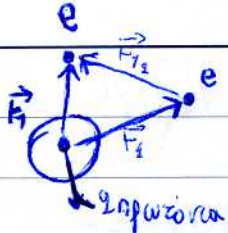


93-3-10



$$r_1 = |\vec{r}_1|$$

$$r_2 = |\vec{r}_2|$$

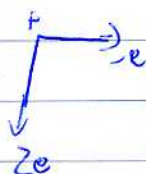
$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_{n-e}^1 + V_{n-e}^2 + V^{e-e} = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 + \frac{ze^2}{r_1} - \frac{ze^2}{r_2} +$$

$$\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

$$E_n = -\frac{me^4}{2\hbar^2 n^2}, \quad n=1,2,3,\dots$$

$$\psi_{200}(r, \theta, \varphi) = \psi_{1s}(r, \theta, \varphi) = \frac{1}{\sqrt{\pi} \cdot a_0} \cdot e^{-r/a_0}$$

$$a_0 = \frac{\hbar^2}{me^2}$$



$$V = -\frac{Ze^2}{r}$$

$$a_0 = \frac{\hbar^2}{Ze}$$

$$\psi_{1s}(r, \theta, \varphi) = \frac{Z^{3/2}}{\sqrt{\pi} \cdot a_0^{3/2}} \cdot e^{-Zr/a_0}$$

Θαρούμε τα $2e^-$ μm - αλληλεπιδρώντα



$$E_1 = -\frac{m \cdot e^4}{2\hbar^2} \cdot 4 = -54.4 \text{ eV} \quad E_{\text{ολ. θερ.}} = -2 \times 54.4 = -108.8 \text{ eV}$$

$$\psi_{1s}(\vec{r}_1) \psi_{1s}(\vec{r}_2)$$

$$\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\pi \cdot a_0^3} e^{-2(k_1 + k_2)/a_0}$$



$$E_2 = -\frac{m e^4}{2\hbar^2} = -13.6 \text{ eV}$$



$$S=1$$

$$(\vec{r}_1, \vec{r}_2)$$

$$\Psi_{\text{αντισυμμετρ.}} = \frac{1}{\sqrt{2}} [\psi_{1s}(\vec{r}_1) \psi_{2s}(\vec{r}_2) - \psi_{2s}(\vec{r}_1) \psi_{1s}(\vec{r}_2)]$$

$$S=0$$

$$\Psi_{\text{συμμετρ.}} = \frac{1}{\sqrt{2}} [\psi_{1s}(\vec{r}_1) \psi_{2s}(\vec{r}_2) + \psi_{2s}(\vec{r}_1) \psi_{1s}(\vec{r}_2)]$$

$$E^{\text{συμμετρ.}} = -13.6_{\text{eV}} - 54.4_{\text{eV}} = -68 \text{ eV} + (\text{κατ.})$$

Με $S=1$, έχουμε μικρότερη ενέργεια ~~από την~~ $S=0$

$$E^{(1)} = \int dV_1 \int dV_2 \Psi(\vec{r}_1, \vec{r}_2) \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} = \frac{5}{8} Z \cdot \frac{me^4}{\hbar^2} \quad (\rightarrow j)$$

$$E_{\text{exp.}} = -108,8 \text{ eV} + \frac{5}{8} \cdot 2 \cdot 27,2 \text{ eV} = -74,8 \text{ eV}$$

$$E_{\text{exp.}}^{\text{exp.}} = -78,6 \text{ eV} \quad \text{Απόκλιση: 5\%}$$

$$H = \left[\frac{\hbar^2 \nabla_1^2}{2m} + \frac{\hbar^2 \nabla_2^2}{2m} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{Z \cdot e^2}{r_1} + \frac{Z \cdot e^2}{r_2} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} \right]$$

Έχει την ίδια μέση ενέργεια με πριν αλλά για $z = \bar{z}$
 $\hbar = m = e = 1$

$$\langle H \rangle = -\bar{z}^2 + \frac{5}{8} \bar{z} + 2(\bar{z} - 2) \cdot \bar{z} = -\bar{z}^2 + \frac{5}{8} \bar{z} + 2\bar{z}^2 - 4\bar{z}$$

$$\frac{d\langle H(\bar{z}) \rangle}{d\bar{z}} = 0 \Rightarrow -2\bar{z} + \frac{5}{8} + 4\bar{z} - 4 = 0 \Rightarrow 2\bar{z} = \frac{27}{8} \Rightarrow \bar{z} = \frac{27}{16}$$

$$E_{\text{min}} = -\bar{z}_{\text{min}}^2 = -77,5 \text{ eV} \quad \text{Απόκλιση: 14\%}$$

ΔΙΑΒΑΣΜΑ ΚΕΦ. 71 ΤΡΑΧΑΝΑΣ

ΟΝΙΚΗ ΣΤΡΟΦΟΡΜΗ ΑΠΟ ΚΕΦ. 70