Complements of the discussion at Tokyo

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1 Normal ordering stuffs

Let me first define the expression of the normal ordering and the contraction. Wick's theorem says

$$
\begin{aligned}
A_1A_2A_3A_4\cdots A_n = &\{A_1A_2A_3A_4\cdots A_n\} \\
&+ C_{12}\{A_3A_4\cdots A_n\} + \text{ all possible single contractions} \\
&+ C_{12}C_{34}\{\cdots A_n\} + \text{ all possible double contractions} \\
&+ \cdots \\
&+ (\text{all fully contracted terms}). \qquad (1)
\end{aligned}
$$

Here, the C_{12} means the contraction, following the relation

$$C_{12} = \langle v| A_1A_2 |v\rangle\,, \qquad (2)$$

where $|v\rangle$ is the true vacuum or filled Fermi sea. As specific cases,

$$
\begin{aligned}
C_{i^\dagger j} &= \langle v| a_i^\dagger a_j |v\rangle = \delta_{ij}n_i \qquad (3)\\
C_{ij^\dagger} &= \langle v| a_i a_j^\dagger |v\rangle = \delta_{ij}\bar{n}_i, \qquad (4)
\end{aligned}
$$

where

$$n_i \equiv \theta(\varepsilon_F - \varepsilon_i) \quad \bar{n}_i \equiv \theta(\varepsilon_i - \varepsilon_F) = 1 - n_i. \qquad (5)$$

The ε_F means the Fermi energy. Thus if one takes the N-ordering with respect to the true vacuum, then always $n_i = 0$.

$$\{a_1^\dagger a_2\} = a_1^\dagger a_2 - C_{1+2} \qquad (6)$$

Now, I will show the relation of N-ordering

$$\{a_3^\dagger a_1\}\{a_4^\dagger a_2\} = \{a_3^\dagger a_1 a_4^\dagger a_2\} + C_{3^\dagger 2}\{a_1a_4^\dagger\} + C_{14^\dagger}\{a_3^\dagger a_2\} + C_{3^\dagger 2}C_{14^\dagger} \qquad (7)$$

To prove the eq. (7), first consider the Wick's theorem for the operator

$$
\begin{aligned}
a_3^\dagger a_1 a_4^\dagger a_2 = &\{a_3^\dagger a_1 a_4^\dagger a_2\} + C_{3^\dagger 1}\{a_4^\dagger a_2\} + C_{4^\dagger 2}\{a_3^\dagger a_1\} + C_{3^\dagger 2}\{a_1a_4^\dagger\} + C_{14^\dagger}\{a_3^\dagger a_2\} \\
&+ C_{3^\dagger 1}C_{4^\dagger 2} + C_{3^\dagger 2}C_{14^\dagger} \qquad (8)\\
&= \{a_3^\dagger a_1 a_4^\dagger a_2\} + C_{3^\dagger 1}(a_4^\dagger a_2 - C_{4^\dagger 2}) + C_{4^\dagger 2}(a_3^\dagger a_1 - C_{3^\dagger 1}) \\
&+ C_{3^\dagger 2}(a_1a_4^\dagger - C_{14^\dagger}) + C_{14^\dagger}(a_3^\dagger a_2 - C_{3^\dagger 2}) \\
&+ C_{3^\dagger 1}C_{4^\dagger 2} + C_{3^\dagger 2}C_{14^\dagger} \qquad (9)\\
&= \{a_3^\dagger a_1 a_4^\dagger a_2\} + C_{3^\dagger 1}a_4^\dagger a_2 + C_{4^\dagger 2}a_3^\dagger a_1 + C_{3^\dagger 2}a_1a_4^\dagger + C_{14^\dagger}a_3^\dagger a_2 \\
&- C_{3^\dagger 1}C_{4^\dagger 2} - C_{3^\dagger 2}C_{14^\dagger} \qquad (10)
\end{aligned}
$$

Next consider

$$
\begin{aligned}
\{a_3^\dagger a_1\}\{a_4^\dagger a_2\} &= (a_3^\dagger a_1 - C_{3^\dagger 1})(a_4^\dagger a_2 - C_{4^\dagger 2}) \\
&= a_3^\dagger a_1 a_4^\dagger a_2 - C_{4^\dagger 2}a_3^\dagger a_1 - C_{3^\dagger 1}a_4^\dagger a_2 + C_{3^\dagger 1}C_{4^\dagger 2} \qquad (11)
\end{aligned}
$$

Inserting the eq. (10) into eq. (11) yields

$$\{a_3^\dagger a_1\}\{a_4^\dagger a_2\} = \{a_3^\dagger a_1 a_4^\dagger a_2\} + C_{3^\dagger 2} a_1 a_4^\dagger + C_{14^\dagger} a_3^\dagger a_2 - C_{14^\dagger} C_{3^\dagger 2} \tag{12}$$

$$= \{a_3^\dagger a_1 a_4^\dagger a_2\} + C_{3^\dagger 2}\{a_1 a_4^\dagger\} + C_{14^\dagger}\{a_3^\dagger a_2\} + C_{14^\dagger} C_{3^\dagger 2}. \tag{13}$$

This is what I wanted to show (eq. (7)). This is in fact general result and a specific case of the Wick's theorem. Regarding the products of 2 or more operator strings that are each N-ordered, we only need to take contractions between the 2 normal-ordered strings of operators that we started with.

2 IM-SRG wave function

The preceding results does not mean that the wave function obtained by the IM-SRG contains only linked contributions. The wave function $|\psi(s)\rangle$ can be given by

$$|\psi(s)\rangle = \mathcal{T}_s \exp\left(\int_0^s \eta(t)dt\right)|\phi\rangle . \tag{14}$$

At the second order in terms of η, it is (assuming η is one body)

$$\left|\psi^{[2]}(s)\right\rangle = \frac{1}{2}\sum_{ijkl}\int_0^s \left[\theta(t-t')\eta_{ij}(t)\{a_i^\dagger a_j\}\eta_{kl}(t')\{a_k^\dagger a_l\} + \theta(t'-t)\eta_{kl}(t')\{a_k^\dagger a_l\}\eta_{ij}(t)\{a_i^\dagger a_j\}\right] dtdt' \,|\phi\rangle . \tag{15}$$

The first term produces

$$\frac{1}{2}\sum_{ijkl}\int_0^s \theta(t-t')\eta_{ij}(t)\eta_{kl}(t')dtdt'\left(\{a_i^\dagger a_j a_k^\dagger a_l\} + C_{i^\dagger l}\{a_j a_k^\dagger\} + C_{jk^\dagger}\{a_i^\dagger a_l\} + C_{jk^\dagger}C_{i^\dagger l}\right)|\phi\rangle . \tag{16}$$

This clearly contains disconnected pieces. Regarding the wave function, the IM-SRG produces unlinked diagrams as other similarity transformation methods do, but there is no unlinked diagrams for evolved operators.

3 Conclusion

- a corollary of Wick's theorem

$$\{a_3^\dagger a_1\}\{a_4^\dagger a_2\} = \{a_3^\dagger a_1 a_4^\dagger a_2\} + C_{3^\dagger 2}\{a_1 a_4^\dagger\} + C_{14^\dagger}\{a_3^\dagger a_2\} + C_{3^\dagger 2}C_{14^\dagger} \tag{17}$$

  is true.

- The im-medium SRG (or usual SRG) produces the unlinked wave functions, but does not for the operators, including Hamiltonians.