

$$\hat{T}=-\frac{1}{2}\nabla^2$$

$$\langle T \rangle = \int \psi^*(\mathbf{r}) \left(-\frac{1}{2} \nabla^2 \right) \psi(\mathbf{r}) d^3 r$$

$$\phi_\zeta(r)=\frac{\zeta^{3/2}}{\sqrt{\pi}a_0^{3/2}}e^{-\zeta r/a_0}$$

$$T=\int \phi_\zeta^*(r) \left(-\frac{1}{2} \nabla^2 \right) \phi_\zeta(r) d^3 r$$

$$\nabla^2 \phi = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\phi}{dr} \right)$$

$$\frac{d\phi_\zeta}{dr}=-\frac{\zeta}{a_0}\phi_\zeta(r)$$

$$\frac{d}{dr} \left(r^2 \frac{d\phi_\zeta}{dr} \right) = -\frac{\zeta}{a_0} \left(2r\phi_\zeta(r) + r^2 \frac{d\phi_\zeta}{dr} \right) = -\frac{2\zeta}{a_0}r\phi_\zeta + \frac{\zeta^2}{a_0^2}r^2\phi_\zeta$$

$$\nabla^2 \phi_\zeta = -\frac{2\zeta}{a_0 r} \phi_\zeta + \frac{\zeta^2}{a_0^2} \phi_\zeta$$

$$\langle T \rangle = -\frac{1}{2} \int \phi_\zeta \nabla^2 \phi_\zeta d^3 r = -\frac{1}{2} \int \phi_\zeta \left(-\frac{2\zeta}{a_0 r} \phi_\zeta + \frac{\zeta^2}{a_0^2} \phi_\zeta \right) d^3 r$$

$$= \frac{1}{2} \int \phi_\zeta^2 \frac{2\zeta}{a_0 r} d^3 r - \frac{1}{2} \int \phi_\zeta^2 \frac{\zeta^2}{a_0^2} d^3 r$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{\zeta}{a_0}, \quad \int \phi_\zeta^2 d^3 r = 1$$

$$\langle T \rangle = \frac{1}{2} \times 2\zeta \times \frac{\zeta}{a_0^2} - \frac{1}{2} \frac{\zeta^2}{a_0^2} = \frac{\zeta^2}{a_0^2} - \frac{\zeta^2}{2a_0^2} = \frac{\zeta^2}{2a_0^2}$$

$$T_{total}=2\times \frac{\zeta^2}{2a_0^2}=\frac{\zeta^2}{a_0^2}$$

$$a_0=1$$

$$T_{total}=\zeta^2$$

$$\psi_T(r_1,r_2)=\frac{\zeta^3}{\pi a_0^3}e^{-\frac{\zeta}{a_0}(r_1+r_2)}$$

$$\hat{V}_{nuclear}=-\frac{2}{r_1}-\frac{2}{r_2}$$

$$\begin{aligned} V_{nuclear} &= \left\langle \psi_T \left| -\frac{2}{r_1} - \frac{2}{r_2} \right| \psi_T \right\rangle = -2 \left\langle \frac{1}{r_1} \right\rangle - 2 \left\langle \frac{1}{r_2} \right\rangle \\ &\left\langle \frac{1}{r_1} \right\rangle = \left\langle \frac{1}{r_2} \right\rangle = \left\langle \frac{1}{r} \right\rangle \end{aligned}$$

$$V_{nuclear}=-4\left\langle \frac{1}{r} \right\rangle$$

$$\left\langle \frac{1}{r} \right\rangle:$$

$$\int_0^\infty r e^{-\alpha r} dr = \frac{1}{\alpha^2} \quad \text{with} \quad \alpha = \frac{2\zeta}{a_0}$$

$$\left\langle \frac{1}{r} \right\rangle = 4\pi \left(\frac{\zeta^3}{\pi a_0^3} \right)^2 \frac{1}{\left(\frac{2\zeta}{a_0} \right)^2} = \frac{\zeta}{a_0}$$

Final result:

$$V_{nuclear} = -4 \frac{\zeta}{a_0}$$

In atomic units where $a_0 = 1$, this simplifies to:

$$V_{nuclear} = -4\zeta$$

$$V_{ee} = \frac{5}{8} \zeta$$

$$E_{\text{trial}}(\zeta) = \zeta^2 - \frac{27}{8} \zeta$$

$$\frac{dE}{d\zeta} = 2\zeta - \frac{27}{8} = 0 \Rightarrow \zeta = \frac{27}{16}$$

Substitute into E_{trial} :

$$E_{\min} = \left(\frac{27}{16} \right)^2 - \frac{27}{8} \cdot \frac{27}{16} = \frac{729}{256} - \frac{729}{128} = -\frac{729}{256}$$

$$E_{\min} \approx -2.8476 \text{ Hartree}$$

$$1 \text{ Hartree} = 27.2114 \text{ eV}$$

$$E_{\min} \approx -2.8476 \times 27.2114 = -77.53 \text{ eV}$$

The energy calculated with the test function is a good approximation for the ground state energy of the helium atom. This number represents the total electronic energy of the system in its most stable (lowest energy) state.