QM1)

(a) normalisation $\int \psi^* \psi dx = 1$

$A^2 \int (3\psi_1 + \psi_3)^2 dx = A^2 \int (9\psi_1^2 + \psi_3^2 + 6\psi_1\psi_3) dx = 1$ [U:1 mark]

wavefunctions are orthonormal so $= A^2(9+1) = 1$ so $A = 1/\sqrt{10}$ [U:1 mark]

prob E_1 is 9/10. so prob $< E_3 >$ is 1/10 [U:1 mark]

$< E >= 9/10E_1 + 1/10E_3 = 9/10E_1 + 9/10E_1 = 1.8E_1$. no measurement can obtain this as its not an eigenvalue [U:1 mark]

(b) $\int \psi_m^* \psi dx = \int \psi_m^* \sum_n c_n \psi_n dx$

$\int \psi_m^* \psi dx = \sum_n c_n \int \psi_m^* \psi_n dx = \sum_n c_n \delta_{mn}$

$\int \psi_m^* \psi dx = c_m$ so $c_n = \int \psi_n^* \psi dx$ [S:1 mark]

$c_1 = \int_0^1 \psi_1^* \psi dx = \sqrt{2}\sqrt{30} \int_0^1 x(1-x)\sin(\pi x) dx$

$= \sqrt{60}(\int_0^1 x \sin \pi x dx - \int_0^1 x^2 \sin \pi x dx) = \sqrt{60}[1/\pi - (1/\pi - 4/\pi^3)] = \sqrt{60}.4/\pi^3$ [U:1 mark]

$c_2 = \int_0^1 \psi_2^* \psi(x) dx = \sqrt{2}\sqrt{30} \int_0^1 x(1-x) \sin 2\pi x dx$

$= \sqrt{60}(\int_0^1 x \sin 2\pi x dx - \int_0^1 x^2 \sin 2\pi x dx) = \sqrt{60}[1/\pi - (1/\pi)] = 0$[U:1 mark]

as expected as $\psi(x)$ is symmetric about $x = 1/2$ so will have a lot of ψ as this is also symmetric about this point but none of ψ_2 as this is antisymmetric about $x = 1/2$. [S:1 mark]

(c) $p = -i\hbar d/dx$ [S:1 mark]

$[x,p]\psi = (xp\psi - px\psi)$ [S:1 mark]

$[x,p]\psi = -i\hbar\Big(xd\psi/dx - d(x\psi)/dx\Big) = -i\hbar\Big(xd\psi/dx - (xd\psi/dx + \psi)\Big) = i\hbar\psi$ [S:2 marks]

(d) $< x >= \int_0^1 2x \sin^2(n\pi x) dx = 2.1/4 = 1/2$

$< p >= -i\hbar \int_0^1 2 \sin(n\pi x) d(\sin(n\pi x)/dx dx$

$= -i\hbar \int_0^1 2 \sin(n\pi x) n\pi \cos(n\pi x) dx = 0$ (could also get these 2 from symmetry) [U:1 mark]

$< x^2 >= \int_0^1 2x^2 \sin^2(n\pi x)dx = 2(\frac{1}{6} - \frac{1}{4\pi^2 n^2}) = \frac{1}{3} - \frac{1}{2\pi^2 n^2}$ [U:1 mark]

$< p^2 >= -\hbar^2 \int_0^1 2\sin(n\pi x)d^2(\sin(n\pi x)/dx^2 dx = \hbar^2 \int_0^1 2n^2\pi^2 \sin^2(n\pi x)n^2\pi^2 = \hbar^2 n^2 \pi^2$ [U:1 mark]

$\Delta x \Delta p = \sqrt{(1/3 - 1/(2n^2\pi^2) - 1/4)(\hbar^2 n^2 \pi^2)} = \hbar\sqrt{n^2\pi^2/12 - 1/2}$ so minimize for $n = 1$ (where its $0.56\hbar$ so still above minimum limit from heisenburg) [U:1 mark]

(e) $dV(r)/dr = -e^2/(4\pi\epsilon_0)d(1/r)/dr = e^2/(4\pi\epsilon_0)1/r^2 = -V(r)/r$

hence $rdV/dr = -V$ so $2 < T >=< rdV/dr >= - < V >$ [U:2 marks]

But $< E >=< T > + < V >=< T > -2 < T >= - < T >$ hence for any eigenstate ψ_{nlm} where $< E >= E_n$ we have $< T >= -E_n$. [U:1 mark]

this is a lot easier than calculating $< T >$ as kinetic energy is a second order differential operator [S:1 mark]

(f)

$$
\begin{aligned}
D(r)dr &= \int_0^{2\pi}\int_0^{\pi} \psi_{211}^* \psi_{211} r^2 \sin\theta dr d\theta d\phi \\
&= \frac{1}{64\pi a^3}\int_0^{2\pi}\int_0^{\pi} \frac{r^4}{a^2} e^{-r/a} \sin^3\theta d\theta d\phi \\
&= \frac{r^4 e^{-r/a}}{64\pi a^5} 2\pi \int_0^{\pi} \sin^3\theta d\theta \\
&= \frac{r^4 e^{-r/a}}{32 a^5}\frac{4}{3} = \frac{r^4 e^{-r/a}}{24 a^5}
\end{aligned}
$$

[S:2 marks]

max when $dD/dr = 0$ so $d(r^4 e^{-r/a})/dr = 0$

$4r^3 e^{-r/a} + -1/a r^4 e^{-r/a} = 0$

$r^3 e^{-r/a}(4 - r/a) = 0$ so at $r = 4a$ [U:2 marks]

(g) $$\frac{(\Delta E)_+}{(\Delta E)_H} = \frac{g_e g_+}{m_+ m_e a_+^3}\frac{m_p m_e a_H^3}{g_e g_p}$$

$$= \frac{g_+}{g_p}\frac{m_p}{m_+}\frac{a_H^3}{a_+^3}$$

[U:2 marks]

$$\frac{a_H}{a_+} = \frac{\mu_+}{\mu_H} = \frac{m_e m_+}{m_e + m_+} \frac{m_e + m_p}{m_e m_p} = \frac{m_e}{2m_e} \frac{m_e + m_p}{m_p} = \frac{1}{2}$$

as $m_e << m_p$ [S:1 mark]

so ratio is $2/5.59 \times 1833 \times (1/2)^3 = 82$ [U:1 mark]

(h) $E_1^1 = 2 \int_{1/2-\Delta/2}^{1/2+\Delta/2} (\alpha/\Delta) \sin^2 \pi x dx$.

$E_1^1 = 2\alpha/(4\pi\Delta)[2\pi\Delta + \sin 2\pi(1/2 - \Delta/2) - \sin 2\pi(1/2 + \Delta/2)]$. [U:1 mark]

$= \alpha/(2\pi\Delta)[2\pi\Delta + \sin(\pi - \Delta\pi) - \sin(\pi + \Delta\pi)] = \alpha/(2\pi\Delta)[2\pi\Delta + 2\sin\Delta\pi]$

$\to \alpha/(2\pi\Delta)[2\pi\Delta + 2\Delta\pi] = 2\alpha$. [U:1 mark]

$E_2^1 = 2 \int_{1/2-\Delta/2}^{1/2+\Delta/2} (\alpha/\Delta) \sin^2 2\pi x dx$.

$= 2\alpha/(8\pi\Delta)[4\pi\Delta + \sin 4\pi(1/2 - \Delta/2) - \sin 4\pi(1/2 + \Delta/2)]$[U:1 mark]

$= \alpha/(4\pi\Delta)[4\pi\Delta - 2\sin(2\pi\Delta)]$

$\to \alpha/(4\pi\Delta)[4\pi\Delta - 4\pi\Delta] = 0$ [U:1 mark]

QM2)

(a)

$$\frac{1}{2m_e a^2} L^2 Y_{lm} = \frac{l(l+1)\hbar^2}{2m_e a^2} Y_{lm}$$

so eigenenergies are

$$E_{lm} = E_l = \frac{l(l+1)\hbar^2}{2m_e a^2}$$

[S:1 mark]

$l = 0$ means $m = 0$ so degeneracy 1 [S:1 mark]

$l = 1$ can have $m = -1, 0, 1$ degeneracy 3 [S:1 mark]

general formula is $2l + 1$ degeneracy [S:1 mark]

(b) $dP = Y_{22}^* Y_{22} \sin\theta d\theta d\phi$ [S:1 mark]

prob within $\pi/3 \leq \theta \leq /\pi/2$ is

$$= \int_0^{2\pi} d\phi \int_{\pi/3}^{\pi/2} Y_{22}^* Y_{22} \sin\theta d\theta d\phi$$

$$= \Big(\frac{15}{32\pi}\Big) \int_0^{2\pi} \int_{\pi/3}^{\pi/2} \sin^2\theta e^{-2i\phi} \sin^2\theta e^{2i\phi} \sin\theta d\theta d\phi$$

[U:1 mark]

$$= \Big(\frac{15}{32\pi}\Big) 2\pi \int_{1/2}^{0} (1-\mu^2)^2 (-d\mu)$$

$$= \Big(\frac{15}{16}\Big) \int_0^{1/2} (1-\mu^2)^2 d\mu = \Big(\frac{15}{16}\Big) [\mu - 2\mu^3/3 + \mu^5/5]_0^{1/2}$$

$$= \Big(\frac{15}{16}\Big) [1/2 - 2(1/2)^3/3 + (1/2)^5/5] = \Big(\frac{15}{16}\Big) (1/2)^5 [2^4 - 2^3/3 + 1/5]$$

$$= \Big(\frac{15}{16.32}\Big) [16 - 8/3 + 1/5] = \frac{203}{480} \frac{15}{16} = 0.396$$

[U:2 marks]

(c) $$L_-(Y_{22}) = N_{22}. - \hbar e^{-i\phi}\Big(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\Big)\sin^2\theta e^{2i\phi}$$

$$= N_{22}. - \hbar e^{-i\phi}\Big(e^{2i\phi}\frac{\partial(\sin^2\theta)}{\partial\theta} - i\cot\theta\sin^2\theta\frac{\partial(e^{2i\phi})}{\partial\phi}\Big)$$

[U:2 marks]

$$= -\hbar N_{22}e^{-i\phi}\Big(e^{2i\phi}2\sin\theta\cos\theta - i\cos\theta\sin\theta 2ie^{2i\phi}\Big)$$

$$= -\hbar N_{22}e^{i\phi}\Big(2\sin\theta\cos\theta + 2\cos\theta\sin\theta\Big)$$

$$= -4\hbar N_{22}\sin\theta\cos\theta e^{i\phi}$$

[U:1 mark]

$= -4\hbar N_{22}Y_{21}/N_{21} = AY_{21}$ [U:1 mark]

(d) $$[L_z, L_-] = [L_z, L_x - iL_y] = [L_z, L_x] - i[L_z, L_y] = i\hbar L_y - i(-i\hbar L_x)$$

$$= -\hbar L_x + i\hbar L_y = -\hbar L_-$$

[U:2 marks]

$$L_z(L_-Y_{lm}) = (L_zL_- - L_-L_z + L_-L_z)Y_{lm} = -\hbar L_-Y_{lm} + L_-L_zY_{lm}$$

$$= (-\hbar + m\hbar)L_-Y_{lm} = (m-1)\hbar(L_-Y_{lm})$$

[U:2 marks]

(e) $L_+L_- = (L_x + iL_y)(L_x - iL_y) = L_x^2 + iL_yL_x - iL_xL_y + L_y^2$ [U:1 mark]
$= L_x^2 + L_y^2 - i(L_xL_y - L_yL_x) = L_x^2 + L_y^2 - i[L_x, L_y] = L_x^2 + L_y^2 - ii\hbar L_z$ [U:1 mark]
$= L^2 - L_z^2 + \hbar L_z$ [U:1 mark]
so eigenvalues $l(l+1)\hbar^2 - m^2\hbar^2 + \hbar m\hbar = \hbar^2[l(l+1) - m(m-1)]$ [U:1 mark]

(a) $\psi_{nx,ny,nz} = X_{nx}(x)Y_{ny}(y)Z_{nz}(z)$ and $V = V_x(x) + V_y(y) + V_z(z)$ so

$$-\frac{\hbar^2}{2m_e}\left(YZ\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + XY\frac{\partial^2 XYZ}{\partial z^2}\right) + (V_x + V_y + V_z)XYZ = EXYZ$$

[S:1 mark]

divide by XYZ to get

$$\left(-\frac{\hbar^2}{2m_e}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + V_x\right) + \left(-\frac{\hbar^2}{2m_e}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + V_y\right) + \left(-\frac{\hbar^2}{2m_e}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} + V_z\right) = E$$

[S:1 mark]

these 3 groups depend only on x, y and z respectively (so we can replace $\partial/\partial x$ with d/dx) so NONE of them can depend on x, y or z - they must be constants which we'll call E_x, E_y, E_z. Then we get the three equations

$$-\frac{\hbar^2}{2m_e}\frac{1}{X}\frac{d^2 X}{dx^2} + V_x = E_x$$

$$-\frac{\hbar^2}{2m_e}\frac{1}{Y}\frac{d^2 Y}{dy^2} + V_y = E_y$$

$$-\frac{\hbar^2}{2m_e}\frac{1}{Z}\frac{d^2 Z}{dz^2} + V_z = E_z$$

where each is the same as the 1D schroedinger equation for the harmonic oscillator. [S:1 mark]

and $E_x + E_y + E_z = E$ so $E = (n_x + 1/2)\hbar\omega + (n_y + 1/2)\hbar\omega + (n_z + 1/2)\hbar\omega = (n_x + n_y + n_z + 3/2)\hbar\omega$ [U:2 marks]

(b) $E^1_{0,0,0} = \int\int\int Ne^{-ax^2/2}e^{-ay^2/2}e^{-az^2/2}\lambda x^2 yz Ne^{-ax^2/2}e^{-ay^2/2}e^{-az^2/2}dxdydz$
[U:1 mark]

$= N^2\lambda\int\int\int x^2 yz e^{-ax^2}e^{-ay^2}e^{-az^2}dxdydz$

$= 0$ as $\int ye^{-ay^2}dy = 0$ (and same in z) [U:1 mark]

(c) $W_{11} = A^2 \int\int\int z^2 e^{-ax^2} e^{-ay^2} e^{-az^2} \lambda x^2 yz dx dy dz = 0$ [U:1 mark]

$W_{22} = A^2 \int\int\int y^2 e^{-ax^2} e^{-ay^2} e^{-az^2} \lambda x^2 yz dx dy dz = 0$

$W_{33} = A^2 \int\int\int x^2 e^{-ax^2} e^{-ay^2} e^{-az^2} \lambda x^2 yz dx dy dz = 0$ [U:1 mark]

$W_{12} = A^2 \int\int\int yz e^{-ax^2} e^{-ay^2} e^{-az^2} \lambda x^2 yz dx dy dz$

$= A^2 \lambda \int x^2 e^{-ax^2} dx \int y^2 e^{-ay^2} dx \int z^2 e^{-az^2} dz$

$= A^2 \lambda \frac{1}{2} \left(\frac{\pi}{a^3}\right)^{1/2} \frac{1}{2} \left(\frac{\pi}{a^3}\right)^{1/2} \frac{1}{2} \left(\frac{\pi}{a^3}\right)^{1/2}$

$= 2a \left(\frac{a}{\pi}\right)^{3/2} \lambda \frac{1}{8} \left(\frac{\pi}{a^3}\right)^{3/2} = \frac{\lambda}{4a^2}$ [U:2 marks]

$W_{13} = A^2 \int\int\int xz e^{-ax^2} e^{-ay^2} e^{-az^2} \lambda x^2 yz dx dy dz = 0$

$W_{23} = A^2 \int\int\int yx e^{-ax^2} e^{-ay^2} e^{-az^2} \lambda x^2 yz dx dy dz = 0$ [U:1 mark]

$W_{ij} = W_{ji}^*$ and all terms are real so $W_{ij} = W_{ji}$ [U:1 mark]

(d) let $b = \lambda/(4a^2)$ then the matrix is

$$\begin{pmatrix} -E^1 & b & 0 \\ b & -E^1 & 0 \\ 0 & 0 & -E^1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

[U:1 mark]

non trivial solution when determinant is zero so

$-E^1(E^1)^2 - b(-bE^1) = 0$ so $E^1[b^2 - (E^1)^2] = 0$ i.e. $E^1 = 0$ and $E^1 = \pm b$. [U:2 marks]

so the degeneracy is completely lifted. [U:1 mark]

for $E^1 = b$ then the matrix becomes

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

so $-b\alpha + b\beta = 0$ so $\alpha = \beta$ and $\gamma = 0$ so $\chi_1 = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$ [U:1 mark]

for $E^1 = -b$ we have $b\alpha + b\beta = 0$ so $\alpha = -\beta$ and $\gamma = 0$ so $\chi_2 = \frac{1}{\sqrt{2}}(\psi_1 - \psi_2)$ [U:1 mark]

fo $E^1 = 0$ the matrix gives all $\alpha, \beta, \gamma = 0$ so $\chi_3 = \psi_3$ as this is the only one which works for all values of E^1. [U:1 mark]