

SOLUTION MANUAL FOR HW # 8

10.5

$$S_{total}^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2(S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z})$$

$$\psi_+ = (\alpha(1)\beta(2) + \beta(1)\alpha(2))/\sqrt{2} \quad \& \quad \psi_- = (\alpha(1)\beta(2) - \beta(1)\alpha(2))/\sqrt{2}$$

$$S_1^2 \alpha(1)\beta(2) = \frac{3\hbar^2}{4} \alpha(1)\beta(2) \quad \& \quad S_1^2 \beta(1)\alpha(2) = \frac{3\hbar^2}{4} \beta(1)\alpha(2)$$

$$S_2^2 \alpha(1)\beta(2) = \frac{3\hbar^2}{4} \alpha(1)\beta(2) \quad \& \quad S_2^2 \beta(1)\alpha(2) = \frac{3\hbar^2}{4} \beta(1)\alpha(2)$$

$$S_{1x}S_{2x} \alpha(1)\beta(2) = \frac{\hbar}{2} \beta(1) \frac{\hbar}{2} \alpha(2) \quad \& \quad S_{1x}S_{2x} \beta(1)\alpha(2) = \frac{\hbar}{2} \alpha(1) \frac{\hbar}{2} \beta(2)$$

$$S_{1y}S_{2y} \alpha(1)\beta(2) = \frac{i\hbar}{2} \beta(1) \frac{-i\hbar}{2} \alpha(2) \quad \& \quad S_{1y}S_{2y} \beta(1)\alpha(2) = \frac{i\hbar}{2} \alpha(1) \frac{-i\hbar}{2} \beta(2)$$

$$S_{1z}S_{2z} \alpha(1)\beta(2) = \frac{\hbar}{2} \alpha(1) \frac{-\hbar}{2} \beta(2) \quad \& \quad S_{1z}S_{2z} \beta(1)\alpha(2) = \frac{\hbar}{2} \beta(1) \frac{-\hbar}{2} \alpha(2)$$

$$S_{total}^2 \psi_+ = S_1^2 (\alpha(1)\beta(2)/\sqrt{2}) + S_1^2 (\beta(1)\alpha(2)/\sqrt{2}) + S_2^2 (\alpha(1)\beta(2)/\sqrt{2}) + S_2^2 (\beta(1)\alpha(2)/\sqrt{2})$$

$$+ (2/\sqrt{2})S_{1x}S_{2x} \alpha(1)\beta(2) + (2/\sqrt{2})S_{1x}S_{2x} \beta(1)\alpha(2) + (2/\sqrt{2})S_{1y}S_{2y} \alpha(1)\beta(2) + (2/\sqrt{2})S_{1y}S_{2y} \beta(1)\alpha(2)$$

$$+ (2/\sqrt{2})S_{1z}S_{2z} \alpha(1)\beta(2) + (2/\sqrt{2})S_{1z}S_{2z} \beta(1)\alpha(2) = 2\hbar^2 \psi_+ \Rightarrow \text{Eigenvalue is } "2\hbar^2".$$

$$S_{total}^2 \psi_- = S_1^2 (\alpha(1)\beta(2)/\sqrt{2}) - S_1^2 (\beta(1)\alpha(2)/\sqrt{2}) + S_2^2 (\alpha(1)\beta(2)/\sqrt{2}) - S_2^2 (\beta(1)\alpha(2)/\sqrt{2})$$

$$+ (2/\sqrt{2})S_{1x}S_{2x} \alpha(1)\beta(2) - (2/\sqrt{2})S_{1x}S_{2x} \beta(1)\alpha(2) + (2/\sqrt{2})S_{1y}S_{2y} \alpha(1)\beta(2) - (2/\sqrt{2})S_{1y}S_{2y} \beta(1)\alpha(2)$$

$$+ (2/\sqrt{2})S_{1z}S_{2z} \alpha(1)\beta(2) - (2/\sqrt{2})S_{1z}S_{2z} \beta(1)\alpha(2) = 0$$

10.9

$$E(\alpha) = \frac{\int \phi H \phi d\tau}{\int \phi \phi d\tau} \quad \& \quad \phi(r) = e^{-\alpha r}$$

a)

$$H = \frac{-\hbar^2}{2m_e r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{e^2}{4\pi\epsilon_0 r} \Rightarrow H\phi = \frac{-\hbar^2}{2m_e r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \phi(r) \right) - \frac{e^2}{4\pi\epsilon_0 r} \phi(r)$$

$$H\phi = \frac{-\hbar^2}{2m_e r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} e^{-\alpha r} \right) - \frac{e^2}{4\pi\epsilon_0 r} e^{-\alpha r} = \frac{\hbar^2}{2m_e r^2} \frac{\partial}{\partial r} \left(r^2 (-\alpha) e^{-\alpha r} \right) - \frac{e^2}{4\pi\epsilon_0 r} e^{-\alpha r}$$

$$= \frac{\alpha \hbar^2}{2m_e r^2} (2r - \alpha r^2) - \frac{e^2}{4\pi\epsilon_0 r} e^{-\alpha r}$$

b)

$$\int \phi H \phi d\tau = \int_0^\infty \int_0^\pi \int_0^{2\pi} \left\{ \frac{\alpha \hbar^2}{2m_e r^2} (2r - \alpha r^2) e^{-2\alpha r} - \frac{e^2}{4\pi\epsilon_0 r} e^{-2\alpha r} \right\} r^2 dr \sin \theta d\theta d\varphi$$

$$= \int_0^\infty \left\{ \frac{\alpha \hbar^2}{2m_e r^2} (2r - \alpha r^2) e^{-2\alpha r} - \frac{e^2}{4\pi\epsilon_0 r} e^{-2\alpha r} \right\} r^2 dr \left(\int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\varphi \right)$$

$$= 4\pi \int_0^\infty \left\{ \frac{\alpha \hbar^2}{2m_e} (2r - \alpha r^2) e^{-2\alpha r} - \frac{e^2}{4\pi\epsilon_0} r e^{-2\alpha r} \right\} dr$$

$$\therefore \int_0^\infty r e^{-2\alpha r} dr = \frac{1}{(2\alpha)^2} \quad \& \quad \int_0^\infty r^2 e^{-2\alpha r} dr = \frac{2!}{(2\alpha)^3}$$

$$= 4\pi \left\{ \frac{\alpha \hbar^2}{m_e} \frac{1}{(2\alpha)^2} - \frac{\alpha^2 \hbar^2}{2m_e} \frac{2!}{(2\alpha)^3} - \frac{e^2}{4\pi\epsilon_0} \frac{1}{(2\alpha)^2} \right\} = \frac{\pi \hbar^2}{2m_e \alpha} - \frac{e^2}{4\epsilon_0 \alpha^2}$$

c)

$$\int \phi \phi d\tau = \int_0^\infty \int_0^\pi \int_0^{2\pi} \left\{ e^{-2\alpha r} \right\} r^2 dr \sin \theta d\theta d\varphi = 4\pi \frac{2!}{(2\alpha)^3} = \pi / \alpha^3$$

d)

$$E(\alpha) = \frac{\int \phi H \phi d\tau}{\int \phi \phi d\tau} = \frac{\frac{\pi \hbar^2}{2m_e \alpha} - \frac{e^2}{4\epsilon_0 \alpha^2}}{\pi / \alpha^3} = \frac{\hbar^2 \alpha^2}{2m_e} - \frac{e^2 \alpha}{4\pi\epsilon_0}$$

$$\frac{dE(\alpha)}{d\alpha} = \frac{\hbar^2 \alpha}{m_e} - \frac{e^2}{4\pi\epsilon_0} = 0 \Rightarrow \alpha = \frac{e^2 m_e}{4\pi\epsilon_0 \hbar^2} \Rightarrow E(\alpha) = \frac{e^4 m_e}{32\pi^2 \epsilon_0^2 \hbar^2} - \frac{e^4 m_e}{16\pi^2 \epsilon_0^2 \hbar^2} = -\frac{e^4 m_e}{32\pi^2 \epsilon_0^2 \hbar^2}$$

e)

Energy is greater than true energy.

10.11

a)

$$Y_1^0(\theta, \phi) = (3/4\pi)^{1/2} \cos \theta$$

$$Y_1^1(\theta, \phi) = (3/8\pi)^{1/2} \sin \theta e^{i\phi}$$

$$Y_1^{-1}(\theta, \phi) = (3/8\pi)^{1/2} \sin \theta e^{-i\phi}$$

$$|Y_1^0(\theta, \phi)|^2 = \left| \left\{ (3/4\pi)^{1/2} \cos \theta \right\} \left\{ (3/4\pi)^{1/2} \cos \theta \right\} \right| = (3/4\pi) \cos^2 \theta$$

$$|Y_1^1(\theta, \phi)|^2 = \left| \left\{ (3/8\pi)^{1/2} \sin \theta e^{i\phi} \right\} \left\{ (3/8\pi)^{1/2} \sin \theta e^{-i\phi} \right\} \right| = (3/8\pi) \sin^2 \theta$$

$$|Y_1^{-1}(\theta, \phi)|^2 = \left| \left\{ (3/8\pi)^{1/2} \sin \theta e^{-i\phi} \right\} \left\{ (3/8\pi)^{1/2} \sin \theta e^{i\phi} \right\} \right| = (3/8\pi) \sin^2 \theta$$

b)

$$\begin{aligned} |Y_1^0(\theta, \phi)|^2 + |Y_1^1(\theta, \phi)|^2 + |Y_1^{-1}(\theta, \phi)|^2 &= (3/4\pi) \cos^2 \theta + (3/8\pi) \sin^2 \theta + (3/8\pi) \sin^2 \theta \\ &= (3/4\pi) \cos^2 \theta + (3/4\pi) \sin^2 \theta = (3/4\pi)(\cos^2 \theta + \sin^2 \theta) = (3/4\pi) \end{aligned}$$

c) Because charge density does not depend on angular part only radial part.

10.21

a) $s^1 d^5$: 7S b) f^3 : $L = 6, S = 3/2, {}^4I$ c) g^2 : $L = 7, S = 1, {}^3J$

10.26

a) 2S b) 2P c) 1S d) 2S e) 1S **f) 4S** g) 2D