Assignment (17)

① $E = \frac{-Z^2}{2n^2}$

n=3

↑↓

e) n=2

↑↓

f) n=1

$E_T = \left[\frac{-Z^2}{2(1)^2}\right][2] + \left[\frac{-Z^2}{2(2)^2}\right][2] + \left[\frac{-Z^2}{2(3)^2}\right][1]$

$E_T = -Z^2\left[1 + \frac{1}{4} + \frac{1}{18}\right] = -Z^2\left[\frac{36+9+2}{36}\right] = \frac{-47}{36}Z^2$

② $\Psi_{He^+}\{\vec{r},t\} = 0.5774\,\Psi_{3s}\{\vec{r},t\} - 0.7071\,\Psi_{3p_1}\{\vec{r},t\} + 0.4082\,\Psi_{3d_2}\{\vec{r},t\}$

a) $\langle E\rangle = \langle \Psi_{He^+}|\hat{H}|\Psi_{He^+}\rangle = \langle 0.5774\Psi_{3s} - 0.7071\Psi_{3p_1} + 0.4082\Psi_{3d_2}|\hat{H}|0.5774\Psi_{3s} - 0.7071\Psi_{3p_1} + 0.4082\Psi_{3d_2}\rangle$

$= \langle 0.5774\Psi_{3s} - 0.7071\Psi_{3p_1} + 0.4082\Psi_{3d_2}|(0.5774)\left(\frac{Z^2}{2(3)^2}\right)\Psi_{3s} - (0.7071)\left(\frac{Z^2}{2(3)^2}\right)\Psi_{3p_1} + (0.4082)\left(\frac{Z^2}{2(3)^2}\right)\Psi_{3d_2}\rangle$

$= \frac{4}{18}\left[(0.5774)^2\langle\Psi_{3s}|\Psi_{3s}\rangle + (0.7071)^2\langle\Psi_{3p_1}|\Psi_{3p_1}\rangle + (0.4082)^2\langle\Psi_{3d_2}|\Psi_{3d_2}\rangle\right]$

$= 0.2222$ a.u.

b) $\langle \hat{L}^2\rangle = \langle\Psi_{He^+}|\hat{L}^2|\Psi_{He^+}\rangle = \langle 0.5774\Psi_{3s} - 0.7071\Psi_{3p_1} + 0.4082\Psi_{3d_2}|\hat{L}^2|0.5774\Psi_{3s} - 0.7071\Psi_{3p_1} + 0.4082\Psi_{3d_2}\rangle$

$= \hbar^2\langle 0.5774\Psi_{3s} - 0.7071\Psi_{3p_1} + 0.4082\Psi_{3d_2}|(0.5774)(0)(1)\Psi_{3s} - (0.7071)(1)(2)\Psi_{3p_1} + (0.4082)(2)(3)\Psi_{3d_2}\rangle$

$= \hbar^2\left[(0.7071^2)(2)\langle\Psi_{3p_1}|\Psi_{3p_1}\rangle + (0.4082)^2(6)\langle\Psi_{3d_2}|\Psi_{3d_2}\rangle\right]$

$= 1.9997\,\hbar^2$

c) $\langle \hat{L}_z\rangle = \langle\Psi_{He^+}|\hat{L}_z|\Psi_{He^+}\rangle$

$= \hbar\left[(0.7071^2)(0)\langle\Psi_{3s}|\Psi_{3s}\rangle + (0.7071)^2(1)\langle\Psi_{3p_1}|\Psi_{3p_1}\rangle + (0.4082)^2(2)\langle\Psi_{3d_2}|\Psi_{3d_2}\rangle\right]$

$= 0.8332\,\hbar$

d) $P\{L^2 = 0\} = \frac{\langle 0.5774\Psi_{3s}|0.5774\Psi_{3s}\rangle}{\langle\Psi_{He^+}|\Psi_{He^+}\rangle} = \frac{0.5774^2}{0.5774^2 + 0.7071^2 + 0.4082^2} = 0.3334$

e) Yes

③ $E^{(1)} = \langle\Psi_0|V\{x\}|\Psi_0\rangle = \int\left(\frac{\sqrt{km}}{\pi\hbar}\right)^{1/2} e^{-(\sqrt{km}/2\hbar\, x^2)(2)}\, cx^4\,dx = C\left(\frac{\sqrt{km}}{\pi\hbar}\right)^{1/2}\int x^4 e^{-(\sqrt{km}/\hbar)x^2}\,dx$

$= C\left(\frac{\sqrt{km}}{\pi\hbar}\right)^{1/2}\frac{3}{\left[2\left(\frac{\sqrt{km}}{\hbar}\right)\right]^2}\sqrt{\frac{\pi}{\frac{\sqrt{km}}{\hbar}}} = C\left(\frac{\sqrt{km}}{\pi\hbar}\right)^{1/2}(3/2^2)\left(\frac{\hbar}{\sqrt{km}}\right)^2\left(\frac{\pi\hbar}{\sqrt{km}}\right)^{1/2} = \frac{3C}{4}\left(\frac{\hbar}{\sqrt{km}}\right)^2$

⑤ ^5I a) $L = 6$

b) $M_L = \pm 6, \pm 5, \pm 4, \pm 3, \pm 2, \pm 1, 0$

c) $S = \frac{5-1}{2} = 2$

d) $M_S = \pm 2, \pm 1, 0$

⑥ $2p^1 3p^1$:

$L = |L_1 - L_2|, \ldots, L_1 + L_2 = \{0, 1, 2\} \rightarrow S, P, D$

$S = |S_1 - S_2|, \ldots, S_1 + S_2 = \{0, 1\} \rightarrow 2S+1 = \{1, 3\}$

$^1S, {}^1P, {}^1D, {}^3S, {}^3P, {}^3D$

* $S = 0$: $J = |L - S|, \ldots, L + S = \{0, 1, 2\} \rightarrow {}^1S_0, {}^1P_1, {}^1D_2$

* $S = 1$: $J = |L - S|, \ldots, L + S = \{\underbrace{|0-1|}_{L=0},\ \underbrace{|1-1|, 1, 2}_{L=1},\ \underbrace{|2-1|, 2, 3}_{L=2}\}$

$^3S_1 \qquad {}^3P_0, {}^3P_1, {}^3P_2 \qquad {}^3D_1, {}^3D_2, {}^3D_3$

$^1S_0, {}^3S_1, {}^1P_1, {}^3P_0, {}^3P_1, {}^3P_2, {}^1D_2, {}^3D_1, {}^3D_2, {}^3D_3$

$2p^2$: from C exercise = $^1S_0, {}^1D_2, {}^3P_0, {}^3P_1, {}^3P_2$

$2p^1 3p^1$ has more terms because it is not limited by Pauli's exclusion principle.

Order

$) = 2$

$) = 1$

ras.

$2\}$

:H

$\vec{r}_2\}$