Aula 1 - Mecânica Quântica (Revisão)

Sistemas de partícula única - 1ª quantização

Forma geral do Hamiltoniano

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + U(\vec{r}) \quad \underline{\text{ou}} \quad \boxed{\hat{H} = \frac{1}{2m}(\vec{p} - q\vec{A})^2 + U(\vec{r})}$$

$$\nabla \times \vec{A} = \vec{B}$$

Eq. de Schrödinger (não relativística!)

$$\boxed{i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle}$$

$$\begin{cases} (|\psi(t)\rangle)^\dagger = \langle\psi(t)| & \text{"bra"} \\ \langle\vec{r}|\psi\rangle = \psi(\vec{r},t) \\ \langle\phi|\psi\rangle = \int d^3\vec{r}\, \phi^*(\vec{r},t)\,\psi(\vec{r},t) \end{cases}$$

$\{|\varphi_\alpha\rangle\} \rightarrow$ base ortonormal do espaço de Hilbert

$$\boxed{|\psi(t)\rangle = \sum_\alpha c_\alpha^{(t)}|\varphi_\alpha\rangle} \; ; \quad \underbrace{\boxed{\langle\varphi_\alpha|\varphi_\beta\rangle = \delta_{\alpha\beta}}}_{\text{ortogonalidade}} \; ; \quad \underbrace{\boxed{\sum_\alpha |\varphi_\alpha\rangle\langle\varphi_\alpha| = \mathbb{1}}}_{\text{completeza}}$$

Operador $\hat{A}$: $\quad A_{\alpha\beta} = \langle\varphi_\alpha|\hat{A}|\varphi_\beta\rangle$

$$\hat{A}^\dagger : (A^\dagger)_{\alpha\beta} = \langle\varphi_\alpha|A^\dagger|\varphi_\beta\rangle \equiv (\langle\varphi_\beta|\hat{A}|\varphi_\alpha\rangle)^* = A_{\beta\alpha}^*$$

$\underline{A = A^\dagger} \rightarrow$ operador Hermitiano ("Observável")

$\hat{A}|\varphi_a\rangle = a|\varphi_a\rangle$; $\boxed{|\langle\varphi_a|\psi\rangle|^2 \rightarrow \text{Probabilidade } P(a) \text{ de se medir "}a\text{" estando o sistema no estado } |\psi\rangle}$

$\rightarrow$ $\boxed{\text{Medição experimental}}$

Sistema no estado $|\psi\rangle$. Então

$$\boxed{|\psi(\vec{r})|^2 d^3\vec{r} = |\langle \vec{r}|\psi\rangle|^2 d^3\vec{r}}$$

$|\psi(\vec{r})|^2 \downarrow$ densidade de probabilidade

$\rightarrow$ Probabilidade $dP(\vec{r})$ de a partícula estar em um volume $d^3\vec{r}$ em torno de $\vec{r}$

Em geral, se um operador $\hat{A}$ tem um espectro contínuo $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle$ então $dP(\alpha) = |\langle\alpha|\psi\rangle|^2 d\alpha$

Exemplo importante: o oscilador harmônico em 1D

Hamiltoniano: $$H = \frac{\hat{p}^2}{2m} + \underbrace{\frac{1}{2}m\omega^2\hat{x}^2}_{\rightarrow U(x)}$$

$[\hat{x},\hat{p}] = i\hbar$; $\boxed{\hat{p}\,\varphi(x) \rightarrow \frac{\hbar}{i}\frac{d}{dx}\varphi(x)}$ (formalmente: $\langle x|\hat{p}|\varphi\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|\varphi\rangle$)

Definimos: $$\begin{cases} \hat{\bar{x}} = \sqrt{\frac{m\omega}{\hbar}}\,\hat{x} \\ \hat{\bar{p}} = \frac{1}{\sqrt{m\hbar\omega}}\,\hat{p} \end{cases} \Rightarrow \boxed{\hat{H} = \frac{\hbar\omega}{2}\left(\hat{\bar{p}}^2 + \hat{\bar{x}}^2\right)}$$

e ainda $$\begin{cases} \hat{a} = \frac{1}{\sqrt{2}}\left(\hat{\bar{x}} + i\hat{\bar{p}}\right) \\ \hat{a}^+ = \frac{1}{\sqrt{2}}\left(\hat{\bar{x}} - i\hat{\bar{p}}\right) \end{cases} \Leftrightarrow \begin{aligned} \hat{\bar{x}} &= \frac{1}{\sqrt{2}}\left(\hat{a}^+ + \hat{a}\right) \\ \hat{\bar{p}} &= \frac{i}{\sqrt{2}}\left(\hat{a}^+ - \hat{a}\right) \end{aligned}$$

Note que: $[\hat{\bar{x}},\hat{\bar{p}}] = \frac{1}{\hbar}[\hat{x},\hat{p}] = i$ logo:

$$[\hat{a},\hat{a}^+] = \frac{1}{2}\left(\cancel{[\bar{x},\bar{x}]} - i[\bar{x},\bar{p}] + i[\bar{p},\bar{x}] + \cancel{[\bar{p},\bar{p}]}\right) = -\frac{2i}{2}[\bar{x},\bar{p}] = 1$$

Escrevendo $\hat{H}$ com termos de $\hat{a}$ e $\hat{a}^+$:

$$\begin{cases} \bar{X}^2 = \frac{1}{2}(\hat{a}^+a^+ + aa + a^+a + aa^+) \\ \bar{P}^2 = -\frac{1}{2}(a^+a^+ + aa - a^+a - aa^+) \end{cases}$$

$$\Rightarrow \hat{H} = \frac{\hbar\omega}{2}(a^+a + \overbrace{aa^+}^{-a^+a+a^+a}) = \frac{\hbar\omega}{2}\Big(2a^+a + \overbrace{(aa^+ - a^+a)}^{=1}\Big)$$

$$\boxed{\hat{H} = \hbar\omega\left(a^+a + \tfrac{1}{2}\right)}$$

Mostra-se também que $[a,a]=0$ e $[a^+,a^+]=0$

Com isso, definimos o operador $\hat{N} = a^+a$ que é hermitiano e comuta com $\hat{H}$ (mostre!). Ou seja, se

$\hat{N}|n\rangle = n|n\rangle$ então $|n\rangle$ é auto-estado de $\hat{H}$ com energia $\boxed{E_n = \hbar\omega(n+\tfrac{1}{2})}$

É possível mostrar (Lista) que $|n\rangle \propto (a^+)^n|0\rangle$ — com n inteiro e positivo

onde $|0\rangle$ é tal que $a|0\rangle = 0$

Na verdade $|n\rangle = \dfrac{(a^+)^n|0\rangle}{\sqrt{n!}}$

Disso decorre que $\begin{cases} a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle \\ a|n\rangle = \sqrt{n}\,|n-1\rangle \end{cases}$

Sistema de N partículas - 1º quantização

Forma geral do Hamiltoniano

$$\hat{H} = \sum_{i=1}^{N} \underbrace{\frac{\hat{P}_i^2}{2m_i} + U_i(\vec{r}_i)}_{H_i^{(1p)}} + \underbrace{V(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N)}_{\text{interação (operador)}}$$

Eq. de Schrödinger

$$\boxed{i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H}|\Psi\rangle}$$

$|\Psi\rangle$: estado das N partículas

Base: $\{|\Psi_{\vec{\alpha}}\rangle\} = \{|\varphi_\alpha^1\rangle\} \otimes \{|\varphi_\alpha^2\rangle\} \otimes \dots \otimes \{|\varphi_\alpha^N\rangle\}$
(exemplo)

Base do esp de Hilbert de N part

Bases de 1p

operador de 1p

$$\boxed{\hat{A}^{1p}|\varphi^i_{\alpha_j}\rangle = \alpha_j|\varphi^i_{\alpha_j}\rangle}$$

estados de 1 partícula

ou $\{|\Psi_\beta\rangle\}$ são auto-estados de um operador de N partículas (por exemplo, um Hamiltoniano $\hat{\mathbb{H}}^{(0)}$)

Exemplo de estado de base (contínua) de N partículas:

$$\underbrace{|\vec{r}_1, \vec{r}_2, \dots \vec{r}_N\rangle}_{\text{estado de N}} = |\vec{r}_1\rangle \otimes |\vec{r}_2\rangle \otimes \dots \otimes |\vec{r}_N\rangle \text{ :}$$

estado de 1p

$$\underbrace{|\langle \vec{r}_1, \vec{r}_2, \vec{r}_3, \dots \vec{r}_N|\Psi\rangle|^2 d^3\vec{r}_1 d^3\vec{r}_2 \dots d^3\vec{r}_N = |\Psi(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N)|^2 \prod_{i=1}^{N} d^3\vec{r}_i}$$

Probabilidade de encontrar N partícula no volume 3N-dim $\prod_{i=1}^{N} d^3\vec{r}_i$ em volta do ponto $(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N)$ do espaço de Hilbert de 3N-dim

Sisteme de N partículas <u>indistinguíveis</u>

Exemplo: elétrons de mesmo spin ("spinless electrons")

Suposições FUNDAMENTAIS
- partículas caracterizadas pelos <u>mesmos números quânticos</u>
- Não é possível, mesmo em princípio, diferenciá-las por medições

⇒ logo, a troca de coordenadas de duas partículas em um estado quântico de N partículas idênticas não pode ser detectada e leva à <u>mesma</u> densidade de probabilidade. → $\boxed{\text{Fato experimental}}$

$$\left|\Psi(\vec{r}_1,\vec{r}_2,\ldots\vec{r}_K\ldots\vec{r}_\ell,\ldots\vec{r}_N)\right|^2 = \left|\Psi(\vec{r}_1,\vec{r}_2,\ldots\vec{r}_\ell\ldots\vec{r}_K,\ldots\vec{r}_N)\right|^2$$

Logo:

$$\Psi(\vec{r}_1\ldots\vec{r}_K\ldots\vec{r}_\ell\ldots\vec{r}_N) = e^{i\theta}\,\Psi(\vec{r}_1\ldots r_\ell\ldots r_K\ldots\vec{r}_N)$$

$\boxed{\text{Fato experimental}}$ ⊛

Mas trocando $\vec{r}_K \Leftrightarrow \vec{r}_\ell$ novamente, voltamos <u>ao mesmo</u> estado

$$\Psi(\vec{r}_1\ldots\vec{r}_K\ldots\vec{r}_\ell\ldots\vec{r}_N) = \underbrace{e^{i\theta}(e^{i\theta}}_{e^{i2\theta}}\Psi(\vec{r}_1\ldots\vec{r}_K\ldots\vec{r}_\ell\ldots\vec{r}_N) \Rightarrow \boxed{e^{i2\theta}=1}$$

ou seja $\boxed{\theta = 0 \quad \underline{\text{ou}} \quad \theta = \pi}$

<u>BOSONS</u> <u>FÉRMIONS</u>

⊛ Em 3D; alguns sistemas em 2D podem admitir $e^{i\theta} \neq \pm 1$ ("anyons"): F. Wilczek PRL <u>49</u> 957 (1982)

Como escrever $\Psi(\vec{r}_1 \dots \vec{r}_N)$ de N part. idênticas em bases de 1p? Por exemplo, no caso de Férmions?

Exemplo $\boxed{N=2}$ Base de 1p: $\{|\varphi_1^{1p}\rangle, |\varphi_2^{1p}\rangle, |\varphi_3^{1p}\rangle\}$

Base de N=2: $\{|\varphi_1^{1p}\rangle \otimes |\varphi_1^{1p}\rangle; |\varphi_1^{1p}\rangle \otimes |\varphi_2^{1p}\rangle; |\varphi_1^{1p}\rangle \otimes |\varphi_3^{1p}\rangle;$
(9 estados) $|\varphi_2^{1p}\rangle \otimes |\varphi_1^{1p}\rangle; |\varphi_2^{1p}\rangle \otimes |\varphi_2^{1p}\rangle; |\varphi_2^{1p}\rangle \otimes |\varphi_3^{1p}\rangle;$
DISTINGUIVEIS $|\varphi_3^{1p}\rangle \otimes |\varphi_1^{1p}\rangle; |\varphi_3^{1p}\rangle \otimes |\varphi_2^{1p}\rangle; |\varphi_3^{1p}\rangle \otimes |\varphi_3^{1p}\rangle\}$

$$\stackrel{!}{=} \{|\varphi_1^{N=2}\rangle, |\varphi_2^{N=2}\rangle, \dots, |\varphi_9^{N=2}\rangle\} \rightarrow 9 \text{ estados.}$$

Qual a diferença entre: $|\varphi_2^{N=2}\rangle = |\varphi_1^{1p}\rangle \otimes |\varphi_2^{1p}\rangle$
$|\varphi_4^{N=2}\rangle = |\varphi_2^{1p}\rangle \otimes |\varphi_1^{1p}\rangle$?

$$\langle x_1 x_2 | \varphi_2^{N=2}\rangle = \langle x_1 | \varphi_1^{1p}\rangle . \langle x_2 | \varphi_2^{1p}\rangle = \varphi_1^{1p}(x_1)\, \varphi_2^{1p}(x_2) = \varphi_2^{N=2}(x_1, x_2)$$

$$\langle x_1 x_2 | \varphi_4^{N=2}\rangle = \langle x_1 | \varphi_2^{1p}\rangle . \langle x_2 | \varphi_1^{1p}\rangle = \varphi_2^{1p}(x_1)\, \varphi_1^{1p}(x_2) = \varphi_4^{N=2}(x_1, x_2)$$

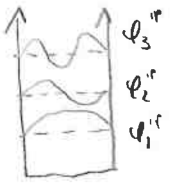
Se $\varphi_1^{1p}(x) = \sqrt{\frac{2}{L}} \operatorname{sen}\left(\frac{\pi x}{L}\right)$ e $\varphi_2(x) = \sqrt{\frac{2}{L}} \operatorname{sen}\left(\frac{2\pi x}{L}\right)$;

$$\varphi_2^{N=2}(x_1, x_2) = \frac{2}{L} \operatorname{sen}\left(\frac{\pi x_1}{L}\right) \operatorname{sen}\left(\frac{2\pi x_2}{L}\right) \neq \frac{2}{L} \operatorname{sen}\left(\frac{2\pi x_1}{L}\right) \operatorname{sen}\left(\frac{\pi x_2}{L}\right) = \varphi_4^{N=2}(x_1, x_2)$$

ou $\varphi_2^{N=2}(x_2, x_1) = \varphi_4^{N=2}(x_1, x_2)$ (DISTINGUÍVEIS) $\Rightarrow \boxed{\varphi_2^{N=2}(x_2, x_1) \neq \varphi_2^{N=2}(x_1, x_2)}$

O que ocorre se as partículas são INDISTINGUÍVEIS?

$\boxed{N=2}$ Férmions (indistinguíveis)



Base de 1p $\{|\varphi_1^{1p}\rangle, |\varphi_2^{2p}\rangle, |\varphi_3^{3p}\rangle\}$ QUANTOS ?

Base de 2p : $\{|\varphi_1^{(A)N=2}\rangle, |\varphi_2^{(A)N=2}\rangle, \dots, |\varphi_K^{(A)N=2}\rangle, \dots\}$

Tem que ser tais que $\langle x_1\, x_2 | \varphi_K^{(A)N=2}\rangle = -\langle x_2\, x_1 | \varphi_K^{(A)N=2}\rangle$

Já que $$\boxed{\Psi^A(x_1, x_2) = \sum_K C_K^{\Psi}\, \varphi_K^{(A)\,N=2}(x_1, x_2) = -\Psi^A(x_2, x_1)}$$

p/ $\forall\, C_K^{\Psi}$ (Todo $\Psi^A(x_1\, x_2)$)

Solução: cada $|\varphi_K^{(A)\,N=2}\rangle$ é formado por uma combinação antisimétrica de **N** estados de 1p distintos.

↳ Determinante de Slater
$$\begin{vmatrix} \varphi_{\nu_1}^{1p}(\vec{r}_1) & \varphi_{\nu_1}^{1p}(\vec{r}_2) & \dots & \varphi_{\nu_1}^{1p}(\vec{r}_N) \\ \varphi_{\nu_2}^{1p}(\vec{r}_1) & \varphi_{\nu_2}^{1p}(\vec{r}_2) & \dots & \varphi_{\nu_2}^{1p}(\vec{r}_N) \\ \vdots & & & \vdots \\ \varphi_{\nu_N}^{1p}(\vec{r}_1) & \varphi_{\nu_N}^{1p}(\vec{r}_2) & \dots & \varphi_{\nu_N}^{1p}(\vec{r}_N) \end{vmatrix}$$

Possibilidades p/ N = 2 e 3 estados de 1p:

NORM + REP KET

$$\begin{vmatrix} \varphi_1^{1p}(x_1) & \varphi_1^{1p}(x_2) \\ \varphi_2^{1p}(x_1) & \varphi_2^{1p}(x_2) \end{vmatrix} = \varphi_1^{1p}(x_1)\,\varphi_2^{1p}(x_2) - \varphi_2^{1p}(x_1)\,\varphi_1^{1p}(x_2) \longrightarrow \frac{1}{\sqrt{2}}\left(|\varphi_1^{1p}\rangle|\varphi_2^{1p}\rangle - |\varphi_2^{1p}\rangle|\varphi_1^{1p}\rangle\right)$$

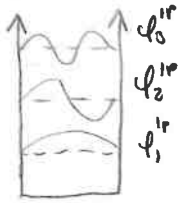
$$\begin{vmatrix} \varphi_1^{1p}(x_1) & \varphi_1^{1p}(x_2) \\ \varphi_3^{1p}(x_1) & \varphi_3^{1p}(x_2) \end{vmatrix} = \varphi_1^{1p}(x_1)\,\varphi_3^{1p}(x_2) - \varphi_3^{1p}(x_1)\,\varphi_1^{1p}(x_2) \longrightarrow \frac{1}{\sqrt{2}}\left(|\varphi_1^{1p}\rangle|\varphi_3^{1p}\rangle - |\varphi_3^{1p}\rangle|\varphi_1^{1p}\rangle\right)$$

$$\begin{vmatrix} \varphi_2^{1p}(x_1) & \varphi_2^{1p}(x_2) \\ \varphi_3^{1p}(x_1) & \varphi_3^{1p}(x_2) \end{vmatrix} = \varphi_2^{1p}(x_1)\,\varphi_3^{1p}(x_2) - \varphi_3^{1p}(x_1)\,\varphi_2^{1p}(x_2) \longrightarrow \frac{1}{\sqrt{2}}\left(|\varphi_2^{1p}\rangle|\varphi_3^{1p}\rangle - |\varphi_3^{1p}\rangle|\varphi_2^{1p}\rangle\right)$$

Base N=2 (Férmions): $\{|\varphi_1^{(A)N=2}\rangle, |\varphi_2^{(A)N=2}\rangle, |\varphi_3^{(A)N=3}\rangle\}$

Serão auto-estados de H ? Nem sempre.

E o caso de $M=2$ bósons?



Base de 1p $\{|\varphi_1^{1p}\rangle, |\varphi_2^{1p}\rangle, |\varphi_3^{1p}\rangle\}$

$$\Psi^S(x_1,x_2) = +\Psi^S(x_2,x_1)$$

$$\Rightarrow \sum C_K^{\Psi}\, \varphi_K^{(S)\,N=2}(x_1,x_2) = \sum C_K^{\Psi}\, \varphi_K^{(S)\,N=2}(x_2,x_1)$$

Base simetrizada: combinações simétrica de N estados de 1p (podem ser iguais). $\Rightarrow$ 6 possibilidades

- $|\varphi_1^{(S)\,N=2}\rangle = |\varphi_1^{1p}\rangle \otimes |\varphi_1^{1p}\rangle \left(\Rightarrow \varphi_1^{(S)\,N=2}(x_1,x_2) = \varphi_1^{1p}(x_1)\,\varphi_1^{1p}(x_2)\right)$

$$|\varphi_2^{(S)\,N=2}\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_1^{1p}\rangle|\varphi_2^{1p}\rangle + |\varphi_2^{1p}\rangle|\varphi_1^{1p}\rangle\right)$$

$$|\varphi_3^{(S)\,N=2}\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_1^{1p}\rangle|\varphi_3^{1p}\rangle + |\varphi_3^{1p}\rangle|\varphi_1^{1p}\rangle\right)$$

- $|\varphi_4^{(S)\,N=2}\rangle = |\varphi_2^{1p}\rangle \otimes |\varphi_2^{1p}\rangle \left(\Rightarrow \varphi_4^{(S)}(x_1,x_2) = \varphi_2^{1p}(x_1)\,\varphi_2^{1p}(x_2)\right)$

$$|\varphi_5^{(S)\,N=2}\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_2^{1p}\rangle|\varphi_3^{1p}\rangle + |\varphi_3^{1p}\rangle|\varphi_2^{1p}\rangle\right)$$

- $|\varphi_6^{(S)\,N=2}\rangle = |\varphi_3^{1p}\rangle \otimes |\varphi_3^{1p}\rangle \left(\Rightarrow \varphi_6^{(S)}(x_1,x_2) = \varphi_3^{1p}(x_1)\,\varphi_3^{1p}(x_2)\right)$