1 a) The radial probabily distribution function is $P(r) = r^2 R_{10}^2(r) = \frac{4}{a^3} r^2 e^{-\frac{2r}{a}}$ where $a = \frac{4\pi\varepsilon_0 \hbar^2}{mZe^2}$

The most probable r corresponds to the point where $P(r)$ is maximized:

$$\frac{\partial P}{\partial r} = 0 \implies \left(2r - \frac{2r^2}{a}\right) e^{-\frac{2r}{a}} = 0 \implies r = a$$

Hence $r = a$ is the most likely outcome

b) $\Psi_{init} = \frac{1}{\sqrt{4\pi}} \cdot \frac{2}{a^{3/2}} e^{-\frac{r}{a}}$ $\qquad a = \frac{4\pi\varepsilon_0 \hbar^2}{2me^2}$

$\Psi_{final} = \frac{1}{\sqrt{4\pi}} \frac{2}{b^{3/2}} e^{-\frac{r}{b}}$ $\qquad b = \frac{4\pi\varepsilon_0 \hbar^2}{me^2}$

$$P = |\langle \Psi_{final} | \Psi_{init} \rangle|^2 = \left| \int_0^\infty \frac{2}{b^{3/2}} \frac{2}{a^{3/2}} e^{-\frac{r}{b}} e^{-\frac{r}{a}} r^2 dr \right|^2 =$$

$$= \left| \frac{4}{a^{3/2} b^{3/2}} \int_0^\infty r^2 e^{-\frac{a+b}{ab} r} dr \right|^2 = \left| \frac{4}{a^{3/2} b^{3/2}} \frac{2}{\left(\frac{a+b}{ab}\right)^3} \right|^2 = 64 \frac{a^3 b^3}{(a+b)^6} =$$

$$= 64 \frac{\left(\frac{1}{2}\right)^3}{\left(\frac{3}{2}\right)^6} = \frac{512}{729} \approx 0.702$$

2 a) Time-evolution of the expectation value $\langle xp_x \rangle$ is given by the generalized Ehrenfest theorem:

$$\underbrace{\frac{d}{dt}\langle xp_x \rangle}_{\substack{0,\text{ because for stationary} \\ \text{states expectation values} \\ \text{do not depend on time}}} = \frac{i}{\hbar}\langle [H, xp_x] \rangle + \underbrace{\left\langle \frac{\partial xp_x}{\partial t} \right\rangle}_{0}$$

Hence we have $\langle [H, xp_x] \rangle = 0$

or $$\langle [T, xp_x] \rangle = -\langle [V, xp_x] \rangle$$

Now

$$\left[\frac{d^2}{dx^2}, x\frac{d}{dx}\right]f = \frac{d^2}{dx^2}x\frac{d}{dx}f - x\frac{d^3}{dx^3}f = \frac{d^2}{dx^2}xf' - xf''' = \frac{d}{dx}(xf''+f') - xf''' = xf'''+f''+f''-xf''' = 2f'',$$ So $\left[\frac{d^2}{dx^2}, x\frac{d}{dx}\right] = 2\frac{d^2}{dx^2}$

On the other hand

$$\left[V(x), x\frac{d}{dx}\right]f = Vx\frac{d}{dx}f - x\frac{d}{dx}Vf = Vxf' - xVf' - xV'f$$

so $$\left[V, x\frac{d}{dx}\right] = -x\frac{\partial V}{\partial x}$$

With that we have

$$-\frac{\hbar^2}{2m}(-i\hbar)\left\langle \left[\frac{d}{dx^2}, x\frac{d}{dx}\right] \right\rangle = -(-i\hbar)\left\langle \left[V, x\frac{d}{dx}\right] \right\rangle$$

or $$2\langle T \rangle = \left\langle x\frac{\partial V}{\partial x} \right\rangle$$

b) Since coordinates x, y, and z are independent and the kinetic energy is proportional to the sum of second derivatives with respect to x, y, and z we obviously have the following relation in 3D

$$2\langle T \rangle = \langle \vec{r} \cdot \nabla_{\vec{r}} V \rangle$$

c) $$\langle \vec{v}^2 \rangle = \left\langle \frac{\vec{p}^2}{m^2} \right\rangle = \frac{2}{m}\langle T \rangle = \frac{1}{m}\langle \vec{r}\cdot\nabla_{\vec{r}}V \rangle = \frac{1}{m}\int |\psi|^2 r \frac{d}{dr}\alpha \ln\frac{r}{r_0}\, d\vec{r} =$$

$$= \frac{\alpha}{m}\underbrace{\int |\psi|^2 d\vec{r}}_{1} = \frac{\alpha}{m}$$

③ a) Using the basis of the eigenstates of S^2 & S_z

$$|1,1\rangle, \; |1,0\rangle, \; |1,-1\rangle$$

or, in vector form:

$$|1,1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |1,-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

we can find the action of the ladder operators S_+ and S_-:

$$S_{\pm}|1,m\rangle = \hbar\sqrt{2 - m(m\pm 1)}\,|1, m\pm 1\rangle$$

$$S_+|1,1\rangle = 0 \qquad S_+|1,0\rangle = \hbar\sqrt{2}\,|1,1\rangle \qquad S_+|1,-1\rangle = \hbar\sqrt{2}\,|1,0\rangle$$

$$S_-|1,1\rangle = \hbar\sqrt{2}\,|1,0\rangle \qquad S_-|1,0\rangle = \hbar\sqrt{2}\,|1,-1\rangle \qquad S_-|1,-1\rangle = 0$$

Hence

$$S_+ = \hbar\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \qquad S_- = \hbar\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

From that we can determine S_x and S_y:

$$S_x = \frac{1}{2}(S_+ + S_-) = \hbar\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

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

S_z has a diagonal form in its own basis:

$$S_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

b) Given the explicit matrix form of S_x and S_z the Hamiltonian is

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

$$= \begin{pmatrix} \beta+\alpha & 0 & \beta \\ 0 & 2\beta & 0 \\ \beta & 0 & \beta-\alpha \end{pmatrix} \quad \text{where} \quad \alpha \equiv A\hbar \quad \beta \equiv \frac{B\hbar^2}{2}$$

Solving for eigenvalues of H yields:

$$\det \begin{pmatrix} \beta+\alpha-E & 0 & \beta \\ 0 & 2\beta-E & 0 \\ \beta & 0 & \beta-\alpha-E \end{pmatrix} = 0 \implies (2\beta - E)(E^2 - 2\beta E - \alpha^2) = 0$$

$$E_1 = 2\beta = B\hbar^2$$

$$E_{2,3} = \beta \pm \sqrt{\beta^2 + \alpha^2} = \frac{B\hbar^2}{2} \pm \sqrt{\frac{B^2\hbar^4}{4} + A^2\hbar^2}$$

(4) The spin part of electron's Hamiltonian is

$$H = \frac{e}{m} \vec{B} \cdot \vec{S} = \mu_B \vec{B} \cdot \vec{\sigma} = \mu_B B \sigma_z = \mu_B B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Its eigenvalues are $E_+ = \mu_B B$ $E_- = -\mu_B B$

If a measurement at time $t=0$ yielded the positive projection on the z-axis then this means that the initial state for subsequent time-evolution is

$$\chi(t=0) = \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Since H is time-independent the general solution is

$$\chi(t) = a \chi_+ e^{-\frac{iE_+ t}{\hbar}} + b \chi_- e^{\frac{-iE_- t}{\hbar}} = \chi_+ e^{-\frac{i\mu_B B t}{\hbar}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-\frac{i\mu_B B t}{\hbar}}$$

The average spin polarization along the x-direction is

$$\langle S_x \rangle = \chi^+(t) S_x \chi(t) = (1 \;\; 0) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$