CEM 993 **Spring 2023**

Assignment No. 2 (20 pts.) **Due Date: February 10, 2023**

1. (3 pts.) Use Wick's theorem to write the expressions (in terms of the n-products with or without contractions) for the operator product $M_1M_2M_3M_4M_5$, where M_i, $i = 1-5$, are the creation or annihilation operators.

2. (4 pts.) Use Wick's theorem to show that

$$X_pX_qX_r^\dagger X_s^\dagger = X_r^\dagger X_s^\dagger X_pX_q + \delta_{pr}X_s^\dagger X_q - \delta_{ps}X_r^\dagger X_q - \delta_{qr}X_s^\dagger X_p + \delta_{qs}X_r^\dagger X_p + \delta_{ps}\delta_{qr} - \delta_{pr}\delta_{qs}. \tag{1}$$

Verify the correctness of Eq. (1) by applying the anticommutation relations for the creation and annihilation operators.

3. (6 pts.) Use Wick's theorem and rules of calculating the expectation values of normal products $n[\ldots]$ with or without contractions relative to the true vacuum to evaluate the following matrix element:

$$\langle\{p_1p_2\}|Z|\{q_1q_2\}\rangle, \tag{2}$$

where

$$Z = \sum_{r,s}\langle r|z|s\rangle X_r^\dagger X_s \tag{3}$$

is a one-body operator and

$$|\{p_1p_2\}\rangle = X_{p_1}^\dagger X_{p_2}^\dagger|0\rangle \tag{4}$$

and

$$|\{q_1q_2\}\rangle = X_{q_1}^\dagger X_{q_2}^\dagger|0\rangle \tag{5}$$

are the 2-fermion Slater determinants (as usual, $|0\rangle$ designates the true vacuum state). Do not use the general Slater rules for matrix elements involving one-body operators derived in class, but, rather, calculate the matrix element given by Eq. (2) directly by applying to it the rules of determining the expectation values of the products of the creation or annihilation operators in the true vacuum state, resulting from Wick's theorem. Once you are done, demonstrate that the resulting expression for the matrix element given by Eq. (2) recovers the Slater rules for the two cases that lead the nonzero results, i.e., $\langle\{p_1p_2\}|Z|\{p_1p_2\}\rangle$ and $\langle\{p_1p_2\}|Z|\{q_1p_2\}\rangle$.

4. (3 pts.) Calculate the following N-products:

   (a) $N[X_aX_bX_i^\dagger X_j^\dagger]$,

   (b) $N[X_iX_jX_a^\dagger X_b^\dagger]$,

   (c) $N[X_iX_aX_j^\dagger X_b^\dagger]$.

5. (4 pts.) Let $\chi(p)$ and $\pi(p)$ be the "step" functions defined as follows:

$$\chi(p) = \begin{cases} 1, & \text{for } p = i \\ 0, & \text{for } p = a \end{cases}, \qquad \pi(p) = \begin{cases} 0, & \text{for } p = i \\ 1, & \text{for } p = a \end{cases}. \tag{6}$$

Show that

(a) $\contraction{}{Y}{_p}{X}Y_p X_q = \chi(q)\delta_{pq}$,

(b) $\contraction{}{Y}{_p}{X}Y_p X_q^\dagger = \pi(q)\delta_{pq}$,

(c) $\contraction{}{Y}{_p^\dagger}{X}Y_p^\dagger X_q = 0$,

(d) $\contraction{}{Y}{_p^\dagger}{X}Y_p^\dagger X_q^\dagger = 0$.

SOLUTIONS

1. We have to apply Wick's theorem to $M_1 M_2 M_3 M_4 M_5$. Thus, we have to consider all possible n-products without and with contractions involving operators M_i, $i=1,\dots,5$, in $M_1 M_2 M_3 M_4 M_5$. We obtain,

$$M_1 M_2 M_3 M_4 M_5 = n[M_1 M_2 M_3 M_4 M_5]$$
$$+ n[\underbrace{M_1 M_2} M_3 M_4 M_5] + n[\underbrace{M_1 M_2 M_3} M_4 M_5]$$
$$+ n[\underbrace{M_1 M_2 M_3 M_4} M_5] + n[\underbrace{M_1 M_2 M_3 M_4 M_5}]$$
$$+ n[M_1 \underbrace{M_2 M_3} M_4 M_5] + n[M_1 \underbrace{M_2 M_3 M_4} M_5]$$
$$+ n[M_1 \underbrace{M_2 M_3 M_4 M_5}] + n[M_1 M_2 \underbrace{M_3 M_4} M_5]$$
$$+ n[M_1 M_2 \underbrace{M_3 M_4 M_5}] + n[M_1 M_2 M_3 \underbrace{M_4 M_5}]$$

$$+ n[M_1 M_2 M_3 M_4 M_5] + n[M_1 M_2 M_3 M_4 M_5]$$

$$+ n[M_1 M_2 M_3 M_4 M_5] + n[M_1 M_2 M_3 M_4 M_5]$$

$$+ n[M_1 M_2 M_3 M_4 M_5] + n[M_1 M_2 M_3 M_4 M_5]$$

$$+ n[M_1 M_2 M_3 M_4 M_5] + n[M_1 M_2 M_3 M_4 M_5]$$

$$+ n[M_1 M_2 M_3 M_4 M_5] + n[M_1 M_2 M_3 M_4 M_5]$$

$$+ n[M_1 M_2 M_3 M_4 M_5] + n[M_1 M_2 M_3 M_4 M_5]$$

$$+ n[M_1 M_2 M_3 M_4 M_5] + n[M_1 M_2 M_3 M_4 M_5]$$

$$+ n[M_1 M_2 M_3 M_4 M_5]$$

Please note that we went here systematically by considering first single contractions and then double contractions. All these cases could be classified using the notation: $M_i M_j \Longrightarrow (ij)$., $i < j$.

For example,

$$n[M_1 M_2 M_3 M_4 M_5] \Longrightarrow (13),$$

$$n[M_1 M_2 M_3 M_4 M_5] \Longrightarrow (13)(25).$$

All single contractions can be listed as pairs,

$$(ij) \; ; \; i = 1-4, \; j > i \, .$$

All double contractions can be listed as double pairs:

$$(ij)(kl) \; ; \; i < j, \; k < l, \; i < k$$

For the single contractions, we get the following pairings:

$$(12), (13), (14), (15),$$

$$(23), (24), (25), (34), (35),$$

$$(45) \; \longrightarrow \text{altogether, } 10 \text{ cases}$$

$$\left[\binom{5}{2} = \frac{5!}{2! \cdot 3!} = 10 \right]$$

For the double contractions, we obtain the following pairings:

(12)(34) (13)(24) (14)(23)
(12)(35) (13)(25) (14)(25)
(12)(45) (13)(45) (14)(35)

(15)(23) (23)(45) (24)(35)
(15)(24)
(15)(34)

(25)(34) → altogether, 15 cases

$$\left[\binom{5}{2\;2} \Big/ 2! = \frac{5!}{2!\,2!\,1!}\cdot\frac{1}{2!} = \frac{5\cdot4\cdot3\cdot2}{2\cdot2\cdot2} = 15 \right]$$

the number of selections of two ordered pairs out of 5 symbols

$(ij)(kl) \Leftrightarrow (kl)(ij)$

[to eliminate repetitions; we MUST HAVE $i<k$

2. $$X_p X_q X_r^\dagger X_s^\dagger = n[X_p X_q X_r^\dagger X_s^\dagger]$$
$$+\; n[\underbrace{X_p X_q X_r^\dagger}_{} X_s^\dagger] + n[\underbrace{X_p X_q X_r^\dagger X_s^\dagger}_{}]$$
$$+\; n[X_p \underbrace{X_q X_r^\dagger}_{} X_s^\dagger] + n[X_p \underbrace{X_q X_r^\dagger X_s^\dagger}_{}]$$

$$+ \, n[X_p X_q X_r^\dagger X_s^\dagger] + n[X_p X_q X_r^\dagger X_s^\dagger]$$

$$= X_r^\dagger X_s^\dagger X_p X_q - X_p X_r^\dagger \, n[X_q X_s^\dagger]$$
$$+ X_p X_s^\dagger \, n[X_q X_r^\dagger] + X_q X_r^\dagger \, n[X_p X_s^\dagger]$$
$$- X_q X_s^\dagger \, n[X_p X_r^\dagger] - X_p X_r^\dagger X_q X_s^\dagger$$
$$+ X_p X_s^\dagger X_q X_r^\dagger \quad =$$

$$= X_r^\dagger X_s^\dagger X_p X_q + \delta_{pr} X_s^\dagger X_q$$
$$- \delta_{ps} X_r^\dagger X_q - \delta_{qr} X_s^\dagger X_p$$
$$+ \delta_{qs} X_r^\dagger X_p - \delta_{pr}\delta_{qs}$$
$$+ \delta_{ps}\delta_{qr} \implies$$ This is exactly Eq. (1).

Verification ($\leftrightarrow$ designates operators that we wish to interchange):

$$X_p X_q X_r^\dagger X_s^\dagger = X_p (\delta_{qr} - X_r^\dagger X_q) X_s^\dagger$$
$$= \delta_{qr} X_p X_s^\dagger - X_p X_r^\dagger X_q X_s^\dagger .$$

$$= \delta_{qr}(\delta_{ps} - X_s^{+} X_p)$$
$$- (\delta_{pr} - X_r^{+} X_p)(\delta_{qs} - X_s^{+} X_q)$$
$$= \delta_{qr}\delta_{ps} - \delta_{qr} X_s^{+} X_p$$
$$- \delta_{pr}\delta_{qs} + \delta_{pr} X_s^{+} X_q$$
$$+ \delta_{qs} X_r^{+} X_p - X_r^{+} X_p X_s^{+} X_q$$
$$= \delta_{qr}\delta_{ps} - \delta_{pr}\delta_{qs} + \delta_{pr} X_s^{+} X_q$$
$$- \delta_{qr} X_s^{+} X_p + \delta_{qs} X_r^{+} X_p$$
$$- X_r^{+}(\delta_{ps} - X_s^{+} X_p) X_q$$
$$= \delta_{qr}\delta_{ps} - \delta_{pr}\delta_{qs} + \delta_{pr} X_s^{+} X_q$$
$$- \delta_{qr} X_s^{+} X_p + \delta_{qs} X_r^{+} X_p$$
$$- \delta_{ps} X_r^{+} X_q + X_r^{+} X_s^{+} X_p X_q$$

$\Rightarrow$ this is exactly Eq. (1).

3. We must consider

$$\langle \{p_1 p_2\} | Z | \{q_1 q_2\} \rangle$$

$$= \sum_{r,s} \langle r|\hat{z}|s\rangle \langle 0| X_{p_2} X_{p_1} X_r^{\dagger} X_s X_{q_1}^{\dagger} X_{q_2}^{\dagger} |0\rangle.$$

Let us focus on $\langle 0| X_{p_2} X_{p_1} X_r^{\dagger} X_s X_{q_1}^{\dagger} X_{q_2}^{\dagger} |0\rangle \equiv A$.

First, let us realize that $X_{p_2} X_{p_1}$ and $X_{q_1}^{\dagger} X_{q_2}^{\dagger}$ are in the normal product forms, so that

$$A = \langle 0| X_{p_2} X_{p_1} X_r^{\dagger} X_s X_{q_1}^{\dagger} X_{q_2}^{\dagger} |0\rangle$$
$$= \langle 0| n[X_{p_2} X_{p_1}] X_r^{\dagger} X_s \, n[X_{q_1}^{\dagger} X_{q_2}^{\dagger}] |0\rangle.$$

We now consider fully contracted terms only, avoiding contractions in $n[X_{p_2} X_{p_1}]$ and $n[X_{q_1}^{\dagger} X_{q_2}^{\dagger}]$. $X_r^{\dagger}$ can only be contracted with X_{p_1} or X_{p_2}. X_s can only be contracted with $X^\dagger_{q_1}$ or $X^\dagger_{q_2}$. This is because the only nonzero contractions relative to true vacuum are of the $XX^\dagger$ type.

This leaves us with only four terms,

$$A = \langle 0| n[X_{p_2} X_{p_1} X^\dagger_r X_s X^\dagger_{q_1} X^\dagger_{q_2}]|0\rangle$$

$$+ \langle 0| n[X_{p_2} X_{p_1} X^\dagger_r X_s X^\dagger_{q_1} X^\dagger_{q_2}]|0\rangle$$

$$+ \langle 0| n[X_{p_2} X_{p_1} X^\dagger_r X_s X^\dagger_{q_1} X^\dagger_{q_2}]|0\rangle$$

$$+ \langle 0| n[X_{p_2} X_{p_1} X^\dagger_r X_s X^\dagger_{q_1} X^\dagger_{q_2}]|0\rangle$$

$$= \delta_{rp_1}\delta_{sq_1}\delta_{p_2q_2} - \delta_{rp_1}\delta_{sq_2}\delta_{p_2q_1}$$

$$- \delta_{rp_2}\delta_{sq_1}\delta_{p_1q_2} + \delta_{rp_2}\delta_{sq_2}\delta_{p_1q_1}$$

Thus,

$$\langle \{p_1 p_2\} | \hat{Z} | \{q_1 q_2\} \rangle$$

$$\begin{aligned}
= \; & \langle p_1 | \hat{z} | q_1 \rangle \langle p_2 | q_2 \rangle \\
- \; & \langle p_1 | \hat{z} | q_2 \rangle \langle p_2 | q_1 \rangle \\
- \; & \langle p_2 | \hat{z} | q_1 \rangle \langle p_1 | q_2 \rangle \\
+ \; & \langle p_2 | \hat{z} | q_2 \rangle \langle p_1 | q_1 \rangle . \qquad (\star)
\end{aligned}$$

The above is a general expression. Let us now consider the two special cases listed in Problem 3. The first one is $\langle \{p_1 p_2\} | \hat{Z} | \{p_1 p_2\} \rangle$, i.e., $q_1 = p_1$, $q_2 = p_2$. Since $p_1 \neq p_2$ and $q_1 \neq q_2$, the only terms that contribute to $\langle \{p_1 p_2 | \hat{Z} | \{p_1 p_2\} \rangle$, according to Eq. $(\star)$ are the first and the last ones. We obtain,

$$\langle \{p_1 p_2\} | Z | \{p_1 p_2\} \rangle = \langle p_1 | \hat{z} | p_1 \rangle + \langle p_2 | \hat{z} | p_2 \rangle,$$

which is exactly what the Slater rule for $\langle \{p_1 \cdots p_N\} | Z | \{p_1 \cdots p_N\} \rangle$ would give for $N = 2$.

The second case is $\langle \{p_1 p_2\} | Z | q_1 p_2\} \rangle$, i.e., $p_1 \neq q_1$, $p_2 = q_2$. Again, since $q_1 \neq p_2$ and $p_1 \neq p_2$, we obtain

$$\langle \{p_1 p_2\} | Z | \{q_1 p_2\} \rangle = \langle p_1 | \hat{z} | q_1 \rangle .$$

The remaining three terms in Eq. (☆) vanish in this case. As in the previous case, we have recovered one of the Slater rules, this time for

$$\langle \{p_1 p_2 \cdots p_N\} | Z | \{q_1 p_2 \cdots p_N\} \rangle,$$

where $q_1 \neq p_1$ and $N = 2$.

4. In order to determine each of the N-products, we must convert the X and $X^\dagger$ operators into the $Y/Y^\dagger$ form and rearrange the resulting operators accordingly.

We obtain,

(a) $N[X_a X_b X_i^\dagger X_j^\dagger]$

$= N[Y_a Y_b Y_i Y_j] = Y_a Y_b Y_i Y_j$

$= X_a X_b X_i^\dagger X_j^\dagger.$

(b) $N[X_i X_j X_a^\dagger X_b^\dagger]$

$= N[Y_i^\dagger Y_j^\dagger Y_a^\dagger Y_b^\dagger]$

$= Y_i^\dagger Y_j^\dagger Y_a^\dagger Y_b^\dagger = X_i X_j X_a^\dagger X_b^\dagger.$

(c) $N[X_i X_a X_j^\dagger X_b^\dagger] =$

$$= N[Y_i^\dagger Y_a Y_j Y_b^\dagger] = Y_i^\dagger Y_b^\dagger Y_a Y_j$$

$$= X_i X_b^\dagger X_a X_j^\dagger .$$

5. (a) $$\overbracket{Y_p X_q} = [\underbrace{\chi(q) + \pi(q)}] \times .$$

$$\times\ \overbracket{Y_p X_q} = \chi(q)\, \overbracket{Y_p X_q} + \pi(q)\, \overbracket{Y_p X_q}$$

$$= \chi(q)\, \underbrace{\overbracket{Y_p Y_q^\dagger}}_{=\delta_{pq}} + \pi(q)\, \underbrace{\overbracket{Y_p Y_q}}_{=0}$$

$$= \chi(q)\, \delta_{pq} .$$

(b) $$\overbracket{Y_p X_q^\dagger} = [\chi(q) + \pi(q)]\, \overbracket{Y_p X_q^\dagger}$$

$$= \chi(q)\, \overbracket{Y_p X_q^\dagger} + \pi(q)\, \overbracket{Y_p X_q^\dagger}$$

$$= \chi(q)\, \underbrace{\overbracket{Y_p\, Y_q}}_{\overset{\shortparallel}{0}} + \pi(q)\, \underbrace{\overbracket{Y_p\, Y_q^{\dagger}}}_{\overset{\shortparallel}{\delta_{pq}}}$$

$$= \pi(q)\, \delta_{pq} .$$

(c) $\overbracket{Y_p^{\dagger}\, X_q} = 0$, since

$$\overbracket{Y_p^{\dagger}\, M} = 0 \quad \text{for } M = Y_q, Y_q^{\dagger}.$$

(d) $\overbracket{Y_p^{\dagger}\, X_q^{\dagger}} = 0$, since

$$\overbracket{Y_p^{\dagger} M} = 0 \quad \text{for } M = Y_q, Y_q^{\dagger}.$$