

Working out the $2p_z$ orbital

This is worked out directly from Atkins:

$$\psi_{2p_z} = R_{21} Y_{10} \quad \text{--- (1)}$$

where $Y_{10} = \frac{1}{2} \left(\frac{3}{\pi} \right)^{1/2} \cos \theta \quad \text{--- (2)}$

$$R_{21} = \frac{1}{a^{3/2}} \left(\frac{1}{2\sqrt{6}} \right) \left(\frac{r}{a} \right) e^{-r/(2a)} \quad \text{--- (3)}$$

So $\psi_{2p_z} = \frac{1}{4} \frac{1}{\sqrt{6}} \left(\frac{3}{\pi} \right)^{1/2} \frac{1}{a^{3/2}} \left(\frac{r}{a} \right) e^{-r/(2a)} \cos \theta$

$$\psi_{2p_z} = \frac{1}{4} \left(\frac{1}{2\pi} \right)^{1/2} \frac{1}{a^{3/2}} \left(\frac{r}{a} \right) e^{-r/(2a)} \cos \theta$$

$$\psi_{2p_z} = \left[\frac{1}{2\sqrt{2}} \cdot \frac{1}{2\pi^{1/2}} \right] \frac{1}{a^{3/2}} \left(\frac{r}{a} \right) e^{-r/(2a)} \cos \theta$$

This is the same as Atkins, page 76.

$$\psi_{2s} = \left[\frac{1}{2\sqrt{2}} \cdot \frac{1}{2\pi^{1/2}} \right] \left(2 - \frac{r}{a} \right) e^{-r/2a}$$