

Variational Calculation for the Helium Atom Ground State Energy

Griffiths QM, 2nd Edition, p. 299

Energy (eV)

-75 (Z = 2, hydrogenic WFs)

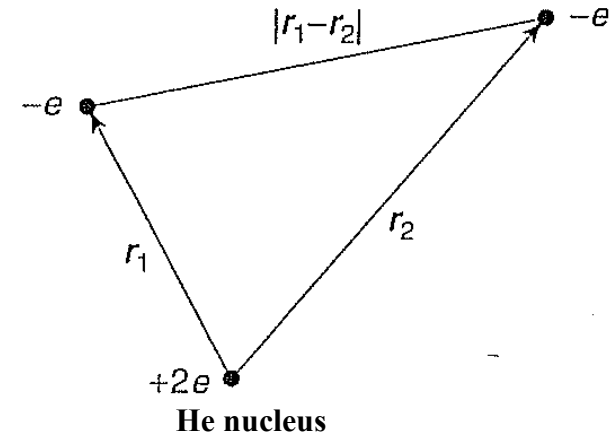
$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) \equiv \psi_{100}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2) = \frac{8}{\pi a^3} e^{-2(r_1+r_2)/a}$$

-77.5 (Variational Z)

$$\psi_1(\mathbf{r}_1, \mathbf{r}_2) \equiv \frac{Z^3}{\pi a^3} e^{-Z(r_1+r_2)/a}$$

-78.975 (experimental)

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0} \left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right)$$



Variational Hamiltonian:

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0} \left(\frac{Z}{r_1} + \frac{Z}{r_2} \right) + \frac{e^2}{4\pi\epsilon_0} \left(\frac{(Z-2)}{r_1} + \frac{(Z-2)}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right)$$

Z is the nucleus screening parameter

$$\langle H \rangle = \left[2Z^2 - 4Z(Z-2) - (5/4)Z \right] E_1 = [-2Z^2 + (27/4)Z] E_1$$

$$\frac{d}{dZ} \langle H \rangle = [-4Z + (27/4)] E_1 = 0 \quad \Rightarrow \quad Z = \frac{27}{16} = 1.69 \quad \text{so} \quad \langle H \rangle = \frac{1}{2} \left(\frac{3}{2} \right)^6 E_1 = -77.5 \text{ eV}$$