(1) Given:

$$\ell^2|\ell m\rangle = \hbar^2 \ell(\ell+1) \quad \text{and} \quad \ell_z|\ell m\rangle = m\hbar|\ell m\rangle$$

Show:

$$\langle \ell_x\rangle = 0, \quad \langle \ell_y\rangle = 0, \quad \langle \ell_x^2\rangle = \langle \ell_y^2\rangle = \frac{\ell(\ell+1)\hbar^2 - m^2\hbar^2}{2}$$

given

$$\ell_+ = \ell_x + i\ell_y$$
$$\ell_- = \ell_x - i\ell_y$$

$$\ell_x = \frac{1}{2}(\ell_+ + \ell_-)$$
$$\ell_y = \frac{1}{2i}(\ell_+ - \ell_-)$$

$$\langle \ell_x\rangle = \langle \ell m|\tfrac{1}{2}(\ell_+ + \ell_-)|\ell m\rangle = \frac{1}{2}\Big[\langle \ell m|\ell_+|\ell m\rangle + \langle \ell m|\ell_-|\ell m\rangle\Big]$$

$$= \frac{1}{2}\Big[c^+_{\ell m}\underbrace{\cancel{\langle \ell m|\ell, m+1\rangle}}_{0} + c^-_{\ell m}\underbrace{\cancel{\langle \ell m|\ell, m-1\rangle}}_{0}\Big]$$

$$= 0$$

$$\langle \ell_y\rangle = \frac{1}{2i}\Big[\underbrace{\cancel{\langle \ell m|\ell_+|\ell m\rangle}}_{0} - \underbrace{\cancel{\langle \ell m|\ell_-|\ell m\rangle}}_{0}\Big]$$

$$= 0$$

$$\langle l_x^2\rangle = \langle l_x l_x\rangle = \frac{1}{4}\langle lm|(l_+ + l_-)(l_+ + l_-)|lm\rangle$$

$$= \frac{1}{4}\Big[\cancelto{0}{\langle lm|l_+ l_+|lm\rangle} + \langle lm|l_+ l_-|lm\rangle + \langle lm|l_- l_+|lm\rangle + \cancelto{0}{\langle lm|l_- l_-|lm\rangle}\Big]$$

$$= \frac{1}{4}\Big[\left(\sqrt{l(l+1)-m(m-1)}\,\hbar\right)\left(\sqrt{l(l+1)-(m-1)(m-1+1)}\,\hbar\right) + \left(\hbar\sqrt{l(l+1)-m(m+1)}\right)\left(\hbar\sqrt{l(l+1)-(m+1)(m+1-1)}\right)\Big]$$

$$= \frac{1}{4}\Big[\hbar^2\big[l(l+1)-m(m-1)\big] + \hbar^2\big[l(l+1)-m(m+1)\big]\Big]$$

$$= \frac{1}{4}\Big[2\hbar^2 l(l+1) - 2m^2\hbar^2\Big] = \frac{\hbar^2 l(l+1) - m^2\hbar^2}{2} \quad \checkmark$$

$$\langle l_y^2\rangle = \langle l_y l_y\rangle = -\frac{1}{4}\langle lm|(l_+ - l_-)(l_+ - l_-)|lm\rangle$$

$$= -\frac{1}{4}\Big[\cancelto{0}{\langle lm|l_+ l_+|lm\rangle} - \langle lm|l_+ l_-|lm\rangle - \langle lm|l_- l_+|lm\rangle + \cancelto{0}{\langle lm|l_- l_-|lm\rangle}\Big]$$

$$= +\frac{1}{4}\Big\{\left(\hbar\sqrt{l(l+1)-m(m-1)}\right)\left(\hbar\sqrt{l(l+1)-(m-1)(m-1+1)}\right) + \left(\hbar\sqrt{l(l+1)-m(m+1)}\right)\left(\hbar\sqrt{l(l+1)-(m+1)(m+1-1)}\right)\Big\}$$

$$= \frac{1}{4}\Big[2\hbar^2 l(l+1) - 2m^2\hbar^2\Big] = \frac{\hbar^2 l(l+1) - m^2\hbar^2}{2} \quad \checkmark$$

(2) [redacted] real spherical harmonics:

$$Y_x = \frac{1}{\sqrt{2}}\left(Y_{1,-1} - Y_{1,1}\right)$$
$$Y_y = \frac{i}{\sqrt{2}}\left(Y_{1,1} + Y_{1,-1}\right)$$
$$Y_z = Y_{1,0}$$

(a) $\langle Y_y | l_y | Y_y \rangle = -\frac{1}{2}\langle Y_{1,1} + Y_{1,-1} | l_y | Y_{1,1} + Y_{1,-1} \rangle$

but $l_y = \frac{1}{2i}\left(l_+ - l_-\right)$ see #3

$$\langle Y_y | l_y | Y_y \rangle = -\frac{1}{4i}\Big[\langle Y_{1,1} + Y_{1,-1} | l_+ | Y_{1,1} + Y_{1,-1}\rangle - \langle Y_{1,1} + Y_{1,-1} | l_- | Y_{1,1} + Y_{1,-1}\rangle\Big]$$

$$= -\frac{1}{4i}\Big[\cancelto{0}{\langle Y_{1,1} | l_+ | Y_{1,1}\rangle} + \langle Y_{1,1} | l_+ | Y_{1,-1}\rangle + \cancelto{0}{\langle Y_{1,-1} | l_+ | Y_{1,1}\rangle} + \cancelto{0}{\langle Y_{1,-1} | l_+ | Y_{1,-1}\rangle} - \cancelto{0}{\langle Y_{1,1} | l_- | Y_{1,1}\rangle} - \cancelto{0}{\langle Y_{1,1} | l_- | Y_{1,-1}\rangle} - \langle Y_{1,-1} | l_- | Y_{1,+1}\rangle - \cancelto{0}{\langle Y_{1,-1} | l_- | Y_{1,-1}\rangle}\Big]$$

$$= -\frac{1}{4i}\Big[\langle Y_{1,1} | l_+ | Y_{1,-1}\rangle - \langle Y_{1,-1} | l_- | Y_{1,1}\rangle\Big]$$

$$= -\frac{1}{4i}\Big[\hbar\sqrt{1(1+1)-(-1)(-1+1)} - \hbar\sqrt{l(l+1)-1(1-1)}\Big]$$

$$= -\frac{1}{4i}(0) = 0$$

(b) $\langle Y_y | l_z | Y_y \rangle = -\frac{1}{2} \langle Y_{1,1} + Y_{1,-1} | l_z | Y_{1,1} + Y_{1,-1} \rangle$

$$= -\frac{1}{2}\Big[\langle Y_{1,1} | l_z | Y_{1,1} \rangle + \langle Y_{1,1} | l_z | Y_{1,-1} \rangle + \langle Y_{1,-1} | l_z | Y_{1,1} \rangle + \langle Y_{1,-1} | l_z | Y_{1,-1} \rangle \Big]$$

$$= -\frac{1}{2}\Big[\hbar + 0 + 0 - \hbar \Big]$$

$$= 0$$

BONUS!

(c) $\langle Y_x | l_+ l_- | Y_x \rangle$

recall: $l_+ l_- = l^2 - l_z^2 + l_z \hbar$

$$\frac{1}{2}\Big[\langle Y_{1,-1} - Y_{1,1} | l^2 - l_z^2 + l_z \hbar | Y_{1,-1} - Y_{1,1} \rangle \Big]$$

$$= \frac{1}{2}\Big[\langle Y_{1,-1} | l_+ l_- | Y_{1,-1} \rangle + \langle Y_{1,1} | l_+ l_- | Y_{1,1} \rangle \Big]$$

other 2 will be zero since $l^2 + l_z$ are diagonal in lm

$$= \frac{1}{2}\Big\{ 1(1+1)\hbar^2 - (-1)^2\hbar^2 + (-1)\hbar^2 + 1(1+1)\hbar^2 - (1)^2\hbar^2 + (1)\hbar^2 \Big]$$

$$= \frac{1}{2}\Big[4\hbar^2 - 2\hbar^2 - \hbar^2 + \hbar^2 \Big]$$

$$= \hbar^2$$

(d) $\langle Y_z | l_x | Y_z \rangle$

recall: $l_x = \frac{1}{2}(l_+ + l_-)$

$$\langle Y_z | l_x | Y_z \rangle = \langle Y_{1,0} | l_x | Y_{10} \rangle = \frac{1}{2} \langle Y_{1,0} | l_+ + l_- | Y_{1,0} \rangle$$

$$= \frac{1}{2} \left[\cancelto{0}{\langle Y_{1,0} | l_+ | Y_{1,0} \rangle} + \cancelto{0}{\langle Y_{1,0} | l_- | Y_{1,0} \rangle} \right]$$

$$= 0$$

(e) $\langle Y_z | l_x^2 + l_y^2 | Y_z \rangle$

recall: $l_x^2 + l_y^2 = l^2 - l_z^2$

$$\langle Y_z | l_x^2 + l_y^2 | Y_z \rangle = \langle Y_{1,0} | l^2 - l_z^2 | Y_{1,0} \rangle$$

$$= \langle Y_{1,0} | l^2 | Y_{1,0} \rangle - \langle Y_{1,0} | l_z^2 | Y_{1,0} \rangle$$

$$= 1(1+1)\hbar^2 - (0)^2 \hbar^2$$

$$= 2\hbar^2$$

(3) Locate the radial nodes of the H atom 3s orbital

$$R_{30} = \frac{2}{3\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2}\underbrace{\left(1 - \frac{2Z}{3a_0}r + \frac{1}{6}\left(\frac{2Z}{3a_0}\right)^2 r^2\right)}_{\text{we need to find the roots of this polynomial}} e^{-Zr/3a_0}$$

$$\frac{\frac{2Z}{3a_0} \pm \sqrt{\left(-\frac{2Z}{3a_0}\right)^2 - 4\left(\frac{1}{6}\right)\left(\frac{2Z}{3a_0}\right)^2(1)}}{2\left(\frac{1}{6}\right)\left(\frac{2Z}{3a_0}\right)^2}$$

$$\frac{9a_0}{2Z}\left(1 \pm \frac{1}{\sqrt{3}}\right)$$

2 roots : $1.9019\,(a_0/Z)$, $7.0981\,(a_0/Z)$

for H, $Z=1$: $1.9019\,a_0$, $7.0981\,a_0$

for Ar^{+17}, $Z=18$: $0.1057\,a_0$, $0.3943\,a_0$

(4) Consider the 2s orbital of a H-like atom

Since we are only interested in $\langle r \rangle$, $\langle r^2 \rangle$, and r_{mp} for this problem, we only need R_{20}.

$$R_{20} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(1 - \frac{1}{2}\frac{Z}{a_0} r\right) e^{-Zr/2a_0}$$

$$\langle r \rangle = \int_0^\infty R_{20}\, r\, R_{20}\, r^2\, dr$$

$$= \frac{1}{2}\left(\frac{Z}{a_0}\right)^3 \left[\int_0^\infty e^{-Zr/a_0} r^3\, dr - \frac{Z}{a_0}\int_0^\infty e^{-Zr/a_0} r^4\, dr \right.$$

$$\left. + \left(\frac{1}{2}\frac{Z}{a_0}\right)^2 \int_0^\infty e^{-Zr/a_0} r^5\, dr \right]$$

Note: $\displaystyle\int_0^\infty x^n e^{-ax}\, dx = \frac{n!}{a^{n+1}}$

$$\langle r \rangle = \frac{1}{2}\left(\frac{Z}{a_0}\right)^3 \left[\frac{3!}{(Z/a_0)^4} - \frac{Z}{a_0}\left[\frac{4!}{(Z/a_0)^5}\right] \right.$$

$$\left. + \left(\frac{1}{2}\frac{Z}{a_0}\right)^2 \left[\frac{5!}{(Z/a_0)^6}\right] \right]$$

$$\langle r \rangle = \frac{1}{2}\left\{ \frac{3!}{(Z/a_0)} - \frac{4!}{(Z/a_0)} + \frac{1}{4}\cdot\frac{5!}{(Z/a_0)} \right\}$$

$$= \frac{a_0}{Z}\left[\frac{6}{2} - \frac{24}{2} + \frac{120}{8} \right]$$

$$= \frac{a_0}{Z}\left[\frac{48}{8} \right] = 6\,\frac{a_0}{Z}$$

$$\langle r^2 \rangle = \int_0^\infty R_{20}\, r^2 R_{20}\, r^2\, dr$$

$$= \frac{1}{2}\left(\frac{Z}{a_0}\right)^3 \left\{ \frac{4!}{(Z/a_0)^5} - \frac{Z}{a_0}\left[\frac{5!}{(Z/a_0)^6}\right] + \frac{1}{4}\left(\frac{Z}{a_0}\right)^2\left[\frac{6!}{(Z/a_0)^7}\right] \right\}$$

$$= \frac{1}{2}\left(\frac{a_0}{Z}\right)^2 \left[24 - 120 + 180 \right]$$

$$= 42\left(\frac{a_0}{Z}\right)^2$$

the most probable radius $r_{mp.}$ is given by the maximum in radial distribution function

$$P(r) = |R_{20}|^2 r^2$$
$$= \frac{1}{2}\left(\frac{Z}{a_0}\right)^3 e^{-Zr/a_0}\left[r^2 - \frac{Z}{a_0}r^3 + \left(\frac{1}{2}\frac{Z}{a_0}\right)^2 r^4\right]$$

$$\frac{dP(r)}{dr} = 0 = e^{-Zr/a_0}\left[2r - \frac{3Z}{a_0}r^2 + \left(\frac{Z}{a_0}\right)^2 r^3\right]$$
$$+ \left(-\frac{Z}{a_0}\right)e^{-Zr/a_0}\left[r^2 - \frac{Z}{a_0}r^3 + \frac{1}{4}\left(\frac{Z}{a_0}\right)^2 r^4\right]$$

$$0 = 2 - \frac{3Z}{a_0}r + \left(\frac{Z}{a_0}\right)^2 r^2 - \frac{Z}{a_0}r + \left(\frac{Z}{a_0}\right)^2 r^2$$
$$- \frac{1}{4}\left(\frac{Z}{a_0}\right)^3 r^3$$

$$= 2 - 4\left(\frac{Z}{a_0}\right)r + 2\left(\frac{Z}{a_0}\right)^2 r^2 - \frac{1}{4}\left(\frac{Z}{a_0}\right)^3 r^3$$

let $\rho = \frac{Z}{a_0}r$

then $0 = 2 - 4\rho + 2\rho^2 - \frac{1}{4}\rho^3$

by successive numerical approx, $\rho = 5.23607$

$\Rightarrow r_{mp} = 5.23607\, a_0/Z$

Note: I chose the root closer to $\langle r \rangle$