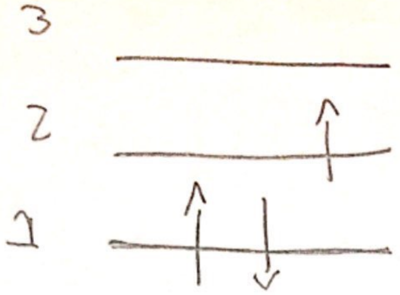


$$|1\bar{1}2\rangle$$

$$\hat{S}^2 = \hat{S}_-\hat{S}_+ + \hat{S}_z + \hat{S}_z^2$$

$$\hat{S}_z = \hat{s}_z(1)\,\hat{\mathbb{I}}(2)\,\hat{\mathbb{I}}(3) + \hat{\mathbb{I}}(1)\,\hat{s}_z(2)\,\hat{\mathbb{I}}(3) + \hat{\mathbb{I}}(1)\,\hat{\mathbb{I}}(2)\,\hat{s}_z(3)$$

$$\hat{S}_z|1\bar{1}2\rangle = |s_z(1)\bar{1}2\rangle + |1\,s_z(\bar{1})\,2\rangle + |1\bar{1}\,s_z(2)\rangle$$

$$= 1/2\,|1\bar{1}2\rangle - 1/2\,|1\bar{1}2\rangle + 1/2\,|1\bar{1}2\rangle$$

$$= \boxed{1/2}\,|1\bar{1}2\rangle$$

$$\hat{S}_z^2|1\bar{1}2\rangle = (1/2)(1/2)\,|1\bar{1}2\rangle$$

$$\hat{S}_-\hat{S}_+(|1\bar{1}2\rangle) = \hat{S}_-\left(\hat{S}_+|1\bar{1}2\rangle\right) =$$

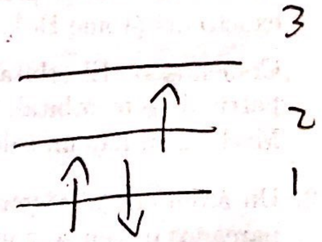
$$= \hat{S}_-\left(0 + |112\rangle + 0\right) = 0$$

$$\hat{S}^2_- |1\bar{1}2\rangle = (1/2 + 1/2 \; 1/2)\,|1\bar{1}2\rangle$$

$$= 1/2\,(1/2+1)\,|1\bar{1}2\rangle$$

$$\boxed{S = 1/2}$$

Energía



$$\langle 1\bar{1}2|H|1\bar{1}2\rangle$$

$\theta_1 = h_{11} + h_{\bar{1}\bar{1}} + h_{22}$, recordar $h_{11} = h_{\bar{1}\bar{1}}$

$$= 2h_{11} + h_{22}$$

$$\theta_2 = J_{1\bar{1}} + J_{12} + J_{\bar{1}2} - K_{12}$$

chequear con la def de J_{ij} : $J_{\bar{1}2} = J_{12}$

$$J_{1\bar{1}} = J_{11}$$

$$\Rightarrow \boxed{\langle H \rangle = 2h_{11} + h_{22} + 2J_{12} + J_{11} - K_{12}}$$

con La tabla

occ $= \{1, \bar{1}, 2\}$

$$\langle \theta_1 \rangle = \sum_i^{occ} \langle i|h|i\rangle$$

$$= h_{11} + h_{\bar{1}\bar{1}} + h_{22}$$

$$\langle \theta_2 \rangle = \frac{1}{2} \sum_i^{occ} \sum_j^{occ} \langle ij||ij\rangle$$

$i = \{1, \bar{1}, 2\}$
$j = \{1, \bar{1}, 2\}$

$$= \frac{1}{2} \sum_i^{occ} \left[\langle i1||i1\rangle + \langle i\bar{1}||i\bar{1}\rangle + \langle i2||i2\rangle \right]$$

$$\langle i1||i1\rangle = \underbrace{\langle 11||11\rangle}_{0} + \underbrace{\langle \bar{1}1||\bar{1}1\rangle}_{0} + \langle 21||21\rangle$$

$$\langle 21|21\rangle - \langle 21|12\rangle$$

$\vdots$

$$\langle i\bar{1}||i\bar{1}\rangle = \underbrace{\langle 1\bar{1}||1\bar{1}\rangle}_{0} + \underbrace{\langle \bar{1}\bar{1}||\bar{1}\bar{1}\rangle}_{0} + \langle 2\bar{1}||2\bar{1}\rangle$$

$$= \langle 2\bar{1}|2\bar{1}\rangle - \underbrace{\langle 2\bar{1}|\bar{1}2\rangle}_{0}$$

x spin

$$= \langle 21|21\rangle$$

and so on ...

| Notas sobre | h_{ij}, K_{ab}, J_{ab} $\boxed{\text{Clase 2}}$

Repaso

$$h_{ij} = \int d^3x \; \phi_i^*(x) \, \hat{h} \, \phi_j(x)$$

$$J_{ab} = \int d^3x_1 \, d^3x_2 \; \phi_a^*(1) \, \phi_b^*(2) \, \hat{\Theta}(1,2) \, \phi_a(1) \, \phi_b(2)$$

depende de x_1 y x_2

$$\equiv \langle ab|ab\rangle$$

$$K_{ab} = \int d^3x_1 \, d^3x_2 \; \phi_a(1) \, \phi_b(2) \, \hat{\Theta}(1,2) \, \phi_a(2) \, \phi_b(1)$$

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

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

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