}),\ \frac{1}{\sqrt{2}}(\psi_{200}-\psi_{210}).}$

$$
\langle \mathbf{p}_e\rangle_4 = -e\frac{1}{\pi a}\frac{1}{64a^4}\int r^2e^{-r/a}\sin^2\theta\left[r\sin\theta\cos\phi\hat{i}+r\sin\theta\sin\phi\hat{j}+r\cos\theta\hat{k}\right]r^2\sin\theta\,dr\,d\theta\,d\phi.
$$

But $\int_0^{2\pi}\cos\phi\,d\phi = \int_0^{2\pi}\sin\phi\,d\phi = 0,\quad \int_0^{\pi}\sin^3\theta\cos\theta\,d\theta = \left|\frac{\sin^4\theta}{4}\right|_0^{\pi} = 0,\quad$ so

$\boxed{\langle \mathbf{p}_e\rangle_4 = 0.\quad \text{Likewise}\quad \langle \mathbf{p}_e\rangle_2 = 0.}$

Now the other two states with non-zero eigenvalues,

$$
\begin{aligned}
\langle \mathbf{p}_e \rangle_\pm &= -\frac{1}{2} e \int (\psi_1 \pm \psi_3)^2 (\mathbf{r}) r^2 \sin\theta \, dr \, d\theta \, d\phi \\
&= -\frac{1}{2} e \frac{1}{2\pi a} \frac{1}{4a^2} \int \left[\left(1 - \frac{r}{2a}\right) \pm \frac{r}{2a} \cos\theta \right]^2 e^{-r/a} r (\sin\theta\cos\phi\, \hat{i} + \sin\theta\sin\phi\, \hat{j} + \cos\theta\, \hat{k}) r^2 \sin\theta \, dr \, d\theta \, d\phi \\
&= -\frac{e}{2} \frac{\hat{k}}{2\pi a} \frac{1}{4a^2} 2\pi \int \left[\left(1 - \frac{r}{2a}\right) \pm \frac{r}{2a} \cos\theta \right]^2 r^3 e^{-r/a} \cos\theta \sin\theta \, dr \, d\theta .
\end{aligned}
$$

But $\int_0^\pi \cos\theta \sin\theta \, d\theta = \int_0^\pi \cos^3\theta \sin\theta \, d\theta = 0$, so only the cross-term survives:

$$
\begin{aligned}
\langle \mathbf{p}_e \rangle_\pm &= -\frac{e}{8a^3} \hat{k} \left(\pm \frac{1}{a} \right) \int \left(1 - \frac{r}{2a}\right) r \cos\theta \, r^3 e^{-r/a} \cos\theta \sin\theta \, dr \, d\theta \\
&= \mp \left(\frac{e}{8a^4} \hat{k} \right) \left[\int_0^\pi \cos^2\theta \sin\theta \, d\theta \right] \int_0^\infty \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} dr = \mp \left(\frac{e}{8a^4} \hat{k} \right) \frac{2}{3} \left[4! a^5 - \frac{1}{2a} 5! a^6 \right] \\
&= \mp e \hat{k} \left(\frac{1}{12a^4} \right) 24a^5 \left(1 - \frac{5}{2}\right) = \boxed{\pm 3ae\hat{k}.}
\end{aligned}
$$

8.1(b) Variational Principle with quartic potential and gaussian trial function (limit on ground state energy)

$$\langle V \rangle = 2\alpha A^2 \int_0^\infty x^4 e^{-2bx^2}\,dx = 2\alpha A^2 \frac{3}{8(2b)^2}\sqrt{\frac{\pi}{2b}} = \frac{3\alpha}{16b^2}\sqrt{\frac{\pi}{2b}}\sqrt{\frac{2b}{\pi}} = \frac{3\alpha}{16b^2}.$$

$$\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2}. \quad \frac{\partial\langle H \rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{3\alpha}{8b^3} = 0 \Longrightarrow b^3 = \frac{3\alpha m}{4\hbar^2};\ b = \left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3}.$$

$$\langle H \rangle_{\min} = \frac{\hbar^2}{2m}\left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3} + \frac{3\alpha}{16}\left(\frac{4\hbar^2}{3\alpha m}\right)^{2/3} = \frac{\alpha^{1/3}\hbar^{4/3}}{m^{2/3}} 3^{1/3} 4^{-1/3}\left(\frac{1}{2}+\frac{1}{4}\right) = \boxed{\frac{3}{4}\left(\frac{3\alpha\hbar^4}{4m^2}\right)^{1/3}}.$$

8.3 Best bound on ground state in $V(x) = -\alpha\delta(x)$ using triangular trial wavefunction

$$\psi(x) = \begin{cases} A(x+a/2), & (-a/2 < x < 0), \\ A(a/2 - x), & (0 < x < a/2), \\ 0, & (\text{otherwise}). \end{cases}$$

$$1 = |A|^2 2\int_0^{a/2} \left(\frac{a}{2} - x\right)^2 dx = -2|A|^2 \frac{1}{3}\left(\frac{a}{2} - x\right)^3 \Big|_0^{a/2} = \frac{2}{3}|A|^2\left(\frac{a}{3}\right)^3 = \frac{a^3}{12}|A|^2; \quad A = \sqrt{\frac{12}{a^3}} \quad (\text{as before}).$$

$$\frac{d\psi}{dx} = \begin{cases} A, & (-a/2 < x < 0), \\ -A, & (0 < x < a/2), \\ 0, & (\text{otherwise}). \end{cases} \qquad \frac{d^2\psi}{dx^2} = A\delta\left(x + \frac{a}{2}\right) - 2A\delta(x) + A\delta\left(x - \frac{a}{2}\right).$$

$$\begin{aligned} \langle T \rangle &= -\frac{\hbar^2}{2m}\int \psi\left[A\delta\left(x + \frac{a}{2}\right) - 2A\delta(x) + A\delta\left(x - \frac{a}{2}\right)\right] dx = \frac{\hbar^2}{2m}2A\psi(0) = \frac{\hbar^2}{m}A^2\frac{a}{2} \\ &= \frac{\hbar^2 a}{2m}\frac{12}{a^3} = 6\frac{\hbar^2}{ma^2} \quad (\text{as before}). \\ \langle V \rangle &= -\alpha\int |\psi|^2\delta(x)\,dx = -\alpha|\psi(0)|^2 = -\alpha A^2\left(\frac{a}{2}\right)^2 = -3\frac{\alpha}{a}. \quad \langle H \rangle = \langle T \rangle + \langle V \rangle = 6\frac{\hbar^2}{ma^2} - 3\frac{\alpha}{a}. \end{aligned}$$

$$\frac{\partial}{\partial a}\langle H \rangle = -12\frac{\hbar^2}{ma^3} + 3\frac{\alpha}{a^2} = 0 \Rightarrow a = 4\frac{\hbar^2}{m\alpha}.$$

$$\langle H \rangle_{\min} = 6\frac{\hbar^2}{m}\left(\frac{m\alpha}{4\hbar^2}\right)^2 - 3\alpha\left(\frac{m\alpha}{4\hbar^2}\right) = \frac{m\alpha^2}{\hbar^2}\left(\frac{3}{8} - \frac{3}{4}\right) = \boxed{-\frac{3m\alpha^2}{8\hbar^2}} > -\frac{m\alpha^2}{2\hbar^2}. \quad \checkmark$$

8.4 a) Show Corollary to variational principle. That is if test wave function is orthogonal to ground state, then $\langle H \rangle \geq E_{1stexcitedstate}$

$\sum_{n=1}^{\infty} c_n \langle \psi_1 | \psi \rangle = c_1 = 0$; the coefficient of the ground state is zero. So

$$\langle H \rangle = \sum_{n=2}^{\infty} E_n |c_n|^2 \geq E_{\text{fe}} \sum_{n=2}^{\infty} |c_n|^2 = E_{\text{fe}}, \text{ since } E_n \geq E_{\text{fe}} \text{ for all } n \text{ except } 1.$$

(b)

$$1 = |A|^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2} dx = |A|^2 \, 2\frac{1}{8b}\sqrt{\frac{\pi}{2b}} \Longrightarrow |A|^2 = 4b\sqrt{\frac{2b}{\pi}}.$$

$$\langle T \rangle = -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} x e^{-bx^2} \frac{d^2}{dx^2}\left(x e^{-bx^2}\right) dx$$

$$\frac{d^2}{dx^2}\left(xe^{-bx^2}\right) = \frac{d}{dx}\left(e^{-bx^2} - 2bx^2 e^{-bx^2}\right) = -2bxe^{-bx^2} - 4bxe^{-bx^2} + 4b^2x^3e^{-bx^2}$$

$$\langle T \rangle = -\frac{\hbar^2}{2m}4b\sqrt{\frac{2b}{\pi}}2\int_0^{\infty}\left(-6bx^2 + 4b^2x^4\right)e^{-2bx^2}dx = -\frac{2\hbar^2 b}{m}\sqrt{\frac{2b}{\pi}}2\left[-6b\frac{1}{8b}\sqrt{\frac{\pi}{2b}} + 4b^2\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}}\right]$$

$$= -\frac{4\hbar^2 b}{m}\left(-\frac{3}{4} + \frac{3}{8}\right) = \frac{3\hbar^2 b}{2m}.$$

$$\langle V \rangle = \frac{1}{2}m\omega^2|A|^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2} x^2 dx = \frac{1}{2}m\omega^2 4b\sqrt{\frac{2b}{\pi}}2\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}} = \frac{3m\omega^2}{8b}.$$

$$\langle H \rangle = \frac{3\hbar^2 b}{2m} + \frac{3m\omega}{8b}; \quad \frac{\partial \langle H \rangle}{\partial b} = \frac{3\hbar^2}{2m} - \frac{3m\omega^2}{8b^2} = 0 \Longrightarrow b^2 = \frac{m^2\omega^2}{4\hbar^2} \Longrightarrow b = \frac{m\omega}{2\hbar}.$$

$$\langle H \rangle_{\min} = \frac{3\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{3m\omega^2}{8}\frac{2\hbar}{m\omega} = \hbar\omega\left(\frac{3}{4} + \frac{3}{4}\right) = \boxed{\frac{3}{2}\hbar\omega.}$$