QU47

$$\langle H\rangle_\phi\Big|_{min} = \frac{\hbar^2}{2m}\left(\frac{3m^2\omega^2}{\hbar^2}\right)^{1/2} + \frac{3}{2}m\omega^2\left(\frac{\hbar^2}{3m\omega^2}\right)^{1/2}$$

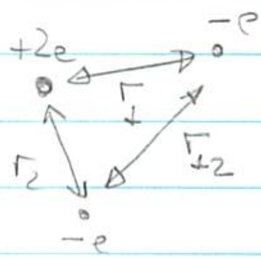
$$= \hbar\omega\left\{\frac{\sqrt{3}}{2} + \frac{3}{2}\frac{1}{\sqrt{3}}\right\} = \sqrt{3}\,\hbar\omega$$

COMPARE: EXACT ANSWER $E_0 = \frac{3}{2}\hbar\omega$

$\frac{3}{2} = 1.5$ $\qquad$ $\sqrt{3} = 1.73$

$\Rightarrow$ 15% HIGH

GROUNDSTATE OF HELIUM



- HAMILTONIAN

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

- PROBLEM: e-e INTERACTION $\Rightarrow$ 3-BODY PROBLEM

- WAVE FUNCTION: $\psi_{m_1,m_2}(r_1, r_2)$

- CAN IGNORE SPIN (G.S. ONLY) $\psi_{m_1 m_2}(r_1, r_2) \sim (\uparrow\downarrow - \downarrow\uparrow) \times \psi(r_1, r_2)$

- VARIATIONAL ANSATZ

$$\psi(r_1, r_2) = \phi(r_1)\,\phi(r_2) \sim e^{-\alpha(r_1 + r_2)}$$

NOTE: EXACT FOR $V_{12} = 0$

QU48

NORMALIZATION

$$\langle\psi|\psi\rangle = \int d^3r_1 \int d^3r_2\, \phi^*(r_1)\phi(r_1)\, \phi^*(r_2)\phi(r_2)$$

$$= \left[\int d^3r_1\, \phi^*(r_1)\phi(r_1)\right]^2$$

AS IN H.O. EXAMPLE

$$= \left[\int d^3r\, e^{-2\alpha r}\right]^2 = \left(\frac{\pi}{\alpha^3}\right)^2 = \frac{\pi^2}{\alpha^6}$$

POTENTIAL ENERGY $\langle V_1\rangle = \langle V_2\rangle$

$$\langle V_2\rangle = \langle\psi|\left(-\frac{2e^2}{r_2}\right)|\psi\rangle$$

$$= -2e^2 \int d^3r_1\, e^{-2\alpha r_1} \int d^3r_2\, \frac{1}{r_2} e^{-2\alpha r_2}$$

$$= (-2e^2)\cdot\left(\frac{\pi}{\alpha^3}\right)\cdot\frac{4\pi}{(2\alpha)^2}\int x\,dx\, e^{-x}$$

$$= (-2e^2)\,\frac{\pi^2}{\alpha^5}$$

INTERACTION

$$\langle V_{12}\rangle = e^2 \int d^3r_1 \int d^3r_2\, e^{-2\alpha(r_1+r_2)}/r_{12}$$

$$= \frac{e^2}{(2\alpha)^5}\int d^3x_1 \int d^3x_2\, e^{-(x_1+x_2)}/x_{12}$$

CAN BE DONE IN SPH. COORDINATES

$$2\pi \int d(\cos\theta) \int x_2^2\,dx_2\, e^{-x_2}/\left[x_1^2+x_2^2+2x_1x_2\cos\theta\right]^{1/2}$$

$$\int d(\cos\theta)\, \frac{1}{[x_1^2+x_2^2+2x_1x_2\cos\theta]^{1/2}} = \frac{1}{x_1x_2}\left[x_1^2+x_2^2+2x_1x_2\cos\theta\right]^{1/2}\Big|_{-1}^{1}$$

$$= \frac{1}{x_1x_2}\left\{|x_1+x_2| - |x_1-x_2|\right\}$$

$$= \begin{cases} 2/x_2 & x_1 < x_2 \\ 2/x_1 & x_2 < x_1 \end{cases}$$

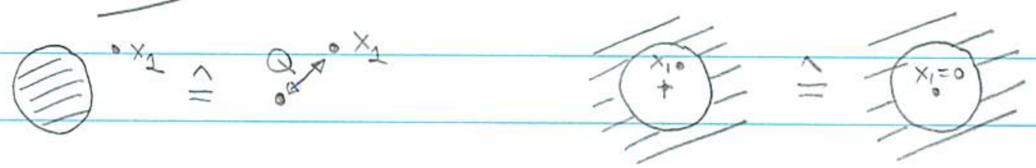
NOTE: YOU CAN GET THIS FROM GAUSS' LAW

$$\int d^3x_2\, \frac{e^{-x_2}}{x_{12}} \equiv \int d^3x_2\, \frac{\rho(x_2)}{x_{12}} \equiv$$ POTENTIAL AT x_1 DUE TO CHARGE DISTRIBUTION $\rho(x_2) \equiv e^{-x_2}$

WRITE

$$\int d^3x_2\, \frac{\rho(x_2)}{x_{12}} = \overbrace{\int d^3x_2\, \frac{\rho(x_2)}{x_{12}}}^{x_2<x_1} + \overbrace{\int d^3x_2\, \frac{\rho(x_2)}{x_{12}}}^{x_1<x_2}$$

$$= \frac{1}{x_1}\int_0^{x_1} d^3x_2\, \rho(x_2) + \int_{x_1}^{\infty} d^3x_2\, \frac{\rho(x_2)}{x_2}$$



POTENTIAL CONSTANT INSIDE

GET $$\int d^3x_2\, \frac{e^{-x_2}}{x_{12}} = 4\pi\left\{\frac{1}{x_1}\int_0^{x_1} x_2^2 dx_2\, e^{-x_2} + \int_{x_1}^{\infty} x_2^2 dx_2\, \frac{1}{x_2} e^{-x_2}\right\}$$

$$= 4\pi\left\{\left(\frac{2}{x_1} - e^{-x_1}\left(\frac{2}{x_1}+2+x_1\right)\right) + e^{-x_1}(1+x_1)\right\}$$

$$= 4\pi\left\{\frac{2}{x_1} - \frac{2}{x_1}e^{-x_1} - e^{-x_1}\right\}$$

QNSO

INTEGRAL OVER x_1

$$\int d^3x_1 \int d^3x_2 \; \frac{e^{-x_1} e^{-x_2}}{x_{12}}$$

$$= (4\pi)^2 \int x_1^2 dx_1 \, e^{-x_1} \left\{ \frac{2}{x_1} - \frac{2}{x_1} e^{-x_1} - e^{-x_1} \right\}$$

$$= (4\pi)^2 \left\{ 2 \int x dx \, e^{-x} - 2 \int x dx \, e^{-2x} - \int x^2 dx \, e^{-2x} \right\}$$

$$= (4\pi)^2 \left\{ 2 \int x dx \, e^{-x} - \frac{1}{2} \int x dx \, e^{-x} - \frac{1}{8} \int x^2 dx \, e^{-x} \right\}$$

$$= (4\pi)^2 \left\{ 2 - \frac{1}{2} - \frac{1}{4} \right\} = (4\pi)^2 \frac{5}{4}$$

$$\rightsquigarrow \langle V_{12} \rangle = e^2 \cdot \frac{\pi^2}{32\alpha^5} \cdot 16\pi^2 \cdot \frac{5}{4} = \frac{5\pi^2}{8\alpha^5} e^2$$

- FINALLY $\langle T_1 \rangle = \langle T_2 \rangle$

$$\langle T_1 \rangle = \int d^3r_1 \left(\frac{\hbar^2}{2m} \right) \left(\vec{\nabla} e^{-\alpha r_1} \right)^2 \int d^3r_2 \, e^{-2\alpha r_2}$$

$$= \frac{\hbar^2}{2m} \cdot \frac{\pi}{\alpha} \cdot \frac{\pi}{\alpha^3} = \frac{\hbar^2}{2m} \frac{\pi^2}{\alpha^4}$$

- Sum

$$\langle H \rangle = \left[2\langle T_1 \rangle + 2\langle V_1 \rangle + \langle V_{12} \rangle \right] \cdot \frac{\alpha^6}{\pi^2}$$

$$= \left[\frac{\hbar^2}{m} \frac{\pi^2}{\alpha^4} - 4e^2 \frac{\pi^2}{\alpha^5} + \frac{5\pi^2}{8\alpha^5} e^2 \right] \cdot \frac{\alpha^6}{\pi^2}$$

$$= \left[\frac{\hbar^2}{m} \frac{\pi^2}{\alpha^4} - \frac{27}{8} e^2 \frac{\pi^2}{\alpha^5} \right] \frac{\alpha^6}{\pi^2} = \frac{\hbar^2}{m} \alpha^2 - \frac{27}{8} e^2 \alpha$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 2\frac{\hbar^2}{m}\alpha - \frac{27}{8}e^2 = 0$$

$$\Rightarrow \quad \alpha = \frac{27}{16}\frac{e^2 m}{\hbar^2}$$

$$\Rightarrow \langle H \rangle = \frac{\hbar^2}{m}\left(\frac{27}{16}\right)^2 \frac{e^4 m^2}{\hbar^4} - \frac{27}{8}\cdot e^2 \cdot \frac{27}{16}\frac{e^2 m}{\hbar^2}$$

$$= -\left(\frac{27}{16}\right)^2 \frac{e^4 m}{\hbar^2}$$

NOTE: NEGLECT INTERACTION $27 \rightarrow 32$

$$\langle H \rangle = -4\frac{e^4 m}{\hbar^2} = -8\frac{e^4 m}{2\hbar^2} = -8 \times 13.6\,eV$$

$$\Rightarrow B_0 = -108.8\,eV$$

$$B_{TRIAL} = -\left(\frac{27}{32}\right)^2 108.8\,eV = \underline{-77.5\,eV}$$

$$B_{EXP} = -\underline{78.97\,eV}$$

NOTE: EXACT ENERGY LOWER; ERROR 2%

ALSO NOTE: CAN INTERPRET RESULTS IN TERMS OF EFFECTIVE CHARGE

$$E_0 = -2 Z_{eff}^2 \frac{e^4 m}{\hbar^2 \cdot 2} \quad \Rightarrow \quad Z_{eff} = \frac{27}{16} \simeq 1.68$$

$\Rightarrow$ SCREENING REDUCES $Z = 2 \rightarrow Z \simeq 1.7$