Homework due Wed, Dec 5 — Chapter 12 Problems 4, 5, 8, 9

$\boxed{12-4}$

$$\left\langle \frac{1}{r} \right\rangle_{n,\ell} = \frac{Z}{a_0 n^2} = \frac{Zme^2}{\hbar^2 n^2}$$

$$\langle H \rangle_{n,\ell} = E_n = -\frac{Z^2}{n^2}\frac{me^4}{2\hbar^2}$$

Here $H = T + V$ where $T = p^2/2m$ = kinetic energy, and $V = -Ze^2/r$ = potential energy. Thus

$$\begin{aligned}\langle T \rangle &= E_n - \langle V \rangle \\ &= -\frac{Z^2}{n^2}\frac{me^4}{2\hbar^2} + Ze^2 \frac{Zme^2}{\hbar^2 n^2} \\ &= \frac{Z^2}{n^2}\frac{me^4}{2\hbar^2}\end{aligned}$$

Note that

$$\langle T \rangle_{n,\ell} = -E_n \quad \text{and} \quad \langle V \rangle_{n,\ell} = 2E_n$$

$$\boxed{\langle T \rangle_{n,\ell} = -\frac{1}{2}\langle V \rangle_{n,\ell}} \quad \text{(Virial theorem)}$$

$\boxed{12-5}$

$$\psi(\vec{x}) = \frac{1}{6}\left[4\,\psi_{100}(r) + 3\,\psi_{211}(\vec{r}) - \psi_{210}(\vec{r}) + \sqrt{10}\,\psi_{21,-1}(\vec{r}) \right]$$

(a) $$\langle H \rangle = \left(\frac{4}{6}\right)^2 E_1 + \left(\frac{3}{6}\right)^2 E_2 + \left(\frac{-1}{6}\right)^2 E_2 + \left(\frac{\sqrt{10}}{6}\right)^2 E_2$$

$$= \frac{16}{36}(-Ry) + \frac{9+1+10}{36}\left(\frac{-Ry}{4}\right)$$

$$= \frac{16+5}{36}(-Ry)$$

$$= -\frac{7}{12} Ry \qquad = -7.93 \text{ eV}$$

(b) $$\langle L^2 \rangle = \left(\frac{4}{6}\right)^2 \cdot 0 + \left[\left(\frac{3}{6}\right)^2 + \left(\frac{-1}{6}\right)^2 + \left(\frac{\sqrt{10}}{6}\right)^2\right] \hbar^2 \cdot 1.2$$

$$= \frac{20 \times 2}{36}\hbar^2 \qquad = \frac{10}{9}\hbar^2$$

(c) $$\langle L_z \rangle = 0 + \left(\frac{3}{6}\right)^2 \hbar + 0 + \left(\frac{\sqrt{10}}{6}\right)^2 (-\hbar)$$

$$= -\frac{1}{36}\hbar$$

$\boxed{12-8}$ The momentum space wave function is

$$\phi(\vec{p}) = \int e^{-i\vec{p}\cdot\vec{x}/\hbar}\, \psi_{210}(\vec{x}) \frac{d^3x}{(2\pi\hbar)^{3/2}} \quad (\text{Eq. } 3.26)$$

Let $\vec{p} = \hbar\vec{k}$ to simplify the calculation.
The 2p state has this wave function

$$\psi_{210}(\vec{x}) = R_{21}(r)\, Y_{10}(\theta,\varphi)$$

$$= \underbrace{\frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0}}_{\text{see } (12-30)} \quad \underbrace{\sqrt{\frac{3}{4\pi}}\cos\theta}_{\text{see } (11-65)}$$

$$= \frac{1}{\sqrt{4\pi}}\left(\frac{Z}{2a_0}\right)^{3/2} \frac{Z}{a_0}\, r e^{-\alpha r} \cos\theta$$

where $\alpha = \dfrac{Z}{2a_0}$

$r\cos\theta = z$

Thus

$$\phi(\vec{p}) = \frac{1}{\sqrt{4\pi}}\left(\frac{Z}{4\pi\hbar a_0}\right)^{3/2} \frac{Z}{a_0} \underbrace{\int e^{-i\vec{k}\cdot\vec{x}}\, z e^{-\alpha r}\, d^3x}_{\leftarrow \text{ call this part } J \rightarrow}$$

Calculate J

$$J = \int e^{-i\vec{k}\cdot\vec{x}}\, z e^{-\alpha r}\, d^3x$$

$$= i\frac{\partial}{\partial k_z} \int e^{-i\vec{k}\cdot\vec{x}}\, e^{-\alpha r}\, d^3x$$

This integral depends only on $|\vec{k}|$ by spherical symmetry.

$$= i\frac{\partial}{\partial k_z} F(k) \quad \text{where} \quad k = \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$$= i\,\frac{dF}{dk}\,\frac{\partial k}{\partial k_z} = i\,\frac{dF}{dk}\,\frac{k_z}{k}$$

$F(k)$ depends only on the magnitude of $\vec{k}$, so we can take $\vec{k}$ in any direction. Let $\vec{k} = k\hat{z}$ to evaluate the integral. That is,

$$F(k) = \int e^{-ikr\cos\theta}\, e^{-\alpha r}\, r^2 dr\, \sin\theta\, d\theta\, d\varphi$$

$$= \int_0^\infty r^2 dr\, e^{-\alpha r} \underbrace{\int_0^\pi e^{-ikr\cos\theta} \sin\theta\, d\theta}_{=\frac{1}{ikr} e^{-ikr\cos\theta}\Big|_{\theta=0}^{\pi}} \underbrace{\int_0^{2\pi} d\varphi}_{2\pi}$$

$$= \frac{1}{ikr}\left\{e^{ikr} - e^{-ikr}\right\}$$

$$= \frac{2\sin kr}{kr}$$

$\therefore F(k)$

$$= \frac{4\pi}{k}\int_0^\infty r\, e^{-\alpha r} \sin kr\, dr$$

$$= \frac{4\pi}{k}\left(-\frac{\partial}{\partial\alpha}\right) \underbrace{\int_0^\infty e^{-\alpha r} \sin kr\, dr}$$

$$= \mathrm{Im} \int_0^\infty e^{-\alpha r} e^{ikr}\, dr$$

$$= \mathrm{Im}\, \frac{1}{\alpha - ik} = \frac{k}{\alpha^2 + k^2}$$

$\therefore F(k)$

$$= \frac{4\pi}{k}\left(-\frac{\partial}{\partial\alpha}\right)\frac{k}{k^2+\alpha^2} = \frac{8\pi\alpha}{(k^2+\alpha^2)^2}$$

Now go back to the equation for J:

$$J = i\,\frac{dF}{dk}\,\frac{k_z}{k}$$

$$= i\,\frac{k_z}{k}\,\frac{-32\pi\, k\alpha}{(k^2+\alpha^2)^3} = \frac{-32\pi i\,\alpha k_z}{(k^2+\alpha^2)^3}$$

Now go back to the equation for $\phi(\vec{p})$:

$$\phi(\vec{p}) = \frac{1}{\sqrt{4\pi}}\left(\frac{Z}{4\pi\hbar a_0}\right)^{3/2}\frac{Z}{a_0}\,(-32\pi i)\,\frac{Z k_z}{2a_0}\,\frac{1}{\left[k^2+(Z/2a_0)^2\right]^3}$$

Finally, recall ~~that~~ $\vec{k} = \vec{p}/\hbar$.

$$\phi(\vec{p}) = -i\,\frac{32\pi}{2\times 16\pi^2}\left(\frac{Z}{a_0}\right)^{7/2}\frac{1}{\hbar^{3/2}}\,\frac{\hbar^3\, p_z/\hbar}{\left[p^2+\left(\frac{Z\hbar}{2a_0}\right)^2\right]^3}$$

$$\boxed{\phi(\vec{p}) = \frac{-i}{\pi}\left(\frac{Z}{a_0}\right)^{7/2}\hbar^{1/2}\,\frac{p_z}{\left[p^2+\left(Z\hbar/2a_0\right)^2\right]^3}}$$