Problem 1

$$E_{n_1n_2n_3} = \frac{\pi^2\hbar^2}{2m_e}\left(\frac{n_1^2}{L^2}+\frac{n_2^2}{L^2}+\frac{n_3^2}{(2L)^2}\right) \text{ with } L = 1\text{Å},\ 2L = 2\text{Å}.$$

$$= \frac{\pi^2\hbar^2}{2m_eL^2}\left(n_1^2+n_2^2+\frac{n_3^2}{4}\right) \equiv E_0\left(n_1^2+n_2^2+\frac{n_3^2}{4}\right)$$

$$E_0 = \frac{\pi^2\hbar^2}{2m_eL^2} = \frac{3.81\,\text{eV}\,\text{Å}^2\cdot\pi^2}{1\,\text{Å}^2} = 37.6\,\text{eV}$$

n_1	n_2	n_3	$n_1^2+n_2^2+\frac{n_3^2}{4}$	E
1	1	1	$2\frac{1}{4} = \frac{9}{4}$	$\frac{9}{4}E_0 = 84.6\,\text{eV}$ ← ground state
1	1	2	3	$3E_0 = 112.8\,\text{eV}$ ← 1st excited state
1	1	3	$2+\frac{9}{4} = 4\frac{1}{4}$	$\frac{17}{4}E_0 = 160\,\text{eV}$ ← 2nd excited state
1	2	1	$5+\frac{1}{4} = 5\frac{1}{4}$	$\frac{21}{4}E_0 = 197.4\,\text{eV}$ } 3rd excited states doubly degenerate
2	1	1	$5\,1/4$	$197.4\,\text{eV}$

(c) Wavefunction is:

$$\psi(x,y,z) = C\sin\frac{n_1\pi}{L}x\,\sin\frac{n_2\pi}{L}y\,\sin\frac{n_3\pi}{2L}z$$

Center of the box: $x = L/2$, $y = L/2$, $z = 2L/2 = L \Rightarrow$

$$\psi\left(\frac{L}{2},\frac{L}{2},L\right) = C\sin\frac{n_1\pi}{2}\sin\frac{n_2\pi}{2}\sin\frac{n_3\pi}{2} \neq 0 \Rightarrow$$

n_1, n_2, n_3 need all be odd. The first state after the ground state satisfying that is $(n_1, n_2, n_3) = (1, 1, 3)$

Problem 2

$$\psi(r,\theta,\phi) = C r^2 e^{-r/3a_0} \sin^2\theta \, e^{-i\phi}$$

(a) Radial wave function has e^{-Zr/na_0}, here $Z=1 \Rightarrow \boxed{n=3}$

$l = 0, 1$ or 2. Cannot be 0 because there is angular dependence. Because of $\sin^2\theta$ factor $\Rightarrow \boxed{l=2}$

Azimuthal part is always $e^{-im_l\phi} \Rightarrow \boxed{m_l=-1}$ (satisfies $-l \le m_l \le l$)

$|L| = \sqrt{l(l+1)}\,\hbar = \sqrt{6}\,\hbar$; $L_z = m_l\hbar = -\hbar$

(b) States with same energy are: all states with $n=3 \Rightarrow$

$n=3$	$l=0$	$m_l=0$	1 state
	$l=1$	$m_l=-1,0,1$	3 states
	$l=2$	$m_l=-2,-1,0,1,2$	5 states

} 9 states total

(c) In a magnetic field

$$\Delta E = -\vec{\mu}\cdot\vec{B} = \mu_z B = -\mu_B m_l B = 5.79\times10^{-5}\times(+1)\cdot 3 \,\text{eV} \Rightarrow$$

$$\boxed{\Delta E = +1.74\times10^{-4}\,\text{eV}}$$

Energy increases because B points in $-z$ direction which is same direction as L_z, since $m_l < 0$, so B is opposite to the magnetic moment due to orbital motion.

Problem 3

$$P(r) = r^2 R(r) \quad ; \quad \langle \tfrac{1}{r} \rangle = \int_0^\infty dr\, \frac{1}{r} \cdot P(r) = \int_0^\infty dr .\, r .\, R^2(r)$$

$$R(r) = \frac{1}{(2a_0)^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$$R^2(r) = \frac{1}{(2a_0)^3} \left(4 - \frac{4r}{a_0} + \frac{r^2}{a_0^2}\right) e^{-r/a_0} \Rightarrow$$

$$\langle \tfrac{1}{r} \rangle = \frac{1}{(2a_0)^3} \int_0^\infty dr \left(4r - \frac{4r^2}{a_0} + \frac{r^3}{a_0^2}\right) e^{-r/a_0} =$$

$$= \frac{1}{(2a_0)^3} \left[4a_0^2 - \frac{4}{a_0} \cdot \frac{2!}{(1/a_0)^3} + \frac{3!}{a_0^2 (1/a_0)^4} \right] =$$

$$= \frac{a_0^2}{(2a_0)^3} [4 - 8 + 6] = \frac{2a_0^2}{8a_0^3} = \frac{1}{4a_0} \Rightarrow \langle \tfrac{1}{r} \rangle = \frac{1}{4a_0}$$

Note that $n = 2 \Rightarrow \langle \frac{1}{r} \rangle = \frac{1}{n^2 a_0}$

Potential energy: $U(r) = -\frac{ke^2}{r} \Rightarrow \langle U(r) \rangle = -ke^2 \langle \frac{1}{r} \rangle \Rightarrow$

$\boxed{\langle U(r) \rangle = \frac{-ke^2}{4a_0}}$ Total energy: $E_{n=2} = -\frac{ke^2}{2a_0} \frac{1}{n^2} = -\frac{ke^2}{8a_0}$

$\Rightarrow$ kinetic energy $\langle K \rangle = E - \langle U \rangle = -\frac{ke^2}{8a_0} + \frac{ke^2}{4a_0} \Rightarrow$

$\boxed{\langle K \rangle = \frac{ke^2}{8a_0}}$

(d) In the Bohr model, the orbit is $r_n = n^2 a_0 = 4a_0$; potential energy is $U(r_n) = -\frac{ke^2}{r_n} = -\frac{ke^2}{4a_0}$, total energy is the same as in the real atom $\Rightarrow$ potential and kinetic energy are both the same as obtained above with the wavefunction.