PROBLEMA (9) DO CAP. 11

ÁTOMO DE HIDROGÉNIO

$$\varphi_\alpha(r) = \begin{cases} C\left(1-\frac{r}{\alpha}\right) & r \le \alpha \\ 0 & r > \alpha \end{cases}$$

$$\vec{\nabla}\varphi_\alpha = \frac{d\varphi_\alpha}{dr}\hat{r}$$

a) $$\langle \varphi_\alpha | T | \varphi_\alpha \rangle = \int_0^\infty \varphi_\alpha^*(r)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\varphi_\alpha(r)\, 4\pi r^2 dr$$

$$= -\frac{\hbar^2}{2m}\int_0^\infty \left[\underbrace{\vec{\nabla}\cdot\left[\varphi_\alpha(r)\left(\vec{\nabla}\varphi_\alpha(r)\right)\right]}_{\varphi_\alpha(r)\nabla^2\varphi_\alpha(r) + (\vec{\nabla}\varphi_\alpha)\cdot(\vec{\nabla}\varphi_\alpha)} - |\vec{\nabla}\varphi_\alpha(r)|^2\right] 4\pi r^2 dr$$

1º TERMO: $$\int \vec{\nabla}\cdot\left[\varphi_\alpha \vec{\nabla}\varphi_\alpha\right] d^3r$$

$$= \int_{S(\infty)} \left(\varphi_\alpha \vec{\nabla}\varphi_\alpha\right)\cdot d\vec{S} = 0$$

$$\langle T \rangle = \frac{\hbar^2}{2m}\int_0^\infty |\vec{\nabla}\varphi_\alpha(r)|^2\, 4\pi r^2 dr$$

$$= \frac{\hbar^2}{2m}\int_0^\alpha \left|-\frac{C}{\alpha}\right|^2 4\pi r^2 dr = \frac{C^2\hbar^2}{2m\cancel{\alpha^2}}\, 4\pi\, \frac{\alpha^{\cancel{3}}}{3}$$

$$\langle T \rangle = \frac{2\pi C^2\hbar^2\alpha}{3m}$$

$$\langle V \rangle = \int_0^\alpha C^2\left(1-\frac{r}{\alpha}\right)^2\left(\frac{-e^2}{\cancel{r}}\right) 4\pi r^{\cancel{2}} dr$$

$$= -4\pi e^2 C^2 \int_0^\alpha \left(1 - \frac{2r}{\alpha} + \frac{r^2}{\alpha^2}\right) r\, dr$$

$$= -4\pi e^2 c^2 \left(\frac{\alpha^2}{2} - \frac{2}{3}\alpha^2 + \frac{\alpha^2}{4} \right)$$

$$= -\cancel{4}\pi e^2 c^2 \alpha^2 \left(\frac{6-8+3}{\cancel{12}\,3} \right)$$

$$= -\frac{\pi}{3} e^2 c^2 \alpha^2$$

$$\frac{\langle H \rangle}{c^2} = \frac{2\pi}{3}\frac{\hbar^2 \alpha}{m} - \frac{\pi}{3} e^2 \alpha^2 = \frac{\pi}{3}\left[\frac{2\hbar^2 \alpha}{m} - e^2 \alpha^2 \right]$$

NORMALIZAÇÃO:

$$1 = \int |\varphi_\alpha(r)|^2 d^3 r = 4\pi \int_0^\alpha c^2 \underbrace{\left(1 - \frac{r}{\alpha}\right)^2}_{\left(1 - \frac{2r}{\alpha} + \frac{r^2}{\alpha^2}\right)} r^2 dr$$

$$= 4\pi c^2 \left[\frac{\alpha^3}{3} - \frac{\alpha^3}{2} + \frac{\alpha^3}{5} \right]$$

$$= 4\pi c^2 \alpha^3 \left[\frac{10 - 15 + 6}{30} \right] = \frac{2\pi}{15} c^2 \alpha^3 = 1$$

$$c^2 = \frac{15}{2\pi \alpha^3}$$

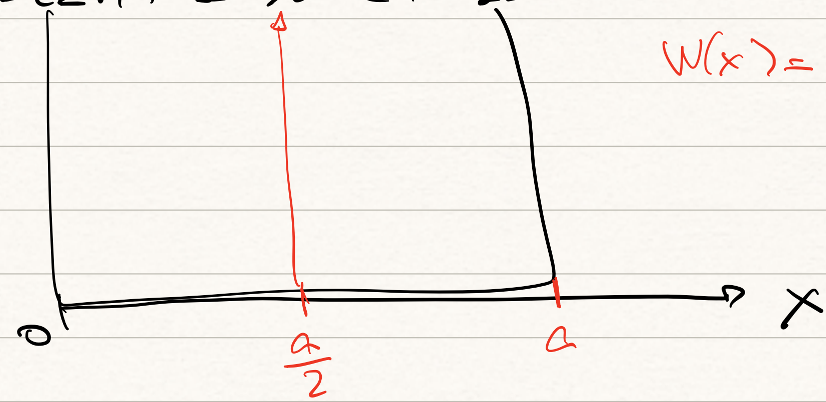
$$\langle H \rangle = \frac{\cancel{\pi}}{\cancel{3}} \frac{\cancel{15}\,5}{2\cancel{\pi}\alpha^3} \left[\frac{2\hbar^2 \alpha}{m} - e^2 \alpha^2 \right] = \frac{5}{2}\left[\frac{2\hbar^2}{m\alpha^2} - \frac{e^2}{\alpha} \right]$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = \frac{5}{2}\left[-\frac{4\hbar^2}{m\alpha^3} + \frac{e^2}{\alpha^2} \right] = 0 \Rightarrow \alpha_0 = \frac{4\hbar^2}{me^2} = 4a_0$$

$$E_0 = \frac{5}{2}\left[\cancel{\frac{2\hbar^2}{m}} \frac{m^2 e^4}{8\,\cancel{16}\,\hbar^4} - \frac{me^4}{4\hbar^2} \right] = \frac{5}{2}\left(\frac{1}{8} - \frac{1}{4} \right)\frac{me^4}{\hbar^2} = -\frac{5}{16}\frac{me^4}{\hbar^2} = -\frac{5}{8} \times (13{,}6\,\text{eV})$$

$0{,}6$

PROBLEMA 1 DO CAP. 11



$W(x) = aW_0\,\delta(x - \frac{a}{2})$

$0 < x < \frac{a}{2}$: $\psi_I(x) = A \sin kx \qquad k = \frac{\sqrt{2mE}}{\hbar}$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + W(x)$$

SE $0 < x < \frac{a}{2}$ OU $\frac{a}{2} < x < a$

$$H\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \psi(x) = A\cos kx + B\sin kx$$

$\frac{a}{2} < x < a$: $\psi_{II}(x) = B\sin kx + C\cos kx$

$$\psi_{II}(a) = 0 \Rightarrow B\sin ka + C\cos ka = 0 \quad (1)$$

$$\psi_I(x = \tfrac{a}{2}) = \psi_{II}(x = \tfrac{a}{2})$$

$$\Rightarrow A\sin\frac{ka}{2} = B\sin\frac{ka}{2} + C\cos\frac{ka}{2} \quad (2)$$

$$\int_{+a/2+\varepsilon}^{\frac{a}{2}-\varepsilon}\left[-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + W_0 a\,\delta(x - \tfrac{a}{2})\psi - E\psi\right]dx = 0$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[\psi'(a/2^+) - \psi'(a/2^-)\right] + W_0 a\,\psi(a/2) = 0 \quad (3)$$