Resumen

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

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

y vimos que:

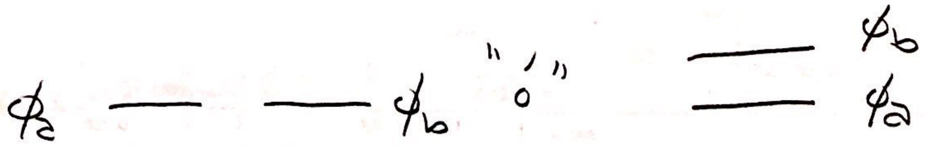
$$\langle \hat{O}_1\rangle = \langle K|\hat{O}_1|K\rangle = \sum_{\alpha}^{N} \overbrace{\langle\alpha|h|\alpha\rangle}^{h_{\alpha\alpha}} \quad ; \quad \alpha \in \{K\}$$

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

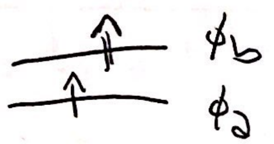
También vimos los casos para $\hat{O}_1$: $\langle K|\hat{O}_1|L\rangle$

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

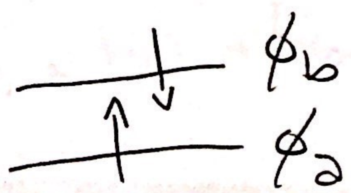
Ejemplo 2 partículas $\{\phi_a, \phi_b\}$



usemos

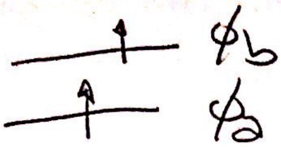


$|\psi\rangle = |ab\rangle$



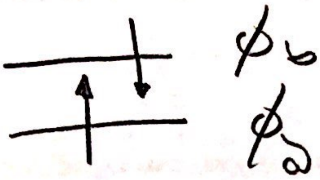
$|\psi\rangle = |a\bar{b}\rangle$

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



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

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



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

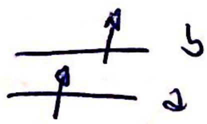
$$h_{\bar{b}\bar{b}} = \int d_1\, \phi_b^*(r_1)\, \beta(1)\, \hat{O}(1)\, \phi_b(1)\, \beta(1) \quad \text{con } \beta(1)\ldots\beta(1) = 1$$

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

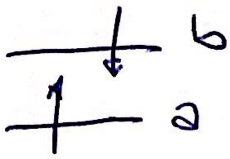
$$\Rightarrow \boxed{h_{bb} \equiv h_{\bar{b}\bar{b}}}$$

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

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

$$\langle O_1\rangle = \sum_{\alpha}^{N} h_{\alpha\alpha} = h_{aa} + h_{\bar{b}\bar{b}}$$

$$\langle O_2\rangle = \frac{1}{2}\sum_{\alpha,\beta}^{N} \langle\alpha\beta||\alpha\beta\rangle = \frac{1}{2}\sum_{\alpha\beta}^{N}\left(\langle a\beta||a\beta\rangle + \langle\bar{b}\beta||\bar{b}\beta\rangle\right)$$

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

·) $\langle aa||aa\rangle \equiv \langle\bar{b}\bar{b}||\bar{b}\bar{b}\rangle = 0$, recién 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 $(1 \Rightarrow 2)$

Hagámoslo según la "tabla":

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

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

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

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

·) $\langle aa || aa \rangle = \langle aa | aa \rangle - \langle aa | aa \rangle \equiv 0$

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

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

·) $\langle ba || ba \rangle = \langle ba | ba \rangle - \langle ba | ab \rangle \leftarrow$ | prop. $1e \to 2$

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

$$\langle \Theta_2 \rangle = \langle ab | ab \rangle - \langle ab | ba \rangle \equiv J_{ab} - K_{ab}$$

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

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

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

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

xspin

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

$$\rightarrow |\Psi\rangle = |a\bar{b}\rangle$$

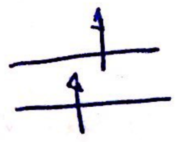
$$E_{|\Psi\rangle} = h_{aa} + \underbrace{h_{\bar{b}\bar{b}}}_{= h_{bb}} + J_{ab}$$

igual que antes.

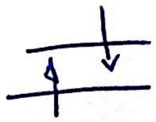
Scanned with CamScanner

Resumen (2)

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



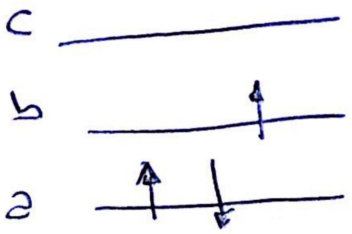
$|\psi_2\rangle = |a\bar{b}\rangle$



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

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

$$\boxed{E_1 < E_2}$$



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

ver: $J_{a\bar{a}} \equiv J_{aa}$

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

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

$$E = 2h_{aa} + h_{bb} + J_{aa} + 2J_{ab} - K_{ab}$$