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1 We actually did this in class!

(a) $\vec{r}\cdot\vec{\nabla} = r\,\hat{r}\cdot\left(\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial\theta} + \frac{\hat{\phi}}{r\sin\theta}\frac{\partial}{\partial\phi}\right)$

$$\boxed{\vec{r}\cdot\vec{\nabla} = r\frac{\partial}{\partial r}}$$

Next we need $\vec{\nabla}\cdot\left(\frac{\vec{r}}{r}\right)$.

Careful, this is an operator. So let's see what it does on a function ψ

$$\vec{\nabla}\cdot\left(\frac{\vec{r}}{r}\psi\right) = \left(\vec{\nabla}\cdot\frac{\vec{r}}{r}\right)\psi + \hat{r}\cdot\vec{\nabla}\psi$$

$$= \left[\sum\frac{\partial}{\partial x_i}\left(\frac{x_i}{r}\right)\right]\psi + \frac{\partial\psi}{\partial r}$$

Where I wrote the first term in Cartesian and used the "boxed" expression for the second term. Thus

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$$\vec{\nabla}\left(\frac{\vec{r}}{r}\psi\right) = \left(\sum\left(\frac{1}{r}\frac{\partial x_i}{\partial x_i} + x_i\frac{\partial(1/r)}{\partial x_i}\right)\right)\psi + \frac{\partial\psi}{\partial r}$$

$$\vec{\nabla}\left(\frac{\vec{r}}{r}\psi\right) = \left[\sum\left(\frac{1}{r} + \frac{-x_i\frac{2x_i}{2r}}{r^2}\right)\right)\psi + \frac{\partial\psi}{\partial r}$$

$$\vec{\nabla}\left(\frac{\vec{r}}{r}\psi\right) = \frac{3}{r}\psi - \sum\frac{x_i^2}{r^3}\psi + \frac{\partial\psi}{\partial r}$$

$$\vec{\nabla}\left(\frac{\vec{r}}{r}\psi\right) = \frac{3}{r}\psi - \frac{r}{r^2}\psi + \frac{\partial\psi}{\partial r}$$

$$\boxed{\vec{\nabla}\left(\frac{\vec{r}}{r}\psi\right) = \left(\frac{2}{r} + \frac{\partial}{\partial r}\right)\psi}$$

Putting the two boxed equations together

$$p_r = \frac{1}{2}\left(\hat{r}\vec{p} + \vec{p}\hat{r}\right) = -\frac{i\hbar}{2}\left(\frac{1}{r}\vec{r}\vec{\nabla} + \vec{\nabla}\frac{\vec{r}}{r}\right) =$$

$$= -\frac{i\hbar}{2}\left(\frac{\partial}{\partial r} + \frac{2}{r} + \frac{\partial}{\partial r}\right) = \boxed{-i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)}$$

About the Hermitian property:

From the previous discussion,

$$\hat{r}\bar{p}' - \bar{p}'\cdot\hat{r} = \frac{2i\hbar}{r}$$

Which means that $(\hat{r}\bar{p}')^{\dagger} = \bar{p}'\hat{r} \neq \hat{r}\bar{p}'$

(b) $$p_r^2\psi = -\hbar^2\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)\psi$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}\right)\psi$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)\psi = -\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\psi$$

2 (a) Note that $\left[r \; \frac{1}{r}\right] = 0 \qquad [p_r \; p_r] = 0$

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Therefore $[p_r \; r] = -i\hbar \left[\frac{\partial}{\partial r} \; r\right] = -i\hbar$

$$\left[p_r \; \frac{1}{r}\right] = -i\hbar \left[\frac{\partial}{\partial r} \; \frac{1}{r}\right] = \frac{i\hbar}{r^2}$$

Then

$$[a_\ell \; a_\ell^+] = \frac{1}{2m\hbar\omega}\Big(-i(\ell+1)\hbar \left[p_r \; \frac{1}{r}\right] + $$
$$+ i m\omega \, [p_r \; r] +$$
$$+ i(\ell+1)\hbar \left[\frac{1}{r} \; p_r\right] +$$
$$- i m\omega \, [r \; p_r] \Big)$$

$$[a_\ell, a_\ell^+] = \frac{1}{2m\hbar\omega}\left[\frac{2\hbar^2(\ell+1)}{r^2} + 2\hbar m\omega\right]$$

$$\boxed{[a_\ell \; a_\ell^+] = \frac{(\ell+1)\hbar}{m\omega r^2} + 1}$$

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(b) $$\hbar\omega a_\ell^+ a_\ell = \frac{1}{2m}\left(-ip_r - (\ell+1)\frac{\hbar}{r} + m\omega r\right)\cdot\left(+ip_r - (\ell+1)\frac{\hbar}{r} + m\omega r\right)$$

$$= \frac{1}{2m}\left(p_r^2 + i(\ell+1)\hbar\, p_r\left(\frac{1}{r}\right) - im\omega p_r r - i(\ell+1)\hbar\frac{1}{r}p_r + (\ell+1)^2\frac{\hbar^2}{r^2} + {} - 2(\ell+1)\hbar m\omega + im\omega r p_r + m^2\omega^2 r^2\right)$$

$$= \frac{1}{2m}\left(p_r^2 + i\hbar(\ell+1)\left[p_r \frac{1}{r}\right] - im\omega\left[p_r\, r\right] + (\ell+1)^2\frac{\hbar^2}{r^2} - 2(\ell+1)\hbar m\omega + m^2\omega^2 r^2\right)$$

$$= \frac{1}{2m}\left(p_r^2 - \frac{\hbar^2(\ell+1)}{r^2} - \hbar m\omega + \frac{\hbar^2(\ell+1)^2}{r^2} + {} - 2(\ell+1)\hbar m\omega + m^2\omega^2 r^2\right)$$

$$\hbar\omega\, a_\ell^\dagger a_\ell = \frac{p_r^2}{2m} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + \frac{1}{2} m\omega^2 r^2 - \left(\ell + \tfrac{3}{2}\right)\hbar\omega$$

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$$\hbar\omega\, a_\ell^\dagger a_\ell = H_\ell - \left(\ell + \tfrac{3}{2}\right)\hbar\omega$$

$$\Longrightarrow \boxed{H_\ell = \hbar\omega\left[a_\ell^\dagger a_\ell + \left(\ell + \tfrac{3}{2}\right)\right]}$$

(c) Take $R_{\ell+1}$ such that $H_{\ell+1} R_{\ell+1} = E R_{\ell+1}$

Then $a_\ell^\dagger H_{\ell+1} R_{\ell+1} = E a_\ell^\dagger R_{\ell+1}$

From lecture $a_\ell H_\ell = H_{\ell+1} a_\ell + \hbar\omega a_\ell$

Taking hermitian conjugate of both sides

$$H_\ell a_\ell^\dagger = a_\ell^\dagger H_{\ell+1} + \hbar\omega a_\ell^\dagger$$

Take both left and right hand side and

make them act on $R_{\ell+1}$

this gives

$$H_\ell\left(a_\ell^{+} R_{\ell+1}\right) = \left(E + \hbar\omega\right)\left(a_\ell^{+} R_{\ell+1}\right)$$

Thus $a_\ell^{+} R_{\ell+1}$ is a state of energy $E+\hbar\omega$ and an eigenfunction of H_ℓ

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3 (a) This is taking what we have done in class and setting $V(r)=0$

(b) $$a_\ell^{+} a_\ell = \frac{1}{2m}\left(p_r^2 + \frac{\hbar^2(\ell+1)^2}{r^2} + i(\ell+1)\left[p_r, \frac{1}{r}\right]\right)$$

The commutator $\left[p_r, \frac{1}{r}\right] = \frac{i\hbar}{r^2}$

from problem 2(a)

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Thus $a_l^+ a_l = \frac{1}{2M}\left[p_r^2 - \frac{\hbar^2(l+1)}{r^2} + \frac{\hbar^2(l+1)^2}{r^2}\right]$

$$\boxed{a_l^+ a_l = \frac{1}{2M}\left(p_r^2 + \frac{l(l+1)\hbar^2}{r^2}\right) = H_l}$$

(c) $[a_l, a_l^+] = \frac{1}{M}\left[-i(l+1)\hbar\left[p_r, \frac{1}{r}\right]\right] = \frac{\hbar^2(l+1)}{Mr^2}$

And also

$$H_{l+1} - H_l = \frac{\hbar^2(l+1)}{2Mr^2}\left[(l+2) - l\right]$$

$$H_{l+1} - H_l = \frac{\hbar^2(l+1)}{Mr^2}$$

So $\boxed{[a_l, a_l^+] = H_{l+1} - H_l}$

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(d) $[a_\ell\, H_\ell] = [a_\ell\, a_\ell^+ a_\ell] =$

$= a_\ell a_\ell^+ a_\ell - a_\ell^+ a_\ell a_\ell = [a_\ell\, a_\ell^+] a_\ell$

$$\boxed{[a_\ell\, H_\ell] = (H_{\ell+1} - H_\ell) a_\ell}$$

$a_\ell H_\ell - \cancel{H_\ell a_\ell} = H_{\ell+1} a_\ell - \cancel{H_\ell a_\ell}$

$a_\ell H_\ell = H_{\ell+1} a_\ell$

Then if we have a solution

$H_\ell R_\ell = E R_\ell$

acting with a_ℓ on both sides gives

$H_{\ell+1}(a_\ell R_\ell) = E(a_\ell R_\ell)$

So $a_\ell R_\ell$ is a soltn with the same E but with $\ell \to \ell+1$

(e) Starting with a solution $(E\ \ell)$ we can build more and more solutions with same E but higher and higher ℓ. This seems like an impossibility since eg classically $L = mvr$ so you'd think that increasing L means increasing $E = \frac{1}{2}mv^2$ and you cannot do that ad infinitum. But there is a "r" factor in L. So as L can become as large as you want without having v become inconsistent with fixed $E = \frac{1}{2}mv^2$, just by increasing r

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4) From the chain rule

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(a) $$\frac{\partial}{\partial \vec{x}_e} = \frac{\partial \vec{X}}{\partial \vec{x}_e}\frac{\partial}{\partial \vec{X}} + \frac{\partial \vec{r}}{\partial \vec{x}_e}\frac{\partial}{\partial \vec{r}} = \frac{m_e}{m_e+m_p}\frac{\partial}{\partial \vec{X}} + \frac{\partial}{\partial \vec{r}}$$

Then taking the dot product of each side with itself

$$\boxed{\nabla_e^2 = \left(\frac{m_e}{m_e+m_p}\right)^2 \nabla_{\vec{X}}^2 + \nabla_r^2 + \frac{2m_e}{m_e+m_p}\frac{\partial^2}{\partial \vec{X}\,\partial \vec{r}}}$$

Doing the same manipulations with $\partial/\partial x_p$ gives

$$\boxed{\nabla_p^2 = \left(\frac{m_p}{m_e+m_p}\right)^2 \nabla_{\vec{X}}^2 + \nabla_r^2 - \frac{2m_p}{m_e+m_p}\frac{\partial^2}{\partial \vec{X}\,\partial \vec{r}}}$$

(b) $$\frac{1}{m_e}\nabla_e^2 + \frac{1}{m_p}\nabla_p^2 = \frac{m_e}{M^2}\nabla_X^2 + \frac{m_p}{M^2}\nabla_X^2 + \left(\frac{1}{m_e}+\frac{1}{m_p}\right)\nabla_r^2$$

where $M = m_p + m_e$

$$= \frac{1}{M}\nabla_X^2 + \frac{1}{\mu}\nabla_r^2$$ where $\mu = \frac{m_e m_p}{M}$

Substituting into the original H we get the desired expression

$$\boxed{\frac{\hbar^2}{2M}\nabla_x^2\psi - \frac{\hbar^2}{2\mu}\nabla_r\psi - \frac{e^2}{4\pi\varepsilon_0 r}\psi = E\psi}$$

(c) $\psi = F(\vec{x})\,\phi(\vec{r})$

Plug into the SE, divide by $F\phi$, get

$$-\frac{1}{F}\frac{\hbar^2}{2M}\nabla_x^2 F - \frac{1}{\phi}\frac{\hbar^2}{2\mu}\nabla_r^2\phi - \frac{e^2}{4\pi\varepsilon_0 r} = E$$

Split it into

$$-\frac{\hbar^2}{2M}\nabla_x^2 F(\vec{x}) = E_k F(\vec{x})$$

$$-\frac{\hbar^2}{2\mu}\nabla_r^2\phi(\vec{r}) - \frac{1}{4\pi\varepsilon_0 r}\phi(r) = E_H\,\phi(\vec{r})$$

with $E = E_K + E_r$

The 1st equation is associated with the motion (kinetic energy) of the center of mass. The second equation is associated with the "binding" of the electron into the H atom

5 (a) $\psi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$

$$\langle r \rangle = \frac{1}{\pi a_0^3} \int d\Omega \int_0^\infty r^3 e^{-2r/a_0} dr$$

$$\langle r \rangle = \frac{4\pi}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0} dr$$

Looking up integral $\int_0^\infty x^n e^{-bx} = \frac{n!}{b^{n+1}}$

$$\langle r \rangle = \frac{4}{a_0^3} \frac{6 a_0^4}{2^4}$$

$$\boxed{\langle r \rangle = \frac{3}{2} a_0}$$

$$\langle r^2 \rangle = \frac{4}{a_0^3} \int_0^\infty r^4 e^{-2r/a_0} \, dr$$

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$$\langle r^2 \rangle = \frac{4}{a_0^3} \frac{24 \, a_0^5}{2^5}$$

$$\boxed{\langle r^2 \rangle = 3a_0^2}$$

(b) Looking up solutions

$$\psi_{n,n-1,m} = \frac{1}{\sqrt{(2n)!}} \left(\frac{2}{na_0}\right)^{3/2} \left(\frac{2r}{na_0}\right)^{n-1} e^{-r/na_0} \, Y_{n-1}^m(\theta,\phi)$$

The normalization of the Y_ℓ^m is taken into account automatically

Thus

$$\langle r \rangle = \frac{1}{(2n)!} \left(\frac{2}{na_0}\right)^{2n+1} \int_0^\infty r^3 \left(\frac{2}{na_0}\right)^{2(n-1)} r^{2n-2} e^{-2r/na_0} \, dr$$

$$\langle r \rangle = \frac{1}{(2n)!}\left(\frac{2}{na_0}\right)^{2n+1} \frac{(2n+1)!}{(2/na_0)^{2n+2}}$$

$$\boxed{\langle r \rangle = \frac{(2n+1)!}{2(2n)!} n a_0 = n\left(n+\frac{1}{2}\right) a_0}$$

Similarly

$$\langle r^2 \rangle = \frac{1}{(2n)!}\left(\frac{2}{na_0}\right)^{2n+1} \frac{(2n+2)!}{(2/na_0)^{2n+3}}$$

$$\boxed{\langle r^2 \rangle = \frac{(2n+2)!}{4(2n)!} n^2 a_0^2 = n^2(n+1)\left(n+\frac{1}{2}\right) a_0^2}$$

(c) $$RMS = \sqrt{n^2(n+1)\left(n+\frac{1}{2}\right) - n^2\left(n+\frac{1}{2}\right)^2} \; a_0$$

$$RMS = n a_0 \sqrt{\left(n+\frac{1}{2}\right)\left(n+1-n-\frac{1}{2}\right)}$$

$$\boxed{RMS = n\sqrt{\frac{1}{2}\left(n+\frac{1}{2}\right)} \, a_0 = \frac{1}{2} n \sqrt{2n+1} \; a_0}$$

(d) For large n, $\langle r \rangle \sim n^2 a_0$

Compare it with $\langle r \rangle = \frac{3}{2} a_0$ for the ground state.

So, for $n = 100$, radius is $\sim 10^4$ larger, volume is $\sim 10^{12}$ larger

(6) Compared with the H atom, everything looks the same in the SE expect that $e^2 \to Ze^2$. Since ~~the~~ the energy eigenvalues come from solving SE, we simply have to replace e with Ze in the Rydberg constant. Now, the Rydberg constant goes like e^4, so

$$\boxed{\begin{aligned} R(Z) &= Z^2 R(Z=1) \\ E(Z) &= Z^2 E(Z=1) \end{aligned}}$$

OTOH, the Bohr radius goes like $\frac{1}{e^2}$

therefore $$\boxed{a_0(Z) = a_0(Z=1)/Z}$$

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