PROBLEMES T3

3.1 Φ osc. harmònic 1D prova

$\Phi_{prova} = Ne^{-cx^2}$ optimitzeu variacionalment c i calculeu la cota sup (W) de la E.

Mètode variacional $W = \langle \Psi | \hat{H} \Psi \rangle \geq E_1$

1. N ?

$\langle \Phi_p | \Phi_p \rangle = 1$; $N^2 = \dfrac{1}{\int_{-\infty}^{+\infty} e^{-2cx^2} dx} = \dfrac{1}{2\int_0^{\infty} e^{-2cx^2} dx} = \dfrac{1}{\cancel{2}} \cdot \left(\cancel{\frac{1}{2}}\right) \left(\sqrt{\frac{\pi}{2c}} \right)^{-1}$

$N = \frac{1}{}\left(\frac{\sqrt{2c}}{\sqrt{\pi}} \right)^{1/2} = \left(\frac{2c}{\pi}\right)^{1/4}$

2.

$W = \left\langle \left(\frac{2c}{\pi}\right)^{1/4} e^{-cx^2} \middle| \hat{H} \left(\frac{2c}{\pi}\right)^{1/4} e^{-cx^2} \right\rangle =$

$W = \left(\frac{2c}{\pi}\right)^{1/2} \int_{-\infty}^{+\infty} e^{-cx^2} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 \right) e^{-cx^2} dx$

$W = \sqrt{\frac{2c}{\pi}}\, 2\int_0^{\infty} e^{-cx^2} \left(-\frac{\hbar^2}{2m}\frac{d}{dx}\left(-2cx \cdot e^{-cx^2} \right) + \frac{1}{2}kx^2 e^{-cx^2} \right) dx$

$W = \sqrt{\frac{2c}{\pi}}\, 2\int_0^{\infty} e^{-cx^2} \left(-\frac{\hbar^2}{2m}\left(-2ce^{-cx^2} + 2cx \cdot 2cx\, e^{-cx^2} \right) + \frac{1}{2}kx^2 e^{-cx^2} \right) dx$

$W = \sqrt{\frac{2c}{\pi}}\, 2\int_0^{\infty} \left(\frac{\hbar^2}{\cancel{2}m} \cdot \cancel{2}c\, e^{-2cx^2} - \frac{\hbar^2}{m} 2c^2x^2 e^{-2cx^2} + \frac{1}{2}kx^2 e^{-2cx^2} \right) dx$

parelles!

$W = \sqrt{\frac{2c}{\pi}} \cdot 2\left[\frac{\hbar^2}{m} c \int_0^{\infty} e^{-2cx^2} dx - \frac{\hbar^2}{m} 2c^2 \int_0^{\infty} x^2 e^{-2cx^2} dx + \frac{1}{2}k \int_0^{\infty} x^2 e^{-2cx^2} dx \right]$

$W = \cancel{\sqrt{\frac{2c}{\pi}}}\, 2\left[\frac{\hbar^2}{m} c \frac{1}{2}\cancel{\sqrt{\frac{\pi}{2c}}} - \frac{\hbar^2}{m} 2c^2 \cdot \frac{1}{2^2 \cdot 2c} \cdot \sqrt{\frac{\cancel{\pi}}{(\cancel{2c})^3}} + \frac{1}{2}k \frac{1}{2(2c)4} \sqrt{\frac{\cancel{\pi}}{(\cancel{2c})^3}} \right]$

$W = \frac{\hbar^2 c}{m} - \frac{\hbar^2 \cdot \cancel{2}c^{\cancel{2}}}{m\, \cancel{4}24} + \frac{k}{2c \cdot 4} = \frac{c\hbar^2}{2m} + \frac{k}{8c}$ ✓✓

c^{-1} -1

$W = \frac{\hbar^2 c}{2m} + \frac{k}{8c}$ Minimitzar! $\frac{dW}{dc} = 0$ $\frac{dW}{dc} = \frac{\hbar^2}{2m} - \frac{k}{8c^2} = 0 \rightarrow \frac{\hbar^2}{2m} = \frac{k}{8c^2}$

$c^2 = \frac{2km}{8\hbar^2} = \frac{\alpha^2}{4} \rightarrow \boxed{c_{opt} = \alpha/2}$ $\boxed{\alpha^2 = \frac{km}{\hbar^2}}$

Es un mínimo?

$\alpha = \frac{\sqrt{km}}{\hbar}$

$c = \frac{\alpha}{2}$

$$\frac{d^2W}{dc^2} = 0 - \frac{k(-2)}{8c^3} = \frac{k}{4c^3} > 0$$

$$W_{óptima} = \frac{\hbar^2 c}{2m} + \frac{k}{8c} = \frac{\hbar^2 \alpha}{4m} + \frac{2k}{8\alpha} = \cancel{\frac{\hbar^2 \sqrt{km}}{4\hbar m} + \frac{2k\hbar^2}{8\sqrt{km}}}$$

$$\cancel{W_{op} = \frac{k}{4} + \frac{1}{4}\frac{\hbar^2}{m} = \frac{k}{4}\left(1 + 1/\alpha\right)}$$

$$\cancel{\frac{\hbar^2}{m} = \frac{k}{\alpha}}$$

noo!

$$\cancel{W_{opt} = \frac{\hbar^2 \alpha}{4m} + \frac{k \cdot \hbar^2}{4m} = \frac{\hbar^2 \alpha + k\hbar^2}{4m} = \frac{\hbar^2}{4m}(\alpha + k)}$$

$$\hbar^2 = \frac{km}{\alpha^2}$$

$$W_{op} = \frac{\hbar^2 \alpha}{4m} + \frac{2k}{8\alpha} = \cancel{\ldots} = \frac{k\cancel{m}\cancel{\alpha}}{4\cancel{m}\alpha^2} + \frac{1k}{4\alpha}$$

$$W_{op} = \frac{k + k}{4\alpha} = \frac{2k}{4\alpha} = \frac{k}{2\alpha} \checkmark$$

$$W_{op} = \frac{k\hbar}{2\sqrt{km}} = \frac{kh}{2 \cdot 2\pi\sqrt{km}} = \frac{1}{2}h \cdot \underbrace{\frac{1}{2\pi} \cdot \frac{\sqrt{k}}{\sqrt{m}}}_{\nu} = \frac{1}{2}h\nu$$

es = exacta

13.2 a) Estat f. át H: $\Psi = N r\, e^{-cr}$ optimitzar c? W_{opt}?

1. N?

$$N^2 = \frac{1}{\int_{-\infty}^{+\infty} r^2 e^{-2cr}\, dr} = \frac{1}{2\int_0^{\infty} r^2 e^{-2cr}\, dr} = \frac{1}{2\cdot\frac{2!}{(2c)^3}}$$

$$N^2 = \frac{8\cdot c^3}{4} = 2c^3 \rightarrow N = \sqrt{2c^3} \qquad \hat{H}(u\,a) = -\frac{1}{2}\nabla^2 - \frac{1}{r}$$

$$2.\ W = \langle \Psi | \hat{H}\Psi\rangle = (2c^3)\int_{-\infty}^{+\infty} r e^{-cr}\cdot\left(-\frac{1}{2}\nabla^2 - \frac{1}{r}\right) r e^{-cr}\, dr$$

$$= 2c^3 \int_{-\infty}^{+\infty} r e^{-cr}\left(-\frac{1}{2}\left(\frac{d^2}{dr} + \frac{2}{r}\frac{d}{dr} - \frac{1}{r}\right) r\, e^{-cr}\, dr \ldots\right.$$

$$= \frac{c^2}{6} - \frac{c}{2} \longrightarrow \frac{dW}{dc} = \frac{2c}{6} - \frac{1}{2} = \frac{1}{3}c - \frac{1}{2} = 0$$

$$\boxed{c_{opt} = \frac{3}{2}} \qquad \frac{d^2W}{dc^2} = \frac{2}{6} > 0 \text{ mínimo!}$$

$$W_{opt} = \frac{9}{4\cdot 6} - \frac{3}{4} = \frac{9}{24} - \frac{18}{24} = -\frac{9}{24} = -\frac{3}{8} \text{ hartree}$$

$$E_{1s} = -\frac{z^2}{2n^2} = -\frac{4}{2\cdot 2^2} = -\frac{4}{8} \text{ hartree}$$

b) $\varphi = N e^{\underbrace{-br^2/a_0^2}\, - cr/a_0}$ $\qquad \phi_{1s} = \left(\frac{z^3}{\pi a^3}\right)^{1/2} e^{-zr/a} = \frac{1}{\sqrt{\pi}} e^{-r}$

dependencia con r^2 exacta no!!

sólo si $b = 0$ y $c = 1$ ok ✓

3.3 $\Psi = N(\Phi_0^{oh} + \Phi_1^{oh}) = N\left(\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} + \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x\, e^{-\alpha x^2/2}\right)$

$N = \frac{1}{\sqrt{\sum |c_i|^2}} = \frac{1}{\sqrt{\left(\frac{\alpha}{\pi}\right)^{1/2} + \left(\frac{4\alpha^3}{\pi}\right)^{1/2}}} = \sqrt[4]{\frac{\pi}{\alpha + 4\alpha^3}} = \left(\frac{\pi}{\alpha+4\alpha^3}\right)^{1/4}$

E? Φ estat fonamental os. anarmònic $\Phi_{n=1}$!!

$V(x) = \underbrace{\frac{1}{2} k x^2}_{\text{normal}} + \frac{\hbar^2 \alpha^{5/2}}{6m} x^3$ (b)

$V(x) = \frac{1}{2} k x^2 + b x^3$; $\Phi^{oa} = \frac{1}{\sqrt{2}} N e^{-\alpha x^2/2} + \frac{1}{\sqrt{2}} x\, e^{-\alpha x^2/2}$

$(\mathbb{H} - W\mathbb{S})\, \mathbb{C} = 0$ ① $\to 0$ ② $\to 1$

1) $\mathbb{A} = \mathbb{H} - W\mathbb{S}$; $\mathbb{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = ($

$H_{11} = \langle \Phi_0^{oa} | \hat{H} \Phi_0^{oa} \rangle = \langle \Phi_0^{oh} | (\hat{T} + \hat{V}) \Phi_0^{oa} \rangle + \langle \Phi_0^{oa} | b x^3 \Phi_0^{oa} \rangle$

$H_{11} = E_0^{oh} \underbrace{\langle \Phi_0^{oa} | \Phi_0^{oa} \rangle}_{① \text{ normalitzada}} + b N^2 \int_{-\infty}^{+\infty} \underset{\uparrow \text{ IMPARELL}}{x^3 e^{-\alpha x^2}} = E_0^{oh} + 0$

$H_{12} = \langle \Phi_0^{oa} | \hat{H} \Phi_1^{oa} \rangle = E_1^{oa} \underset{0}{\langle \Phi_0^{oa} | \Phi_1^{oa} \rangle} + b \int_{-\infty}^{+\infty} x \cdot x^3 \left(\frac{\alpha}{\pi} \cdot \frac{4\alpha^3}{\pi}\right)^{1/4} e^{-\alpha x^2} dx$

$H_{12} = 0 + b\left(\frac{4\alpha^4}{\pi^2}\right)^{1/4} 2 \int_0^{+\infty} x^4 e^{-\alpha x^2} dx = \frac{1 \cdot 3}{2^3} \sqrt{\frac{\pi}{\alpha^5}}$

$H_{12} = 2b\alpha \sqrt{\frac{2}{\pi}} \cdot \frac{3}{8} \cdot \sqrt{\frac{\pi}{\alpha^5}} = \frac{\cancel{2}\hbar^2 \cancel{\sqrt{\alpha^5}}}{\cancel{6}m} \cdot \frac{3\alpha}{8 \cancel{\sqrt{\alpha^5}}} = \boxed{\frac{\hbar^2 \alpha}{8m}} = H_{21}$ hermiticitat

$H_{22} = \langle \Phi_1^{oa} | \hat{H} \Phi_1^{oa} \rangle = E_1^{oa} \underset{1}{\langle \Phi_1 | \Phi_1 \rangle} + \langle \Phi_1 | b x^3 \Phi_1 \rangle$

$H_{22} = E_1^{oa} + b \int_{-\infty}^{+\infty} \left(\frac{4\alpha^3}{\pi}\right)^{1/2} \cdot \underbrace{x^3 \cdot x^2}_{\text{imparell}} \cdot e^{-\alpha x^2} dx$

$\mathbb{H} = \begin{pmatrix} \underset{1/2 h\nu}{E_0^{oa}} & \hbar^2\alpha/8m \\ \frac{\hbar^2 \alpha}{8m} & \underset{3/2 h\nu}{E_1} \end{pmatrix}$ $S_{rs} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$$H_{12} = \frac{\hbar\sqrt{km}}{8m} = \frac{h}{8\,2\pi}\sqrt{\frac{km}{m}} = \frac{1}{8}h\nu$$

$$H_{12} = \frac{1}{4}E_0$$

3 (II)

$$\begin{pmatrix} E_0 - W & \frac{\hbar^2\alpha}{8m} \\ \frac{\hbar^2\alpha}{8m} & 3E_0 - W \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0$$

$$(\varepsilon - W)(3\varepsilon - W) - \frac{1}{4}\varepsilon\cdot\frac{1}{4}\varepsilon = 0$$

$$3\varepsilon^2 - \varepsilon W - 3W\varepsilon + W^2 - \frac{1}{16}\varepsilon^2 = 0 \qquad \varepsilon = E = \frac{1}{2}h\nu =$$

$$W^2 - 4\varepsilon W + \varepsilon^2\left(3 - \frac{1}{16}\right) = 0 \qquad ??$$

$\boxed{3.5}$ $E_p \rightarrow V(x) = \frac{1}{2}kx^2 + px^3 + qx^4$ — Mètode pertorbacional !!

E_0? $\hat{H} = \hat{H}^0 + \hat{H}'$

$$E = \langle \Phi_0 | \hat{H}\Phi_0 \rangle = \langle \Phi_0 | \hat{H}^0 \Phi_0 \rangle + \langle \Phi_0 | \hat{H}' \Phi_0 \rangle$$

$$E^{(1)} = E_0 + \int_{-\infty}^{+\infty} \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\left(px^3 + qx^4\right) e^{-\alpha x^2/2}\,dx$$

$$E^{(1)} = \frac{1}{2}h\nu + \left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{+\infty} e^{-\alpha x^2}\left(px^3 + qx^4\right)dx$$

$$E = \frac{1}{2}h\nu + N\int_{-\infty}^{+\infty} \cancel{px^3 e^{-\alpha x^2}} + qx^4 e^{-\alpha x^2}\,dx$$

$$E = \frac{1}{2}h\nu + N\cdot 2q\int_0^{\infty} x^4 e^{-\alpha x^2}dx = \frac{1}{2}h\nu + 2Nq\cdot\frac{1\cdot 3}{2^{3}}\sqrt{\frac{\pi}{\alpha^5}}$$

$$E = \frac{1}{2}h\nu + \cancel{2}q\left(\frac{\alpha}{\pi}\right)^{1/2}\cdot\frac{3}{\cancel{8}4}\sqrt{\frac{\pi}{\alpha^5}} = \frac{1}{2}h\nu + \frac{3}{4}q\sqrt{\frac{\alpha}{\alpha^{5}}} = \underbrace{\frac{1}{2}h\nu}_{} + \underbrace{\frac{3}{4}\frac{q}{\alpha^2}}_{}$$

$$\hbar = \frac{h}{2\pi}$$

$$E = \frac{1}{2}\frac{\hbar\,2\pi}{2\pi}\sqrt{\frac{k}{m}\frac{m}{m}} + 3q/4\alpha^2 = \frac{1}{2}\frac{\hbar\sqrt{km}}{m} = \frac{\hbar^2\alpha}{2m} + 3q/4\alpha^2$$

$$\alpha = \frac{\sqrt{km}}{\hbar}$$

$$\Delta\Psi = N\hat{A}\sum c_i\phi_i = N\sum(c_i\hat{A}\phi_i) = N(\sum c_i a\phi_i)$$

$\boxed{3.6}$ $V(x) = -b\sin\frac{\pi x}{a}$ $\quad x \in (0,a)$ $\Big\}$ partícula caixa!

$V(x) = \infty$ $\quad x \notin (0,a)$

$E_1 = \frac{1^2 h^2}{8ma^2} = \frac{h^2}{8ma^2}$

$\Phi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$

$$\hat{H} = \underset{\substack{\downarrow \\ E_1}}{\hat{H}^0} + H' = \hat{H}^0 - b\sin\frac{\pi x}{a}$$

$$E = E_1 - \langle \Phi_1(x) | b\sin\frac{\pi x}{a}\,\Phi_1(x)\rangle$$

$$E = E_1 - \int_0^a \frac{2}{a}\cdot b\sin\frac{\pi x}{a}\left(\sin\frac{\pi x}{a}\right)^2 dx$$

$$E = E_1 - \frac{2b}{a}\int_0^a \sin^3\frac{\pi x}{a}\,dx$$

$$E = E_1 - \frac{2b}{a}\left(-\sin^2(\pi/a\, x)\cos \right. \ldots$$