PROBLEMES T2

2.1 Electró en estat fonamental $(n=1)$ caixa de potencial 1D de $\ell = 10^{-10}$ m i compareu-la amb $E_2 - E_1$.

$$E_n = \frac{n^2 h^2}{8ma^2} \rightarrow E_1 = \frac{h^2}{8m_e \ell^2} = \frac{(6{,}626 \cdot 10^{-34}\ J \cdot s)^2}{8 \cdot 9{,}109 \cdot 10^{-31}\ kg \cdot (10^{-10}\ m)^2} =$$

$$\frac{(6{,}626)^2}{8\ 9{,}101 \cdot 100} \cdot \frac{10^{-68}}{10^{-31}\ 10^{-20}} = 6{,}03 \cdot 10^{-3} \cdot 10^{-17} = \underline{6{,}02 \cdot 10^{-18}\ J}$$

3x

$$E_2 = 4E_1 \rightarrow E_2 - E_1 = 4E_1 - E_1 = 3E_1 = 1{,}807 \cdot 10^{-17}\ J = \underline{18 \cdot 10^{-18}\ J}$$

b) Ecin clàssica pilota $m = 50\,g$ $v = 20\,m/s$ pista $L = 5\,m$ n? ¿caixa potencial?

$$E_{cin} = T = \frac{1}{2} m v^2 = \frac{0{,}05\,kg}{2} \left(20 \frac{m}{s}\right)^2 = 10\ J$$

$$n = \sqrt{\frac{E_n \cdot 8m \cdot a^2}{h^2}} = \sqrt{\frac{10\,J \cdot 8 \cdot 50 \cdot 10^{-3}\,kg \cdot 5\,m^2}{(6{,}626 \cdot 10^{-34}\ J \cdot s)^2}} = \underline{1{,}5 \cdot 10^{34}}$$

$$\Delta E_{E_n \to E_{n+1}} = \frac{E_{n+1} - E_n}{E_n}$$

$E_{n+1} = ?$

$$\Delta E = \frac{E_{n+1} - 10}{10} = \frac{\frac{(n+1)^2 \cancel{h^2}}{\cancel{8ma^2}} - \frac{n^2 \cancel{h^2}}{\cancel{8ma^2}}}{\frac{n^2 \cancel{h^2}}{\cancel{8ma^2}}} = \frac{(n+1)^2 - n^2}{n^2} =$$

$$\Delta E = \frac{-2{,}277 \cdot 10^{68}}{2{,}277 \cdot 10^{68}} = 0\ !! \rightarrow \underline{1{,}3 \cdot 10^{-34}}$$

✓

2.8 $t=0$ ψ

osc. harmònic 1D

2.2 $\hat{H} = \left(-\frac{\hbar^2}{2m}\right)\left(\frac{d^2}{dx^2} - \alpha^2 x^2\right)$ on $\alpha = \sqrt{km}/\hbar$

a) Normalitzar $\Phi(x) = x e^{-\alpha x^2/2}$

$\langle \Phi | \Phi \rangle = 1 \rightarrow \langle N\Phi | N\Phi \rangle = \int_{-\infty}^{+\infty} N\Phi^* N\Phi \, dx$

$= N^2 \int_{-\infty}^{+\infty} x^2 e^{-\alpha x^2} dx = N^2 \cdot 2 \int_0^{\infty} x^2 e^{-\alpha x^2} dx = 2N^2 \cdot \frac{1}{2^2}\sqrt{\frac{\pi}{\alpha^3}}$ ($2n \to n=1$)

$= 2N^2 \frac{1}{4}\sqrt{\frac{\pi}{\alpha^3}} = 1$; $N = \sqrt{\frac{2\alpha^{3/2}}{\pi^{1/2}}} = \left(\frac{2^2 \alpha^3}{\pi}\right)^{1/4} = \left(\frac{4\alpha^3}{\pi}\right)^{1/4}$ ✓

b) $\Phi(x)$ és pròpia de $\hat{H}$?

$\hat{H}\Phi = \left(-\frac{\hbar^2}{2m}\right)\cdot\left(\frac{4\alpha^3}{\pi}\right)^{1/4}\left(\frac{d^2}{dx^2} - \alpha^2 x^2\right)\left(x e^{-\alpha x^2/2}\right)$

$\hat{H}\Phi = \underbrace{-\frac{\hbar^2}{2m}\left(\frac{4\alpha^3}{\pi}\right)^{1/4}}_{a'}\left[\frac{d}{dx}\left(e^{-\alpha x^2/2} + x\left(-\frac{2\alpha}{2}x\right)e^{-\alpha x^2/2}\right) - \alpha^2 x^3 e^{-\alpha x^2/2}\right]$

$\hat{H}\Phi = a'\left[\underbrace{-\alpha x e^{-\alpha x^2/2} - \alpha x e^{-\alpha x^2/2} - \alpha x e^{-\alpha x^2/2}}_{3} \cancel{- \alpha x^2(-\alpha x)e^{-\alpha x^2/2} - \alpha^2 x^3 e^{-\alpha x^2/2}}\right]$

$\hat{H}\Phi = a'\left[-3\alpha x e^{-\alpha x^2/2}\right] = +\frac{\hbar^2}{2m}\left(\frac{4\alpha^3}{\pi}\right)^{1/4} \cdot 3\alpha x e^{-\alpha x^2/2}$

$\hat{H}\Phi = \frac{\hbar^2}{2m} 3\alpha \underbrace{\left(\frac{4\alpha^3}{\pi}\right)^{1/4} x e^{-\alpha x^2/2}}_{\Phi} = \boxed{\frac{3\hbar^2\alpha}{2m}}\Phi$ $\boxed{E = \frac{3\hbar\alpha}{2m}}$

c) $\langle x \rangle_{\Phi(x)}$ valor esperat $= \langle \psi | \hat{A} \psi \rangle$

$\langle x \rangle_{\Phi(x)} = \langle \Phi | x \Phi \rangle = \int_{-\infty}^{+\infty} x^3 e^{-\alpha x^2} dx = \cancel{2\int_0^{\infty} x^3 e^{-\alpha x^2} dx}$

↑

Funció senar $f(-x) = -f(x)$

No és de quadrat integrable $\rightarrow \langle x \rangle_{\Phi(x)} = 0$ //

✓

Φ osc. harm 1D en $t=0$ $\rightarrow$ $\Psi(x;0) = \frac{1}{\sqrt{5}}\Phi_0(x) + \frac{1}{\sqrt{2}}\Phi_2(x) + c_3\Phi_3(x)$

on $\{\Phi_0, \Phi_1 \ldots\}$ f. pròpies normalitzades $\hat{H}$:

$E_n = \left(n+\frac{1}{2}\right)h\nu \quad n = 0, 1, 2 \ldots$

a) Valor c_3 ? $\mathbb{R}$; >0 i que $\Psi(x;0) \Rightarrow$ normalitzada

$N=1$; $N = \frac{1}{\sqrt{\sum |c_i|^2}} = 1$; $\sqrt{\sum |c_i|^2} = 1$; $\sqrt{\frac{1}{5}+\frac{1}{2}+c_3^2} = 1$

$\frac{1}{5}+\frac{1}{2}+c_3^2 = 1$; $c_3^2 = \frac{1}{1} - \frac{1}{5} - \frac{1}{2} = \frac{3}{10}$ $\rightarrow$ $\boxed{c_3 = \sqrt{3/10}}$ ✓

b) En $t=0$

Podem obtenir $\rightarrow$

$E_0 = 1/2\, h\nu$ $\quad P(\hat{H}\rightarrow E_0) = 1/5$ ✓

$E_2 = 5/2\, h\nu$ $\quad P(\hat{H}\rightarrow E_2) = 1/2$ ✓

$E_3 = 7/2\, h\nu$ $\quad P(\hat{H}\rightarrow E_3) = 3/10$ ✓

Valor esp ?

~~$\langle H \rangle_\psi = \Sigma$~~ $\langle H \rangle_\psi = \sum |c_i|^2 a_i = \frac{1}{5}\cdot\frac{1}{2}h\nu + \frac{1}{2}\cdot\frac{5}{2}h\nu + \frac{3}{10}\cdot\frac{7}{2}h\nu$

$\langle H \rangle_\psi = h\nu\left(\frac{1}{10}+\frac{5}{4}+\frac{21}{20}\right) = \frac{12}{5}h\nu$ ✓

c) Ψ ? en $t>0$? si el sistema evoluciona lliurement ?

Solució en variables separables de eq. Schrodinger depenent del temps per a estats estacionaris i sistemes conservatius:

$\Psi(x_1 \ldots x_n; t) = \Phi(x_1, \ldots x_n)\cdot e^{-iEt/\hbar}$

$\Psi(x;t) = \Psi(x;0)\, e^{-iEt/\hbar} = \frac{1}{\sqrt{5}} e^{-iE_0t/\hbar} + \frac{1}{\sqrt{2}} e^{-iE_2t/\hbar}\Phi_2(x) + \frac{\sqrt{3}}{\sqrt{10}} e^{-iE_3t/\hbar}\Phi_3(x)$

Valors esperats ? Prob ? Valors propis són iguals

Una vegada mesurem torna a obtenir VP. amb seguretat!!

d) $\Phi(x;t)$ si $E = 5/2\, h\nu$ $\rightarrow$ $\Psi(x;t) = \frac{1}{\sqrt{2}}\Phi_2(x)\, e^{-iE_2t/\hbar}$

Valors que podem obtenir $E_2 = 5/2\, h\nu$ $\quad P = 1$

$\langle H \rangle_\psi = h\nu\, \frac{5}{2}\cdot 1 = 5/2\, h\nu$

~~2.3~~ ~~Mec. clàssica m, 1D $E_T = \frac{1}{2} h\nu$~~

2.5 Δx i Δp to osc. harmònic 1D : $\Phi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$

$$\Delta_{\Phi_0} x = \sqrt{\langle x^2 \rangle_{\Phi_0} - \langle x \rangle_{\Phi_0}^2}$$

$$\langle x^2 \rangle_{\Phi_0} = \langle \Phi_0 | x^2 \Phi_0 \rangle = \int_{-\infty}^{+\infty} (a/\pi)^{2/4} x^2 e^{-\alpha x^2} dx = \left(\frac{a}{\pi}\right)^{1/4} 2 \int_0^{\infty} x^2 e^{-\alpha x^2}$$

$$\langle x^2 \rangle_{\Phi_0} = \left(\frac{\alpha}{\pi}\right)^{1/2} 2 \cdot \frac{1 \cdot 1}{2^2} \sqrt{\frac{\pi}{\alpha^3}} = \frac{\alpha^{1/2}}{\alpha^{3/2}} \cdot \frac{\cancel{\pi^{1/2}}}{\cancel{\pi^{1/2}}} \cdot \frac{1}{2} = 2\alpha^{(1/2 - 3/2)} \cancel{\pi^{(2/4 - 1/4)}}$$

$$\langle x^2 \rangle_{\Phi_0} = \cancel{\frac{2 (\pi)^{1/4}}{(\alpha^5)^{1/4}}} = \cancel{2\left(\frac{\pi}{\alpha^5}\right)^{1/4}} \qquad \langle x^2 \rangle_{\Phi_0} = 2^{-1}\alpha^{-1} \Rightarrow \frac{1}{2\alpha}$$

$$\langle x \rangle_{\Phi_0}^2 = (\langle \Phi_0 | x \Phi_0 \rangle)^2 = \int_{-\infty}^{+\infty} N x e^{-\alpha x^2} dx = 0$$

$$\Delta_{\Phi_0} x = \sqrt{\frac{1}{2\alpha} - 0} = 1/\sqrt{2\alpha} \qquad \boxed{\Delta_{\Phi_0} x = \frac{1}{\sqrt{2\alpha}}}$$

$$\Delta_{\Phi_0} p = \sqrt{\langle p^2 \rangle_{\Phi_0} - \underbrace{(\langle p \rangle_{\Phi_0})^2}_{=0}}$$

$$\langle p^2 \rangle_{\Phi_0} = \langle \Phi_0 | \hat{p}_x^2 \Phi_0 \rangle = \left(\frac{\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{+\infty} e^{-\alpha x^2/2} p_x \left(-i\hbar \cancel{f} - \alpha x\right) e^{-\alpha x^2/2} dx$$

$$= \left(\frac{\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{+\infty} e^{-\alpha x^2/2} \hat{p}_x \left(+ i\hbar \alpha x e^{-\alpha x^2/2}\right) dx \Big\} =$$

$$\left[(-i\hbar^2)\right] \alpha \left(e^{-ax^2/2} + x(-\alpha x) e^{-\alpha x^2/2}\right) dx$$

$$= -\left(\frac{\alpha}{\pi}\right)^{1/2} (i\hbar)^2 \alpha \int_{-\infty}^{+\infty} \left(e^{-\alpha x^2/2}\right)\left(e^{-\alpha x^2/2} - \alpha x^2 e^{-\alpha x^2/2}\right) dx$$

$$= -\left(\frac{\alpha}{\pi}\right)^{1/2} \alpha (i\hbar)^2 \int_{-\infty}^{+\infty} e^{-\alpha x^2} - \alpha x^2 e^{-\alpha x^2} dx$$

$$= -\frac{\alpha}{\pi}$$

.....

osc. har. 3D k_x i k_y i k_z.

$$V(x,y,z) = \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2 + \frac{1}{2}k_z z^2$$ isòtrop si $k_x = k_y = k_z = k$

a) E 1° i 2° nivell 1° nivell $= E_{000}$ i $E_{100} = E_{010} = E_{001}$

$$E_{000} = h\nu_x\left(v_0 + \frac{1}{2}\right) + h\nu_y\left(v_0 + \frac{1}{2}\right) + h\nu_z\left(v_0 + \frac{1}{2}\right)$$ si $v=0$

$$E_{000} = \frac{3}{2}h\nu \quad \boxed{\nu_x = \nu_y = \nu_z} \qquad d=1$$

$$E_{100} = h\nu\left(1 + \frac{1}{2}\right) + 1\,h\nu = \boxed{5/2\, h\nu} \qquad d=3 \quad = E_{010} = E_{001}$$

b) Ψ? 1° nivell excitat?

$$\Psi_{100}(x,y,z) = \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x\, e^{-\alpha x^2/2} + \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha y^2/2} + \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha z^2/2}$$

Anar variant $v=1 \to y$ i $\to z$.

2.7 Àtom H (estat fonamental) $\mu \simeq m_e$.

$$E_n = -\frac{Z}{2n^2}\frac{e^2}{4\pi\varepsilon_0 a} = -\frac{Z}{2n^2}\text{ u.a} \qquad \Phi_{1s} = \left(\frac{Z^3}{\pi a^3}\right)^{1/2} e^{-Zr/a}$$

a) $|\Psi|^2 (a_0, \theta, \varphi)$? $Z=1$

$$|\Phi_{1s}|^2 = \left|\left(\frac{Z^3}{\pi a^3}\right)^{1/2} e^{-Z r/a}\right|^2 = \left(\frac{1}{\pi a_0^3}\left(e^{-a_0/a_0}\right)^2\right)$$

$$a = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2} \rightarrow |\Phi_{1s}|^2 = \left(\frac{1}{\pi a_0^3}e^{-\frac{a_0}{a_0}}\right)^2 = \frac{1}{\pi a_0^3}e^{-2a_0/a_0} =$$

$$|\Phi_{1s}|^2 = \frac{1}{a_0^3\pi}e^{-2} = 2{,}908\cdot 10^{29}\ m^{-3}$$

b) Major $|\Phi|^2$ de trobar e^-?

$|\Phi|^2_{màx}$ al centre $r=0$.

$$|\Phi_{1s}(0,\theta,\varphi)|^2 = \left(\left(\frac{1}{\pi a_0^3}\right)^{1/2} \underset{1}{e^{-Z\cdot 0}}\right)^2 = \frac{1}{\pi a_0^3} = 2{,}15\cdot 10^{30}\ m^{-3}$$

UA

c) $P(r < 2\cancel{a_0}) = 1 - P(r \geq 2\cancel{a_0})$

$$P(r \geq 2\cancel{a_0}) = \int_{2a_0}^{\infty}\int_0^{\pi}\int_0^{2\pi} |\Phi_{1s}|^2 \, r^2 \sin\theta \, dr \, d\theta \, d\varphi$$

$$P(r \geq 2a_0) = \int_{2a_0}^{\infty} \frac{1}{\pi \cancel{a_0^3}} e^{-2r/a_0} r^2 \, dr \cdot 4\pi$$

$$= \frac{4\cancel{\pi}}{\cancel{\pi a_0^3}}\int_{2a_0}^{\infty} r^2 e^{-2r/a_0} dr = \cancel{\frac{4 \cdot 2!}{\left(\frac{2}{a_0}\right)^3 a_0^3} e^{-\frac{2}{a_0}\cdot 2a_0}\left(1 + \frac{2\cdot 2a_0}{a_0} + \frac{4 a_0^2 \cdot 4}{a_0^2 \cdot 2!}\right)}$$

$$= \cancel{\frac{4 \cdot 2}{\frac{8 \cdot a_0^3}{a_0^3}} e^{-4}(1 + 4 + 8)} = 13e^{-4} = 0{,}76 \checkmark\checkmark$$

$$= 4\cancel{\pi}\int_2^{\infty} \frac{1}{\cancel{\pi}} e^{-2r} r^2 \, dr = 4\int_2^{\infty} r^2 e^{-2r} dr$$

$$= 4 \cdot \frac{2!}{2^3} e^{-2\cdot 2}\left(1 + 2\cdot 2 + \frac{4\cdot 4}{2!}\right) = \frac{\cancel{8}}{\cancel{8}} e^{-4}(1 + 4 + 8) = 13\cdot e^{-4}$$

$13e^{-4} = 0{,}24$ $\quad P = 1 - 0{,}24 = \underline{0{,}76}$ ✓ $\quad$ c) $0{,}76$ ✓

d) P (r nucli prohibida)

$E < V$

$$-\frac{Z^2 e^2}{2n^2 \cancel{4\pi\varepsilon_0}} < -\frac{Z e^2}{\cancel{4\pi\varepsilon_0} r} \rightarrow -\frac{Z}{2n^2} < -\frac{1}{r}$$

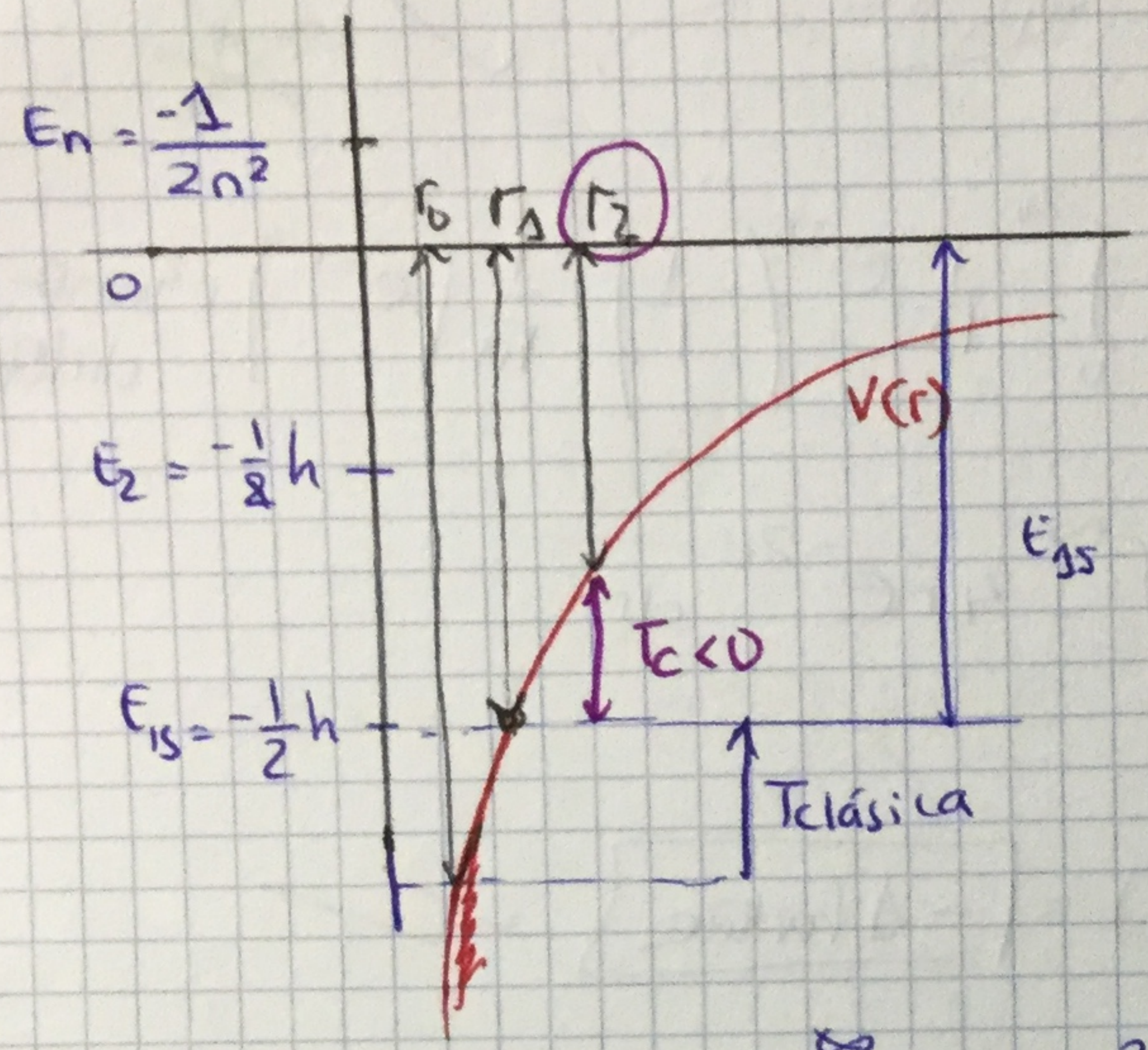
$$\frac{Z}{2n^2} > \frac{1}{r} \; ; \; r > \frac{2n^2}{Z} \rightarrow r > \frac{2\cdot 1}{1} \rightarrow \boxed{r > 2}$$

Abans hem calculat $\boxed{P(r \geq 2) = 0{,}24}$ ✓

$P(r < 2) = 0{,}76$ (apartat c)

2.7(II)

d) P (d nuclei prohibida clásicament) ?



$V(r_1) = E_1 \rightarrow T_c = 0$

En $V(r_2)$

$-\frac{1}{r} = -\frac{1}{2}$ $\quad r_1 = 2ua = 2a_0$

$$P(r>2a_0) = \int_2^{\infty} \left(\frac{1}{\cancel{\pi}} e^{-2r}\right) r^2 \cancel{\sin\theta}\, 4\cancel{\pi}\, dr$$

$$4\int_2^{\infty} r^2 e^{-2r}\, dr = \frac{2!}{2^3} e^{-2\cdot 2}\left(1 + 2\cdot 2 + \frac{4\,4}{2}\right) \cdots \cancel{2^2}$$

$$= \frac{4}{4} e^{-4}\left(1+4+8\right) = \frac{13}{\cancel{4}} e^{-4}\, ua$$

e) p_x , E_p , T esperados!! No tengo lim simétricos/ no puedo hacer par/imp/ $r = \sqrt{x^2+y^2+z^2}$

$$\langle p_x \rangle = \langle \phi_{1S} | \hat{p_x}\, \phi_{1S} \rangle = \int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} \frac{1}{\sqrt{\pi}} e^{-r}\left(-i\frac{d}{dx}\right)\underbrace{\frac{1}{\sqrt{\pi}} e^{-r}}_{\phi_{1S}} \underbrace{r^2 \sin\theta\, dr\, d\theta\, d\varphi}_{dV} =$$

Mezcla polares / cartesianas,
sólo estamos integrando (r) 0 - ∞ // si hacemos cartesianas:

$$= \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-r_{cart}}\left(-i\, e^{-\sqrt{x^2+y^2+z^2}}\left(-\frac{2x+0+0}{2\sqrt{x^2+y^2+z^2}}\right)\right) dx\,dy\,dz$$

límites simétricos!
= FUNCIÓN IMPAR $(-x)$ $\quad f(-x) = -f(x)$ $\quad \langle p_x \rangle = 0$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty} +i\, e^{-2\sqrt{x^2+y^2+z^2}} \cdot \frac{(2x)}{2\sqrt{x^2+y^2+z^2}}\, dx\,dy\,dz = \underline{\underline{0}}$$

Previsible? Valor esperado (promedio de medidas) mido v(electrón)

si $\langle p_x \rangle > 0$ e^- se mueve hacia la derecha de x (se va alejando)

Pero como tenemos estado ligado e^- al un núcleo si mido

v salen tantos >0 como <0 $\rightarrow$ $\langle p_x \rangle = 0$ ✓

e) $\langle V \rangle$? $\langle \Phi_{1s} | V \Phi_{1s} \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\sqrt{\pi}} e^{-r} \left(-\frac{1}{r}\right) \frac{1}{\sqrt{\pi}} \left(e^{-r}\right) r^2 \sin\theta \, dr d\theta d\varphi$

$V = -\frac{1}{r}$

$$= \cancel{\int_0^\infty \int_0^\pi \int_0^{2\pi}} -\frac{1}{\cancel{\pi}} r e^{-2r} \cdot 4\cancel{\pi} \, dr = \int_0^\infty -4 r e^{-2r} dr$$

$$= -4 \int_0^\infty r e^{-2r} dr = \frac{1!}{2^2} \cdot (-\cancel{4}) = \boxed{-1 \text{ hartree}}$$ ✓

$\langle T \rangle$? $\langle \Phi_{1s} | T \Phi_{1s} \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\sqrt{\pi}} e^{-r} \left(-\frac{\hbar^2}{2m} \nabla^2\right) \frac{1}{\sqrt{\pi}} e^{-r} r^2 \sin\theta \, dr d\theta d\varphi$

Estado propio obtenemos E_{1s} ... L^2 $\frac{d^2}{d\theta}$ ...

$E_{1s} = \langle \Phi_{1s} | \hat{H} \Phi_{1s} \rangle$

$$\langle \Phi_{1s} | \hat{H} \Phi_{1s} \rangle = \langle \Phi_{1s} | (T+V) \Phi_{1s} \rangle = \langle \Phi_{1s} | T \Phi_{1s} \rangle + \langle \Phi_{1s} | \hat{V} \Phi_{1s} \rangle = E_{1s}$$

$E_{1s} = -\frac{1}{2}$ hartree $= \langle \Phi_{1s} | T \Phi_{1s} \rangle - 1$ hartree

$\rightarrow \langle \Phi_{1s} | T \Phi_{1s} \rangle = \left(-\frac{1}{2} + 1\right)$ hartree $= 0{,}5$ hartree ✓

f) v cuadrática media e^-) $\cancel{\text{St}}$ + llum buit?

$$v = \sqrt{\langle v^2 \rangle} = \sqrt{\langle \Phi_{1s} | \hat{V}^2 \Phi_{1s} \rangle} = \sqrt{\iiint \frac{1}{\sqrt{\pi}} e^{-r} \left(\frac{1}{m_e}\right) \frac{1}{\sqrt{\pi}} e^{-r} r^2 \sin\theta \, dr d\theta d\varphi}$$

$p^2 = m^2 v^2$

$$= \sqrt{\int \frac{1}{\cancel{\pi}} e^{-2r} r^2 \, 4\cancel{\pi} \, dr} = \sqrt{\int_0^\infty r^2 e^{-2r} dr}$$

$\langle T \rangle = 0{,}5 h$

$\langle T \rangle = \langle \frac{1}{2} m v^2 \rangle = \frac{1}{2} m_e \langle v^2 \rangle$

Átomos + pesados velocidades comparable a c (luz)

$\langle v^2 \rangle = \frac{2 \langle T \rangle}{m_e} = \frac{1 \text{ hartree}}{m_e} = 1 h$

$\rightarrow v = 0{,}0073c$

$\sqrt{\langle v^2 \rangle} = \sqrt{2 \langle T \rangle}$

$v = 2{,}1877 \cdot 10^6$ m/s $c = 2{,}998 \cdot 10^8$ m/s

$\langle p_x \rangle$, E_p , T ? $\Phi_{1s} = \frac{1}{\sqrt{\pi}} e^{-r}$

$\langle p_x \rangle_\Phi = \langle \Phi | \hat{A} \Phi \rangle$

$\langle p \rangle = \int_{-\infty}^{+\infty} \frac{1}{(\sqrt{\pi})^2} e^{-r} (-i\hbar)(-g) e^{-r} dr = 0$

Impar

$\boxed{r = \sqrt{x^2+y^2+z^2}}$?

$\langle V \rangle = \int_{-\infty}^{+\infty} \frac{1}{\pi} e^{-r} \cancel{\frac{1}{2} k x^2} e^{-r} dV$

$V_{e^-} = -\frac{1}{r} \rightarrow \langle V \rangle = \frac{-1}{\pi} \int e^{-2r} \cdot \frac{1}{r} \cdot r^2 \sin\theta \, dr \, d\theta \, d\varphi.$

$\langle V \rangle = -\int_0^\infty \frac{1}{\pi} r e^{-2r} \sin\theta \, dr \, d\theta \, d\varphi = -\frac{4\cancel{\pi}}{\cancel{\pi}} \int_0^\infty r e^{-2r} dr$

$= -4 \frac{1!}{2^2} e^{-0} (1 + 0 + 0 \dots) = -1$ hartree

$\langle T \rangle =$ molt dif. D^2

$E_{1s} = \langle \Phi_{1s} | \hat{H} \Phi_{1s} \rangle = -\frac{z^2}{2n^2} = -\frac{1}{2}$ hartree

$T = H - V = -\frac{1}{2} + 1 = 1/2$ hartree.

$\boxed{2.8}$ $t=0$ $\qquad \psi = N(\phi_{2s} - \phi_{2p_z})$

a) Estat estacionari? ~~Sí~~ ps són pròpies de H.

b) pròpia $\hat{L}_z$? $\hat{L}^2$?

$\hat{L}^2 = \ell(\ell+1)\hbar^2 \qquad \ell(2s)=0, \quad \ell(2p)=1 \Big\} \cancel{\hat{L}^2}$

$\hat{L}_z = m\hbar \rightarrow m(2s)=0, \quad m(p_z)=0$

c) $P(L^2 \rightarrow 2\hbar^2)\ \psi$? $\qquad 2\hbar^2 = \ell(\ell+1)\hbar^2 \rightarrow \boxed{\ell=1} \rightarrow 2p_z$

$P = (\langle\phi|\psi\rangle)^2 = \cancel{\left(\left(\frac{1^5}{2^5\pi}\right)^{1/2} r\cos\theta e^{-2r/2}\right.}$

$\psi = \frac{1}{\sqrt{2}}(\phi_{2s} - \phi_{2p_z}) \qquad \boxed{P = \frac{1}{2}}$

d) $L_z \rightarrow \boxed{m=0}$

$\boxed{\text{e) } P\ e^-\ (z>0)\ ?}$??

f) $S^2 = 3/4\ \hbar^2 \qquad P = 1$

$S_z = +1/2\,\hbar \qquad P = 1/2$

$S_z = -1/2\,\hbar \qquad P = 1/2$