Modelo simple de la molécula de hidrógeno, H_2

Dos núcleos con carga +e (c/u) a la distancia 2x

Dos electrones formando una distribución de carga uniforme, de forma esférica de radio r_0.

$$\frac{4\pi \mathbf{r}_0^3}{3}\rho = -2\mathbf{e} \qquad \therefore \qquad \boldsymbol{\rho} = \frac{-3\mathbf{e}}{2\pi \mathbf{r}_0^3}$$

$$\mathbf{E} = \frac{-2\mathbf{e}}{4\pi\varepsilon_0}\frac{\mathbf{x}}{\mathbf{r}_0^3}$$

$$\mathbf{F} = \frac{-2\mathbf{e}^2}{4\pi\varepsilon_0}\frac{\mathbf{x}}{\mathbf{r}_0^3} + \frac{\mathbf{e}^2}{4\pi\varepsilon_0(2\mathbf{x})^2}$$

$$\frac{\mathbf{dF}}{\mathbf{dx}} = \frac{-2\mathbf{e}^2}{4\pi\varepsilon_0\mathbf{r}_0^3} - \frac{2\mathbf{e}^2}{4\pi\varepsilon_0 \cdot 4\mathbf{x}^3} < 0$$

$$\mathbf{F}(\mathbf{x}_0) = 0 \qquad \Rightarrow \qquad \frac{2\,\mathbf{x}_0}{\mathbf{r}_0^3} = \frac{1}{4\,\mathbf{x}_0^2}$$

$$\mathbf{x}_0^3 = \frac{\mathbf{r}_0^3}{8} \qquad \Rightarrow \qquad \mathbf{x}_0 = \frac{\mathbf{r}_0}{2}$$

Energía electrostática de una distribución discreta de cargas

$q_1, q_2, q_3, \quad . \quad . \quad . \quad . \quad q_N$

Primera carga : $\mathbf{W}_1 = 0$

Segunda carga : $$\mathbf{W}_2 = \mathbf{q}_2 \mathbf{V}_2(\vec{\mathbf{r}}_2) = \frac{1}{4\pi\varepsilon_0} \frac{\mathbf{q}_1 \mathbf{q}_2}{|\vec{\mathbf{r}}_2 - \vec{\mathbf{r}}_1|}$$

Tercera carga : $$\mathbf{W}_3 = \mathbf{q}_3 \mathbf{V}_3(\vec{\mathbf{r}}_3) = \frac{1}{4\pi\varepsilon_0} \left[\frac{\mathbf{q}_1 \mathbf{q}_3}{|\vec{\mathbf{r}}_3 - \vec{\mathbf{r}}_1|} + \frac{\mathbf{q}_2 \mathbf{q}_3}{|\vec{\mathbf{r}}_3 - \vec{\mathbf{r}}_2|} \right]$$

j - ésima carga : $$\mathbf{W}_\mathbf{j} = \mathbf{q}_\mathbf{j} \mathbf{V}_\mathbf{j}(\vec{\mathbf{r}}_\mathbf{j}) = \frac{\mathbf{q}_\mathbf{j}}{4\pi\varepsilon_0} \sum_{\mathbf{i}=1}^{\mathbf{j}-1} \frac{\mathbf{q}_\mathbf{i}}{|\vec{\mathbf{r}}_\mathbf{j} - \vec{\mathbf{r}}_\mathbf{i}|}$$

$$\text{j-ésima carga:} \qquad \mathbf{W_j = q_j V_j(\vec{r}_j) = \frac{q_j}{4\pi\varepsilon_0} \sum_{i=1}^{j-1} \frac{q_i}{|\vec{r}_j - \vec{r}_i|}}$$

$$\text{Energía total:} \qquad \mathbf{W = \sum_{j=1}^{N} W_j = \frac{1}{4\pi\varepsilon_0} \sum_{j=1}^{N} \sum_{i<j}^{N} \frac{q_i q_j}{|\vec{r}_j - \vec{r}_i|}}$$

Para evitar i < j:

$$\text{Energía total:} \qquad \mathbf{W = \frac{1}{2} \frac{1}{4\pi\varepsilon_0} \sum_{j=1}^{N} \sum_{i\neq j}^{N} \frac{q_i q_j}{|\vec{r}_j - \vec{r}_i|}}$$

Ejemplo: Para N = 3

$$\mathbf{W = \frac{1}{2} \frac{1}{4\pi\varepsilon_0} \sum_{j=1}^{N} q_j \sum_{i\neq j}^{N} \frac{q_i}{|\vec{r}_j - \vec{r}_i|} = \frac{1}{2} \sum_{j=1}^{N} q_j V_j}$$

Otra forma de demostrarlo: Supong. $q_i' = xq_i$ q_i = carga final $0 \leq x \leq 1$

$$\mathbf{dW = \sum_{i=1}^{N} V_i^{'} dq_i^{'} = \sum_{i=1}^{N} V_i^{'} q_i dx}$$

$V_i' = xV_i$

$$\mathbf{dW = \sum_{i=1}^{N} V_i q_i x dx}$$

$$\mathbf{W = \sum_{i=1}^{N} V_i q_i \int_0^1 x dx} = \frac{1}{2} \mathbf{\sum_{i=1}^{N} V_i q_i}$$

Distribución continua de carga: $\sum \;\longrightarrow\; \int$

$$W = \frac{1}{2}\int_V V(\vec{r})\,\rho(\vec{r})\,d^3r$$

$$W = \frac{1}{2}\frac{1}{4\pi\varepsilon_0}\int_V \rho(\vec{r})\,d^3r \int_V \frac{\rho(\vec{r}')\,d^3r'}{|\vec{r}-\vec{r}'|} \qquad = \frac{1}{2}\frac{1}{4\pi\varepsilon_0}\int\int \frac{\rho(\vec{r})\,\rho(\vec{r}')\,d^3r\,d^3r'}{|\vec{r}-\vec{r}'|}$$

pero $\rho(\vec{r}) = \varepsilon_0 \nabla \cdot \vec{\mathbf{E}}$ (ley de Gauss)

$$W = \frac{\varepsilon_0}{2}\int_V \nabla \cdot \vec{E}(\vec{r})\,V(\vec{r})\,d^3r$$

$$\text{Identidad}: \quad \nabla\cdot\left(V\vec{E}\right) = V\nabla\cdot\vec{E} + \vec{E}\cdot\nabla V$$

$$W = \frac{\varepsilon_0}{2}\int_V \nabla\cdot\left(V\vec{E}\right) d^3r - \frac{\varepsilon_0}{2}\int_V \vec{E}\cdot\nabla V d^3r$$

$$\text{Aplicar teorema de Gauss}: \quad \int_V \nabla\cdot\left(V\vec{E}\right) d^3r = \int_S V\vec{E}\cdot d\vec{S}$$

$$W = \frac{\varepsilon_0}{2}\int_S V\vec{E}\cdot d\vec{S} + \frac{\varepsilon_0}{2}\int_V \left|\vec{E}\right|^2 d^3r \quad = \frac{\varepsilon_0}{2}\int_V \left|\vec{E}\right|^2 d^3r$$

$$r \to \infty \qquad 0$$

$$\text{Densidad de energía} = \frac{\varepsilon_0\left|\vec{E}\right|^2}{2}$$

Ejemplo: Radio clásico del electrón

Energía = mc^2 = energía electrostática

1.- Modelo: Carga eléctrica distribuída en la superficie de la esfera

$$W = \frac{\varepsilon_0}{2}\int_V \left|\vec{E}\right|^2 d^3r = \frac{\varepsilon_0}{2}4\pi\int_{r_1}^{\infty} r^2 dr \cdot \left(\frac{e}{4\pi\varepsilon_0 r^2}\right)^2$$

$$W = \frac{4\pi\varepsilon_0 e^2}{2(4\pi\varepsilon_0)^2}\int_{r_1}^{\infty}\frac{dr}{r^2} = \frac{e^2}{2\cdot 4\pi\varepsilon_0}\cdot\frac{1}{r_1} \quad = mc^2$$

$$r_1 = \frac{1}{2}\cdot\frac{e^2}{4\pi\varepsilon_0 mc^2}$$

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$$e = 1.6 \cdot 10^{-19}\ \text{C}, \qquad m = 0.9 \cdot 10^{-30}\ \text{Kg}, \qquad \frac{1}{4\pi\varepsilon_0} = 9 \cdot 10^{9}\ \text{Nm}^2/\text{C}^2,$$

$$c = 3 \cdot 10^{8}\ \text{m/seg}$$

$$r_1 = \frac{1}{2} \cdot 2.84 \cdot 10^{-15}\ \text{m} = 1.42 \cdot 10^{-15}\ \text{m}$$

2.- Modelo: Carga eléctrica distribuída en el volumen de una esfera de radio r_2

$$E = \frac{-er}{4\pi\varepsilon_0 r_2^3} \qquad r \le r_2$$

$$W = \frac{\varepsilon_0}{2} 4\pi \int_0^{r_2} \frac{r^2 dr \cdot e^2 r^2}{(4\pi\varepsilon_0)^2 r_2^6} + \frac{\varepsilon_0}{2} 4\pi \int_{r_2}^{\infty} r^2 dr \cdot \left(\frac{e}{4\pi\varepsilon_0 r^2} \right)^2$$

$$W = \frac{1}{2} \cdot \frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{r_2^6} \int_0^{r_2} r^4 dr + \frac{1}{2} \cdot \frac{e^2}{4\pi\varepsilon_0} \int_{r_2}^{\infty} \frac{dr}{r^2}$$

$$W = \frac{1}{2} \cdot \frac{e^2}{4\pi\varepsilon_0 r_2} \cdot \frac{6}{5} = \frac{3}{5} \cdot \frac{e^2}{4\pi\varepsilon_0 r_2} \quad = mc^2$$

$$r_2 = \frac{3}{5} \cdot \frac{e^2}{4\pi\varepsilon_0 mc^2} \qquad\qquad \frac{r_2}{r_1} = \frac{3/5}{1/2} = \frac{6}{5} = 1.2$$