AULA 20

Aplicações para Sistemas de Muitos Corpos (cap. 22)

1. Momento angular em um sistema de partículas Idênticas

$\vec{J}$ é deste tipo $\quad K = \sum_{kl} a_k^\dagger a_l \langle k|K|l\rangle$

$$\vec{J} = \sum_{\substack{\alpha\alpha' \\ JJ' \\ mm'}} a^\dagger_{\alpha J M}\, a_{\alpha' J' m'} \langle \alpha J M|\vec{J}|\alpha' J' m'\rangle$$

O que sabemos sobre isto?

$$\langle \alpha J M|\vec{J}|\alpha' J' m'\rangle = \langle \alpha J M|\vec{J}|\alpha J m'\rangle\, \delta_{\alpha\alpha'}\delta_{JJ'}$$

$$\therefore \boxed{\vec{J} = \sum_{\alpha J}\sum_{mm'} a^\dagger_{\alpha J M}\, a_{\alpha J m'} \langle jM|\vec{J}|jm'\rangle}$$

$|jm\rangle$ caracteriza o estado de 1-partícula (o papel do $|K_i\rangle$)

$J^2 = \vec{J}\cdot\vec{J}$ acopla momentos angulares das partículas

$$J^2 \neq j_1^2 + j_2^2 + \ldots$$

Estado de 2-partículas autoestados de J_z e J^2 com autovalores $m\hbar$ e $J(J+1)\hbar^2$

$$|j_1 j_2 j m\rangle = \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle$$

o que significa isto: Que tal 2 partículas, uma com j_1 e outra com j_2 dando um estado global com momento angular j e componente m

na linguagem de 2ª quantização

$|j_1 j_2 m_1 m_2\rangle = |j_1 m_1\rangle \otimes |j_2, m_2\rangle$ estará relacionado a

$a^+_{j_2 m_2} a^+_{j_1 m_1} |\underline{0}\rangle$ (uma partícula em $j_1 m_1$ e outra em $j_2 m_2$)

assim que tal:

$$\boxed{\Psi^{(2)}_{JM} = C \sum_{m_1 m_2} a^+_{j_2 m_2 \alpha_2} a^+_{j_1 m_1 \alpha_1} |0\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle}$$

Normalização

$$1 = \left(\Psi^{(2)}_{JM}, \Psi^{(2)}_{JM}\right) = |C|^2 \sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \langle 0 | a_{j_1 m_1' \alpha_1} a_{j_2 m_2' \alpha_2} a^+_{j_2 m_2 \alpha_2} a^+_{j_1 m_1 \alpha_1} |0\rangle$$
$$\langle j_1 j_2 j m | j_1 j_2 m_1' m_2'\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle$$

$$= |C|^2 \sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \langle 0 | a_{j_1 m_1' \alpha_1} \left(\delta_{m_2 m_2'} \pm a^+_{j_2 m_2 \alpha_2} a_{j_2 m_2' \alpha_2}\right) a^+_{j_1 m_1 \alpha_1} |0\rangle$$
$$\langle \quad \rangle \langle \quad \rangle$$

caso $\alpha_1 \neq \alpha_2$ ou $j_1 \neq j_2$

$$= |C|^2 \sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \delta_{m_1' m_1} \delta_{m_2' m_2} \langle j_1 j_2 j m | j_1 j_2 m_1' m_2' \rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle$$

$$= |C|^2 \sum_{m_1 m_2} \langle j_1 j_2 j m | j_1 j_2 m_1 m_2 \rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle$$

$$= |C|^2 \quad \therefore \quad \boxed{C = 1}$$

O caso $\alpha_1 = \alpha_2$ e $j_1 = j_2$ fica para vocês

2. Momento angular e operadores de "spin 1/2 de Bósons"

Se postularmos um bóson fictício com spin 1/2 e com nenhuma outra propriedade dinâmica, o momento angular total poderia ser tirado de:

$$\vec{J} = \sum_{\alpha} \sum_{j} \sum_{m m'} a^{+}_{j m' \alpha} a_{j m \alpha} \langle j m' | \vec{J} | j m \rangle$$

$j = 1/2$ sem α (nenhuma outra propriedade dinâmica)

$m = \pm 1/2 \quad m' = \pm 1/2 \quad \vec{J} = (S_x, S_y, S_z)$

$\doteq \frac{\hbar}{2} \vec{\sigma}$ matriz de Pauli

$$\vec{J} = \frac{\hbar}{2} \sum_{m m'} a^{+}_{m'} \vec{\sigma}_{m' m} a_m$$

$$= \frac{\hbar}{2} \begin{pmatrix} a^{+}_{1/2} & a^{+}_{-1/2} \end{pmatrix} \vec{\sigma} \begin{pmatrix} a_{1/2} \\ a_{-1/2} \end{pmatrix}$$

note que

$$J_+ = J_x + i J_y$$

e $J_- = J_x - J_y$

fornece

$$\sigma_+ = \sigma_x + i\sigma_y$$

$$\sigma_- = \sigma_x - i\sigma_y$$

e com isso poderíamos definir

$$J_+ = \frac{\hbar}{2}\begin{pmatrix} a^\dagger_{1/2} & a^\dagger_{-1/2}\end{pmatrix}\left\{\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}}_{\sigma_x} + i\underbrace{\begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}}_{\sigma_y}\right\}\begin{pmatrix} a_{1/2} \\ a_{-1/2}\end{pmatrix}$$

$$= \frac{\hbar}{2}\underbrace{\begin{pmatrix} a^\dagger_{1/2} & a^\dagger_{-1/2}\end{pmatrix}}_{1\times 2}\underbrace{\begin{pmatrix} 0 & 2 \\ 0 & 0\end{pmatrix}}_{2\times 2}\begin{pmatrix} a_{1/2} \\ a_{-1/2}\end{pmatrix} = \hbar\begin{pmatrix} 0 & a^\dagger_{1/2}\end{pmatrix}\begin{pmatrix} a_{1/2} \\ a_{-1/2}\end{pmatrix}$$

$$= \hbar \underset{\substack{\downarrow \\ \text{cria } +1/2}}{a^\dagger_{1/2}}\ \underset{\substack{\downarrow \\ \text{some } -1/2}}{a_{-1/2}} \quad \text{(muda m em +1)}$$

Similarmente, pode-se obter

$$J_- = \hbar \underset{\substack{\downarrow \\ \text{cria } -1/2}}{a^\dagger_{-1/2}}\ \underset{\substack{\downarrow \\ \text{some } 1/2}}{a_{1/2}} \quad \text{(muda m em -1)}$$

$$J_z = \frac{\hbar}{2}\left(\underbrace{a^\dagger_{1/2}a_{+1/2}}_{\text{conta } 1/2} - \underbrace{a^\dagger_{-1/2}a_{-1/2}}_{\text{conta } -1/2}\right) \quad \text{(diferença de "m")}$$

lembre que

$$J^2 = J_x^2 + J_y^2 + J_z^2$$

$$= \left(\frac{J_+ + J_-}{2}\right)^2 + \left(\frac{J_+ - J_-}{2i}\right)^2 + J_z^2$$

$$= J_z^2 + \frac{J_+^2}{4} + \frac{J_-^2}{4} + \frac{J_+J_- + J_-J_+}{4}$$

$$- \frac{J_+^2}{4} - \frac{J_-^2}{4} - \frac{(J_+J_- + J_-J_+)}{-4}$$

$$= J_z^2 + \frac{J_+J_- + J_-J_+}{2}$$

$$\therefore \; J^2 = \frac{\hbar^2}{4}\left(a^+_{1/2} a_{1/2} - a^+_{-1/2} a_{-1/2}\right)^2 + \frac{\hbar^2}{2}\Big(\underbrace{a^+_{1/2} a_{-1/2}}_{J_+/\hbar} \underbrace{a^+_{-1/2} a_{1/2}}_{J_-/\hbar}$$

$$+ \underbrace{a^+_{-1/2} a_{1/2}}_{J_-/\hbar} \underbrace{a^+_{1/2} a_{-1/2}}_{J_+/\hbar}\Big)$$

os dois ultimos termos

$$\frac{\hbar^2}{2}\left\{ a^+_{1/2} a_{-1/2} \left(a_{1/2} a^+_{-1/2}\right) + a^+_{-1/2} a_{1/2} \left(a_{-1/2} a^+_{1/2}\right) \right\} =$$

regra de comutação de Bosons

$$\frac{\hbar^2}{2}\left\{ a^+_{1/2} \left(a_{1/2} a_{-1/2}\right) a^+_{-1/2} + a^+_{-1/2} \left(a_{-1/2} a_{1/2}\right) a^+_{1/2} \right\}$$

$$= \frac{\hbar^2}{2}\left\{ a^+_{1/2} a_{1/2} \left(1 + a^+_{-1/2} a_{-1/2}\right) + a^+_{-1/2} a_{-1/2} \left(1 + a^+_{1/2} a_{1/2}\right) \right\}$$

$$= \frac{\hbar^2}{2}\left(a^{+}_{1/2} a_{+1/2} + a^{+}_{-1/2} a_{-1/2} \right) + \underbrace{\frac{\hbar^2}{2}}_{2\frac{\hbar^2}{4}}\left(a^{+}_{1/2} a_{1/2} a^{+}_{-1/2} a_{-1/2} \right.$$

$$\left. + a^{+}_{-1/2} a_{-1/2} a^{+}_{+1/2} a_{+1/2} \right)$$

o primeiro termo de J^2 é:

$$\frac{\hbar^2}{4}\left(\left(a^{+}_{1/2} a_{1/2}\right)^2 + \left(a^{+}_{-1/2} a_{-1/2}\right)^2 - a^{+}_{1/2} a_{+1/2} a^{+}_{-1/2} a_{-1/2} \right.$$

$$\left. - a^{+}_{-1/2} a_{-1/2} a^{+}_{1/2} a_{1/2} \right)$$

que somado à expressão acima fica

$$J^2 = \frac{\hbar^2}{4}\left(a^{+}_{1/2} a_{1/2} + a^{+}_{-1/2} a_{-1/2} \right)^2 + \frac{\hbar^2}{2}\left(a^{+}_{1/2} a_{1/2} + a^{+}_{-1/2} a_{-1/2} \right)$$

$$= \frac{\hbar^2}{4} N^2 + \frac{\hbar^2}{2} N = \hbar^2 \frac{N}{2}\left(\frac{N}{2} + 1\right)$$

onde $N = a^{+}_{1/2} a_{1/2} + a^{+}_{-1/2} a_{-1/2} = N_+ + N_-$

Esperamos que $J = \frac{n}{2}$ $\therefore$ $\boxed{n = n_+ + n_- = 2J}$ J inteiro ou semi-inteiro

O autovalor do J_z $\frac{\hbar}{2}(n_+ - n_-) = \hbar M$

$\therefore$ $\boxed{n_+ - n_- = 2M}$

$\therefore \quad n_+ = J + M \qquad n_- = J - M$

O que é $|n_+ n_-\rangle$?

é autoket de $N_+ |n_+ n_-\rangle = n_+ |n_+ n_-\rangle$

é autoket de $N_- |n_+ n_-\rangle = n_- |n_+ n_-\rangle$

é autoket de $J^2 | n_+ n_-\rangle = \hbar^2 \left(\frac{N_+ + N_-}{2} \right) \left(\frac{N_+ + N_-}{2} + 1 \right) | n_+ n_- \rangle$

$$= \hbar^2 \left(\frac{n_+ + n_-}{2} \right) \left(\frac{n_+ n_-}{2} + 1 \right) | n_+ n_- \rangle$$

$$= \hbar^2 \frac{2J}{2} \left(\frac{2J}{2} + 1 \right) | n_+ n_- \rangle$$

$$= J (J+1) \hbar^2 | n_+ n_- \rangle$$

é autoket de $J_z |n_+ n_-\rangle = \frac{\hbar}{2} \left(N_+ - N_- \right) |n_+ n_-\rangle$

$$= \frac{\hbar}{2} \left(n_+ - n_- \right) | n_+ n_- \rangle$$

$$= \frac{\hbar}{2} 2m |n_+ n_-\rangle = M\hbar |n_+ n_-\rangle$$

$\therefore \boxed{|JM\rangle = |n_+ n_-\rangle}$ onde $\langle n_+ n_- | n_+ n_- \rangle = 1$

mas $a^\dagger_{-1/2} |n_+ 0\rangle = \sqrt{0+1} |n_+ 1\rangle = \sqrt{1!} |n_+ 1\rangle$

$$(a^\dagger_{-1/2})^2 |n_+ 0\rangle = \sqrt{0+1}\sqrt{1+1} |n_+ 2\rangle = \sqrt{2!} |n_+ 2\rangle$$

$$(a^\dagger_{-1/2})^{n_-} |n_+ 0\rangle = \sqrt{n_-!} |n_+ n_-\rangle$$

$$\therefore \quad (a^\dagger_{1/2})^{n_+} (a^\dagger_{-1/2})^{n_-} |00\rangle = \sqrt{n_+!}\sqrt{n_-!} |n_+ n_-\rangle$$

$$\therefore \ |n_+ n_-\rangle = \frac{1}{\sqrt{n_+!\,n_-!}} \left(a^+_{1/2}\right)^{n_+} \left(a^+_{-1/2}\right)^{n_-} |00\rangle$$

$$\therefore \boxed{|JM\rangle = \frac{1}{\sqrt{(J+M)!\,(J-M)!}} \left(a^+_{1/2}\right)^{J+M} \left(a^+_{-1/2}\right)^{J-M} |00\rangle}$$

Teoria de Perturbação de 1ª ordem em sistemas de Muitos Corpos

$$\mathcal{H} = \sum_{ij} a_i^+ a_j \langle i|H_0|j\rangle + \frac{1}{2}\sum_{qrst} a_q^+ a_r^+ a_s a_t \langle qr|V|ts\rangle$$

suponha H_0 diagonal

$$\langle i|H_0|j\rangle = \varepsilon_i \delta_{ij}$$

$$\mathcal{H} = \sum_i \varepsilon_i a_i^+ a_i + \frac{1}{2}\sum_{qrst} a_q^+ a_r^+ a_s a_t \langle qr|V|ts\rangle$$

e TP 1ª ordem $\quad \mathcal{H}_0 \qquad\qquad V$

p/ um estado $|n_1 n_2 \ldots\rangle$ autoestado de $\mathcal{H}_0$

$$\mathcal{H}_0|n_1 n_2\ldots\rangle = \left(\sum_i \varepsilon_i n_i\right)|n_1 n_2 \ldots\rangle$$

$$\therefore E_{n_1 n_2\ldots} = \sum_i \varepsilon_i n_i + \frac{1}{2}\sum_{qrst} \langle n_1 n_2 \ldots| a_q^+ a_r^+ a_s a_t |n_1 n_2\ldots\rangle \langle qr|V|ts\rangle$$

Calculando

$$\langle n_1 n_2 \dots | a_q^+ a_r^+ a_s a_t | n_1 n_2 \dots \rangle$$

Suponha $q = r$

$$\langle n_1 n_2 | (a_r^+)^2 a_s a_t | n_1 n_2 \dots \rangle = 0$$ se $t \neq s$ pois $(a_r^+)^2$ não pode recompor ambos ao mesmo tempo

$$= 0$$ se $t = s \neq r$

só é $\neq 0$ se $r = s = t$ e dá:

$$\langle n_1 n_2 | (a_q^+)^2 (a_q)^2 | n_1 n_2 \dots \rangle$$

$$= \sqrt{n_q}\sqrt{n_q - 1}\sqrt{(n_q-2)+1}\sqrt{(n_q-1)+1} = n_q(n_q - 1)$$

$q \neq r$

$\langle n_1 n_2 | a_q^+ a_r^+ a_s a_t | n_1 n_2 \rangle$ agora

ou $q = s$ e $r = t$

$$\langle n_1 n_2 | a_q^+ a_r^+ a_q a_r | n_1 n_2 \rangle = \pm \langle n_1 n_2 | a_q^+ a_q a_r^+ a_r | n_1 n_2 \dots \rangle$$

$$= \pm n_q n_r$$

ou $q = t$ e $r = s$

$$\langle n_1 n_2 | a_q^+ a_r^+ a_r a_q | n_1 n_2 \rangle = (\pm)(\pm) n_q n_r = n_q n_r$$

$$\therefore E_{n_1 n_2 \dots} = \sum \varepsilon_i n_i + \frac{1}{2}\sum_{q \neq r} n_q n_r \langle q r | V | q r \rangle$$

direto

Bosons

$$\pm \frac{1}{2}\sum_{q \neq r} n_q n_r \langle q r | V | r q \rangle$$

férmions

troca

$$+ \frac{1}{2}\sum_{q} n_q(n_q - 1) \langle q q | V | q q \rangle$$

pois $n_q = 0$ ou 1

$= 0$ p/ férmions

Como descrever um átomo?

que tal $\prod a^{+}_{n_i l_i m_i m_s} |0\rangle$

n_i — Nº Quântico radial; l_i — L^2; m_i — L_z; m_s — S_z

$$|\psi^{(2)}_{n_1 l_1 n_2 l_2} (L S M_L M_S)\rangle$$

$$= \sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \langle \underbrace{l_1 l_2 m_1 m_2}_{\text{parte orbital}} \; \underbrace{1/2\, 1/2\, m_1' m_2'}_{\text{parte de spin}} | l_1 l_2 L M_L \; 1/2\, 1/2\, S M_S \rangle$$

$$a^{+}_{n_2 l_2 m_2 m_2'} \, a^{+}_{n_1 l_1 m_1 m_1'} |0\rangle$$

inspirado no caso anterior

$$\psi^{(2)}_{JM} = C \sum_{m_1 m_2} a^{+}_{j_2 m_2 \alpha_2} a^{+}_{j_1 m_1 \alpha_1} \langle j_1 j_2 m_1 m_2 | j_1 j_2 J M \rangle \psi^{(0)}$$

Estado fundamental do átomo de Hélio

$(1s)^2$

$$|\psi^{(2)}_{1010} (0000)\rangle = a^{+}_{100-1/2} \, a^{+}_{100 1/2} |\underline{0}\rangle$$

Estados tripletos $(1s)(n\ell)$

$$|\Psi^{(2)}_{10n\ell}(\ell 1 m_L 1)\rangle = \sum_{\substack{m \\ m_1' m_2'}} \langle 0 \ell 0 m | 0 \ell \ell M_L \rangle \langle \tfrac12 \tfrac12 m_1' m_2' | \tfrac12 \tfrac12 1 1 \rangle$$

tripleto $\;\; L$

$$a^{+}_{n\ell m m_2'} \, a^{+}_{100 1/2} |\underline{0}\rangle$$

note $M_L = m$

$m_1' = m_2' = 1/2$

$$|\Psi^{(2)}_{10n\ell}(\ell 1 m 1)\rangle = a^{+}_{n\ell m 1/2} \, a^{+}_{100 1/2} |\underline{0}\rangle$$

mostre que

$$|\Psi^{(2)}_{10n\ell}(\ell 1 m 0)\rangle = \frac{1}{\sqrt{2}} \left(a^{+}_{n\ell m,-1/2} \, a^{+}_{100,1/2} + a^{+}_{n\ell m, 1/2} \, a^{+}_{100,-1/2} \right) |\underline{0}\rangle$$

$$|\Psi^{(2)}_{10n\ell}(\ell 1 m -1)\rangle = a^{+}_{n\ell m -1/2} \, a^{+}_{100 -1/2} |\underline{0}\rangle$$

e o singleto

$$|\Psi^{(2)}_{10n\ell}(\ell 0 m 0)\rangle = \frac{1}{\sqrt{2}} \left(a^{+}_{n\ell m,-1/2} \, a^{+}_{100,1/2} - a^{+}_{n\ell m,+1/2} \, a^{+}_{100,-1/2} \right) |\underline{0}\rangle$$