NO.

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H atom

$$\psi_1 = \sqrt{\frac{1}{\pi a_0^3}}\, e^{-\frac{r}{a_0}} \qquad \psi_2 = \sqrt{\frac{1}{32\pi a_0^3}}\,\left(2-\frac{r}{a_0}\right)e^{-\frac{r}{2a_0}}$$

$$\psi_{trial} = C_1\psi_1 + C_2\psi_2 \quad , \quad S_{11}=S_{22}=0 \quad S_{12}=S_{21}=0$$

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

$$H_{11} = (\gamma-1)bcR \quad H_{22} = \frac{1}{4}(\gamma-1)bcR \quad H_{12}=H_{21} = \frac{16\gamma}{27\sqrt{2}}bcR \qquad \gamma = \frac{m_e}{m_p}$$

$\frac{\hbar^2}{2a_0^2 m_e}$ $\qquad$ $2bcR$: Hartree energy $= \frac{\hbar^2}{a_0^2 m_e}$

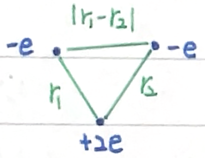
$$\begin{vmatrix} H_{11}-ES_{11} & H_{12}-ES_{12} \\ H_{21}-ES_{21} & H_{22}-ES_{22} \end{vmatrix} = \begin{vmatrix} H_{11}-E & H_{12} \\ H_{21} & H_{22}-E \end{vmatrix} = 0$$

$$E = \frac{1}{8}(\gamma-1)(5+3\sqrt{1+2\Gamma^2})bcR \quad , \quad \Gamma = \frac{2^6\gamma}{3^4(\gamma-1)}$$

$$= -0.999\ 46bcR$$

$$\Rightarrow \begin{cases} C_1(H_{11}-E)+C_2H_{21}=0 \\ C_1H_{12}+C_2(H_{22}-E)=0 \end{cases} \quad , \quad \begin{cases} C_1 \approx 1.000\ 00 \\ C_2 \approx -0.000\ 54 \end{cases}$$

The Ground State of Helium



$$H = -\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - \frac{e^2}{4\pi\epsilon_0}(\ \cdots\ r_1 \quad r_2 \quad |\vec{r}_1-\vec{r}_2|)$$

if we ignore e-e repulsion

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

$$E = \langle\psi|\hat{H}|\psi\rangle = 2E_{1s}(Z=2) = 2(-13.6)\times 2^2 = -108.8\,eV \quad (\text{Experiment} : -78.975\,eV)$$

37.77%

to improve accuracy

$$\left\langle \frac{1}{|r_1-r_2|}\right\rangle = \left(\frac{8}{\pi a^3}\right)^2 \int\int \frac{e^{-\frac{4(r_1+r_2)}{a}}}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}\, d^3r_2\, d^3r_1$$

$$① = \int \frac{e^{-\frac{4r_2}{a}}}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta}}\, r_2^2\sin\theta_2\, dr_2\, d\theta_2\, d\phi_2$$

assume r_1 fixed

$$① = 2\pi\int_0^\infty e^{-\frac{4(r_1+r_2)}{a}}\left[\int_0^\pi \frac{\sin\theta_2}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}\,d\theta_2\right] r_2^2\,dr_2 = 2\pi\int_0^\infty e^{-\frac{4r_2}{a}} \frac{1}{r_1r_2}\left[(r_1+r_2)-|r_1-r_2|\right] r_2^2\,dr_2$$

$$② = \frac{1}{r_1r_2}\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}\,\Big|_0^\pi = \frac{1}{r_1r_2}\left(\sqrt{r_1^2+r_2^2+2r_1r_2} - \sqrt{r_1^2+r_2^2-2r_1r_2}\right)$$

$$= 4\pi\left(\frac{1}{r_1}\int_0^{r_1} e^{-0}\, r_2^2\,dr_2 + \int_{r_1}^\infty e^{-0}\, r_2\,dr_2\right)$$

$$= \frac{1}{r_1r_2}\left[(r_1+r_2)-|r_1-r_2|\right] = \begin{cases} \frac{2}{r_1}, & r_2<r_1 \\ \frac{2}{r_2}, & r_2>r_1 \end{cases}$$

$$= \frac{\pi a^3}{8r_1}\left[1-\left(1+\frac{2r_1}{a}\right)e^{-\frac{4r_1}{a}}\right]$$

$$\Rightarrow ① = 4\pi e^{-\frac{4r_1}{a}}\left(\frac{1}{r_1}\int_0^{r_1} r_2^2 e^{-\frac{4r_2}{a}}\,dr_2 + \int_{r_1}^\infty r_2 e^{-\frac{4r_2}{a}}\,dr_2\right) \quad \frac{1}{r_1}\int_0^{r_1} r_2^2 e^{-\frac{4r_2}{a}}\,dr_2 \ ?$$

$$= \frac{1}{r_1}\left[-\frac{a}{4}r_2^2 e^{-\frac{4r_2}{a}} + \frac{a}{2}\left(\frac{a}{4}\right)^2 e^{-\frac{4r_2}{a}}\left(-\frac{4r_2}{a}-1\right)\right]\Big|_0^{r_1}$$

$$= -\frac{a}{4r_1}\left(r_1^2 e^{-\frac{4r_1}{a}} + \frac{ar_1}{2}e^{-\frac{4r_1}{a}} + \frac{a^2}{8}e^{-\frac{4r_1}{a}} - \frac{a^2}{8}\right)$$