PHYS2581 Foundations2A: QM2 7 solution

(a) $E^1_{1,0,0} = \int_0^\pi \int_0^{2\pi} \int_0^\infty \frac{1}{a^3\pi} e^{-2r/a} eE_{ext} r\cos\theta r^2 \sin\theta dr d\theta d\phi$
$= 2\pi/(\pi a^3) \int_0^\pi \cos\theta \sin\theta \int_0^\infty r^3 e^{-2r/a} dr = 0$ as over $0 \to \pi$, sin is symmetric about $\pi/2$ and cos is antisymmetric about $\pi/2$.

(b) diagonals:
$W_{11} = \ldots \int_0^\pi \cos\theta \sin\theta d\theta = 0$
$W_{22} = \ldots \int_0^\pi \cos\theta \sin^2\theta \sin\theta d\theta = 0$
$W_{33} = \ldots \int_0^\pi \cos\theta \cos^2\theta \sin\theta d\theta = 0$
$W_{44} = \ldots \int_0^\pi \cos\theta \sin^2\theta \sin\theta d\theta = 0$
off diagonals: smart way
only W_{13} will be non-zero as this is the only one where the m quantum number is the same. we have $\psi_{nlm} = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi)$ and we are integrating over all ϕ so $\psi_{nlm} H'(\theta) \psi_{nl'm'} dV \propto \delta(m - m')$
off diagonals: long way
$W_{12} = \ldots \int_0^{2\pi} e^{i\phi} d\phi = 0$
$W_{14} = \ldots \int_0^{2\pi} e^{-i\phi} d\phi = 0$
$W_{23} = \ldots \int_0^{2\pi} e^{-i\phi} d\phi = 0$
$W_{24} = \ldots \int_0^{2\pi} e^{-2i\phi} d\phi = 0$
$W_{34} = \ldots \int_0^{-\pi} e^{-2i\phi} d\phi = 0$

$$W_{13} = \int\int\int \frac{1}{\sqrt{2\pi a}} \frac{1}{2a}\Big(1 - \frac{r}{2a}\Big) e^{-r/2a} eE_{ext} r\cos\theta \frac{1}{\sqrt{2\pi a}} \frac{1}{4a^2} r e^{-r/2a} \cos\theta r^2 \sin\theta dr d\theta d$$

$$= \frac{eE_{ext}}{16\pi a^4} \int\int\int \Big(1 - \frac{r}{2a}\Big) r^4 e^{-r/a} \cos^2\theta \sin\theta dr d\theta d\phi$$

$$= 2\pi \frac{eE_{ext}}{16\pi a^4} \int\int \Big(1 - \frac{r}{2a}\Big) r^4 e^{-r/a} \cos^2\theta \sin\theta dr d\theta$$

$$= \frac{eE_{ext}}{8a^4} \frac{2}{3} \int \Big(1 - \frac{r}{2a}\Big) r^4 e^{-r/a} dr = \frac{eE_{ext}}{12a^4} \Big(\int r^4 e^{-r/a} dr - \frac{1}{2a} \int r^5 e^{-r/a} dr \Big)$$

$$= \frac{eE_{ext}}{12a^4}\Big(\frac{4!}{(1/a)^5} - \frac{1}{2a}\frac{5!}{(1/a)^6}\Big) = \frac{eE_{ext}}{12a^4}(4.3.2a^5 - 5.4.3a^5)$$

$$= \frac{eaE_{ext}}{12}(12 - 60) = -3eaE_{ext}$$

and all $W_{ij} = W_{ji}^*$

(c) so we have

$$-3aeE_{ext}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = E^1\begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix}$$

let $\lambda = E^1/-3aeE_{ext}$ so we have

$$\begin{pmatrix} -\lambda & 0 & 1 & 0 \\ 0 & -\lambda & 0 & 0 \\ 1 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

solve - determinant=0.

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

$$-\lambda. - \lambda(-\lambda^2) + -. - \lambda. - \lambda = \lambda^2(\lambda^2 - 1)$$

hence we have values $\lambda = 0, 0, 1, -1$ so it splits into 3 separate levels with energy shift $E_2^1 = 0, -3aeE_{ext}, 3aeE_{ext}$

(d) eigenvectors with $E_2^1 = 0$ are $|2>$ and $|4>$

eigenvector with $\lambda = 1$ (hence $E_2^1 = -3eaE_{ext}$) are

$$\begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

so $-\alpha + \gamma = 0$ or $\alpha = \gamma$ and $\chi = \frac{1}{\sqrt{2}}(|1 > +|3 >)$

$\lambda = -1$ so $E_2^1 = 3aeE_{ext}$ is

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

so $\alpha + \gamma = 0$ or $\gamma = -\alpha$ and $\chi = \frac{1}{\sqrt{2}}(|1 > -|3 >)$