Derivation of Wick's theorem and the Schwinger term

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1 Wick's theorem

Let $|k\rangle$ be a basis of the one-particle Hilbert space, and write the fermion creation and annihilation operators as $\psi_k^\dagger, \psi_k$. Write the energy as E_k, and abbreviate the conditions $E_k > 0$ and $E_k < 0$ on the index k simply as $k > 0$ and $k < 0$. Let $|0\rangle$ be the vacuum satisfying $\psi_k |0\rangle = 0$ for every k. Define the ground state by

$$|\mathrm{GS}\rangle = \prod_{k<0} \psi_k^\dagger |0\rangle \tag{1}$$

and introduce the normal ordering

$$\ddagger\, \psi_k^\dagger \psi_l \,\ddagger = \begin{cases} -\psi_l \psi_k^\dagger & (k = l < 0), \\ \psi_k^\dagger \psi_l & (\text{else}). \end{cases} \tag{2}$$

For operators involving two or more fermion operators, we also reorder them so that $\ddagger\, \mathcal{O} \,\ddagger |GS\rangle = 0$. A minus sign is produced when the order is exchanged. Notice that

$$\ddagger\, \psi_k^\dagger \psi_l \,\ddagger = -\ddagger\, \psi_l \psi_k^\dagger \,\ddagger. \tag{3}$$

More generally, a minus sign appears when fermion operators are exchanged inside the normal ordering. For example, for fermion creation and annihilation operators $A_1, \dots, A_N$ and a permutation $\sigma \in S_N$,

$$\ddagger\, A_{\sigma_1} \cdots A_{\sigma_N} \,\ddagger = (-1)^\sigma \ddagger\, A_1 \cdots A_N \,\ddagger. \tag{4}$$

For fermion creation and annihilation operators, define the contraction by

$$\contraction{}{A}{}{B}AB := AB - \ddagger\, AB \,\ddagger. \tag{5}$$

Introducing the notation

$$\delta_{kl>0} := \begin{cases} \delta_{kl} & (k = l > 0) \\ 0 & (\text{else}) \end{cases}, \quad \delta_{kl<0} := \begin{cases} \delta_{kl} & (k = l < 0) \\ 0 & (\text{else}), \end{cases} \tag{6}$$

we have

$$\contraction{}{\psi_k^\dagger}{}{\psi_l}\psi_k^\dagger \psi_l = \psi_k^\dagger \psi_l - \begin{cases} -\psi_l \psi_k^\dagger & (k = l < 0) \\ 0 & (\text{else}) \end{cases} = \delta_{kl<0}, \tag{7}$$

$$\contraction{}{\psi_l}{}{\psi_k^\dagger}\psi_l \psi_k^\dagger = \psi_l \psi_k^\dagger - \ddagger\, \psi_l \psi_k^\dagger \,\ddagger = \delta_{kl} - \psi_k^\dagger \psi_l + \ddagger\, \psi_k^\dagger \psi_l \,\ddagger = \delta_{kl} - \contraction{}{\psi_k^\dagger}{}{\psi_l}\psi_k^\dagger \psi_l = \delta_{kl} - \delta_{kl<0} = \delta_{kl>0}, \tag{8}$$

$$\contraction{}{\psi_k^\dagger}{}{\psi_l^\dagger}\psi_k^\dagger \psi_l^\dagger = \contraction{}{\psi_k}{}{\psi_l}\psi_k \psi_l = 0. \tag{9}$$

Notice that all of these are c-numbers. The contraction has a nonzero value when AB is not in normal order. Normal ordering changes only by a sign when the order of the operators inside it is exchanged, but the contraction depends on the order of the operators.

Next we prove Wick's theorem. Introduce notation that simultaneously includes normal ordering and contractions. For a set of fermion creation and annihilation operators $A_1, \ldots, A_N$, specify n pairs by

$$p_1, \ldots, p_{2n}, \tag{10}$$

$$p_1 < p_3 < \cdots p_{2n-1}, \tag{11}$$

$$p_{2j-1} < p_{2j}, \quad j = 1, \ldots, n. \tag{12}$$

Write an arbitrary ordered set of the complement $\{1, \ldots, N\} \backslash \{p_1, \ldots, p_{2n}\}$ as

$$q_1, \ldots, q_{N-2n}. \tag{13}$$

Define the normally ordered product with the contractions specified by $p_1, \ldots, p_{2n}$ as

$$C_{\{p_i\}_{i=1}^{2n}}(A_1 \cdots A_N) := \operatorname{sgn} \begin{pmatrix} 1 & \cdots & N \\ p_1 & \cdots p_{2n} q_1 \cdots & q_{N-2n} \end{pmatrix} \times \prod_{j=1}^{n} \wick{\c A_{p_{2j-1}} \c A_{p_{2j}}} \times \ddagger\, A_{q_1} \cdots A_{q_{N-2n}} \,\ddagger. \tag{14}$$

Notice that the right-hand side is independent of the choice of $q_1, \ldots, q_{N-2n}$. Wick's theorem states that

$$A_1 \cdots A_N = \sum_{n=0}^{\lfloor N/2 \rfloor} \sum_{\{p_i\}_{i=1}^{2n}} C_{\{p_i\}_{i=1}^{2n}} (A_1 \cdots A_N) \,. \tag{15}$$

For hand calculations, it is convenient to compute in the form

$$A_1 \cdots A_N = \ddagger\, A_1 \cdots \,\ddagger + \sum_{\text{singles}} \ddagger \cdots \wick{\c A_i \cdots \c A_j} \cdots \ddagger + \sum_{\text{doubles}} \ddagger \cdots \wick{\c1 A_i \cdots \c2 A_j \cdots \c1 A_k \cdots \c2 A_l} \cdots \ddagger + \cdots \,. \tag{16}$$

We prove this by induction. The case $N = 2$ is exactly the definition of contraction. Assume the statement holds for $N = M$. Then

$$A_0 A_1 \cdots A_M = A_0 \sum_{n=0}^{\lfloor M/2 \rfloor} \sum_{\{p_i\}_{i=1}^{2n}} C_{\{p_i\}_{i=1}^{2n}}(A_1 \cdots A_N). \tag{17}$$

Each term is

$$\operatorname{sgn} \begin{pmatrix} 1 & \cdots & N \\ p_1 & \cdots p_{2n} q_1 \cdots & q_{N-2n} \end{pmatrix} \times \prod_{j=1}^{n} \wick{\c A_{p_{2j-1}} \c A_{p_{2j}}} \times A_0 \ddagger\, A_{q_1} \cdots A_{q_{N-2n}} \,\ddagger. \tag{18}$$

Now choose $q_1 \cdots q_{N-2n}$ to be the order that gives normal ordering,

$$\ddagger\, A_{q_1} \cdots A_{q_{N-2n}} \,\ddagger = A_{r_1} \cdots A_{r_k} A_{s_1} \cdots A_{s_l}, \quad (k + l = N - 2n), \tag{19}$$

where $A_{r_1}, \ldots, A_{r_k}$ are either $\psi^\dagger_{a>0}$ or $\psi_{a<0}$, and $A_{s_1}, \ldots, A_{s_l}$ are either $\psi^\dagger_{a<0}$ or $\psi_{a>0}$. Then

$$A_0 \ddagger\, A_{q_1} \cdots A_{q_{N-2n}} \,\ddagger = A_0 A_{r_1} \cdots A_{r_k} A_{s_1} \cdots A_{s_l}. \tag{20}$$

If A_0 is either $\psi^\dagger_{a>0}$ or $\psi_{a<0}$, no new contraction appears, and the assertion follows. If A_0 is either $\psi^\dagger_{a<0}$ or $\psi_{a>0}$, new contractions appear. Indeed,

$$\begin{aligned} A_0 A_{r_1} \cdots A_{r_k} &= \ddagger\, A_0 A_{r_1} \cdots A_{r_k} \,\ddagger + \wick{\c A_0 \c A_{r_1}} A_{r_2} \cdots A_{r_k} - \wick{\c A_0 \c A_{r_2}} A_{r_1} \cdots A_{r_k} \\ &\quad + \cdots + (-1)^{k-1} \wick{\c A_0 \c A_{r_k}} A_{r_1} \cdots A_{r_{k-1}}, \end{aligned} \tag{21}$$

so the contractions involving A_0 are added. This proves the claim.

2 Schwinger term

Write $\psi_a^\dagger$ and ψ_a as a' and a, respectively. We compute the product $\ddagger\, a'b \,\ddagger\ddagger\, c'd\, \ddagger$ of two normally ordered one-body operators. A direct computation gives

$$\begin{aligned}\ddagger\, a'b \,\ddagger\ddagger\, c'd\, \ddagger &= \ddagger\, a'bc'd + \wick{\c1{a}'bc'\c1{d}} + \wick{a'\c1{b}\c1{c}'d} + \wick{\c2{a}'\c1{b}\c1{c}'\c2{d}}\, \ddagger \\ &= \ddagger\, a'bc'd\, \ddagger + \delta_{ad<0} \ddagger\, bc' \,\ddagger + \delta_{bc>0} \ddagger\, a'd\, \ddagger + \delta_{ad<0}\delta_{bc>0}. \end{aligned} \tag{22}$$

This means that contractions within the already normally ordered pairs of indices $a'b$ and $c'd$ are not included in the sum over possible contractions. For a matrix $A = A_{ab}$ on the one-particle Hilbert space, define

$$Q(A) := \sum_{ab} A_{ab} \ddagger\, a'b\, \ddagger. \tag{23}$$

Also introduce the projections

$$P_+ = \sum_{a>0} |a\rangle \langle a|, \quad P_- = \sum_{a<0} |a\rangle \langle a|, \tag{24}$$

and the notation

$$A_{\epsilon\epsilon'} = P_\epsilon A P_{\epsilon'}, \quad \epsilon, \epsilon' \in \{+, -\}. \tag{25}$$

Then

$$\begin{aligned} Q(A)Q(B) &= \sum_{abcd} A_{ab} B_{cd} (\ddagger\, a'bc'd\, \ddagger + \delta_{ad<0} \ddagger\, bc'\, \ddagger + \delta_{bc>0} \ddagger\, a'd\, \ddagger + \delta_{ad<0}\delta_{bc>0}) && (26) \\ &= Q_2(A \otimes B) + Q(AP_+B - BP_-A) + \mathrm{tr}\,(A_{-+}B_{+-}). && (27) \end{aligned}$$

Here we have written

$$Q_2(A \otimes B) = \sum_{abcd} A_{ab} B_{cd} \ddagger\, a'bc'd\, \ddagger. \tag{28}$$

That is, for

$$Q_{0,2}(A \otimes B) = \sum_{abcd} A_{ab} B_{cd} a'bc'd, \tag{29}$$

we have

$$Q_2(A \otimes B) = \ddagger\, Q_{0,2}(A \otimes B)\, \ddagger. \tag{30}$$

Since one may exchange the order of operators inside the normal ordering, note that

$$Q_2(A \otimes B) = Q_2(B \otimes A). \tag{31}$$

The operator $Q_{0,2}(A \otimes B)$ does not have this property.

The commutator is

$$\begin{aligned} [Q(A), Q(B)] &= Q(AP_+B - BP_-A) + \mathrm{tr}\,(A_{-+}B_{+-}) - (A \leftrightarrow B) && (32) \\ &= Q(AP_-B - BP_-A - BP_-A + AP_-B) + \mathrm{tr}\,(A_{-+}B_{+-} - B_{-+}A_{+-}) && (33) \\ &= Q([A, B]) + S_2(A, B). && (34) \end{aligned}$$

Here

$$S_2(A, B) := \mathrm{tr}\,(A_{-+}B_{+-} - B_{-+}A_{+-}) \tag{35}$$

is called the Schwinger term.

3 Higher products

In the same way, the product of three one-body operators is

$$\begin{aligned}
&\ddagger\, a'b \,\ddagger\ddagger\, c'd \,\ddagger\ddagger\, e'f \,\ddagger \\
&= \ddagger a'bc'de'f \\
&+ \wick{\c1{a}'bc'\c1{d}e'f} + \wick{\c1{a}'bc'de'\c1{f}} + \wick{a'\c1{b}\c1{c}'de'f} + \wick{a'\c1{b}c'd\c1{e}'f} + \wick{a'b\c1{c}'de'\c1{f}} + \wick{a'bc'\c1{d}\c1{e}'f} \\
&+ \wick{\c1{a}'\c2{b}\c2{c}'\c1{d}e'f} + \wick{\c1{a}'\c2{b}c'\c1{d}\c2{e}'f} + \wick{\c1{a}'b\c2{c}'\c1{d}e'\c2{f}} + \wick{\c1{a}'\c2{b}\c2{c}'de'\c1{f}} + \wick{\c1{a}'\c2{b}c'd\c2{e}'\c1{f}} + \wick{a'\c1{b}\c1{c}'\c2{d}\c2{e}'f} + \wick{a'\c1{b}\c2{c}'d\c1{e}'\c2{f}} + \wick{a'b\c1{c}'\c2{d}\c2{e}'\c1{f}} \\
&+ \wick{\c1{a}'\c2{b}\c3{c}'\c1{d}\c2{e}'\c3{f}} + \wick{\c1{a}'\c2{b}\c2{c}'\c3{d}\c3{e}'\c1{f}}\ddagger
\end{aligned} \tag{36}$$

$$\begin{aligned}
&= \ddagger\, a'bc'de'f \,\ddagger \\
&+ \ddagger\, \delta_{ad<0}bc'e'f + \delta_{af<0}bc'de' + \delta_{bc>0}a'de'f + \delta_{be>0}a'c'df + \delta_{cf<0}a'bde' + \delta_{de>0}a'bc'f \,\ddagger \\
&+ \ddagger\delta_{ad<0}\delta_{bc>0}e'f - \delta_{ad<0}\delta_{be>0}c'f - \delta_{ad<0}\delta_{cf<0}be' + \delta_{af<0}\delta_{bc>0}de' \\
&+ \delta_{af<0}\delta_{be>0}c'd + \delta_{bc>0}\delta_{de>0}a'f + \delta_{be>0}\delta_{cf<0}a'd + \delta_{cf<0}\delta_{de>0}a'b\ddagger \\
&- \delta_{ad<0}\delta_{be>0}\delta_{cf<0} + \delta_{af<0}\delta_{bc>0}\delta_{de>0}.
\end{aligned} \tag{37}$$

From this, we obtain

$$\begin{aligned}
&Q(A)Q(B)Q(C) \\
&= Q_3(A\otimes B\otimes C) \\
&- Q_2(BP_-A\otimes C) - Q_2(CP_-A\otimes B) + Q_2(AP_+B\otimes C) + Q_2(AP_+C\otimes B) - Q_2(CP_-B\otimes A) + Q_2(BP_+C\otimes A) \\
&+ Q(C)\mathrm{tr}\,(AP_+BP_-) - Q(BP_-AP_+C) + Q(CP_-BP_-A) - Q(CP_-AP_+B) \\
&+ Q(B)\mathrm{tr}\,(AP_+CP_-) + Q(AP_+BP_+C) + Q(AP_+CP_-B) + Q(A)\mathrm{tr}\,(BP_+CP_-) \\
&- \mathrm{tr}\,(AP_+CP_-BP_-) + \mathrm{tr}\,(AP_+BP_+CP_-).
\end{aligned} \tag{38}$$

Rearranging,

$$\begin{aligned}
&Q(A)Q(B)Q(C) \\
&= Q_3(A\otimes B\otimes C) \\
&+ Q_2(AP_+B\otimes C) + Q_2(AP_+C\otimes B) + Q_2(BP_+C\otimes A) \\
&- Q_2(BP_-A\otimes C) - Q_2(CP_-A\otimes B) - Q_2(CP_-B\otimes A) \\
&- Q(BP_-AP_+C) + Q(CP_-BP_-A) - Q(CP_-AP_+B) + Q(AP_+BP_+C) + Q(AP_+CP_-B) \\
&+ Q(C)\mathrm{tr}\,(AP_+BP_-) + Q(B)\mathrm{tr}\,(AP_+CP_-) + Q(A)\mathrm{tr}\,(BP_+CP_-) \\
&- \mathrm{tr}\,(AP_+CP_-BP_-) + \mathrm{tr}\,(AP_+BP_+CP_-)
\end{aligned} \tag{39}$$

$$\tag{40}$$

or equivalently

$$\begin{aligned}
&Q(A)Q(B)Q(C) \\
&= Q_3(A\otimes B\otimes C) \\
&+ Q_2((AP_+B - BP_-A)\otimes C) + Q_2((AP_+C - CP_-A)\otimes B) + Q_2((BP_+C - CP_-B)\otimes A) \\
&- Q(BP_-AP_+C) + Q(CP_-BP_-A) - Q(CP_-AP_+B) + Q(AP_+BP_+C) + Q(AP_+CP_-B) \\
&+ Q(C)\mathrm{tr}\,(AP_+BP_-) + Q(B)\mathrm{tr}\,(AP_+CP_-) + Q(A)\mathrm{tr}\,(BP_+CP_-) \\
&- \mathrm{tr}\,(AP_+CP_-BP_-) + \mathrm{tr}\,(AP_+BP_+CP_-)
\end{aligned} \tag{41}$$

is obtained.

4 3-bracket

Let us compute the completely antisymmetric product

$$[Q(A^1), Q(A^2), Q(A^3)] = \epsilon_{xyz}Q(A^x)Q(A^y)Q(A^z). \tag{42}$$

We have

$$\begin{aligned}
[Q(A^1), Q(A^2), Q(A^3)] &= \frac{1}{2}\epsilon_{xyz} Q(A^x)[Q(A^y), Q(A^z)] \qquad (43)\\
&= \frac{1}{2}\epsilon_{xyz} Q(A^x)\left(Q([A^y, A^z]) + S_2(A^y, A^z)\right) \qquad (44)\\
&= \frac{1}{2}\epsilon_{xyz}\Big(Q_2(A^x \otimes [A^y, A^z]) + Q(A^x P_+ [A^y, A^z] - [A^y, A^z] P_- A^x)\\
&+ \mathrm{tr}\,(A^x_{-+}[A^y, A^z]_{+-}) + Q(A^x)\mathrm{tr}\,(A^y_{-+}A^z_{+-} - A^z_{-+}A^y_{+-})\Big). \qquad (45)
\end{aligned}$$

5 4-bracket

Let us compute the completely antisymmetric product

$$[Q(A^1), Q(A^2), Q(A^3), Q(A^4)] = \epsilon_{xyzw} Q(A^x) Q(A^y) Q(A^z) Q(A^w). \qquad (46)$$

We have

$$\begin{aligned}
&[Q(A^1), Q(A^2), Q(A^3), Q(A^4)]\\
&= \frac{1}{4}\epsilon_{xyzw}[Q(A^x), Q(A^y)][Q(A^z), Q(A^w)] \qquad (47)\\
&= \frac{1}{4}\epsilon_{xyzw}\left(Q([A^x, A^y]) + S_2(A^x, A^y)\right)\left(Q([A^z, A^w]) + S_2(A^z, A^w)\right) \qquad (48)\\
&= \frac{1}{4}\epsilon_{xyzw}\Big(Q_2([A^x, A^y] \otimes [A^z, A^w]) + Q([A^x, A^y] P_+ [A^z, A^w] - [A^z, A^w] P_- [A^x, A^y])\\
&+ \mathrm{tr}\,([A^x, A^y]_{-+}[A^z, A^w]_{+-}) + Q([A^x, A^y])\mathrm{tr}\,(A^z_{-+}A^w_{+-} - A^w_{-+}A^z_{+-}) + Q([A^z, A^w])\mathrm{tr}\,(A^x_{-+}A^y_{+-} - A^y_{-+}A^x_{+-})\\
&+ \mathrm{tr}\,(A^x_{-+}A^y_{+-} - A^y_{-+}A^x_{+-})\mathrm{tr}\,(A^z_{-+}A^w_{+-} - A^w_{-+}A^z_{+-})\Big). \qquad (49)
\end{aligned}$$