PROBLEMES QF III : T1

1.1. Suposant que f_1 i f_2 NORMALITZADES + REALS no són ortogonals $\langle f_1 | f_2 \rangle \neq 0$

Normalitzeu $\varphi_+ = f_1 + f_2$ i $\varphi_- = f_1 - f_2$ i comproveu que són ortogonals !!

Normalitzar : $\langle \varphi_+ | \varphi_+ \rangle = 1 \rightarrow \langle N(f_1 + f_2) | N(f_1 + f_2) \rangle = 1$

$\int_{-\infty}^{+\infty} N^2 (f_1 + f_2)(f_1 + f_2) dV = 1$; $N^2 \langle f_1 + f_2 | f_1 + f_2 \rangle = 1$

NO CAL

$$\boxed{\langle f_1 | f_2 \rangle \neq 0 = S_{12}}$$

$\left.\begin{array}{l} \langle f_1 | f_1 \rangle = 1 \\ \langle f_2 | f_2 \rangle = 1 \end{array}\right\}$ normalitzades

$N^2 (\langle f_1 | f_1 \rangle + \langle f_1 | f_2 \rangle + \langle f_2 | f_1 \rangle + \langle f_2 | f_2 \rangle) = 1$

$N^2 (1 + S_{12} + 1 + S_{12}) = 1$; $\boxed{N_+ = \frac{1}{\sqrt{2 + 2S_{12}}}}$ ✓

b)

$\langle \varphi_- | \varphi_- \rangle = 1$; $\langle N(f_1 - f_2) | N(f_1 - f_2) \rangle = 1$

$\langle f_1 | f_2 \rangle = S_{12}$

$\langle f_1 | f_1 \rangle = \langle f_2 | f_2 \rangle = 1$

$N^2 \langle f_1 - f_2 | f_1 - f_2 \rangle = 1$

$N^2 (\langle f_1 | f_1 \rangle - \langle f_1 | f_2 \rangle - \langle f_2 | f_1 \rangle + \langle f_2 | f_2 \rangle) = 1$

$N^2 = \frac{1}{(1 - 2S_{12} + 1)} \Rightarrow \boxed{N_- = \frac{1}{\sqrt{2 - 2S_{12}}}}$ ✓

Són ortogonals? $\langle \phi | \psi \rangle = 0$?

$\langle \varphi_+ | \varphi_- \rangle = 0$? $\rightarrow \langle N_+(f_1 + f_2) | N_-(f_1 - f_2) \rangle = N_+ N_- \langle f_1 + f_2 | f_1 - f_2 \rangle$

$\frac{1}{\sqrt{2+2S_{12}}} \cdot \frac{1}{\sqrt{2-2S_{12}}} (\langle f_1 | f_1 \rangle - \langle f_1 | f_2 \rangle + \langle f_2 | f_1 \rangle - \langle f_2 | f_2 \rangle) =$

$\frac{1}{\sqrt{(2 + 2S_{12})(2 - 2S_{12})}} (\cancel{1} - \cancel{S_{12}} + \cancel{S_{12}} - \cancel{1}) = 0$ Són ortogonals !!

Normalitzar : $\langle \phi | \phi \rangle = 1$

$\langle \psi | \psi \rangle = 1$

Ortogonal : $\langle \phi | \psi \rangle = 0$

Ortonormal (conjunt) : normalitzades + ortogonals

$\boxed{1.2}$ Normalitzeu:

a) $\phi = e^{-\alpha x^2/2}$ osc. harmònic 1D:

$\langle \phi | \phi \rangle = 1$; $\langle N e^{-\alpha x^2/2} | N e^{-\alpha x^2/2} \rangle = 1$

$N^2 \int_{-\infty}^{+\infty} \left(\left(e^{-\alpha x^2/2}\right)^* e^{-\alpha x^2/2} \right) dx = 1$; $N^2 \int_{-\infty}^{+\infty} e^{-\alpha x^2} dx = 1$

$N^2 \cdot 2 \underbrace{\int_0^{\infty} e^{-\alpha x^2} dx}_{\text{formulari:}} = 1$ És parella $\boxed{f(-x) = f(x)}$ $\rightarrow \int_{-\infty}^{+\infty} = 2\int_0^{+\infty}$

si fós senar $f(-x) = -f(x)$ $\int_{-\infty}^{+\infty} = 0$ Àrea no integrable

$\cancel{\int_0^{\infty} x^n e^{-ax^2} dx} = \frac{1 \cdot 3 \cdots \cancel{(2n-1)}}{\cancel{2^{n+1}}} \sqrt{\frac{\pi}{a^{2n+1}}}$ No! Fer-ho calculadora!

$\int_0^{\infty} e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$

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

b) $\psi = e^{-r/a}$ origen al Nucli $\int_0^{\infty}$

$\langle N e^{-r/a} | N e^{-r/a} \rangle = 1$

$N^2 \iiint_{-\infty}^{+\infty} e^{-2r/a} dV = 1 \longrightarrow$ passar coordenades esfèriques!!

$N^2 \int_{\cancel{-\infty}\,0}^{+\infty} r^2 e^{-2r/a} dr \underbrace{\int_0^{\pi} \sin\theta \, d\theta}_{2} \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} = 1$

origen coord. (0,0)

$N^2 \cdot \cancel{2} \int_0^{\infty} r^2 e^{-2r/a} dr \cdot (4\pi) = 1 \rightarrow N^2 8\pi \cdot \frac{2!}{\left(\frac{2}{a}\right)^3} = 1$

$N^2 \cdot \cancel{8} \cdot \pi \frac{\cancel{2} a^3}{\cancel{8}} = 1$; $N = \frac{1}{\sqrt{\cancel{2}\pi a^3}}$ $\rightarrow \boxed{N = (\pi a^3)^{1/2}}$ ✓

1.3 $\{f_1, f_2 \dots f_n\}$ conjunt no ortonormal. Comproveu que:

$$\varphi_a = \sum_{i=1}^{n} c_i f_i \rightarrow \langle \varphi_a | \varphi_a \rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} c_i^* c_j S_{ij} = 1 \quad \text{on} \quad \boxed{\langle f_i | f_j \rangle = S_{ij}}$$

$\langle f_i | f_j \rangle \neq 0 = S_{ij}$ ortogonal $\quad \langle f_i | f_i \rangle \neq 1$ no normalitzades!

$$1 = \langle \varphi_a | \varphi_a \rangle = \langle N \sum_{i=1}^{n} c_i f_i | N \sum_{j=1}^{n} c_j f_j \rangle = \cancel{N^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \langle c_i f_i | c_j f_j \rangle =$$

$$= \cancel{N^2} \sum_{i=1}^{n} \sum_{j=1}^{n} c_i^* c_j \underbrace{\langle f_i | f_j \rangle}_{S_{ij}} = \cancel{N^2} \sum_{i=j}^{n} \sum_{j=1}^{n} c_i^* c_j S_{ij} = 1 \quad \checkmark$$

δ_{ij} si $i = j \rightarrow 1$

δ_{ij} si $i \neq j \rightarrow 0$

si són normalitzades : $\langle f_i | f_i \rangle = 1$

$i = j$ $\quad$ Reals

$$\langle \varphi_a | \varphi_a \rangle = \underbrace{\sum_{i=1}^{n} \underbrace{c_i^* c_i}}_{\text{Mòdul}} \underbrace{\langle f_i | f_i \rangle}_{1} = 1$$

$$\langle \varphi_a | \varphi_a \rangle = \sum_{i=1}^{n} c_i^* c_i = \sum_{i=1} |c_i|^2$$

si $i \neq j \rightarrow \underline{\delta_{ij} = 0}$

δ_{ij} elimina 1Σ.

1.4 $\hat{x}$ i $\hat{p}_x$ són hermítics? $\quad$ Hermiticitat: $\langle \hat{A} \Phi | \Psi \rangle = \langle \Phi | \hat{A} \Psi \rangle$

$\cancel{[\hat{x}, \hat{p}_x]}$

$$\langle \hat{x} \Phi | \Psi \rangle = \int_{-\infty}^{+\infty} x \Phi^* \Psi \, dx = \cancel{\frac{d\Phi^*}{dx} \frac{d\Psi}{dx}} \quad \frac{x^2}{2} \int_{-\infty}^{+\infty} \Phi^* \Psi \, dx$$

$$\langle \Phi | \hat{x} \Psi \rangle = \int_{-\infty}^{+\infty} \Phi^* x \Psi \, dx = x^2/2 \int_{-\infty}^{+\infty} \Phi^* \Psi \, dx$$

$$\langle \hat{p}_x \Phi | \Psi \rangle = \int_{-\infty}^{+\infty} \left(-i\hbar \frac{d\Phi}{dx} \right)^* \Psi \, dx = i\hbar \int_{-\infty}^{+\infty} \left(\frac{d\Phi}{dx} \right)^* \Psi \, dx = \hbar \left(\Phi^* + \int_{-\infty}^{+\infty} \Psi \, dx \right.$$

$$\langle \Phi | \hat{p}_x \Psi \rangle = \int_{-\infty}^{+\infty} \Phi^* \left(-i\hbar \frac{d\Psi}{dx} \right) dx = (-i\hbar) \left(\int_{-\infty}^{+\infty} \Phi^* \, dx + \cancel{\int_{-\infty}^{+\infty}} \quad \Psi \right.$$

??

$\boxed{1.5}$ Demostreu :

$\hat{A}\Phi = a\Phi$

a) Valors propis $\hat{A}$ (hermític) són $\mathbb{R}$:

Condició d'hermiticitat : $\langle \hat{A}\Phi | \Phi \rangle = \langle \Phi | \hat{A}\Phi \rangle$

$\langle a\Phi | \Phi \rangle = \langle \Phi | a\Phi \rangle$

$a^* \langle \cancel{\Phi | \Phi} \rangle = a \langle \cancel{\Phi | \Phi} \rangle \rightarrow \boxed{a^* = a}$ han de ser $\mathbb{R}$ sinó a^* canviaria de signe!

b) $\left.\begin{array}{l} \hat{A}\Phi = a_1 \Phi \\ \hat{A}\Psi = a_2 \Psi \end{array}\right\}$ $a_1 \neq a_2$ són ortogonals?

$\langle \hat{A}\Phi | \Psi \rangle = \langle \Phi | \hat{A}\Psi \rangle$

$\langle a_1 \Phi | \Psi \rangle = \langle \Phi | a_2 \Psi \rangle \rightarrow a_1^* \langle \Phi | \Psi \rangle = a_2 \langle \Phi | \Psi \rangle$

si $a_1 \neq a_2$ i a_1 és real (apartat a) l'única manera de

que siguin = és que $\underline{\langle \Phi | \Psi \rangle = 0}$ ortogonals.

c) Qualsevol comb. lineal de funcions pròpies $\hat{A}$ degenerades

tmb é pròpia de $\hat{A}$ amb = a.

$\hat{A}\Phi_i = a\Phi_i$

$\Psi = N \sum c_i \Phi_i \rightarrow \hat{A}\Psi = N\hat{A} \sum c_i \Phi_i = N \sum c_i \hat{A}\Phi_i = N \sum c_i a \Phi_i$

$\hat{A}\Psi = a \underbrace{N \sum c_i \Phi_i}_{\Psi} = \underline{\underline{a\Psi}}$

$\boxed{1.6}$ $[\hat{x}, \hat{p_x}] = i\hbar$

$[\hat{x}, \hat{p_x}] = \hat{x}\hat{p_x} - \hat{p_x}\hat{x}$

$\hat{x}\hat{p_x}\Psi = -x i\hbar \frac{d\Psi}{dx}$

$\hat{p_x}\hat{x}\Psi = \hat{p_x}(x\Psi) = -i\hbar\Psi - i\hbar x \frac{d\Psi}{dx}$

$\hat{x}\hat{p_x}\Psi - \hat{p_x}\hat{x}\Psi = \cancel{-i\hbar \frac{d\Psi}{dx}} + i\hbar\Psi + \cancel{i\hbar \frac{d\Psi}{dx}}$

$[\hat{x}, \hat{p_x}]\Psi = i\hbar\Psi \rightarrow \boxed{[\hat{x}, \hat{p_x}] = i\hbar}$