Quantum Mechanics 9½/10 MegAnn Noah

17.3.1 Use dipole selection rules to show that H' has the above form and carry out the evaluation of Δ.

The dipole transition selection rules are:

$$\Delta l = \pm 1 \quad \Delta m = 0, \pm 1$$

These selection rules are a consequence of the properties of the spherical harmonics.

$\langle 200|H'|200\rangle = 0$ because $\Delta l = 0$ is forbidden

$\langle 200|H'|210\rangle = \Delta$ $\Delta l = +1$ $\Delta m = 0$ is allowed

$\langle 200|H'|211\rangle = 0$ because of orthogonality conditions $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r) Y_l^m(\theta,\phi)$ when $l = 1,0$ and $m = +1$ or $m = -1$ the $e^{mi\phi}$ term results in the integral being zero

$$\langle 21m_1|21m_2\rangle = \int \psi^*_{21m_1}\psi_{21m_2}\, d\tau = \iint f(r,\theta)\int^{2\pi} e^{-m_1 i\phi} e^{m_2 i\phi}\, d\phi = \iint f(r,\theta)\int_0^{2\pi} e^{(m_2-m_1)i\phi}\, d\phi = 0$$

$\langle 200|H'|21\text{-}1\rangle = 0$ orthogonality $\Delta m \neq 0$ and $l = 1$ or 0

$\langle 210|H'|200\rangle = \Delta$ ~~orthogonality $\Delta m \neq 0$ and $l = 1$ or~~ $\Delta l \neq 0$

$\langle 210|H'|210\rangle = 0$ $\Delta l = 0$

$\langle 210|H'|211\rangle = 0$ $\Delta l = 0$

$\langle 210|H'|21\text{-}1\rangle = 0$ $\Delta l = 0$

$\langle 211|H'|200\rangle = 0$ $\Delta m \neq 0$, $l = 1,0$ orthogonality of $\int_0^{2\pi} e^{(m_2-m_1)i\phi}\, d\phi = 0$

$\langle 211|H'|210\rangle = 0$ $\Delta l = 0$

$\langle 211|H'|211\rangle = 0$ $\Delta l = 0$

$\langle 211|H'|21\text{-}1\rangle = 0$ $\Delta l = 0$

$\langle 21\text{-}1|H'|200\rangle = 0$ $\Delta m \neq 0$, $l = 1,0$ orthogonality of $\int_0^{2\pi} e^{(m_2-m_1)i\phi}\, d\phi = 0$

$\langle 21\text{-}1|H'|210\rangle = 0$ $\Delta l = 0$

$\langle 21\text{-}1|H'|211\rangle = 0$ $\Delta l = 0$

$\langle 21\text{-}1|H'|21\text{-}1\rangle = 0$ $\Delta l = 0$

$$Y_0^0(\theta,\phi) = \left(\frac{1}{4\pi}\right)^{1/2} \quad Y_1^0(\theta,\phi) = \frac{1}{2}\left(\frac{3}{\pi}\right)^{1/2}\cos\theta \quad H' = e\mathcal{E}z = e\mathcal{E}r\cos\theta$$

$$\rho = \frac{2r}{na_0} = \frac{r}{a_0} \quad R(\rho) = \rho^l e^{-\frac{1}{2}\rho} L_{n+l}^{2l+1}(\rho) \quad R_{20} = e^{-\rho/2}(1-\rho) = e^{-r/2a_0}\left(1-\frac{2r}{2a_0}\right) \quad R_{21} = e^{-\rho/2}\rho = e^{-r/2a_0}(r/a_0)$$

$$\langle 200|H'|210\rangle = \langle 210|H'|200\rangle = \int Y_0^{0*} Y_1^0 R_{20} R_{21}\, e\mathcal{E} r\cos\theta\, d\tau$$

$$= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \left(\frac{1}{4\pi}\right)^{1/2} \frac{1}{2}\left(\frac{3}{\pi}\right)^{1/2}\cos\theta\, e^{-r/2a_0}\left(1-r/a_0\right)e^{-r/2a_0}(r/a_0)\, e\mathcal{E} r\cos\theta\, r^2\sin\theta\, dr\, d\theta\, d\phi$$

$\mu = \cos\theta$, $d\mu = -\sin\theta\, d\theta$

$$= \frac{1}{2}\sqrt{\frac{3}{4}}\frac{e\mathcal{E}}{\pi}\int_0^{2\pi} d\phi \int_0^{\pi}\cos^2\theta\sin\theta\, d\theta \int_0^{\infty} e^{-r/a_0}\left(\frac{r^4}{a_0} - \frac{r^5}{a_0^2}\right) dr = e\mathcal{E}\sqrt{\frac{3}{4}}\int_{-1}^{+1}\mu^2\, d\mu \int_0^{\infty} e^{-r/a_0}\left(\frac{r^4}{a_0} - \frac{r^5}{a_0^2}\right) dr$$

$$= e\mathcal{E}\sqrt{\frac{3}{4}}\left(\frac{2}{3}\right) a_0^4 \int_0^{\infty} e^{-\rho}\rho^4(2-\rho)\, d\rho = \frac{\mathcal{E}\mathcal{E}a_0^4}{\sqrt{3}}\left[\Gamma(4) - \Gamma(5)\right] = \frac{\mathcal{E}\mathcal{E}a_0^4}{\sqrt{3}}\Big[\rightarrow$$

NOTE BOOK

from http://xbeams.chem.yale.edu/~batista/vvv/node21.html

$$\psi_{2s} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{2a_0}\right)^{3/2}(1 - r/2a_0)e^{-r/2a_0} \qquad \psi_{2p\phi} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{2a_0}\right)^{5/2} r e^{-r/2a_0}\cos\theta$$

$$H' = +|e|\mathcal{E} r\cos\theta \qquad d\tau = r^2\sin\theta\, dr\, d\theta\, d\phi$$

$$\langle 200|H'|210\rangle = \langle 210|H'|200\rangle = +\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \frac{1}{\sqrt{\pi}}\left(\frac{1}{2a_0}\right)^{3/2}(1 - r/a_0)e^{-r/2a_0}|e|\mathcal{E}r\cos\theta\frac{1}{\sqrt{\pi}}\left(\frac{1}{2a_0}\right)^{5/2} r e^{-r/2a_0}\cos\theta\, d\tau$$

$$= +\frac{1}{\pi}\left(\frac{1}{2a_0}\right)^4 |e|\mathcal{E}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}(1 - r/a_0)e^{-r/2a_0}r\cos\theta\, r e^{-r/2a_0}\cos\theta\, r^2\sin\theta\, d\theta\, dr\, d\phi$$

$$= +\frac{|e|\mathcal{E}}{\pi 2^4 a_0^4}\int_0^{2\pi}d\phi\int_0^{\pi}\cos^2\theta\sin\theta\, d\theta\int_0^{\infty}(1 - r/a_0) r^4 e^{-r/a_0}\, dr$$

$$= +\frac{|e|\mathcal{E}}{\pi 2^4 a_0^4}\frac{2\pi}{2a_0}\int_{-1}^{+1}\mu^2 d\mu\int_0^{\infty}(2a_0 - r)r^4 e^{-r/a_0}\, dr \qquad \mu = \cos\theta,\ d\mu = -\sin\theta\, d\theta$$

$$= +\frac{|e|\mathcal{E}}{2^4 a_0^5}\left(\frac{2}{3}\right)\int_0^{\infty}(2a_0 - a_0\rho)(a_0^4\rho^4)e^{-\rho}a_0\, d\rho \qquad \rho = \left(\frac{r}{a_0}\right) \quad r = a_0\rho$$

$$= +\frac{|e|\mathcal{E}}{2^4 a_0^5}\left(\frac{2}{3}\right)a_0^6\int_0^{\infty}(2 - \rho)\rho^4 e^{-\rho}\, d\rho$$

$$= +\frac{|e|\mathcal{E}a_0}{2^3\cdot 3}\left[\int_0^{\infty}(2\rho^4)e^{-\rho}d\rho - \int_0^{\infty}\rho^5 e^{-\rho}d\rho\right] \qquad \int_0^{\infty}x^n e^{-ax}dx = \frac{\Gamma(n+1)}{a^{n+1}}$$

p. 109 Shaum's

$$= +\frac{|e|\mathcal{E}a_0}{2^3\cdot 3}\left[2\Gamma(5) - \Gamma(6)\right] \qquad \Gamma(x+1) = x\Gamma(x)$$

$$= +\frac{|e|\mathcal{E}a_0}{2^3\cdot 3}\left[2\cdot 4\Gamma(4) - 5\Gamma(5)\right]$$

$$= +\frac{|e|\mathcal{E}a_0}{2^3\cdot 3}\left[2\cdot 4\cdot 3\Gamma(3) - 5\cdot 4\Gamma(4)\right]$$

$$= +\frac{|e|\mathcal{E}a_0}{2^3\cdot 3}\left[2\cdot 4\cdot 3\cdot 2\Gamma(2) - 5\cdot 4\cdot 3\Gamma(3)\right]$$

$$= +\frac{|e|\mathcal{E}a_0}{2^3\cdot 3}\left[2\cdot 4\cdot 3\cdot 2\cdot\Gamma(1) - 5\cdot 4\cdot 3\cdot 2\Gamma(2)\right] \qquad \Gamma(2) = \Gamma(1) = 1$$

$$= +\frac{|e|\mathcal{E}a_0}{2^3\cdot 3}\left[2\cdot 4\cdot 3\cdot 2 - 5\cdot 4\cdot 3\cdot 2\right]$$

$$= +|e|\mathcal{E}a_0\left[2 - 5\right] = -3|e|\mathcal{E}a_0$$

17.3.2 Consider a spin-1 particle (with no orbital DOF). Let $H = AS_z^2 + B(S_x^2 - S_y^2)$ where S_i are the 3x3 spin matrices and $A >> B$. Treating the B term as a perturbation, find the eigenstates of $H^0 = AS_z^2$ that are stable under the perturbation. Calculate the energy shifts to first order in B. How are these related to the exact answers?

in the S_z basis: (found on-line)

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad S_y = \frac{-i\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad S_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad S_+ = \sqrt{2}\hbar\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad S_- = \sqrt{2}\hbar\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$H' = B(S_x^2 - S_y^2) = B\left[\frac{\hbar^2}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} - \frac{i^2\hbar^2}{2}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}\right]$$

$$H' = \frac{B\hbar^2}{2}\left[\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} + \begin{pmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{pmatrix}\right] = \frac{B\hbar^2}{2}\left[\begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 0 \end{pmatrix}\right] = B\hbar^2\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$V = \begin{bmatrix} \langle 1|H'|1\rangle & \langle 1|H'|0\rangle & \langle 1|H'|-1\rangle \\ \langle 0|H'|1\rangle & \langle 0|H'|0\rangle & \langle 0|H'|-1\rangle \\ \langle -1|H'|1\rangle & \langle -1|H'|0\rangle & \langle -1|H'|-1\rangle \end{bmatrix}$$

$$\langle 1|H'|1\rangle = [1\ 0\ 0]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = B\hbar^2 [1\ 0\ 0]\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 0$$

$$\langle 1|H'|0\rangle = [1\ 0\ 0]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = B\hbar^2 [1\ 0\ 0]\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

$$\langle 1|H'|-1\rangle = [1\ 0\ 0]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = B\hbar^2 [1\ 0\ 0]\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = B\hbar^2$$

$$\langle 0|H'|1\rangle = [0\ 1\ 0]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = B\hbar^2 [0\ 1\ 0]\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 0$$

$$\langle 0|H'|0\rangle = [0\ 1\ 0]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = B\hbar^2 [0\ 1\ 0]\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

$$\langle 0|H'|-1\rangle = [0\ 1\ 0]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = B\hbar^2 [0\ 1\ 0]\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = 0$$

$$\langle -1|H'|1\rangle = [0\ 0\ 1]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = B\hbar^2 [0\ 0\ 1]\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = B\hbar^2$$

$$\langle -1|H'|0\rangle = [0\ 0\ 1]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = B\hbar^2 [0\ 0\ 1]\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

$$\langle -1|H'|-1\rangle = [0\ 0\ 1]\, B\hbar^2\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = B\hbar^2 [0\ 0\ 1]\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = 0$$

→

$$V = \begin{bmatrix} \langle 1|H'|1\rangle & \langle 1|H'|0\rangle & \langle 1|H'|-1\rangle \\ \langle 0|H'|1\rangle & \langle 0|H'|0\rangle & \langle 0|H'|-1\rangle \\ \langle -1|H'|-1\rangle & \langle -1|H'|0\rangle & \langle -1|H'|-1\rangle \end{bmatrix} = \begin{bmatrix} 0 & 0 & B\hbar^2 \\ 0 & 0 & 0 \\ B\hbar^2 & 0 & 0 \end{bmatrix}$$

$$V = B\hbar^2 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

The eigenvalues of H' are the roots of ~~det~~ $\det(V - \lambda I)$

$$\begin{vmatrix} -\lambda & 0 & B\hbar^2 \\ 0 & -\lambda & 0 \\ B\hbar^2 & 0 & -\lambda \end{vmatrix} = 0$$

$$-\lambda^3 + \lambda B^2\hbar^4 = 0$$

$$-\lambda(\lambda^2 - B^2\hbar^4) = 0$$

$$\lambda(\lambda - B\hbar^2)(\lambda + B\hbar^2) = 0$$

$$\lambda = 0, \pm B\hbar^2 \quad \text{3 roots}$$

these are the shifts in energy

$$\varphi = a|1\rangle + b|0\rangle + c|-1\rangle$$

$$\begin{bmatrix} -\lambda & 0 & B\hbar^2 \\ 0 & -\lambda & 0 \\ B\hbar^2 & 0 & -\lambda \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = 0$$

$$\begin{bmatrix} -\lambda a + B\hbar^2 c \\ -\lambda b \\ aB\hbar^2 - \lambda c \end{bmatrix} = 0$$

for $\lambda = 0$: $\begin{bmatrix} B\hbar^2 c \\ 0 \\ aB\hbar^2 \end{bmatrix} = 0$ ~~$B\hbar^2(c|1\rangle + a|-1\rangle)$~~ $c=0$ $a=0$ $b=$ anything

~~normalize~~ normalize $B=1$: $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = |0\rangle$

$\lambda = B\hbar^2$: $\begin{bmatrix} -B\hbar^2 a + B\hbar^2 c \\ -B\hbar^2 b \\ aB\hbar^2 - B\hbar^2 c \end{bmatrix} = B\hbar^2 \begin{bmatrix} -a+c \\ -b \\ a-c \end{bmatrix} = 0 \therefore a=c,\ b=0$ stable

$\Rightarrow \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \Rightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle)$

$\lambda = -B\hbar^2$: $\begin{bmatrix} B\hbar^2 a + B\hbar^2 c \\ -B\hbar^2 b \\ aB\hbar^2 + B\hbar^2 c \end{bmatrix} = 0 = B\hbar^2 \begin{bmatrix} a+c \\ b \\ a+c \end{bmatrix} \therefore a = -c,\ b = 0$

$\Rightarrow \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \Rightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle)$

The stable eigenstates are:

$E^{(1)} = +B\hbar^2 \quad \varphi = \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle) \qquad E^{(1)} = 0 \quad \varphi = |0\rangle \qquad E^{(1)} = -B\hbar^2 \quad \varphi = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle)$

How are these related to the exact answers?

$H = H^0 + H'$

$$H^0 = AS_z^2 = A\hbar^2\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix} = A\hbar^2\begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}$$

$$H' = B\hbar^2\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}$$

$$H = H^0 + H' = A\hbar^2\begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix} + B\hbar^2\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix} = \hbar^2\begin{pmatrix}A&0&B\\0&0&0\\B&0&A\end{pmatrix}$$

Example 10.7 in Schaum's asks a similar problem (not a spin problem...)

The eigenvalues of H are the roots of the equation $\det(H-\lambda I)=0$

$$\begin{vmatrix}\hbar^2A-\lambda&0&B\hbar^2\\0&-\lambda&0\\\hbar^2B&0&\hbar^2A-\lambda\end{vmatrix}=0$$

$$-\lambda(A\hbar^2-\lambda)^2 + \lambda B^2\hbar^4 = 0$$

$$\lambda(A^2\hbar^4 - 2A\hbar^2\lambda + \lambda^2 - B^2\hbar^4) = 0$$

$$\lambda(\lambda^2 - 2A\hbar^2\lambda + (A^2-B^2)\hbar^4) = 0$$

$$\lambda = 0 \qquad \lambda = \left(\frac{2A \pm \sqrt{4A^2-4(A^2-B^2)}}{2}\right)\hbar^2 = A\hbar^2 \pm \sqrt{A^2-(A^2-B^2)}\,\hbar^2 = (A\pm B)\hbar^2$$

$$\lambda = 0, (A+B)\hbar^2, (A-B)\hbar^2$$

The exact energy levels are:

$E_+ = A\hbar^2 + B\hbar^2$
$E_0 = 0$
$E_- = A\hbar^2 - B\hbar^2$

The eigenvectors are:

$\varphi = a|1\rangle + b|0\rangle + c|-1\rangle$

$$\begin{pmatrix}A\hbar^2-A\hbar^2-B\hbar^2&0&B\hbar^2\\0&-A\hbar^2-B\hbar^2&0\\B\hbar^2&0&A\hbar^2-A\hbar^2-B\hbar^2\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = \begin{bmatrix}-B\hbar^2a+cB\hbar^2\\b(-A\hbar^2-B\hbar^2)\\aB\hbar^2-cB\hbar^2\end{bmatrix} = 0 \Rightarrow a=c \Rightarrow \begin{bmatrix}1\\0\\1\end{bmatrix} \Rightarrow \frac{1}{\sqrt2}\begin{bmatrix}1\\0\\1\end{bmatrix}$$

for $E_+ = A\hbar^2 + B\hbar^2$ the eigenvector is $\varphi_+ = \frac{1}{\sqrt2}(|1\rangle + |-1\rangle)$

~~$\begin{pmatrix}0&0&B\hbar^2\\0&-A\hbar^2&0\\B\hbar^2&0&0\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = \begin{bmatrix}B\hbar^2c\\-A\hbar^2b\\B\hbar^2a\end{bmatrix} = 0 \therefore a=b=c=0$ anything $\Rightarrow$ ... $\frac{1}{\sqrt3}(|1\rangle+|0\rangle+|-1\rangle)$~~ not a state?

$$\begin{pmatrix}A\hbar^2&0&B\hbar^2\\0&0&0\\\hbar^2B&0&A\hbar^2\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = \begin{pmatrix}aA\hbar^2+B\hbar^2c\\0b\\\hbar^2Ba+B\hbar^2c\end{pmatrix} \Rightarrow b = \text{anything} \Rightarrow$$

$a\hbar^2A + B\hbar^2c = 0$
$a\hbar^2B + A\hbar^2c = 0$

for $E_0 = 0$

$$\varphi_0 = \begin{bmatrix}0\\1\\0\end{bmatrix} = |0\rangle$$

$\Rightarrow$

for $E_- = A\hbar^2 - B\hbar^2$

$$\begin{pmatrix} A\hbar^2 - A\hbar^2 + B\hbar^2 & 0 & B\hbar^2 \\ 0 & -A\hbar^2 + B\hbar^2 & 0 \\ B\hbar^2 & 0 & A\hbar^2 - A\hbar^2 + B\hbar^2 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} B\hbar^2(a+c) \\ (-A\hbar^2 + B\hbar^2)b \\ B\hbar^2(a+c) \end{pmatrix} = 0 \Rightarrow \begin{matrix} b = 0 \\ a = -c \end{matrix}$$

So the eigenvector is $\varphi_- = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle)$

Compare

	perturbations: shift	eigenstate	Exact Solutions: exact energy	eigenstate
E_+	$+B\hbar^2$	$1/\sqrt{2}(\|1\rangle + \|-1\rangle)$	$A\hbar^2 + B\hbar^2$	$1/\sqrt{2}(\|1\rangle + \|-1\rangle)$
E_0	0	$\|0\rangle$	0	$\|0\rangle$
E_-	$-B\hbar^2$	$\frac{1}{\sqrt{2}}(\|1\rangle - \|-1\rangle)$	$A\hbar^2 - B\hbar^2$	$1/\sqrt{2}(\|1\rangle - \|-1\rangle)$

17.3.3 Consider the case where H^0 includes the Colomb plus spin-orbit interaction and H' is the effect of a weak magnetic field $\vec{B} = B\hat{k}$. Using the appropriate bases, show that the 1st order shift is related to j_z by $E' = (eB/2mc)(1 \pm 1/(2l+1))j_z \quad j = l \pm 1/2$

found a solution on-line...

$\hat{H}' = -\mu_z \hat{B}$ with $\mu_z = \frac{e}{2m_e c}\hat{L}_z + \frac{ge}{2m_e c}\hat{S}_z = \frac{e}{2m_e c}(\hat{L}_z + 2\hat{S}_z) = \frac{-e}{2m_e c}(\hat{J}_z + \hat{S}_z)$

$\hat{H}' = \frac{-eB}{2mc}(\hat{J}_z + \hat{S}_z)$

$E' = \langle \hat{H}' \rangle = \frac{-eB}{2m_e c}\langle \hat{J}_z + \hat{S}_z \rangle_{j = l \pm 1/2, m} = \frac{-eB}{2m_e c}[m\hbar + \langle S_z \rangle] = \frac{-eB}{2m_e c}[j_z + \langle S_z \rangle]$

Use Clebsh-Gordon coefficients to get $|j = l \pm 1/2, m\rangle$ in the S_z basis

$|j = l \pm 1/2, m\rangle = C_+|m_l = m - 1/2, m_s = 1/2\rangle + C_-|m_l = m + 1/2, m = -1/2\rangle$

$\langle S_z \rangle = \frac{\hbar}{2}|C_+|^2 - \frac{\hbar}{2}|C_-|^2 = \frac{\hbar}{2(2l+1)}\left[l \pm m + 1/2 - l \pm m - 1/2\right] = \frac{\pm m\hbar}{2l+1} = \frac{\pm j_z}{(2l+1)}$

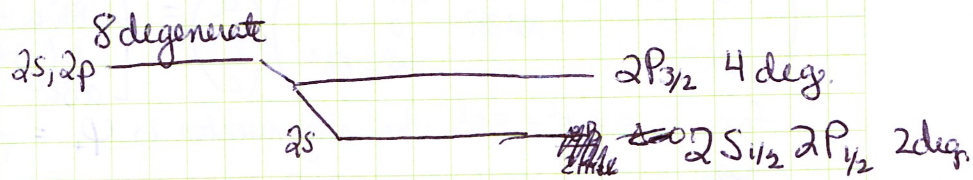
$\Rightarrow E_{shift} = \frac{-eB}{2m_e c}\left[1 \pm \frac{1}{2l+1}\right] j_z$

Sketch the levels for $n = 2$ level assuming $E^l \ll E^l_{f.s.}$

no field   field

2s $n = 2 \quad l = 0 \quad m = 0$

2p $n = 2 \quad l = 1 \quad m = \{-1, 0, +1\}$



n=2 energy shift Δ

$l = 0, m = 0 \quad -eB/2m_e c[1 \pm 1]0 = 0$

$l = 1, m = -1 \quad eB/2m_e c[1 + 1/3] = 2eB/3m_e c$

$l = 1, m = 0 \quad 0$

$l = 1, m = +1 \quad -eB/2m_e c[1 - 1/3] =$.

17.3.4 Tricks

(1) Compute $\langle 1/r \rangle_{nlm}$. Consider $\langle \lambda/r \rangle$ as first order correction due to perturbation λ/r.
Solve by $e^2 \to e^2 - \lambda$ $\therefore$ $E(\lambda) = -(e^2-\lambda)^2 m/2n^2\hbar^2$ from $E_n = \frac{-me^4}{2\hbar^2 n^2} = \frac{-m(e^2)^2}{2\hbar^2 n^2} = \frac{-m(e^2-\lambda)^2}{2\hbar^2 n^2}$

$E^1 = me^2\lambda/n^2\hbar^2 = \langle \lambda/r \rangle \Rightarrow \langle 1/r \rangle = 1/n^2 a_0$ (13.1.36)
because $a_0 = \hbar^2/me^2$

$$E(\lambda) = E^0 + E^1 + \cdots = E(\lambda=0) + \lambda (dE/d\lambda)_{\lambda=0} + \cdots$$

$$E(\lambda) = -(e^2-\lambda)^2 m/n\hbar^2 2$$

$$dE/d\lambda = +2(e^2-\lambda)m/n\hbar^2 2$$

$$\left(dE/d\lambda\right)_{\lambda=0} = \frac{2e^2 m}{2n\hbar^2} = \frac{e^2 m}{n\hbar^2}$$

$$E^1 = \lambda\left(\frac{dE}{d\lambda}\right)_{\lambda=0} = \lambda\frac{e^2 m}{n\hbar^2}$$

$$E^1 = \langle \lambda/r \rangle = \frac{\lambda e^2 m}{n\hbar^2}$$

$$\boxed{\langle 1/r \rangle_{nlm} = \frac{e^2 m_e}{n\hbar^2}}$$

m_e = mass of electron

(2) Compute $\langle \lambda/r^2 \rangle$

perturbation: $\frac{\hbar^2 l(l+1)}{2m_e r^2} + \frac{\lambda}{r^2} = \frac{\hbar^2 l'(l'+1)}{2m_e r^2} = \frac{\hbar^2}{2m_e r^2}\left[l(l+1) + \frac{2m_e\lambda}{\hbar^2}\right]$

$E(l') = \frac{-me^4}{2\hbar^2(k+l'+1)^2}$ $k = 0,1,2,\ldots$ $l = 0,1,2,\ldots$ $l'(l'+1) = l(l+1) + \frac{2m_e\lambda}{\hbar^2}$ ①

① $\Rightarrow l' = f(\lambda)$

$E = E^0 + E^1$

① $\Rightarrow \frac{d\lambda}{dl'} = \frac{\hbar^2}{2m_e}(2l'+1)$

$E^1(l') = ~~l'\left(\frac{dE}{dl'}\right)_{l'=0}~~ = \lambda\left(\frac{dE}{d\lambda}\right)_{\lambda=0} = \lambda\left(\frac{dE}{dl'}\right)_{l'=l}\left(\frac{dl'}{d\lambda}\right)_{l'=l}$

① if $\lambda=0$, $l'=l$

$\frac{dE}{dl'} = \frac{me^4}{\hbar^2(k+l'+1)^3}$ $\left(\frac{dE}{dl'}\right)_{l'=l} = \frac{me^4}{\hbar^2(k+l+1)^3}$ $\left(\frac{dl'}{d\lambda}\right) = \left(\frac{\hbar^2(2l'+1)}{2m_e}\right)^{-1}$ $\left(\frac{dl'}{d\lambda}\right)_{l'=l} = \left(\frac{\hbar^2(2l+1)}{2m_e}\right)^{-1}$

~~$E^1(l') = \left\langle\frac{\lambda}{r^2}\right\rangle = \lambda\left(\frac{dE}{dl'}\right)_{l'=l}\left(\frac{dl'}{d\lambda}\right)_{l'=l} = \lambda\frac{me^4}{\hbar^2(k+l+1)^3}\frac{\hbar^2(2l+1)}{2m_e} = \lambda e^4\frac{(2l+1)}{(k+l+1)^3}$~~

$n = (k+l+1)$ $E^1(l') = \left\langle\frac{\lambda}{r^2}\right\rangle = \lambda\left(\frac{dE}{dl'}\right)_{l'=l}\left(\frac{dl'}{d\lambda}\right)_{l'=l} = \frac{\lambda me^4}{\hbar^2(k+l+1)^3}\frac{2m_e}{\hbar^2(2l+1)}$

$$\left\langle\frac{\lambda}{r^2}\right\rangle = \lambda\frac{m_e^2 e^4}{\hbar^4}\frac{1}{n^3}\frac{1}{(2l+1)} = \frac{\lambda}{n^3(l+1/2)a_0^2} \Rightarrow \left\langle\frac{1}{r^2}\right\rangle = \frac{1}{n^3 a_0^2(l+1/2)}$$

(3) $\langle 1/r^3 \rangle$

$$p_r = -i\hbar\left(\frac{d}{\partial r} + \frac{1}{r}\right) \qquad H_r = \frac{-\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\right) = \frac{p_r^2}{2m}$$

$$\langle [H, p_r] \rangle = 0$$

~~$\langle Hp_r \rangle - \langle p_r H \rangle =$~~

$$\langle Hp_r - p_r H \rangle = \langle n | Hp_r - p_r H | n \rangle = \text{~~}E_n \langle n | p_r - p_r | n \rangle\text{~~} = 0 = 0$$

$\therefore$ ~~$\left\langle \frac{1}{r^3} \right\rangle = \left\langle \frac{1}{r} \right\rangle \left\langle \frac{1}{r^2} \right\rangle = \left(\frac{1}{\hbar a_0}\right)\left(\frac{1}{n^3}\right)$~~

$$E_n \langle n | p_r | n \rangle - \langle n | p_r H | n \rangle$$

$$H = H^0 + H^1 = \frac{p_r^2}{2m} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$

$$p_r H = \frac{p_r^3}{2m} + \left(\frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\right)\frac{\hbar^2 \ell(\ell+1)}{2mr^2} = \frac{p_r^3}{2m}$$

$$E_n \langle p_r \rangle = \langle p_r^3 \rangle \Rightarrow$$ ~~$E_n = \langle \frac{1}{r} \rangle$~~

$\Rightarrow$ ~~$E_n \langle \frac{1}{r} \rangle = \langle \frac{1}{r^3} \rangle$~~ $\qquad \langle p_r^3 \rangle = E_n \langle p_r \rangle$

~~$E_n = -\frac{1}{2}\left(\frac{e^2}{r}\right)_{nem}$~~ $\qquad \Rightarrow \left\langle \frac{1}{r^3} \right\rangle = \frac{E_n}{\hbar^2}\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{a_0\, \ell(\ell+1)}\left\langle \frac{1}{r^2} \right\rangle$

(4) Find the mean kinetic energy

$$\langle T \rangle = \text{~~}\langle \frac{p^2}{2m} \rangle\text{~~} \left\langle \frac{p^2}{2\mu} \right\rangle = \left\langle \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} \right\rangle =$$

$$\langle T \rangle = \left\langle \frac{p_r^2}{2\mu} \right\rangle + \frac{\hbar^2 \ell(\ell+1)}{2\mu}\left\langle \frac{1}{r^2} \right\rangle \quad \times$$

Special problem was done in the last set.

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