

Q10-12

This way the repulsive interactions are counted twice.

P10-8

a)

$$\begin{aligned}
 -\frac{\hbar^2}{2m_e} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} e^{-\alpha r} \right) - \frac{e^2}{4\pi\epsilon_0 r} e^{-\alpha r} &= -\frac{\hbar^2}{2m_e} \frac{1}{r^2} \frac{\partial}{\partial r} (-\alpha r^2 e^{-\alpha r}) - \frac{e^2}{4\pi\epsilon_0 r} e^{-\alpha r} \\
 &= -\frac{\hbar^2}{2m_e} \frac{1}{r^2} (-2\alpha r e^{-\alpha r} + \alpha^2 r^2 e^{-\alpha r}) - \frac{e^2}{4\pi\epsilon_0 r} e^{-\alpha r} = \\
 &= \frac{\alpha \hbar^2}{2m_e} \frac{1}{r^2} (2r - \alpha r^2) e^{-\alpha r} - \frac{e^2}{4\pi\epsilon_0 r} e^{-\alpha r}
 \end{aligned}$$

b)

$$\begin{aligned}
 \frac{\hbar^2 \alpha}{2m_e} \left(2 \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty r e^{-2\alpha r} dr - \alpha \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty r^2 e^{-2\alpha r} dr \right) \\
 - \frac{e^2}{4\pi\epsilon_0} \left(\int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty r e^{-2\alpha r} dr \right) \\
 = \frac{4\pi \hbar^2 \alpha}{2m_e} \left(2 \int_0^\infty r e^{-2\alpha r} dr - \alpha \int_0^\infty r^2 e^{-2\alpha r} dr \right) - \frac{4\pi e^2}{4\pi\epsilon_0} \int_0^\infty r e^{-2\alpha r} dr \\
 = \frac{2\pi \hbar^2 \alpha}{m_e} \left(\frac{1}{2\alpha^2} - \frac{1}{4\alpha^2} \right) - \frac{e^2}{\epsilon_0} \frac{1}{4\alpha^2} = \frac{\pi \hbar^2}{2m_e \alpha} - \frac{e^2}{4\alpha^2 \epsilon_0}
 \end{aligned}$$

c)

$$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty r^2 e^{-2\alpha r} dr = 4\pi \int_0^\infty r^2 e^{-2\alpha r} dr = 4\pi \frac{2}{2^3 \alpha^3} = \frac{\pi}{\alpha^3}$$

d)

$$\frac{d}{d\alpha} \left(\frac{\hbar^2 \alpha^2}{2m_e} - \frac{e^2 \alpha}{4\pi\epsilon_0} \right) = 0 \Rightarrow \frac{\hbar^2 \alpha}{m_e} - \frac{e^2}{4\pi\epsilon_0} = 0 \Rightarrow \alpha_{optimal} = \frac{m_e e^2}{4\pi\epsilon_0 \hbar^2}$$

e)

$$E(\alpha_{optimal}) = \left(\frac{\hbar^2 \alpha^2}{2m_e} - \frac{e^2 \alpha}{4\pi\epsilon_0} \right) = -\frac{m_e e^4}{32\pi^2 \epsilon_0^2 \hbar^2}$$

$E(\alpha_{optimal})$ is equal to the true energy because the trial wave function has the same form as the true wave function.

P10-9

The orange line (the middle line) is correct. For the second ionization energy, the alkali metals have the maximum for each row of the periodic table.

P11-19

[] represents one orbital:

$$s^1 d^5 \rightarrow [1] [1][1][1][1][1] \rightarrow L=0, S=3 \rightarrow {}^7S_3$$

$$f^3 \rightarrow [1][1][1][0][0][0][0] \rightarrow L=6, S=3/2 \rightarrow {}^4I_{9/2}$$

$$g^2 \rightarrow [1][1][0][0][0][0][0][0][0] \rightarrow L=7, S=1 \rightarrow {}^3K_6$$

Note that (from Wikipedia):

L =	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
	S	P	D	F	G	H	I	K	L	M	N	O	Q	R	T	U	V

P11-21

$$\psi_{triplet} = \frac{1}{\sqrt{2}} [1s(1)2s(2) - 2s(1)1s(2)] \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)]$$

By expanding the determinants in Example 10.2 and comparing to the triplet wave function, then:

$$\psi_{triplet} = \frac{1}{\sqrt{2}} [\psi_1(1,2) + \psi_4(1,2)]$$

P11-38

$$F (2p^5) \rightarrow [2][2][1] \rightarrow {}^2P_{3/2}$$

$$Na (3s^1) \rightarrow [1] \rightarrow {}^2S_{1/2}$$

$$P (3p^3) \rightarrow [1][1][1] \rightarrow {}^4S_{3/2}$$