Wick’s theorem for matrix elements

Consider two non-orthogonal states $|\Psi_1\rangle$ and $|\Psi_2\rangle$

$$\langle\Psi_2|\Psi_1\rangle \neq 0$$

For any operator, the following decomposition holds:

$$\hat{A} = \hat{A}_0 + \hat{A}_+ + \hat{A}_-$$

where

$$\begin{array}{ll} 1^\circ & \hat{A}_0 \ = \text{const.}, \\ 2^\circ & \hat{A}_-|\Psi_1\rangle = 0, \\ 3^\circ & \langle\Psi_2|\hat{A}_+ = 0. \end{array}$$

Let us introduce:

$$\hat{P} \equiv \frac{|\Psi_1\rangle\langle\Psi_2|}{\langle\Psi_2|\Psi_1\rangle}$$

$$\begin{aligned} \hat{P}^2 &= \hat{P}, \\ \hat{P}|\Psi_1\rangle &= |\Psi_1\rangle, \\ \langle\Psi_2|\hat{P} &= \langle\Psi_2| \end{aligned}$$

$$
\text{(X)} \qquad
\begin{aligned}
\hat{A}_0 &= \frac{\langle\Psi_2|\hat{A}|\Psi_1\rangle}{\langle\Psi_2|\Psi_1\rangle} \;, \\
\hat{A}_- &= \left(\hat{A} - \frac{\langle\Psi_2|\hat{A}|\Psi_1\rangle}{\langle\Psi_2|\Psi_1\rangle}\right)(1-\hat{P}) \;, \\
\hat{A}_+ &= (1-\hat{P})\hat{A}\hat{P}
\end{aligned}
$$

Homework:

(i) Demonstrate that the above decomposition is correct

(ii) $\hat{J}_x, \hat{J}_y, \hat{J}_z$ are angular momentum components. Decompose $\hat{J}_x^2$ and $\hat{J}_y^2$ according to (X). Assume

$$|\Psi_1\rangle = |\Psi_2\rangle = |JJ\rangle$$

where

$$
\begin{aligned}
\hat{J}^2|JJ\rangle &= J(J+1)|JJ\rangle \\
\hat{J}_z|JJ\rangle &= J|JJ\rangle
\end{aligned}
$$

(iii) Using Wick's theorem, calculate

$$\langle JJ|\hat{J}_x^2\hat{J}_y^2|JJ\rangle$$

If all the contractions of operators appearing in the product are numbers, then the matrix element

$$\langle \Phi_2 | \hat{A}_1 \ldots \hat{A}_n | \Phi_1 \rangle$$

divided by the scalar product $\langle \Phi_2 | \Phi_1 \rangle$

can be written as a liner combination of products of all possible contractions and self-contractions

$$\begin{aligned} \overbracket{\hat{A}} &= \frac{\langle \Phi_2 | \hat{A} | \Phi_1 \rangle}{\langle \Phi_2 | \Phi_1 \rangle} \quad , \\ \overbracket{\hat{A}\hat{B}} &= \frac{\langle \Phi_2 | \hat{A}\hat{B} | \Phi_1 \rangle}{\langle \Phi_2 | \Phi_1 \rangle} - \frac{\langle \Phi_2 | \hat{A} | \Phi_1 \rangle \langle \Phi_2 | \hat{B} | \Phi_1 \rangle}{\langle \Phi_2 | \Phi_1 \rangle^2} \quad . \end{aligned}$$

$$\frac{\langle \Phi_2 | \hat{A}\hat{B} | \Phi_1 \rangle}{\langle \Phi_2 | \Phi_1 \rangle} = \overbracket{\hat{A}\hat{B}} + \overbracket{\hat{A}}\ \overbracket{\hat{B}}$$

Wick's theorem in the Fock's space

We want to find all the many-body states for which Wick's theorem holds. Since we shall be dealing with fermions, *c=-1*, and

$$\overbracket{\hat{A}\hat{B}} = \{\hat{A}_-, \hat{B}\}$$

Every operator in the Fock's space can be written as a product of creation and annihilation operators. In general, every operation takes the form:

$$\sum_{mn=0}^{M} \hat{O}(m,n),$$

m creation and n annihilation operators in normal order

(m,n) is called "operator's signature"

Let us now calculate

$$\left\{\hat{O}(m,n), a_\nu^+\right\} = \hat{O}'(m,n-1) + \underbrace{\hat{O}'(m+1,n)}_{\text{differs from zero only if } m+n \text{ even !}},$$

(demonstrate!)

In general, the annihilating part of the annihilating operator can be written as:

$$a_{\mu-} = \sum_{mn=0}^{M} \hat{T}(m,n),$$

$$\overbracket{a_\mu a_\nu^+} = \left\{ \sum_{mn}^{M} \hat{T}(m,n), a_\nu^+ \right\}$$

This expression will become a constant - signature (0,0) - only if $a_{\mu-}$ can be written as a sum of (0,1) and (*m*,0) operators (*m*-odd). By the same token, the contraction

$$\overbracket{a_\mu a_\nu} = \left\{ \sum_{mn}^{M} \hat{T}(m,n), a_\nu \right\}$$

becomes a constant only if $a_{\mu-}$ can be written as a sum of (1,0) and (0,*n*) operators (*n*-odd). Both conditions imply that $a_{\mu-}$ can only contain terms (0,1) and (1,0), i.e., it has be a linear combination of creation and annihilation operators. A similar conclusion holds for $a_{\mu-}^+$. Therefore, we can write:

$$\begin{aligned} a_{\mu-} &= \sum_{\nu} \left[(1-\rho)_{\mu\nu} a_\nu - \kappa_{\mu\nu} a_\nu^+ \right] \quad , \\ a_{\mu-}^+ &= \sum_{\nu} \left(\rho'^{T}_{\mu\nu} a_\nu^+ + \kappa'^{*}_{\mu\nu} a_\nu \right) \quad . \end{aligned}$$

and, similarly:

$$\begin{aligned} a_{\mu+} &= \sum_\nu \left(\rho_{\mu\nu} a_\nu + \kappa_{\mu\nu} a_\nu^+\right) - x_\mu \quad , \\ a_{\mu+}^+ &= \sum_\nu \left[(1-\rho'^T)_{\mu\nu} a_\nu^+ - \kappa'^*_{\mu\nu} a_\nu\right] - y_\mu^* \quad , \end{aligned}$$

where

$$\begin{aligned} x_\mu &= \overbracket{a_\mu} \quad , \\ y_\mu^* &= \overbracket{a_\mu^+} \quad . \end{aligned}$$

we shall soon demonstrate that self-contractions vanish!

Using the above expressions, one obtains:

$$\begin{aligned} \overbracket{a_\mu a_\nu^+} &= (1-\rho)_{\mu\nu}, \\ \overbracket{a_\mu a_\nu} &= -\kappa_{\mu\nu}, \\ \overbracket{a_\mu^+ a_\nu^+} &= \kappa'^*_{\mu\nu}, \\ \overbracket{a_\mu^+ a_\nu} &= \rho'^T_{\mu\nu} \end{aligned}$$