

Drawings That We Use in Many-Body Physics

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1 Slater determinants

Drawing the reference state will result in a drawing of nothing. A single-excited reference state is two vertical arrows

$$\Phi_i^a = \begin{array}{c} | \\ | \\ \text{i} \nearrow \\ | \\ | \\ \text{a} \searrow \\ | \\ | \end{array} , \quad (1)$$

while the double-excited Slater determinant consists of four vertical arrows,

$$\Phi_{ij}^{ab} = \begin{array}{c} | \\ | \\ \text{i} \nearrow \\ | \\ | \\ \text{a} \searrow \\ | \\ | \\ \text{j} \nearrow \\ | \\ | \\ \text{b} \searrow \\ | \\ | \end{array} . \quad (2)$$

The horizontal positions of the lines have no significance. If we want to indicate a bra or ket form we draw a couple of horizontal lines,

$$|\Phi_i^a\rangle = \{\hat{a}^\dagger \hat{i}\} |0\rangle = \begin{array}{c} | \\ | \\ \text{i} \nearrow \\ | \\ | \\ \text{a} \searrow \\ | \\ | \end{array} , \quad \langle \Phi_i^a| = \langle 0| \{\hat{i}^\dagger \hat{a}\} = \begin{array}{c} \overline{\overline{|}} \\ \overline{\overline{|}} \\ \text{i} \nearrow \\ | \\ | \\ \text{a} \searrow \\ | \\ | \end{array} , \quad (3)$$

where $\{ABC\dots\}$ is a normal ordered product relative to the Fermi vacuum. A double-excited ket state could be drawn like

$$\left| \phi_{ij}^{ab} \right\rangle = \{ \hat{a}^\dagger \hat{b}^\dagger \hat{j} \hat{i} \} |0\rangle = \{ (\hat{a}^\dagger \hat{i}) (\hat{b}^\dagger \hat{j}) \} |0\rangle = \begin{array}{cccc} & & & \\ & & & \\ & & & \\ & & & \\ \text{i} \uparrow & \downarrow \text{a} & \text{j} \uparrow & \downarrow \text{b} \\ \hline \hline \end{array} \quad (4)$$

This drawing could, however, also mean $\left| \phi_{ij}^{ba} \right\rangle$. The use of diagrams will be independent of this ambiguity, as long as one remains consistent. To be precise one can introduce dotted/dashed lines,

$$\left| \phi_{ij}^{ab} \right\rangle = \{ \hat{a}^\dagger \hat{b}^\dagger \hat{j} \hat{i} \} |0\rangle = \{ (\hat{a}^\dagger \hat{i}) (\hat{b}^\dagger \hat{j}) \} |0\rangle = \begin{array}{cccc} & & & \\ & & & \\ & & & \\ & & & \\ \text{i} \uparrow & \downarrow \text{a} & \text{j} \uparrow & \downarrow \text{b} \\ \hline \hline \end{array} \cdot \quad (5)$$

These indicate what index letters should be above and below one another.

2 One-Particle Operators

The one-electron operator on normal-ordered form is given by

$$\hat{U}_N = \sum_{pq} \langle p | \hat{u} | q \rangle \{ \hat{p}^\dagger \hat{q} \}, \quad (6)$$

acting on a singly excited Slater determinant

$$|\Phi_i^a\rangle = \{ \hat{a}^\dagger \hat{i} \} |0\rangle, \quad (7)$$

id est

$$\sum_{pq} \langle p | \hat{u} | q \rangle \{ \hat{p}^\dagger \hat{q} \} \{ \hat{a}^\dagger \hat{i} \} |0\rangle. \quad (8)$$

There are four different terms arising from this expression, depending on whether p and q represents particles or holes. Beginning with a *particle-particle* term,

$$\begin{aligned} \langle b | \hat{u} | c \rangle \{ \hat{b}^\dagger \hat{c} \} \{ \hat{a}^\dagger \hat{i} \} |0\rangle &= \langle b | \hat{u} | c \rangle \{ \hat{b}^\dagger \hat{c} \hat{a}^\dagger \hat{i} \} |0\rangle + \langle b | \hat{u} | c \rangle \{ \hat{b}^\dagger \hat{c} \hat{a}^\dagger \hat{i} \} |0\rangle \\ &= \langle b | \hat{u} | c \rangle \hat{b}^\dagger \hat{a}^\dagger \hat{i} \hat{c} |0\rangle + \langle b | \hat{u} | c \rangle \delta_{ac} \{ \hat{b}^\dagger \hat{i} \} \\ &= 0 + \langle b | \hat{u} | c \rangle \delta_{ac} |\Phi_i^a\rangle, \end{aligned} \quad (9)$$

giving non-zero contributions of the type

$$\langle b | \hat{u} | a \rangle \{ \hat{b}^\dagger \hat{a} \} | \Phi_i^a \rangle = \langle b | \hat{u} | a \rangle | \Phi_i^b \rangle. \quad (10)$$

We can draw a graphical representation of this contraction process,

$$\langle b | \hat{u} | c \rangle \{ \hat{b}^\dagger \hat{c} \} : \times \text{---} \text{---} \text{---} \rightarrow \times \text{---} \text{---} \text{---} \delta_{ac} \rightarrow \times \text{---} \text{---} \text{---} \quad (11)$$

$| \Phi_i^a \rangle :$

Now, let's consider a *hole-hole* term acting on the same single-excited Slater determinant,

$$\begin{aligned} \langle j | \hat{u} | k \rangle \{ \hat{j}^\dagger \hat{k} \} \{ \hat{a}^\dagger \hat{i} \} | 0 \rangle &= \langle j | \hat{u} | k \rangle \{ \hat{j}^\dagger \hat{k} \hat{a}^\dagger \hat{i} \} | 0 \rangle + \langle j | \hat{u} | k \rangle \{ \overline{\hat{j}^\dagger \hat{k} \hat{a}^\dagger \hat{i}} \} | 0 \rangle \\ &= - \langle j | \hat{u} | k \rangle \{ \hat{k} \hat{a}^\dagger \hat{i} \hat{j}^\dagger \} | 0 \rangle + \delta_{ij} \langle i | \hat{u} | k \rangle \{ \hat{k} \hat{a}^\dagger \} | 0 \rangle \quad (12) \\ &= 0 - \delta_{ij} \langle i | \hat{u} | j \rangle \{ \hat{a}^\dagger \hat{k} \} | 0 \rangle \\ &= -\delta_{ij} \langle i | \hat{u} | j \rangle | \Phi_k^a \rangle, \end{aligned}$$

meaning we are only left with non-zero contributions of the type,

$$\langle i | \hat{u} | j \rangle \{ \hat{i}^\dagger \hat{k} \} | \Phi_i^a \rangle = - \langle i | \hat{u} | k \rangle | \Phi_k^a \rangle. \quad (13)$$

One can make a diagrammatic representation of this contraction as well,

$$\langle b | \hat{u} | c \rangle \{ \hat{b}^\dagger \hat{c} \} : \times \text{---} \text{---} \text{---} \rightarrow \times \text{---} \text{---} \text{---} \delta_{ij} \rightarrow \times \text{---} \text{---} \text{---} \quad (14)$$

$| \Phi_i^a \rangle :$