HW 1 - Solutions

1.1

1.1.1

$$\mu_p = \frac{m_{e^-} m_{e^+}}{m_{e^-} + m_{e^+}} = \frac{m_{e^\pm}^2}{2 m_{e^\pm}} = \frac{m_{e^-}}{2}$$

mass of electron and positron are identical!

$$a_0' = \frac{4\pi \varepsilon_0 \hbar^2}{\mu_p e^2} = \frac{8\pi \hbar^2 \varepsilon_0}{m_e e^2} = 1.06 \cdot 10^{-10} \, m$$

$$E_p = -\frac{z^2 \hbar^2}{2 a_0^2 \mu_p} \frac{1}{n^2} \overset{(z=1, n=1)}{=\!=} -\frac{2 (1.054 \cdot 10^{-34} \, Js)^2}{2 (1.06 \cdot 10^{-10} m)^2 \cdot 9.11 \cdot 10^{-31} kg}$$

$$= 1.086 \cdot 10^{-18} \left[\frac{kg \, m^4 \, s^2}{s^4 \, m^2 \, kg} \right]$$

$$= 1.086 \cdot 10^{-18} \left[\frac{kg \, m^2}{s^2} \right]$$

$$= 1.086 \cdot 10^{-18} \, J$$

$$= 6.78 \, eV$$

Compare to H:

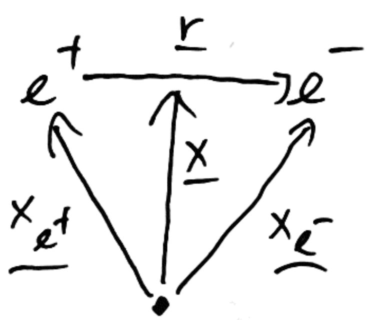
$$\mu_p = \frac{m_e}{2} \qquad \mu_H = \frac{m_p m_e}{m_p + m_e} \approx m_e \quad \text{with } m_p \approx 2000 m_e$$

$$a_0^P = 2 a_0^H$$

$$E_P = \frac{1}{2} E_H$$

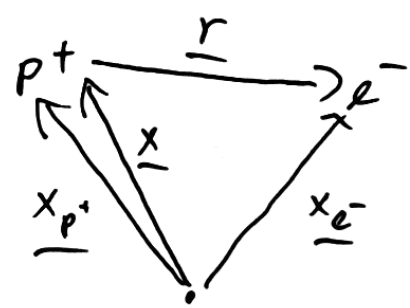
1.1.2

Positronium



- center of mass $\underline{X}$ half way in between e^+ and e^-
- e^+ and e^- both orbit $\underline{X}$ with $|\underline{r}| \sim a_0^P$

Hydrogen



- C. O. m. $\underline{X}$ very close to p^+
- e^- orbits p^+ with $|\underline{r}| = a_0^H$

1.2

1.2.1 $$E(\alpha) = \frac{\langle \Psi(\alpha) | H | \Psi(\alpha) \rangle}{\langle \Psi(\alpha) | \Psi(\alpha) \rangle}$$

$\rightarrow$ minimum provides upper bound

denominator:

$$\langle \Psi(\alpha) | \Psi(\alpha) \rangle = 4\pi N^2 \int_0^\infty e^{-2(r/\alpha)^2} r^2 \, dr$$

with $x = \sqrt{2}\frac{r}{\alpha} \rightsquigarrow r = \frac{\alpha x}{\sqrt{2}}$, $dx = \frac{\sqrt{2}}{\alpha} dr$

$$\langle \Psi(\alpha) | \Psi(\alpha) \rangle = 4\pi N^2 \left(\frac{\alpha}{\sqrt{2}}\right)^3 \int_0^\infty x^2 e^{-x^2} dx = 4\pi N^2 \left(\frac{\alpha^3}{8\sqrt{2}}\right)$$

numerator: $H = T + V$, $T = -\frac{1}{2}\nabla^2$, $V = -\frac{1}{r}$

(in Hartree units)

$$\langle \Psi(\alpha) | T | \Psi(\alpha) \rangle = -\frac{1}{2} \int \Psi^*(\alpha) \nabla^2 \Psi(\alpha) \, dr$$

$$= -\frac{1}{2} 4\pi N^2 \int_0^\infty r^2 e^{-(r/\alpha)^2} \left[\frac{1}{r_2} \frac{d}{dr} r^2 \frac{d}{dr} \right] e^{-(r/\alpha)^2} dr$$

$$= -\frac{1}{2} 4\pi N^2 \int_0^\infty e^{-(r/\alpha)^2} \frac{d}{dr} \left(-\frac{2r^3}{\alpha^2} \right) e^{-(r/\alpha)^2} dr$$

$$= \frac{4\pi N^2}{\alpha^2} \int_0^\infty e^{-(r/\alpha)^2} \frac{d}{dr} r^3 e^{-(r/\alpha)^2} dr$$

$$= \frac{4\pi N^2}{\alpha^2} \int_0^\infty e^{-(r/\alpha)^2} \left(3r^2 - \frac{2r^4}{\alpha^2}\right) e^{-(r/\alpha)^2} dr$$

$$= \frac{4\pi}{\alpha^2} N^2 \int_0^\infty \left(3r^2 - \frac{2r^4}{\alpha^2}\right) e^{-2(r/\alpha)^2} dr$$

again use $x = \sqrt{2}\frac{r}{\alpha}$

$$= \frac{12\pi}{\alpha^2 N^2} \left(\frac{\alpha}{\sqrt{2}}\right)^3 \int_0^\infty x^2 e^{-x^2} dx - \frac{8\pi N^2}{\alpha^4} \left(\frac{\alpha}{\sqrt{2}}\right)^5 \int_0^\infty x^4 e^{-x^2} dx$$

$$= 4\pi N^2 \alpha \frac{6\sqrt{\pi}}{32\sqrt{2}}$$

$$\Rightarrow \frac{\langle \psi(\alpha) | T | \psi(\alpha) \rangle}{\langle \psi(\alpha) | \psi(\alpha) \rangle} = \underline{\underline{\frac{3}{2\alpha^2}}}$$

$$\langle \psi(\alpha) | V | \psi(\alpha) \rangle = -4\pi N^2 \int_0^\infty r^2 e^{-2(r/\alpha)^2} \frac{1}{r} dr$$

$$= -4\pi N^2 \left(\frac{\alpha}{\sqrt{2}}\right)^2 \int_0^\infty x e^{-x^2} dx$$

$$= -4\pi N^2 \left(\frac{\alpha^2}{4}\right)$$

$$\Rightarrow \frac{\langle \psi(\alpha) | V | \psi(\alpha) \rangle}{\langle \psi(\alpha) | \psi(\alpha) \rangle} = -\frac{1}{\alpha}\sqrt{\frac{8}{\pi}}$$

$$E(\alpha) = \frac{3}{2\alpha^2} - \frac{1}{\alpha}\sqrt{\frac{8}{\pi}} \quad \Rightarrow \quad \frac{dE(\alpha)}{d\alpha} = 0$$

$$-\frac{3}{\alpha^3} + \frac{2\sqrt{2}}{\sqrt{\pi}\,\alpha^2} = 0$$

$$\Rightarrow \alpha_{min} = \frac{3\sqrt{\pi}}{2\sqrt{2}} = 3\sqrt{\frac{\pi}{8}}$$

$$E_{min} = \frac{3}{2\alpha_{min}^2} - \frac{1}{\alpha_{min}}\sqrt{\frac{8}{\pi}}$$

$$= \frac{3}{2}\,\frac{8}{9\pi} - \frac{8}{3\pi} = -\frac{4}{3\pi} = -0.42 \text{ Hartrees} > -0.5 \text{ Hartrees}$$

in eV: $-11.54\,eV > -13.6\,eV$

not bad!