

PYU33P15: Atomic Physics

Problem Set 1 due 26/11/2021

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JS Theoretical Physics

Q1.

$$\frac{\mu v^2}{r} = \frac{Z e^2}{4 \pi \varepsilon_0 r^2} \quad (\text{equating the centripetal and Coulomb forces})$$

$$E = K + U \quad (\text{total energy expression})$$

$$= \frac{\mu v^2}{2} - \int \frac{Z e^2}{4 \pi \varepsilon_0 r^2} (-\hat{r} \cdot \hat{r}) dr \quad (\text{substituting } K \text{ and } U)$$

$$= \frac{\mu v^2}{r} \frac{r}{2} + \frac{Z e^2}{4 \pi \varepsilon_0} \int \frac{dr}{r^2} \quad (\text{rewriting and simplifying})$$

$$= \frac{Z e^2}{8 \pi \varepsilon_0 r} - \frac{Z e^2}{4 \pi \varepsilon_0 r} \quad (\text{substituting and computing the integral})$$

$$= -\frac{Z e^2}{8 \pi \varepsilon_0 r}$$

$$\mu v r = n \hbar, n = 1, 2, \dots \quad (\text{assuming quantised angular momentum in integer values of } \hbar)$$

$$\mu^2 v^2 r^2 = n^2 \hbar^2 \quad (\text{squaring both sides})$$

$$\frac{\mu v^2}{r} \mu r^3 = n^2 \hbar^2 \quad (\text{rewriting})$$

$$\frac{Z e^2}{4 \pi \varepsilon_0 r^2} \mu r^3 = n^2 \hbar^2 \quad (\text{substituting})$$

$$r = \frac{4 \pi \varepsilon_0 \hbar^2 n^2}{\mu Z e^2} \quad (\text{rearranging for } r)$$

$$E = -\frac{Z e^2}{8 \pi \varepsilon_0} \frac{\mu Z e^2}{4 \pi \varepsilon_0 \hbar^2 n^2} \quad (\text{substituting } r \text{ into the expression for } E)$$

$$= -\frac{\mu Z^2 e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2 n^2} \quad (\text{simplifying})$$

$$\Delta E_{i \rightarrow f} = E_f - E_i$$

$$= \frac{\mu Z^2 e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

$$\Delta E_{2 \rightarrow 1} = \frac{\mu Z^2 e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \left(\frac{1}{2^2} - \frac{1}{1^2} \right) \quad (\text{substituting } n_i = 2, n_f = 1)$$

$$= -\frac{3 \mu Z^2 e^4}{128 \pi^2 \varepsilon_0^2 \hbar^2}$$

$$\begin{aligned}
\lambda_{2 \rightarrow 1} &= \frac{h c}{-\Delta E_{2 \rightarrow 1}} && \text{(using } E = \frac{h c}{\lambda} \text{)} \\
&= 2 \pi \hbar c \frac{128 \pi^2 \varepsilon_0^2 \hbar^2}{3 \mu Z^2 e^4} && \text{(substituting)} \\
&= \frac{256 \pi^3 \varepsilon_0^2 \hbar^3 c}{3 \mu Z^2 e^4} && \text{(simplifying)}
\end{aligned}$$

$$\lambda_{\min} \leq \lambda_{2 \rightarrow 1} \leq \lambda_{\max}$$

$$\frac{1}{\lambda_{\min}} \geq \frac{3 \mu Z^2 e^4}{256 \pi^3 \varepsilon_0^2 \hbar^3 c} \geq \frac{1}{\lambda_{\max}}$$

$$\frac{256 \pi^3 \varepsilon_0^2 \hbar^3 c}{3 \mu e^4 \lambda_{\min}} \geq Z^2 \geq \frac{256 \pi^3 \varepsilon_0^2 \hbar^3 c}{3 \mu e^4 \lambda_{\max}}$$

$$\frac{16 \pi^{\frac{1}{2}} \varepsilon_0 \hbar^{\frac{3}{2}} c^{\frac{1}{2}}}{3^{\frac{1}{2}} \mu^{\frac{1}{2}} e^2 \lambda_{\min}^{\frac{1}{2}}} \geq Z \geq \frac{16 \pi^{\frac{1}{2}} \varepsilon_0 \hbar^{\frac{3}{2}} c^{\frac{1}{2}}}{3^{\frac{1}{2}} \mu^{\frac{1}{2}} e^2 \lambda_{\max}^{\frac{1}{2}}}$$

$$142.3 \geq Z \geq 3.1,$$

where $\mu \approx m_e$ and $\lambda_{\min}, \lambda_{\max} = 0.06 \text{ \AA}, 125 \text{ \AA}$. Since Z is explicitly an integer value, Z ranges from 4 to 142.

Q2.

$$\Delta E_{i \rightarrow f} = \frac{\mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \quad \text{(as before with } Z = 1 \text{)}$$

$$\begin{aligned}
\Delta E_{3 \rightarrow 2} &= \frac{\mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \left(\frac{1}{3^2} - \frac{1}{2^2} \right) && \text{(substituting } n_i = 3, n_f = 2 \text{)} \\
&= \frac{5 \mu e^4}{1152 \pi^2 \varepsilon_0^2 \hbar^2}
\end{aligned}$$

$$\begin{aligned}
\lambda_{3 \rightarrow 2} &= \frac{h c}{-\Delta E_{3 \rightarrow 2}} \\
&= \frac{2304 \pi^3 \varepsilon_0^2 \hbar^3 c}{5 \mu e^4}
\end{aligned}$$

$$\begin{aligned}
\Delta \lambda_{3 \rightarrow 2} &= \left| \frac{2304 \pi^3 \varepsilon_0^2 \hbar^3 c}{5 \mu_1 e^4} - \frac{2304 \pi^3 \varepsilon_0^2 \hbar^3 c}{5 \mu_2 e^4} \right| \\
&= \frac{2304 \pi^3 \varepsilon_0^2 \hbar^3 c}{5 e^4} \left| \frac{m_e + m_p}{m_e m_p} - \frac{m_e + m_p + m_n}{m_e (m_p + m_n)} \right| \\
&\text{(substituting } \mu_1, \mu_2 \text{ as the reduced mass of the hydrogen and deuterium electron)} \\
&\approx 0.179 \text{ nm}
\end{aligned}$$

Q3.

(a)

$$\Delta E_{i \rightarrow f} = \frac{9 \mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \quad \text{(as before with } Z = 3 \text{)}$$

$$\begin{aligned}
|\Delta E_{2 \rightarrow 1}| &\leq |\Delta E_{\text{Lyman}}| \leq |\Delta E_{\infty \rightarrow 1}| \\
\left| \frac{9 \mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \left(\frac{1}{2^2} - \frac{1}{1^2} \right) \right| &\leq |\Delta E_{\text{Lyman}}| \leq \left| \frac{9 \mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \left(0 - \frac{1}{1^2} \right) \right| \\
\frac{27 \mu e^4}{128 \pi^2 \varepsilon_0^2 \hbar^2} &\leq |\Delta E_{\text{Lyman}}| \leq \frac{9 \mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \\
2 \pi \hbar c \frac{128 \pi^2 \varepsilon_0^2 \hbar^2}{27 \mu e^4} &\geq \frac{2 \pi \hbar c}{|\Delta E_{\text{Lyman}}|} \geq 2 \pi \hbar c \frac{32 \pi^2 \varepsilon_0^2 \hbar^2}{9 \mu e^4} \\
\frac{256 \pi^3 \varepsilon_0^2 \hbar^3 c}{27 \mu e^4} &\geq \lambda_{\text{Lyman}} \geq \frac{64 \pi^3 \varepsilon_0^2 \hbar^3 c}{9 \mu e^4},
\end{aligned}$$

and so (assuming there are 3 protons and 4 neutrons in an atom of doubly ionised lithium and so $\mu = \frac{m_e(3m_p+4m_n)}{m_e+3m_p+4m_n}$), the wavelength ranges from **10.126 nm to 13.501 nm**.

(b)

$$\begin{aligned}
E &= -\frac{9 \mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2} \quad (\text{as before with } Z = 3, n = 1) \\
|E| &\approx 1.962 \times 10^{-17} \text{ J} \approx 122.422 \text{ eV}
\end{aligned}$$

Q4.

(a)

$$\begin{aligned}
\vec{F}(r) &= -\frac{G m M}{r^2} \hat{r} \\
U(r) &= -\int \vec{F} \cdot d\vec{r} \\
&= \int \frac{G m M}{r^2} dr \\
&= -\frac{G m M}{r}
\end{aligned}$$

(b)

If we compare the potential energy function for the earth-sun system to that of the Hydrogen atom, we can convert expressions such as the Bohr radius and Bohr formula as needed for the earth-sun system.

$$\begin{aligned}
U_{\text{hydrogen}}(r) \rightarrow U_{\text{earth-sun}}(r) &\implies -\frac{e^2}{4 \pi \varepsilon_0 r} \rightarrow -\frac{G m M}{r} \implies \frac{e^2}{4 \pi \varepsilon_0} \rightarrow G m M \\
a_0 = \frac{4 \pi \varepsilon_0 \hbar^2}{\mu e^2} &= \left(\frac{\mu}{\hbar^2} \frac{e^2}{4 \pi \varepsilon_0} \right)^{-1} \rightarrow \left(\frac{\mu}{\hbar^2} G m M \right)^{-1} = \frac{\hbar^2}{G m M \mu} = a_g
\end{aligned}$$

Thus the gravitational Bohr radius is given by $a_g = \frac{\hbar^2}{G m M \mu} \approx 2.349 \times 10^{-138}$.

$$E_{n,\text{hydrogen}} = -\frac{\mu e^4}{32 \pi^2 \varepsilon_0^2 \hbar^2 n^2} = -\frac{e^2}{4 \pi \varepsilon_0} \left(\frac{4 \pi \varepsilon_0 \hbar^2}{\mu e^2} \right)^{-1} \frac{1}{2 n^2} \rightarrow -G m M a_g^{-1} \frac{1}{2 n^2} = -\frac{G m M}{2 a_g n^2} = E_{n,\text{gravitational}}$$

Equating this expression of the energy of the earth-sun system to the classical result $-\frac{G m M}{2 r_0}$ gives us

$$a_g n^2 = r_0, \text{ i.e. } n = \sqrt{\frac{r_0}{a_g}}.$$

(c)

$$\begin{aligned}
\Delta E_{i \rightarrow f} &= \frac{G m M}{2 a_g} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \\
\Delta E_{n \rightarrow n-1} &= \frac{G m M}{2 a_g} \left(\frac{1}{n^2} - \frac{1}{(n-1)^2} \right) \\
&= \frac{G m M}{2 a_g n^2} \left(1 - \frac{1}{\left(1 - \frac{1}{n}\right)^2} \right) \\
&= \frac{G m M}{2 a_g n^2} \left(1 - 1 - \frac{2}{n} - \frac{3}{n^2} - \frac{4}{n^3} - \dots \right) \quad \left(\text{expanding } \frac{1}{\left(1 - \frac{1}{n}\right)^2} \text{ in a Taylor series about } \infty \right) \\
&\approx -\frac{G m M}{a_g n^3} \quad \left(\text{neglecting terms of } n^{-2} \text{ and lower} \right) \\
&= -G m M \frac{G m M \mu}{\hbar^2} \frac{1}{r_0^{\frac{3}{2}}} \frac{\hbar^3}{(G m M \mu)^{\frac{3}{2}}} \quad \left(\text{substituting } n \text{ and } a_g \right) \\
&= \frac{\hbar \sqrt{G m M}}{r_0^{\frac{3}{2}} \sqrt{\mu}} \\
|\Delta E_{n \rightarrow n-1}| &\approx 2.1 \times 10^{-41} \text{ J}
\end{aligned}$$

$$\begin{aligned}
\lambda_{n \rightarrow n-1} &= \frac{2 \pi \hbar c}{-\Delta E_{n \rightarrow n-1}} \\
&\approx \frac{2 \pi \hbar^2 n^3}{G^2 m^2 M^2 \mu} \\
&\approx 0.9999 \text{ lightyears}
\end{aligned}$$

Q5.

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

$$\begin{aligned}
R_{nl}(r) &= \frac{1}{r} (\kappa r)^{l+1} e^{-\kappa r} \nu(\kappa r) \\
R_{1,0}(r) &= \frac{1}{r} \kappa r e^{-\kappa r} c_0 \\
&= c_0 \kappa e^{-\kappa r}
\end{aligned}$$

$$\begin{aligned}
\kappa &= \frac{\sqrt{-2 m E}}{\hbar} \\
&= \frac{1}{\hbar} \sqrt{\frac{2 m^2}{2 \hbar^2} \left(\frac{e^2}{4 \pi \varepsilon_0} \right)^2} \quad \left(\text{for } n = 1 \right) \\
&= \frac{m e^2}{4 \pi \varepsilon_0 \hbar^2} \\
&= \frac{1}{a_0} \\
\Rightarrow R_{1,0}(r) &= \frac{c_0}{a_0} e^{-\frac{r}{a_0}}
\end{aligned}$$

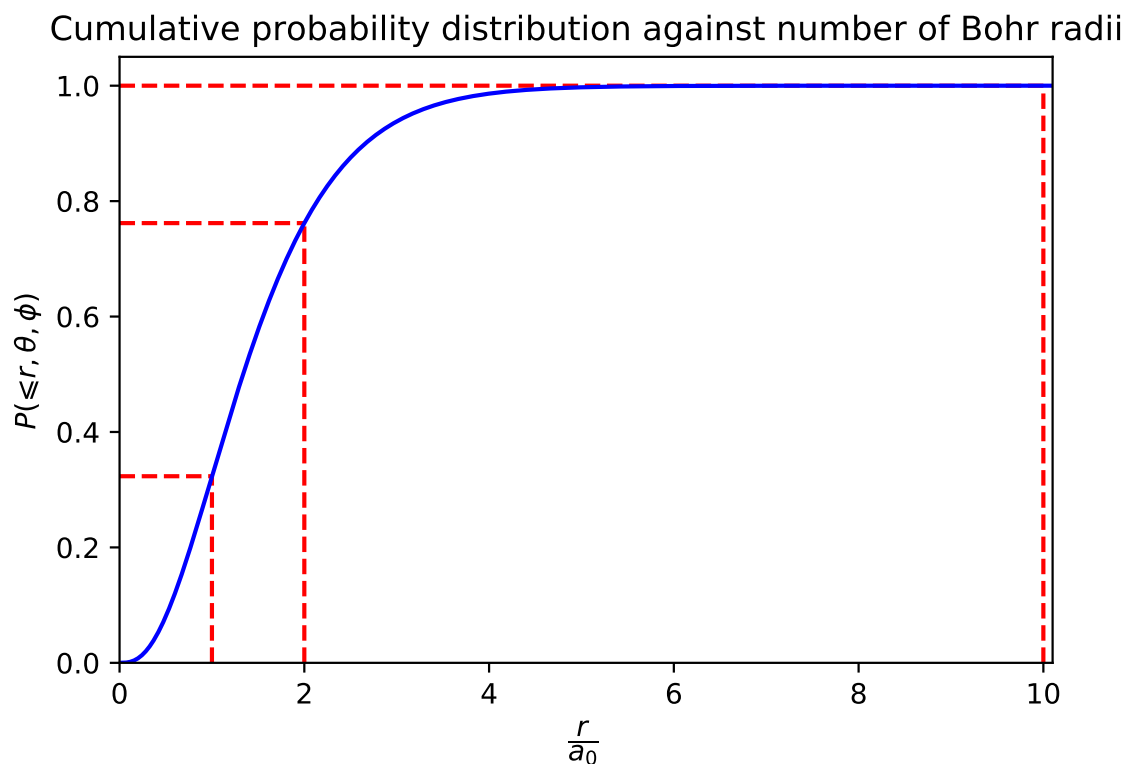
$$\begin{aligned}
1 &= \int_0^\infty |R_{1,0}(r)|^2 dr \\
&= \int_0^\infty \frac{|c_0|^2}{a_0^2} e^{-\frac{2r}{a_0}} \\
&= \frac{|c_0|^2}{a_0^2} \frac{a_0^3}{4} \\
\Rightarrow |c_0| &= \frac{2}{\sqrt{a_0}}
\end{aligned}$$

$$\begin{aligned}
Y_l^m &= (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m|)^2}{(l+|m|)^2}} e^{im\phi} P_l^m(\cos\theta) \\
Y_0^0 &= \frac{1}{\sqrt{4\pi}} = \frac{1}{2\sqrt{\pi}} \\
\Rightarrow \psi_{1,0,0}(r, \theta, \phi) &= \frac{c_0}{2a_0\sqrt{\pi}} e^{-\frac{r}{a_0}}
\end{aligned}$$

$$\begin{aligned}
P(\leq r, \theta, \phi) &= \int_0^r |\psi_{1,0,0}(r, \theta, \phi)|^2 dV \\
&= \int_0^r \frac{|c_0|^2}{4a_0^2\pi} e^{-\frac{2r}{a_0}} 4\pi^2 r dr \\
&\quad \text{(substituting } \psi_{1,0,0} \text{ and } dV = 4\pi r^2 dr, \text{ i.e. volume of shell of radius } r \text{ and thickness } dr) \\
&= \int_0^r \frac{4r^2}{a_0^3} e^{-\frac{2r}{a_0}} dr \quad \text{(substituting } |c_0|) \\
&= 4 \int_0^{\frac{r}{a_0}} \rho^2 e^{-\rho} d\rho \quad (r = a_0 \rho, dr = a_0 d\rho) \\
&= 4 \left(-\frac{\rho^2 e^{-2\rho}}{2} \Big|_0^{\frac{r}{a_0}} + \int_0^{\frac{r}{a_0}} \rho e^{-2\rho} d\rho \right) \quad \text{(integration by parts with } u = \rho^2, dv = e^{-2\rho} d\rho) \\
&= 4 \left(-\frac{r^2 e^{-\frac{2r}{a_0}}}{2a_0^2} + 0 - \frac{\rho e^{-2\rho}}{2} \Big|_0^{\frac{r}{a_0}} + \frac{1}{2} \int_0^{\frac{r}{a_0}} e^{-2\rho} d\rho \right) \\
&\quad \text{(integration by parts with } u = \rho, dv = e^{-2\rho} d\rho) \\
&= 4 \left(-\frac{r^2 e^{-\frac{2r}{a_0}}}{2a_0^2} - \frac{r e^{-\frac{2r}{a_0}}}{2a_0} - \frac{e^{-2\rho}}{4} \Big|_0^{\frac{r}{a_0}} \right) \\
&= 4 \left(-\frac{r^2 e^{-\frac{2r}{a_0}}}{2a_0^2} - \frac{r e^{-\frac{2r}{a_0}}}{2a_0} - \frac{e^{-\frac{2r}{a_0}}}{4} + \frac{1}{4} \right) \\
&= 1 - e^{-\frac{2r}{a_0}} \left(1 + \frac{2r}{a_0} \left(1 + \frac{r}{a_0} \right) \right)
\end{aligned}$$

$$\begin{aligned}
P(\leq a_0, \theta, \phi) &= 1 - e^{-\frac{2a_0}{a_0}} \left(1 + \frac{2a_0}{a_0} \left(1 + \frac{a_0}{a_0} \right) \right) \quad P(\leq 2a_0, \theta, \phi) = 1 - e^{-\frac{4a_0}{a_0}} \left(1 + \frac{4a_0}{a_0} \left(1 + \frac{2a_0}{a_0} \right) \right) \\
&= 1 - \frac{5}{e^2} \approx 0.323 \quad = 1 - \frac{13}{e^4} \approx 0.762
\end{aligned}$$

$$\begin{aligned}
P(\leq 10a_0, \theta, \phi) &= 1 - e^{-\frac{20a_0}{a_0}} \left(1 + \frac{20a_0}{a_0} \left(1 + \frac{10a_0}{a_0} \right) \right) \\
&= 1 - \frac{221}{e^{20}} \approx 0.9999995
\end{aligned}$$



Q6.

$$\begin{aligned}
[H, L_x] f &= \left[\frac{\vec{P}^2}{2m} + V(\vec{r}), L_x \right] f \\
&= \frac{1}{2m} [\vec{P}^2, L_x] f + [V(\vec{r}), L_x] f \\
&= \frac{1}{2m} \left(\vec{P} [P_y \hat{x} + P_y \hat{y} + P_z \hat{z}, Y P_z - Z P_y] + [P_y \hat{x} + P_y \hat{y} + P_z \hat{z}, Y P_z - Z P_y] \vec{P} \right) f \\
&\quad + [V(\vec{r}), Y P_z - Z P_y] f \\
&= \frac{1}{2m} \left(\vec{P} ([P_y, Y P_z] \hat{y} + [P_z, -Z P_y] \hat{z}) + ([P_y, Y P_z] \hat{y} + [P_z, -Z P_y] \hat{z}) \vec{P} \right) f \\
&\quad + [V(\vec{r}), Y] P_z f + Y [V(\vec{r}), P_z] f - [V(\vec{r}), Z] P_y f - Z [V(\vec{r}), P_y] f \\
&= \frac{1}{2m} \left(\vec{P} (-i \hbar P_z \hat{y} + i \hbar P_y \hat{z}) + (-i \hbar P_z \hat{y} + i \hbar P_y \hat{z}) \vec{P} \right) f - i \hbar \left(V(\vec{r}) Y \frac{\partial}{\partial Z} f - Y V(\vec{r}) \frac{\partial}{\partial Z} f \right. \\
&\quad \left. + Y V(\vec{r}) \frac{\partial}{\partial Z} f - Y \frac{\partial}{\partial Z} V(\vec{r}) f - V(\vec{r}) Z \frac{\partial}{\partial Y} f + Z V(\vec{r}) \frac{\partial}{\partial Y} f - Z V(\vec{r}) \frac{\partial}{\partial Y} f + Z \frac{\partial}{\partial Y} V(\vec{r}) f \right) \\
&= \frac{i \hbar}{2m} (-P_y P_z + P_z P_y - P_y P_z + P_z P_y) f - i \hbar \left(V(\vec{r}) Y \frac{\partial f}{\partial Z} - Y V(\vec{r}) \frac{\partial f}{\partial Z} + Y V(\vec{r}) \frac{\partial f}{\partial Z} \right. \\
&\quad \left. - Y \frac{\partial V(\vec{r})}{\partial Z} f - Y V(\vec{r}) \frac{\partial f}{\partial Z} - V(\vec{r}) Z \frac{\partial f}{\partial Y} + Z V(\vec{r}) \frac{\partial f}{\partial Y} - Z V(\vec{r}) \frac{\partial f}{\partial Y} + Z \frac{\partial V(\vec{r})}{\partial Y} f + Z V(\vec{r}) \frac{\partial f}{\partial Y} \right) \\
&= 0 - i \hbar \left(V(\vec{r}) Y \frac{\partial f}{\partial Z} - Y \frac{\partial V(\vec{r})}{\partial Z} f - Y V(\vec{r}) \frac{\partial f}{\partial Z} - V(\vec{r}) Z \frac{\partial f}{\partial Y} + Z \frac{\partial V(\vec{r})}{\partial Y} f + Z V(\vec{r}) \frac{\partial f}{\partial Y} \right) \\
[H, L_x] &= -i \hbar \left(-Y \frac{\partial V(\vec{r})}{\partial Z} + Z \frac{\partial V(\vec{r})}{\partial Y} \right) \\
&= i \hbar (\vec{R} \times \nabla V)_x
\end{aligned}$$

Similarly, $[H, L_y] = i \hbar (\vec{R} \times \nabla V)_y$ and $[H, L_z] = i \hbar (\vec{R} \times \nabla V)_z$, and so

$$\begin{aligned}
[H, \vec{L}] &= i \hbar \vec{R} \times \nabla V \\
\frac{d \langle \vec{L} \rangle}{dt} &= \frac{i}{\hbar} \langle [H, \vec{L}] \rangle + \left\langle \frac{\partial \vec{L}}{\partial t} \right\rangle \\
&= -\vec{R} \times \nabla V + 0 \\
&= \vec{R} \times (-\nabla V)
\end{aligned}$$

$$\begin{aligned}
V(\vec{r}) &= V(r) \\
\Rightarrow \nabla V &= \frac{\partial V(r)}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial V(r)}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial V(r)}{\partial \phi} \hat{\phi} \\
&= \frac{\partial V(r)}{\partial r} \hat{r} + 0 \\
\Rightarrow \frac{d \langle \vec{L} \rangle}{dt} &= \vec{R} \times \frac{\partial V(r)}{\partial r} \hat{r} \\
&= (\vec{R} \times \hat{r}) \left(-\frac{\partial V(r)}{\partial r} \right) \\
&= 0
\end{aligned}$$