Operadores de 2 cuerpos

$$\hat{O}_2 = \sum_{i,j>i}^{N} \hat{g}(i,j) \qquad \text{por ejemplo } \hat{g}(i,j) = \frac{1}{r_{ij}}$$

En este caso, $\frac{1}{|\vec{r}_{ij}|}$ es simétrico.

(dim 3)

$$\hat{O}_2 = \hat{g}(1,2)\,\mathbb{1}(3) + \hat{g}(1,3)\,\mathbb{1}(2) + \mathbb{1}(1)\,\hat{g}(2,3)$$

(dim 2)

$$\hat{O}_2 = \hat{g}(1,2)$$

Veamos $\langle O_2 \rangle$ para un estado de 2 partículas.

$$|ab\rangle^{(AS)} = \frac{1}{\sqrt{2}}\left(\phi_a(1)\phi_b(2) - \phi_b(1)\phi_a(2)\right)$$

$$\langle ab|\hat{O}_2|ab\rangle = \int \frac{1}{\sqrt{2}}\left(\phi_a^*(1)\phi_b^*(2) - \phi_b^*(1)\phi_a^*(2)\right) \cdot$$

$$\frac{1}{\sqrt{2}}\left(\hat{g}(1,2)\,\phi_a(1)\phi_b(2) - \hat{g}(1,2)\,\phi_b(1)\phi_a(2)\right) d_1 d_2$$

distribuyo)

$$\langle O_2 \rangle = \frac{1}{2}\left(\cdots\right)$$

① α

$$\text{I)} \int d_1 d_2\, \phi_a^*(1)\, \phi_b^*(2) \frac{1}{r_{12}} \phi_a(1)\, \phi_b(2)$$

$$- \int d_1 d_2\, \phi_a^*(1)\, \phi_b^*(2)\, \hat{g}(1,2)\, \phi_b(1)\, \phi_a(2)$$

$\langle ab|ba \rangle$

$$- \int d_1 d_2\, \phi_b^*(1)\, \phi_a^*(2)\, \hat{g}(1,2)\, \phi_a(1)\, \phi_b(2)$$

$\phi_b(2)\, \phi_a(1) \qquad \phi_a(2)\, \phi_b(1) \rightarrow ab|ba$

$$+ \int d_1 d_2\, \phi_b^*(1)\, \phi_a^*(2)\, g(1,2)\, \phi_b(1)\, \phi_a(2)$$

= $e_1 \leftrightarrow e_2$

= $e_1 \leftrightarrow e_2$

$(d_1 \leftrightarrow d_2)$

$$\phi_b^*(2)\, \phi_a^*(1)\, g(2,1)\, \phi_b(2)\, \phi_a(1)$$

$$= \phi_a^*(1)\, \phi_b^*(2)\, g(1,2)\, \phi_a(1)\, \phi_b(2)$$

$$\Rightarrow \langle O_2 \rangle = \frac{1}{2} \left[2 \int d_1 d_2\, a(1) b(2)\, g(1,2)\, \boxed{a(1)\, b(2)} - 2 \int d_1 d_2\, a(1)\, b(2)\, g(1,2)\, \boxed{b(1)\, a(2)} \right]$$

$$\langle O_2 \rangle = \langle ab|ab \rangle - \langle ab|ba \rangle$$

② (β)

Notación (y no tanto...)

$$\langle ab|ab\rangle = \int d_1 d_2\, \phi_a^*(1)\, \phi_b^*(2)\, g(1,2)\, \phi_a(1)\, \phi_b(2)$$

$$= \int d_1 d_2\, |\phi_a(1)|^2 \frac{1}{r_{12}} |\phi_b(2)|^2 \equiv J_{ab}$$

$$\langle ab|ba\rangle = \int d_1 d_2\, \phi_a^*(1)\, \phi_b^*(2)\, \frac{1}{r_{12}}\, \phi_b(1)\, \phi_a(2)$$

$$\equiv K_{ab}$$

J_{ab} es como interacción de coulomb entre las nubes $|\phi_a(1)|^2$ y $|\phi_b(2)|^2$

K_{ab} viene del hecho de que la función de onda es antisimétrica ante el intercambio de 2 part. no tiene un análogo "clásico".

$$\langle \hat{O}_2\rangle = \langle ab|\hat{O}_2|ab\rangle = \langle ab||ab\rangle$$

$$\langle ab||ab\rangle \equiv \langle ab|ab\rangle - \langle ab|ba\rangle$$

$$J_{aa} - K_{aa}$$

Resumen

Sabemos que $\hat{H} = \hat{O}_1 + \hat{O}_2$. De modo que

$$\langle H\rangle = \langle \hat{O}_1\rangle + \langle \hat{O}_2 \rangle \quad ; \quad |K\rangle = |\dots mm\dots\rangle$$

y vimos que:

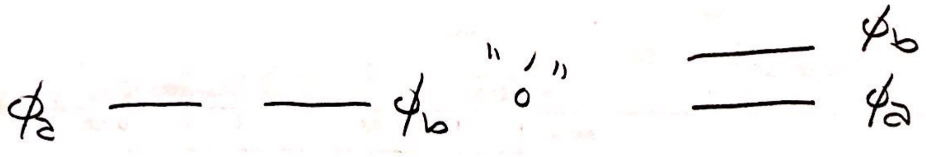
$$\langle \hat{O}_1\rangle = \langle K|\hat{O}_1|K\rangle = \sum_{\alpha}^{N} \overbrace{\langle\alpha|h|\alpha\rangle}^{h_{\alpha\alpha}} \quad ; \quad \alpha \in \{K\}$$

$$\langle \hat{O}_2\rangle = \langle K|\hat{O}_2|K\rangle = \frac{1}{2} \sum_{\alpha}^{N}\sum_{\beta}^{N} \underbrace{\langle\alpha\beta||\alpha\beta\rangle}_{J_{\alpha\beta}-K_{\alpha\beta}}$$

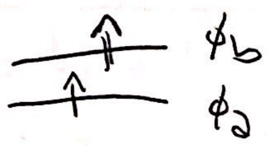
También vimos los casos para $\hat{O}_1$: $\langle K|\hat{O}_1|L\rangle$

Por ahora enfocamos en los valores medios de $\hat{H}$, o sea $|K\rangle \equiv |L\rangle$.

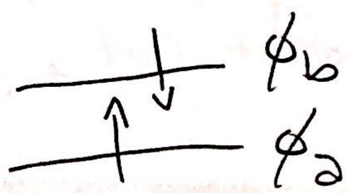
Ejemplo 2 partículas $\{\phi_a, \phi_b\}$



usemos

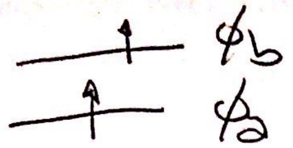


$|\psi\rangle = |ab\rangle$



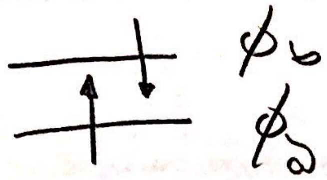
$|\psi\rangle = |a\bar{b}\rangle$

$$|\psi\rangle = |ab\rangle$$



$$\boxed{E_{|ab\rangle} = h_{aa} + h_{bb} + J_{ab} - K_{ab}}$$

$$|\psi\rangle = |a\bar{b}\rangle$$



$$E_{|a\bar{b}\rangle} = h_{aa} + h_{\bar{b}\bar{b}} + J_{a\bar{b}} - \cancel{K_{a\bar{b}}} \to 0$$

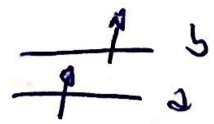
$$h_{\bar{b}\bar{b}} = \int d_1\, \phi_b^*(r_1)\, \beta(1)\, \hat{\theta}(1)\, \phi_b(1)\, \beta(1) \qquad \underbrace{\beta(1)\cdots\beta(1)}_{=1}$$

$$= \int d_1\, \phi_b^*(1)\, \hat{\theta}(1)\, \phi_b(1) \equiv h_{bb}$$

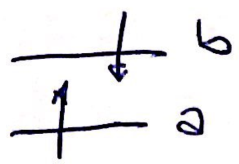
$$\Rightarrow \boxed{h_{bb} \equiv h_{\bar{b}\bar{b}}}$$

* chequeen : $J_{a\bar{b}} = J_{ab}$ y que $K_{a\bar{b}} = 0$

$$\Rightarrow E_{|ab\rangle} = h_{aa} + h_{bb} + J_{ab} - K_{ab}$$



$$E_{|a\bar{b}\rangle} = h_{aa} + h_{bb} + J_{ab}$$



~~Veremos $\langle\psi|H|\psi\rangle$~~

Veamos $\langle\psi|\hat{H}|\psi\rangle$ con $|\psi\rangle = |a\bar{b}\rangle$

$|\psi\rangle = |a\bar{b}\rangle \qquad \alpha = \{a, \bar{b}\}$

$$\langle \Theta_1 \rangle = \sum_{\alpha}^{N} h_{\alpha\alpha} = h_{aa} + h_{\bar{b}\bar{b}}$$

$$\langle \Theta_2 \rangle = \frac{1}{2} \sum_{\alpha,\beta}^{N} \langle \alpha\beta||\alpha\beta\rangle = \frac{1}{2} \sum_{\alpha\beta}^{N} \left(\langle a\beta||a\beta\rangle + \langle \bar{b}\beta||\bar{b}\beta\rangle \right)$$

$$= \frac{1}{2} \left[\langle aa||aa\rangle + \langle a\bar{b}||a\bar{b}\rangle + \langle \bar{b}a||\bar{b}a\rangle + \langle \bar{b}\bar{b}||\bar{b}\bar{b}\rangle \right]$$

.) $\langle aa||aa\rangle \equiv \langle \bar{b}\bar{b}||\bar{b}\bar{b}\rangle = 0$, recien lo vimos

.) $\langle a\bar{b}||a\bar{b}\rangle = \langle a\bar{b}|a\bar{b}\rangle - \langle a\bar{b}|\bar{b}a\rangle$

integro en spin. $\langle a\bar{b}|a\bar{b}\rangle \equiv \langle ab|ab\rangle$

. $\langle a\bar{b}|\bar{b}a\rangle = 0$

.) idem $\langle \bar{b}a||\bar{b}a\rangle$

$$= \langle \bar{b}a|\bar{b}a\rangle - \underbrace{\langle \bar{b}a|a\bar{b}\rangle}_{0} = \langle ba|ba\rangle$$

$$= \langle ab|ab\rangle$$

. parte (1 ⟷ 2)

Hagámoslo según la "tabla":

$|\psi\rangle = |ab\rangle \qquad \alpha \equiv \{a, b\}$

$$\langle \theta_1 \rangle = \sum_{\alpha}^{N} h_{\alpha\alpha} = h_{aa} + h_{bb}$$

$$\langle \theta_2 \rangle = \frac{1}{2}\sum_{\alpha,\beta}^{N} \langle \alpha\beta || \alpha\beta \rangle = \frac{1}{2} \sum_{\beta}^{N} \left(\langle a\beta || a\beta \rangle + \langle b\beta || b\beta \rangle \right)$$

$$= \frac{1}{2}\left(\cancel{\langle aa || aa \rangle} + \langle ab || ab \rangle + \langle ba || ba \rangle + \cancel{\langle bb || bb \rangle} \right)$$

• $\langle aa || aa \rangle = \langle aa | aa \rangle - \langle aa | aa \rangle \equiv 0$

$\langle bb || bb \rangle = 0$

• $\langle ab || ab \rangle = \langle ab | ab \rangle - \langle ab | ba \rangle$ ⊛

• $\langle ba || ba \rangle = \langle ba | ba \rangle - \langle ba | ab \rangle$ ← prop. 1e⁻ 2

$= \langle ab | ab \rangle - \langle ab | ba \rangle$ ⊛

$$\langle \theta_2 \rangle = \langle ab | ab \rangle - \langle ab | ba \rangle \equiv J_{ab} - K_{ab}$$

$$\Rightarrow \langle H \rangle_{|\psi\rangle} = E_{|ab\rangle} = h_{aa} + h_{bb} + J_{ab} - K_{ab}$$

$$\Rightarrow \langle O_2 \rangle = \frac{1}{2}\Big[\cancel{\langle aa \| aa \rangle}^{0} + \langle a\bar{b} \| a\bar{b} \rangle + \langle \bar{b}a \| \bar{b}a \rangle + \cancel{\langle b\bar{b} \| b\bar{b} \rangle}^{0}\Big]$$

$$= \frac{1}{2}\Big[\langle a\bar{b} | a\bar{b} \rangle - \overbrace{\langle a\bar{b} | \bar{b}a \rangle}^{0} + \langle \bar{b}a | \bar{b}a \rangle - \underbrace{\langle \bar{b}a | a\bar{b} \rangle}_{0}\Big]$$

xspin

$$\langle O_2 \rangle = \frac{1}{2}\Big(\langle ab | ab \rangle + \underbrace{\langle ba | ba \rangle}_{\langle ab | ab \rangle}\Big) \leftarrow 1 \leftrightarrow 2$$

$$\langle O_2 \rangle = \langle ab | ab \rangle \equiv J_{ab}$$

$$\Rightarrow |\psi\rangle = |a\bar{b}\rangle$$

b

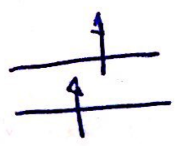
a

$$E_{|\psi\rangle} = h_{aa} + \underbrace{h_{\bar{b}\bar{b}}}_{= h_{bb}} + J_{ab}$$

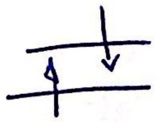
] just for 2 rates.

Scanned with CamScanner

Resumen (2)



$|\psi_1\rangle = |ab\rangle$

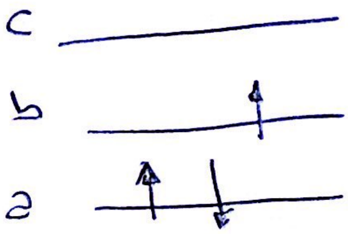


$|\psi_2\rangle = |a\bar{b}\rangle$

$$E_1 = \langle ab|\hat{H}|ab\rangle = h_{aa} + h_{bb} + J_{ab} - K_{ab}$$

$$E_2 = \langle a\bar{b}|\hat{H}|a\bar{b}\rangle = h_{aa} + h_{bb} + J_{ab}$$

$$\boxed{E_1 < E_2}$$



$$E = h_{aa} + h_{\bar{a}\bar{a}} + h_{bb} + J_{a\bar{a}} + J_{ab} + J_{\bar{a}b} - K_{ab}$$

ver: $J_{a\bar{a}} \equiv J_{aa}$ | $E = 2h_{aa} + h_{bb} + J_{aa} + 2J_{ab} - K_{ab}$

$J_{\bar{a}b} = J_{ab}$

$h_{\bar{a}\bar{a}} = h_{aa}$