The non-equilibrium Green function method

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Chapter 1

Basic issues

1.1 Time evolution operator

The time evolution operator $\hat{U}_{\mathbf{s}}(t, t_0)$ in the Schrodinger representation is defined by

$$|\Psi_{\mathbf{s}}(t)\rangle = \hat{U}_{\mathbf{s}}(t, t_0)|\Psi_{\mathbf{s}}(t_0)\rangle, \tag{1.1}$$

where $|\Psi_{\mathbf{s}}(t)\rangle$ and $|\Psi_{\mathbf{s}}(t_0)\rangle$ are the ket vectors of the states in the Schrodinger representation at time t and t_0, respectively. The time evolution operator $\hat{U}_{\mathbf{s}}(t, t_0)$ must satisfy the following three conditions:

(1) Unitarity

Consider the conservation of the probability:

$$\langle\Psi_{\mathbf{s}}(t_0)|\Psi_{\mathbf{s}}(t_0)\rangle = \langle\Psi_{\mathbf{s}}(t)|\Psi_{\mathbf{s}}(t)\rangle = \langle\Psi_{\mathbf{s}}(t_0)|\hat{U}_{\mathbf{s}}^{\dagger}(t, t_0)\hat{U}_{\mathbf{s}}(t, t_0)|\Psi_{\mathbf{s}}(t_0)\rangle. \tag{1.2}$$

This is assured by imposing the unitarity of $\hat{U}_{\mathbf{s}}(t, t_0)$:

$$\hat{U}_{\mathbf{s}}^{\dagger}(t, t_0)\hat{U}_{\mathbf{s}}(t, t_0) = \hat{U}_{\mathbf{s}}(t, t_0)\hat{U}_{\mathbf{s}}^{\dagger}(t, t_0) = 1, \tag{1.3}$$

where 1 is the identity operator. **If** the inverse operator $\hat{U}_{\mathbf{s}}^{-1}(t, t_0)$ of $\hat{U}_{\mathbf{s}}(t, t_0)$ can be defined, by multiplying both the sides by $\hat{U}_{\mathbf{s}}^{-1}(t, t_0)$, we obtain

$$\hat{U}_{\mathbf{s}}^{\dagger}(t, t_0) = \hat{U}_{\mathbf{s}}^{-1}(t, t_0). \tag{1.4}$$

Also, **if** the time evolution of $\Psi_{\mathbf{s}}$ in the reverse time

$$|\Psi_{\mathbf{s}}(t_0)\rangle = \hat{U}_{\mathbf{s}}(t_0, t)|\Psi_{\mathbf{s}}(t)\rangle \tag{1.5}$$

is defined, by putting Eq. (1.1) into Eq. (1.5) we get

$$|\Psi_{\mathbf{s}}(t_0)\rangle = \hat{U}_{\mathbf{s}}(t_0, t)\hat{U}_{\mathbf{s}}(t, t_0)|\Psi_{\mathbf{s}}(t_0)\rangle. \tag{1.6}$$

Since it is expected to be $\hat{U}_{\mathbf{s}}(t_0, t)\hat{U}_{\mathbf{s}}(t, t_0) = 1$, by noting Eqs. (1.3) and (1.4), we conclude

$$\hat{U}_{\mathbf{s}}(t_0, t) = \hat{U}_{\mathbf{s}}^{\dagger}(t, t_0) = \hat{U}_{\mathbf{s}}^{-1}(t, t_0). \tag{1.7}$$

(2) Associativity

It is natural to consider that the time evolution of $|\Psi_{\mathbf{s}}(t_0)\rangle$ from t_0 to t_2 coincides with that from t_0 to t_1 and subsequently from t_1 to t_2, where $t_0 < t_1 < t_2$. That is,

$$\hat{U}_{\mathbf{s}}(t_2, t_0) = \hat{U}_{\mathbf{s}}(t_2, t_1)\hat{U}_{\mathbf{s}}(t_1, t_0). \tag{1.8}$$

(3) Continuity

It is assumed that the state changes continously as a function of time:

$$|\Psi_{\mathbf{s}}(t_0 + dt)\rangle = \hat{U}_{\mathbf{s}}(t_0 + dt, t_0)|\Psi_{\mathbf{s}}(t_0)\rangle. \tag{1.9}$$

Thus,

$$\lim_{dt\to 0} \hat{U}_{\mathbf{s}}(t_0 + dt, t_0) = 1. \tag{1.10}$$

Let us now look for an expression satisfying above three conditions. An expression for $\hat{U}_{\mathbf{s}}(t_0+dt, t_0)$ which satisfies above three conditions approximately within small time interval dt is given by

$$\hat{U}_{\mathbf{s}}(t_0 + dt, t_0) = 1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0)dt. \tag{1.11}$$

The unitarity is confirmed as:

$$\begin{aligned}
\hat{U}^{\dagger}_{\mathbf{s}}(t_0 + dt, t_0)\hat{U}_{\mathbf{s}}(t_0 + dt, t_0) &= (1 + \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0)dt)(1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0)dt), \\
&= 1 + \frac{\hat{H}_{\mathbf{s}}(t_0)}{\hbar}dt^2, \\
&\simeq 1.
\end{aligned} \tag{1.12}$$

The associativity is confirmed as:

$$\begin{aligned}
\hat{U}_{\mathbf{s}}(t_0 + dt_1 + dt_2, t_0 + dt_1)\hat{U}_{\mathbf{s}}(t_0 + dt_1, t_0) &= (1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0 + dt_1)dt_2)(1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0)dt_1), \\
&= \left(1 - \frac{i}{\hbar}\left(\hat{H}_{\mathbf{s}}(t_0) + \frac{\partial \hat{H}_{\mathbf{s}}(t_0)}{\partial t}dt_1 + \cdots\right)dt_2\right)\left(1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0)dt_1\right), \\
&= 1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0)(dt_1 + dt_2) + O(dt^2), \\
&\simeq \hat{U}_{\mathbf{s}}(t_0 + dt_1 + dt_2, t_0).
\end{aligned} \tag{1.13}$$

The continuity is confirmed as:

$$\lim_{dt\to 0}\left(1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t_0)dt\right) = 1. \tag{1.14}$$

Thus, we have confirmed that the expression Eq. (1.11) surely satisfies the three conditions mentioned above within small time interval. Using the expression Eq. (1.11), we now derive an equation governing the time evolution of the time evolution operator. Considering the associativity, we can write

$$\begin{aligned}
\hat{U}_{\mathbf{s}}(t + dt, t_0) &= \hat{U}_{\mathbf{s}}(t + dt, t)\hat{U}_{\mathbf{s}}(t, t_0), \\
&\simeq \left(1 - \frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t)dt\right)\hat{U}_{\mathbf{s}}(t, t_0).
\end{aligned} \tag{1.15}$$

Rearranging the above equation gives

$$\frac{\hat{U}_{\mathbf{s}}(t + dt, t_0) - \hat{U}_{\mathbf{s}}(t, t_0)}{dt} = -\frac{i}{\hbar}\hat{H}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t, t_0). \tag{1.16}$$

So, we get the equation:

$$i\hbar\frac{\partial}{\partial t}\hat{U}_{\mathbf{s}}(t,t_0) = \hat{H}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t,t_0). \tag{1.17}$$

This is the equation governing the time evolution of the time evolution operator in the Schrodinger representation. By differentiating both the sides of Eq. (1.1) with respect to time t and mutiplying $i\hbar$, we obtain

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\mathbf{s}}(t)\rangle = \left(i\hbar\frac{\partial}{\partial t}\hat{U}_{\mathbf{s}}(t,t_0)\right)|\Psi_{\mathbf{s}}(t_0)\rangle. \tag{1.18}$$

Replacing the time derivarive in the parenthesis of the right hand side by Eq. (1.17), the time dependent Schrodinger equation can be obtained as:

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\mathbf{s}}(t)\rangle = \hat{H}_{\mathbf{s}}(t)|\Psi_{\mathbf{s}}(t)\rangle. \tag{1.19}$$

1.2 Density matrix

Let us consider a mixed ensemble that electrons populate states $\Psi_{\mathbf{s},k}$ where each proportion is $w_k (k = 1, 2, \cdots)$. The sum of the proportions in the population is unity:

$$\sum_k w_k = 1. \tag{1.20}$$

The ensemble average of an operator $\hat{A}(t)$ is defined by

$$\begin{aligned}
[A(t)] &= \sum_k w_k \langle\Psi_{\mathbf{s},k}|\hat{A}_{\mathbf{s}}(t)|\Psi_{\mathbf{s},k}\rangle, \\
&= \sum_{i,j}\sum_k w_k \langle\Psi_{\mathbf{s},k}|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{s}}(t)|\chi_j\rangle\langle\chi_j|\Psi_{\mathbf{s},k}\rangle, \\
&= \sum_{i,j}\langle\chi_j|\left[\sum_k w_k|\Psi_{\mathbf{s},k}\rangle\langle\Psi_{\mathbf{s},k}|\right]|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{s}}(t)|\chi_j\rangle, \\
&= \sum_{i,j}\langle\chi_j|\hat{\rho}_{\mathbf{s}}(t)|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{s}}(t)|\chi_j\rangle, \\
&= \mathrm{tr}(\hat{\rho}_{\mathbf{s}}(t)\hat{A}_{\mathbf{s}}(t)).
\end{aligned} \tag{1.21}$$

with the definition of the density matrix operator:

$$\hat{\rho}_{\mathbf{s}}(t) = \sum_k w_k|\Psi_{\mathbf{s},k}(t)\rangle\langle\Psi_{\mathbf{s},k}(t)|, \tag{1.22}$$

where the trace in Eq. (1.21) is interpreted as the trace for the matrix form of the operators using certain complete basis set. Considering that $\Psi_{\mathbf{s},k}$ follows Eq. (1.19) and **assuming** that w_k is independent of time, the time derivative of Eq. (1.22) leads to

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{\rho}_{\mathbf{s}}(t) &= \sum_k w_k\left[\left(i\hbar\frac{\partial}{\partial t}|\Psi_{\mathbf{s},k}\rangle\right)\langle\Psi_{\mathbf{s},k}| + |\Psi_{\mathbf{s},k}\rangle\left(i\hbar\frac{\partial}{\partial t}\langle\Psi_{\mathbf{s},k}|\right)\right], \\
&= \sum_k w_k\left[\hat{H}_{\mathbf{s}}|\Psi_{\mathbf{s},k}\rangle\langle\Psi_{\mathbf{s},k}| - |\Psi_{\mathbf{s},k}\rangle\langle\Psi_{\mathbf{s},k}|\hat{H}_{\mathbf{s}}\right], \\
&= -[\hat{\rho}_{\mathbf{s}}(t), \hat{H}_{\mathbf{s}}(t)].
\end{aligned} \tag{1.23}$$

In the thermal equilibrium, it can be considered to be $\frac{\partial}{\partial t}\hat{\rho}_{\mathbf{s}}(t) = 0$. This leads to $[\hat{\rho}_{\mathbf{s}}, \hat{H}_{\mathbf{s}}] = 0$, and means that $\hat{\rho}_{\mathbf{s}}$ and $\hat{H}_{\mathbf{s}}$ can be simultaneously diagonalized using the eigenstates of $\hat{H}_{\mathbf{s}}$. Using the eigenstates a quantity σ, related to the entropy $S = k_{\mathrm{B}}\sigma$, can be written as

$$\begin{aligned} \sigma &= -\mathrm{tr}(\hat{\rho}_{\mathbf{s}} \ln(\hat{\rho}_{\mathbf{s}})), \\ &= -\sum_k \rho_{kk} \ln(\rho_{kk}), \end{aligned} \tag{1.24}$$

where ρ_{kk} is the diagonal term of the matrix form, and equl to w_k in Eq. (1.20). In the complete random ensemble, the σ takes the maximum, and it turns out to be $\sigma = \ln(N)$, since $\rho_{kk} = \frac{1}{N}$ where N is the number of states. On the other hand for the pure ensemble σ takes the minimum, and $\sigma = 0$. In the thermal equilibrium, it can be considered that σ may take a maximum under two conditions:

$$\sum_k \rho_{\mathbf{s},kk} = 1 \tag{1.25}$$

and

$$\begin{aligned} [\hat{H}_{\mathbf{s}}] &= \mathrm{tr}(\hat{\rho}_{\mathbf{s}}\hat{H}_{\mathbf{s}}), \\ &= \sum_k \rho_{kk} E_k \equiv U, \end{aligned} \tag{1.26}$$

where E_k is the eigenenergy of $\hat{H}_{\mathbf{s}}$, and U is a constant. The density matrix, giving the maximum, can be found by minimizing the following function F using Lagrange's multiplier method:

$$F = -\sigma + \gamma\left(\sum_k \rho_{kk} - 1\right) + \beta\left(\sum_k \rho_{kk}E_k - U\right), \tag{1.27}$$

where γ and β are the multipliers. $\frac{F}{\rho_{ii}} = 0$ gives

$$\rho_{ii} = \frac{\exp(-\beta E_i)}{\exp(\gamma + 1)}. \tag{1.28}$$

$\frac{F}{\gamma} = 0$ gives

$$\sum_k \rho_{kk} = 1. \tag{1.29}$$

Putting Eq. (1.28) into Eq. (1.29) yields

$$\exp(\gamma + 1) = \sum_k \exp(-\beta E_k). \tag{1.30}$$

Replacing $\exp(\gamma + 1)$ by Eq. (1.30), we obtain

$$\rho_{ii} = \frac{\exp(-\beta E_i)}{\sum_k \exp(-\beta E_k)}. \tag{1.31}$$

Noting that $\sum_k \exp(-\beta E_k) = \mathrm{tr}(\exp(-\beta H_{\mathbf{d}})) = \mathrm{tr}(\exp(-\beta V H_{\mathbf{d}} V^{\dagger})) = \mathrm{tr}(\exp(-\beta \hat{H}_{\mathbf{s}}))$, $V\rho_{\mathbf{d}}V^{\dagger} = \rho_{\mathbf{s}}$, and $V\exp(-\beta H_{\mathbf{d}})V^{\dagger} = \exp(-\beta H_{\mathbf{s}})$, where V is the unitary matrix which diagonalizes $H_{\mathbf{s}}$, and $H_{\mathbf{d}}$ is a matrix of which diagonal terms are E_k, and $\rho_{\mathbf{d}}$ a matrix of which diagonal terms are ρ_{kk}, we can write the density matrix in the thermal equilibrium as

$$\rho_{\mathbf{s}} = \frac{\exp(-\beta H_{\mathbf{s}})}{\mathrm{tr}(\exp(-\beta \hat{H}_{\mathbf{s}}))}. \tag{1.32}$$

1.3 Field operator

A creation operator $\hat{a}^\dagger$ and destruction operator $\hat{a}$ defined for the Fermion satisfy the following anti-commutation relations:

$$\{\hat{a}_{\mathbf{s},i}, \hat{a}^\dagger_{\mathbf{s},j}\} = \delta_{ij}, \tag{1.33}$$
$$\{\hat{a}_{\mathbf{s},i}, \hat{a}_{\mathbf{s},j}\} = \{\hat{a}^\dagger_{\mathbf{s},i}, \hat{a}^\dagger_{\mathbf{s},j}\} = 0, \tag{1.34}$$

where $\{\hat{a}, \hat{b}\} \equiv \hat{a}\hat{b} + \hat{b}\hat{a}$. Using the operators, a field operator $\hat{\Psi}_\mathbf{s}(\mathbf{r})$ is defined by

$$\begin{aligned} \hat{\Psi}_\mathbf{s}(\mathbf{r}) &= \sum_i \Psi_{\mathbf{s},i}(\mathbf{r}, t_0)\hat{a}_{\mathbf{s},i}, \\ \hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}) &= \sum_i \Psi^\dagger_{\mathbf{s},i}(\mathbf{r}, t_0)\hat{a}^\dagger_{\mathbf{s},i}, \end{aligned} \tag{1.35}$$

where we considered $\Psi_{\mathbf{s},i}(\mathbf{r}, t_0)$ being eigenstates of $H_\mathbf{s}(t_0)$ as one-particle wave functions. The anti-commutation relation for the field operator can be found as:

$$\begin{aligned} \hat{\Psi}_\mathbf{s}(\mathbf{r})\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}') + \hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}')\hat{\Psi}_\mathbf{s}(\mathbf{r}) &= \sum_{i,j} \Psi_{\mathbf{s},i}(\mathbf{r}, t_0)\Psi^\dagger_{\mathbf{s},j}(\mathbf{r}', t_0)\left(\hat{a}_{\mathbf{s},i}\hat{a}^\dagger_{\mathbf{s},j} + \hat{a}^\dagger_{\mathbf{s},j}\hat{a}_{\mathbf{s},i}\right), \\ &= \sum_{ij} \Psi_{\mathbf{s},i}(\mathbf{r}, t_0)\Psi^\dagger_{\mathbf{s},j}(\mathbf{r}', t_0)\{\hat{a}_{\mathbf{s},i}, \hat{a}^\dagger_{\mathbf{s},j}\}, \\ &= \sum_i \Psi_{\mathbf{s},i}(\mathbf{r}, t_0)\Psi^\dagger_{\mathbf{s},i}(\mathbf{r}', t_0), \\ &= \delta(\mathbf{r} - \mathbf{r}'). \end{aligned} \tag{1.36}$$

Therefore,

$$\{\hat{\Psi}_{\mathbf{s},i}(\mathbf{r}, t_0), \hat{\Psi}^\dagger_{\mathbf{s},i}(\mathbf{r}', t_0)\} = \delta(\mathbf{r} - \mathbf{r}'). \tag{1.37}$$

The similar analysis leads to

$$\{\hat{\Psi}_{\mathbf{s},i}(\mathbf{r}, t_0), \hat{\Psi}_{\mathbf{s},i}(\mathbf{r}', t_0)\} = \{\hat{\Psi}^\dagger_{\mathbf{s},i}(\mathbf{r}, t_0), \hat{\Psi}^\dagger_{\mathbf{s},i}(\mathbf{r}', t_0)\} = 0. \tag{1.38}$$

It is also noted that the second quantized Hamiltonian $\hat{H}$ using the operators $\hat{a}^\dagger$ and $\hat{a}$ can be rewritten by the field operators as follows:

$$\begin{aligned} \hat{H}_\mathbf{s} &= \sum_{ij} \hat{a}^\dagger_{\mathbf{s},i}\left[\int d\mathbf{r}\Psi^\dagger_{\mathbf{s},i}(\mathbf{r}, t_0)\hat{v}_1(\mathbf{r}, t)\Psi_{\mathbf{s},j}(\mathbf{r}, t_0)\right]\hat{a}_{\mathbf{s},j} \\ &\quad + \frac{1}{2}\sum_{ijkl} \hat{a}^\dagger_{\mathbf{s},i}\hat{a}^\dagger_{\mathbf{s},j}\left[\int\int d\mathbf{r}d\mathbf{r}'\Psi^\dagger_{\mathbf{s},i}(\mathbf{r}, t_0)\Psi^\dagger_{\mathbf{s},j}(\mathbf{r}', t_0)\hat{v}_2(\mathbf{r}, \mathbf{r}', t)\Psi_{\mathbf{s},k}(\mathbf{r}', t_0)\Psi_{\mathbf{s},l}(\mathbf{r}, t_0)\right]\hat{a}_{\mathbf{s},k}\hat{a}_{\mathbf{s},l} \end{aligned} \tag{1.39}$$
$$\begin{aligned} &= \int d\mathbf{r}\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}, t_0)\hat{v}_1(\mathbf{r}, t)\hat{\Psi}_\mathbf{s}(\mathbf{r}, t_0) \\ &\quad + \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}, t_0)\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}', t_0)\hat{v}_2(\mathbf{r}, \mathbf{r}', t)\hat{\Psi}_\mathbf{s}(\mathbf{r}', t_0)\hat{\Psi}_\mathbf{s}(\mathbf{r}, t_0), \end{aligned} \tag{1.40}$$

where $\hat{v}_1$ and $\hat{v}_2$ are one- and two-particle time dependent operators. In the Schrodinger representationm, the field operator is not time dependent, while $\hat{v}_1$ and $\hat{v}_2$ can be time dependent. Thus, we see

$$\begin{aligned} \frac{\partial}{\partial t}\hat{\Psi}_\mathbf{s}(\mathbf{r}) &= 0, \\ \frac{\partial}{\partial t}\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}) &= 0, \end{aligned} \tag{1.41}$$

1.4 Representation

We discuss three kind of representations: Schrodinger, Heisenberg, and interaction representations. To avoid confusion, the representation is denoted by a subscript, i.e., **s**, **h**, and **i** stand for the Schrodinger, Heisenberg, and interaction representations, respectively.

(1) Schrodinger representation

In the Schrodinger representation, the expectation value of an operator $\hat{A}_{\mathbf{s}}(t)$ is given by

$$\langle\Psi_{\mathbf{s}}(t)|\hat{A}_{\mathbf{s}}(t)|\Psi_{\mathbf{s}}(t)\rangle = \langle\Psi_{\mathbf{s}}(t_0)|\hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\hat{A}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t,t_0)|\Psi_{\mathbf{s}}(t_0)\rangle. \tag{1.42}$$

If $\hat{A}_{\mathbf{s}}(t)$ is time dependent, the time derivative of the operator $\hat{A}_{\mathbf{s}}(t)$ can be considered:

$$\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t) = \frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t). \tag{1.43}$$

(2) Heisenberg representation

In the right hand side of the Eq. (1.42), it is possible to consider that the operator $\hat{A}_{\mathbf{s}}(t)$ is evolved by the time evolution operator $\hat{U}_{\mathbf{s}}$ instead of the wave function. This change of view defines the Heisenberg representation of $\hat{A}$ as:

$$\hat{A}_{\mathbf{h}}(t) = \hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\hat{A}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t,t_0). \tag{1.44}$$

In this Heisenberg representation, the wave function, $\Psi_{\mathbf{h}}(t) \equiv \Psi_{\mathbf{s}}(t_0)$, is clearly independent of time. Thus we see

$$i\hbar\frac{\partial}{\partial t}\Psi_{\mathbf{h}}(t) = 0. \tag{1.45}$$

So, $U_{\mathbf{h}}(t,t_0) = 1$, and

$$i\hbar\frac{\partial}{\partial t}U_{\mathbf{h}}(t,t_0) = 0. \tag{1.46}$$

Differentiating $\hat{A}_{\mathbf{h}}(t)$ and multiplying $i\hbar$, and utilizing Eq. (1.17), we find

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{h}}(t) &= \left(i\hbar\frac{\partial}{\partial t}\hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\right)\hat{A}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t,t_0) + \hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\left(i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t)\right)\hat{U}_{\mathbf{s}}(t,t_0) + \hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\hat{A}_{\mathbf{s}}(t)\left(i\hbar\frac{\partial}{\partial t}\hat{U}_{\mathbf{s}}(t,t_0)\right), \\
&= -\hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\hat{H}_{\mathbf{s}}(t)\hat{A}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t,t_0) + \hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\hat{A}_{\mathbf{s}}(t)\hat{H}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t,t_0) + \hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\left(i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t)\right)\hat{U}_{\mathbf{s}}(t,t_0), \\
&= -\hat{H}_{\mathbf{h}}(t)\hat{A}_{\mathbf{h}}(t) + \hat{A}_{\mathbf{h}}(t)\hat{H}_{\mathbf{h}}(t) + \hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\left(i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t)\right)\hat{U}_{\mathbf{s}}(t,t_0), \\
&= [\hat{A}_{\mathbf{h}}(t),\hat{H}_{\mathbf{h}}(t)] + \hat{U}^{\dagger}_{\mathbf{s}}(t,t_0)\left(i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t)\right)\hat{U}_{\mathbf{s}}(t,t_0).
\end{aligned} \tag{1.47}$$

If $\hat{A}_{\mathbf{s}}$ is independent of time, Eq. (1.47) is simplified as

$$i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{h}}(t) = [\hat{A}_{\mathbf{h}}(t),\hat{H}_{\mathbf{h}}(t)]. \tag{1.48}$$

Let us consider to write $\hat{H}$ in the Heisenberg representation. The first term in the right side of Eq. (1.39) is transformed using Eq. (1.44) as

$$
\begin{aligned}
&\hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\left(\sum_{ij}\hat{a}_{\mathbf{s},i}^{\dagger}\left[\int d\mathbf{r}\Psi_{\mathbf{s},i}^{\dagger}(\mathbf{r},t_0)\hat{v}_1(\mathbf{r},t)\Psi_{\mathbf{s},i}(\mathbf{r},t_0)\right]\hat{a}_{\mathbf{s},j}\right)\hat{U}_{\mathbf{s}}(t,t_0)\\
&=\sum_{ij}\hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},i}^{\dagger}\hat{U}_{\mathbf{s}}(t,t_0)\hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\left[\int d\mathbf{r}\Psi_{\mathbf{s},i}^{\dagger}(\mathbf{r},t_0)\hat{v}_1(\mathbf{r},t)\Psi_{\mathbf{s},i}(\mathbf{r},t_0)\right]\hat{U}_{\mathbf{s}}(t,t_0)\hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},j}\hat{U}_{\mathbf{s}}(t,t_0),\\
&=\sum_{i,j}\hat{a}_{\mathbf{h},i}^{\dagger}(t)\left[\int d\mathbf{r}\Psi_{\mathbf{s},i}^{\dagger}(\mathbf{r},t_0)\hat{v}_1(\mathbf{r},t)\Psi_{\mathbf{s},i}(\mathbf{r},t_0)\right]\hat{a}_{\mathbf{h},j}(t),\\
&=\int d\mathbf{r}\hat{\Psi}_{\mathbf{h}}^{\dagger}(t)(\mathbf{r},t)\hat{v}_1(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r},t),
\end{aligned}
$$

where we defined

$$
\begin{aligned}
\hat{a}_{\mathbf{h},i}^{\dagger}(t) &= \hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},i}^{\dagger}\hat{U}_{\mathbf{s}}(t,t_0),\\
\hat{a}_{\mathbf{h},i}(t) &= \hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},i}\hat{U}_{\mathbf{s}}(t,t_0),
\end{aligned}
\tag{1.49}
$$

and

$$
\begin{aligned}
\hat{\Psi}_{\mathbf{h}}(\mathbf{r},t) &= \sum_i \Psi_{\mathbf{s},i}(\mathbf{r},t_0)\hat{a}_{\mathbf{h},i}(t),\\
\hat{\Psi}_{\mathbf{h}}^{\dagger}(\mathbf{r},t) &= \sum_i \Psi_{\mathbf{s},i}^{\dagger}(\mathbf{r},t_0)\hat{a}_{\mathbf{h},i}^{\dagger}(t).
\end{aligned}
\tag{1.50}
$$

By doing the same analysis for the second term in the right side of Eq. (1.39), the total Hamiltonian in the Heisenberg representation is written by

$$\hat{H}_{\mathbf{h}} = \hat{H}_{\mathbf{h},1} + \hat{H}_{\mathbf{h},2}, \tag{1.51}$$

where $\hat{H}_{\mathbf{h},1}$ and $\hat{H}_{\mathbf{h},2}$ are one- and two-particle Hamiltonians in the Heisenberg representation defined by

$$\hat{H}_{\mathbf{h},1} = \int d\mathbf{r}\hat{\Psi}_{\mathbf{h}}^{\dagger}(\mathbf{r},t)\hat{v}_1(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r},t) \tag{1.52}$$

and

$$\hat{H}_{\mathbf{h},2} = \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\hat{\Psi}_{\mathbf{h}}^{\dagger}(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}^{\dagger}(\mathbf{r}',t)\hat{v}_2(\mathbf{r},\mathbf{r}',t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}',t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r},t). \tag{1.53}$$

The anticommutation relations for $\hat{a}_{\mathbf{h},i}^{\dagger}$ and $\hat{a}_{\mathbf{h},i}$ are confirmed as follows:

$$
\begin{aligned}
\{\hat{a}_{\mathbf{h},i},\hat{a}_{\mathbf{h},j}^{\dagger}\} &= \hat{a}_{\mathbf{h},i}\hat{a}_{\mathbf{h},j}^{\dagger}+\hat{a}_{\mathbf{h},j}^{\dagger}\hat{a}_{\mathbf{h},i},\\
&= \hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},i}\hat{U}_{\mathbf{s}}(t,t_0)\hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},j}^{\dagger}\hat{U}_{\mathbf{s}}(t,t_0)+\hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},j}^{\dagger}\hat{U}_{\mathbf{s}}(t,t_0)\hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\hat{a}_{\mathbf{s},i}\hat{U}_{\mathbf{s}}(t,t_0),\\
&= \hat{U}_{\mathbf{s}}^{\dagger}(t,t_0)\{\hat{a}_{\mathbf{s},i},\hat{a}_{\mathbf{s},j}^{\dagger}\}\hat{U}_{\mathbf{s}}(t,t_0),\\
&= \delta_{ij}.
\end{aligned}
\tag{1.54}
$$

As well,

$$\{\hat{a}_{\mathbf{h},i},\hat{a}_{\mathbf{h},j}\} = \{\hat{a}_{\mathbf{h},i}^{\dagger},\hat{a}_{\mathbf{h},j}^{\dagger}\} = 0. \tag{1.55}$$

The anticommutation relation for $\hat{\Psi}^\dagger_{\mathbf{h},i}$ and $\hat{\Psi}_{\mathbf{h},i}$ is confirmed using Eq. (1.54) as follows:

$$\begin{aligned}
\{\hat{\Psi}_\mathbf{h}(\mathbf{r},t), \hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}',t)\} &= \sum_{i,j} \Psi_{\mathbf{s},i}(\mathbf{r},t_0)\Psi^\dagger_{\mathbf{s},j}(\mathbf{r}',t_0)\left(\hat{a}_{\mathbf{h},i}\hat{a}^\dagger_{\mathbf{h},j} + \hat{a}^\dagger_{\mathbf{h},j}\hat{a}_{\mathbf{h},i}\right), \\
&= \sum_i \Psi_{\mathbf{s},i}(\mathbf{r},t_0)\Psi^\dagger_{\mathbf{s},i}(\mathbf{r}',t_0) \\
&= \delta(\mathbf{r}-\mathbf{r}').
\end{aligned} \tag{1.56}$$

As well,

$$\{\hat{\Psi}_\mathbf{h}(\mathbf{r},t), \hat{\Psi}_\mathbf{h}(\mathbf{r}',t)\} = \{\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r},t), \hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}',t)\} = 0. \tag{1.57}$$

The time derivative of the field operator given by Eq. (1.50) can be obtained by making use of Eq. (1.47). So, first let us consider $[\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t), \hat{H}_\mathbf{h}(\mathbf{r},t)]$. Noting that v_1 and v_2 are Hermitian so that

$$\int d\mathbf{r}\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r},t_0)\hat{v}_1(\mathbf{r},t)\hat{\Psi}_\mathbf{s}(\mathbf{r},t_0) = \int d\mathbf{r}\left(\hat{v}_1(\mathbf{r},t)\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r},t_0)\right)\hat{\Psi}_\mathbf{s}(\mathbf{r},t_0) \tag{1.58}$$

and

$$\begin{aligned}
&\int\int d\mathbf{r}d\mathbf{r}'\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r},t_0)\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}',t_0)\hat{v}_2(\mathbf{r},\mathbf{r}',t)\hat{\Psi}_\mathbf{s}(\mathbf{r}',t_0)\hat{\Psi}_\mathbf{s}(\mathbf{r},t_0) = \\
&\qquad \int\int d\mathbf{r}d\mathbf{r}'\left(\hat{v}_2(\mathbf{r},\mathbf{r}',t)\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r},t_0)\hat{\Psi}^\dagger_\mathbf{s}(\mathbf{r}',t_0)\right)\hat{\Psi}_\mathbf{s}(\mathbf{r}',t_0)\hat{\Psi}_\mathbf{s}(\mathbf{r},t_0),
\end{aligned} \tag{1.59}$$

we can evaluate $[\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t), \hat{H}_\mathbf{h}(\mathbf{r},t)]$ as follows:

$$\begin{aligned}
\left[\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t), \hat{H}_\mathbf{h}(t)\right] &= \int d\mathbf{r}\hat{v}_1(\mathbf{r},t)\left[\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t), \hat{\Psi}^\dagger_\mathbf{h}(t)(\mathbf{r},t)\hat{\Psi}_\mathbf{h}(\mathbf{r},t)\right] \\
&\quad +\frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\hat{v}_2(\mathbf{r},\mathbf{r}',t)\left[\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t), \hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r},t)\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}',t)\hat{\Psi}_\mathbf{h}(\mathbf{r}',t)\hat{\Psi}_\mathbf{h}(\mathbf{r},t)\right], \\
&= \hat{v}_1(\mathbf{r}'',t)\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t) + \frac{1}{2}\left\{\int d\mathbf{r}'\hat{v}_2(\mathbf{r}'',\mathbf{r}',t)\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}',t)\hat{\Psi}_\mathbf{h}(\mathbf{r}',t)\right\}\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t) \\
&\quad +\frac{1}{2}\left\{\int d\mathbf{r}\hat{v}_2(\mathbf{r},\mathbf{r}'',t)\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r},t)\hat{\Psi}_\mathbf{h}(\mathbf{r},t)\right\}\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t), \\
&= \left\{\hat{v}_1(\mathbf{r}'',t) + \int d\mathbf{r}'\hat{v}_2(\mathbf{r}'',\mathbf{r}',t)\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}',t)\hat{\Psi}_\mathbf{h}(\mathbf{r}',t)\right\}\hat{\Psi}_\mathbf{h}(\mathbf{r}'',t),
\end{aligned} \tag{1.60}$$

where for the above derivation from the first to second lines we utilized Eqs. (1.56) and (1.57), and the following relations:

$$\left[\hat{A},\hat{B}\hat{C}\right] = \left\{\hat{A},\hat{B}\right\}\hat{C} - \hat{B}\left\{\hat{A},\hat{C}\right\}, \tag{1.61}$$

$$\left[\hat{A},\hat{B}\hat{C}\hat{D}\hat{E}\right] = \left\{\hat{A},\hat{B}\right\}\hat{C}\hat{D}\hat{E} - \hat{B}\left\{\hat{A},\hat{C}\right\}\hat{D}\hat{E} - \hat{B}\hat{C}\left\{\hat{A},\hat{D}\right\}\hat{E} + \hat{B}\hat{C}\hat{D}\left\{\hat{A},\hat{E}\right\}. \tag{1.62}$$

The contribution to the time derivative of the field operator in the Heisenberg representation, corresponding to the second term in Eq. (1.48), is strictly zero because of Eq. (1.41). Therefore, the first term only survives in Eq. (1.48), and consequently the time derivative of field operator in the Heisenberg representation is given by

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}_\mathbf{h}(\mathbf{r},t) = \left\{\hat{v}_1(\mathbf{r},t) + \int d\mathbf{r}'\hat{v}_2(\mathbf{r},\mathbf{r}',t)\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}',t)\hat{\Psi}_\mathbf{h}(\mathbf{r}',t)\right\}\hat{\Psi}_\mathbf{h}(\mathbf{r},t). \tag{1.63}$$

The ensemble average of an operator $\hat{A}(t)$ is written by the density matrix in the Heisenberg representation as:

$$\begin{aligned}
[A(t)] &= \sum_k w_k \langle \Psi_{\mathbf{s},k}(t_0)|\hat{U}_{\mathbf{s}}^\dagger(t,t_0)\hat{A}_{\mathbf{s}}(t)\hat{U}_{\mathbf{s}}(t,t_0)|\Psi_{\mathbf{s},k}(t_0)\rangle, \\
&= \sum_k w_k \langle \Psi_{\mathbf{s},k}(t_0)|\hat{A}_{\mathbf{h}}(t)|\Psi_{\mathbf{s},k}(t_0)\rangle, \\
&= \sum_{i,j}\sum_k w_k \langle \Psi_{\mathbf{s},k}(t_0)|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{h}}(t)|\chi_j\rangle\langle\chi_j|\Psi_{\mathbf{s},k}(t_0)\rangle, \\
&= \sum_{i,j}\langle\chi_j|\left[\sum_k w_k|\Psi_{\mathbf{s},k}(t_0)\rangle\langle\Psi_{\mathbf{s},k}(t_0)|\right]|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{h}}(t)|\chi_j\rangle, \\
&= \sum_{i,j}\langle\chi_j|\hat{\rho_{\mathbf{h}}}(t)|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{h}}(t)|\chi_j\rangle, \\
&= \mathrm{tr}(\rho A)
\end{aligned} \tag{1.64}$$

with the definition of the density matrix operator in the Heisenberg representation:

$$\hat{\rho_{\mathbf{h}}}(t) = \sum_k w_k |\Psi_{\mathbf{s},k}(t_0)\rangle\langle\Psi_{\mathbf{s},k}(t_0)|. \tag{1.65}$$

Thus, we see that the the density matrix operator in the Heisenberg representation is independent of time:

$$\frac{\partial}{\partial t}\hat{\rho_{\mathbf{h}}}(t) = 0. \tag{1.66}$$

(3) Interaction representation

Suppose that the Hamiltonian $\hat{H}_{\mathbf{s}}$ is decomposed into a time independent part $\hat{H}_{\mathbf{s},0}$ and a time dependent part $\hat{H}_{\mathbf{s},1}$.

$$\hat{H}_{\mathbf{s}} = \hat{H}_{\mathbf{s},0} + \hat{H}_{\mathbf{s},1}(t). \tag{1.67}$$

In this case, let us consider to express the expectation value in a interaction representation:

$$\begin{aligned}
\langle\Psi_{\mathbf{s}}(t)|\hat{A}_{\mathbf{s}}(t)|\Psi_{\mathbf{s}}(t)\rangle &= \langle\Psi_{\mathbf{s}}(t)|\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{A}_{\mathbf{s}}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{s}}(t)\rangle, \\
&= \langle\Psi_{\mathbf{i}}(t)|\hat{A}_{\mathbf{i}}(t)|\Psi_{\mathbf{i}}(t)\rangle,
\end{aligned} \tag{1.68}$$

where we defined the wave function $\Psi_{\mathbf{i}}(t)$ and the operator $\hat{A}_{\mathbf{i}}(t)$ in the interaction representation as:

$$|\Psi_{\mathbf{i}}(t)\rangle = \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{s}}(t)\rangle, \tag{1.69}$$

$$\hat{A}_{\mathbf{i}}(t) = \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{A}_{\mathbf{s}}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}. \tag{1.70}$$

The equations (1.69) and (1.70) present the relation between the Schrodinger and interaction representations for the state vector and the operator. Differentiating the wave function defined by Eq. (1.69) with respect to time, and multiplying it by $i\hbar$, we obtain

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}|\Psi_{\mathbf{i}}(t)\rangle &= i\hbar\frac{\partial}{\partial t}\left(\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{s}}(t)\rangle\right), \\
&= -\hat{H}_{\mathbf{s},0}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{s}}(t)\rangle + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\left[i\hbar\frac{\partial}{\partial t}\hat{U}_{\mathbf{s}}(t,t_0)\right]|\Psi_{\mathbf{s}}(t_0)\rangle, \\
&= -\hat{H}_{\mathbf{s},0}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{s}}(t)\rangle + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s}}\hat{U}_{\mathbf{s}}(t,t_0)|\Psi_{\mathbf{s}}(t_0)\rangle, \\
&= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s},1}(t)|\Psi_{\mathbf{s}}(t)\rangle, \\
&= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s},1}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{s}}(t)\rangle, \\
&= \hat{H}_{\mathbf{i},1}(t)|\Psi_{\mathbf{i}}(t)\rangle,
\end{aligned} \tag{1.71}$$

where we defined

$$\hat{H}_{\mathbf{i},1}(t) = \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s},1}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}. \tag{1.72}$$

In the derivation of Eq. (1.71), we used $\hat{H}_{\mathbf{s},0}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t} = \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s},0}$. This is a consequence of the fact that if a function can be Taylor expanded, the following commutation relation is proven:

$$\hat{A}f(\hat{A}) = f(\hat{A})\hat{A}. \tag{1.73}$$

Differentiating the operator defined by Eq. (1.70) with respect to time, and multiplying it by $i\hbar$, we obtain

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{i}}(t) &= -\hat{H}_{\mathbf{s},0}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{A}_{\mathbf{s}}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t} + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\left(i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t)\right)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t} + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{A}_{\mathbf{s}}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s},0}, \\
&= \hat{A}_{\mathbf{i}}(t)\hat{H}_{\mathbf{s},0} - \hat{H}_{\mathbf{s},0}\hat{A}_{\mathbf{i}}(t) + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\left(i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t)\right)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}, \\
&= [\hat{A}_{\mathbf{i}}(t), \hat{H}_{\mathbf{s},0}] + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\left(i\hbar\frac{\partial}{\partial t}\hat{A}_{\mathbf{s}}(t)\right)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}.
\end{aligned} \tag{1.74}$$

By doing the same analysis as for the Heisenberg representation, we can define the creation, destruction, and field operators as follows:

$$\begin{aligned}
\hat{a}^{\dagger}_{\mathbf{i},i}(t) &= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{a}^{\dagger}_{\mathbf{s},i}\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}, \\
\hat{a}_{\mathbf{i},i}(t) &= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{a}_{\mathbf{s},i}\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t},
\end{aligned} \tag{1.75}$$

$$\begin{aligned}
\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}, t) &= \sum_i \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}, t_0)\hat{a}^{\dagger}_{\mathbf{i},i}(t), \\
\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t) &= \sum_i \Psi_{\mathbf{s},i}(\mathbf{r}, t_0)\hat{a}_{\mathbf{i},i}(t).
\end{aligned} \tag{1.76}$$

$$\begin{aligned}
\{\hat{a}_{\mathbf{i},i}, \hat{a}^{\dagger}_{\mathbf{i},j}\} &= \delta_{ij}, \\
\{\hat{a}_{\mathbf{i},i}, \hat{a}_{\mathbf{i},j}\} &= \{\hat{a}^{\dagger}_{\mathbf{i},i}, \hat{a}^{\dagger}_{\mathbf{i},j}\} = 0,
\end{aligned} \tag{1.77}$$

$$\begin{aligned}
\{\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t), \hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}', t)\} &= \delta(\mathbf{r} - \mathbf{r}'), \\
\{\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t), \hat{\Psi}_{\mathbf{i}}(\mathbf{r}', t)\} &= \{\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}, t), \hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}', t)\} = 0.
\end{aligned} \tag{1.78}$$

Using the field operator in the interaction representation, we can write the Hamiltonian as:

$$\hat{H}_{\mathbf{i}} = \hat{H}_{\mathbf{i},0} + \hat{H}_{\mathbf{i},1} \tag{1.79}$$

with

$$\begin{aligned}
\hat{H}_{\mathbf{i},0} &= \int d\mathbf{r}\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}, t)\hat{v}_{1,0}(\mathbf{r})\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t) \\
&\quad + \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}, t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}', t)\hat{v}_{2,0}(\mathbf{r}, \mathbf{r}')\hat{\Psi}_{\mathbf{i}}(\mathbf{r}', t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t),
\end{aligned} \tag{1.80}$$

$$\begin{aligned}
\hat{H}_{\mathbf{i},1} &= \int d\mathbf{r}\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}, t)\hat{v}_{1,1}(\mathbf{r}, t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t) \\
&\quad + \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}, t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}', t)\hat{v}_{2,1}(\mathbf{r}, \mathbf{r}', t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}', t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t),
\end{aligned} \tag{1.81}$$

where $\hat{v}_{1,0}$ and $\hat{v}_{2,0}$ are time independent one-particle and two-particle potentials, respectively, and $\hat{v}_{1,1}$ and $\hat{v}_{2,1}$ are time dependent one-particle and two-particle potentials, respectively.

The time derivative of the field operator given by Eq. (1.76) can be obtained by making use of Eq. (1.74). Since in this case the second term in Eq. (1.74) is zero due to Eq. (1.41), we only have to consider $[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t), \hat{H}_{\mathbf{s},0}(\mathbf{r}, t)]$. Noting that

$$\hat{H}_{\mathbf{i},0}(t) = \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s},0}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t} = \hat{H}_{\mathbf{s},0}(t)\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t} = \hat{H}_{\mathbf{s},0}(t), \tag{1.82}$$

and using Eqs. (1.61) and (1.62), we can evaluate $[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t), \hat{H}_{\mathbf{s},0}(\mathbf{r}, t)]$ as follows:

$$\begin{aligned}
[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t), \hat{H}_{\mathbf{s},0}(\mathbf{r}, t)] &= [\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t), \hat{H}_{\mathbf{i},0}(\mathbf{r}, t)], \\
&= \int d\mathbf{r}\hat{v}_{1,0}(\mathbf{r})\left[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t), \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}, t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t)\right] \\
&\quad + \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\hat{v}_{2,0}(\mathbf{r}, \mathbf{r}')\left[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t), \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}, t)\hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}', t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}', t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t)\right], \\
&= \left\{\hat{v}_{1,0}(\mathbf{r}'', t) + \int d\mathbf{r}'\hat{v}_{2,0}(\mathbf{r}'', \mathbf{r}', t)\hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}', t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}', t)\right\}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t).
\end{aligned} \tag{1.83}$$

Thus, we can write

$$i\hbar\frac{\partial\hat{\Psi}_{\mathbf{i}}(\mathbf{r}, t)}{\partial t} = \left\{\hat{v}_{1,0}(\mathbf{r}'', t) + \int d\mathbf{r}'\hat{v}_{2,0}(\mathbf{r}'', \mathbf{r}', t)\hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}', t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}', t)\right\}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'', t). \tag{1.84}$$

Using Eq. (1.68), the ensemble average of an operator $\hat{A}(t)$ is written by the density matrix in the interaction representation as:

$$\begin{aligned}
[A(t)] &= \sum_k w_k\langle\Psi_{\mathbf{s},k}(t)|\hat{A}_{\mathbf{s}}(t)|\Psi_{\mathbf{s},k}(t)\rangle, \\
&= \sum_k w_k\langle\Psi_{\mathbf{i},k}(t)|\hat{A}_{\mathbf{i}}(t)|\Psi_{\mathbf{i},k}(t)\rangle, \\
&= \sum_{i,j}\sum_k w_k\langle\Psi_{\mathbf{i},k}(t)|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{i}}(t)|\chi_j\rangle\langle\chi_j|\Psi_{\mathbf{i},k}(t)\rangle, \\
&= \sum_{i,j}\langle\chi_j|\left[\sum_k w_k|\Psi_{\mathbf{i},k}(t)\rangle\langle\Psi_{\mathbf{i},k}(t)|\right]|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{i}}(t)|\chi_j\rangle, \\
&= \sum_{i,j}\langle\chi_j|\hat{\rho}_{\mathbf{i}}(t)|\chi_i\rangle\langle\chi_i|\hat{A}_{\mathbf{i}}(t)|\chi_j\rangle, \\
&= \mathrm{tr}(\rho A)
\end{aligned} \tag{1.85}$$

with the definition of the density matrix operator in the interaction representation:

$$\hat{\rho}_{\mathbf{i}}(t) = \sum_k w_k|\Psi_{\mathbf{i},k}(t)\rangle\langle\Psi_{\mathbf{i},k}(t)|. \tag{1.86}$$

Noting that $\Psi_{\mathbf{i},k}$ obeys Eq. (1.74) and **assuming** that w_k is independent of time, the time derivative of Eq. (1.86) leads to

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{\rho}_{\mathbf{i}}(t) &= \sum_k w_k\left[\left(i\hbar\frac{\partial}{\partial t}|\Psi_{\mathbf{i},k}\rangle\right)\langle\Psi_{\mathbf{i},k}| + |\Psi_{\mathbf{i},k}\rangle\left(i\hbar\frac{\partial}{\partial t}\langle\Psi_{\mathbf{i},k}|\right)\right], \\
&= \sum_k w_k\left[\hat{H}_{\mathbf{i},1}|\Psi_{\mathbf{i},k}\rangle\langle\Psi_{\mathbf{i},k}| - |\Psi_{\mathbf{i},k}\rangle\langle\Psi_{\mathbf{i},k}|\hat{H}_{\mathbf{i},1}\right], \\
&= -[\hat{\rho}_{\mathbf{i}}(t), \hat{H}_{\mathbf{i},1}(t)].
\end{aligned} \tag{1.87}$$

The time evolution operator in the interaction representation can be found by starting from Eq. (1.69)

$$\begin{aligned}
|\Psi_{\mathbf{i}}(t)\rangle &= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{s}}(t)\rangle, \\
&= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{U}_{\mathbf{s}}(t,t_0)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t_0}\left(\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t_0}|\Psi_{\mathbf{s}}(t_0)\rangle\right), \\
&= \hat{U}_{\mathbf{i}}(t,t_0)|\Psi_{\mathbf{i}}(t_0)\rangle
\end{aligned}$$

with the definion:

$$\hat{U}_{\mathbf{i}}(t,t_0) = \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{U}_{\mathbf{s}}(t,t_0)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t_0}. \tag{1.88}$$

Differentiating Eq. (1.88) with respect to time, and multiplying it by $i\hbar$, we obtain the equation govering the time evoultion of the time evoultion operator in the interaction representation:

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{U}_{\mathbf{i}}(t,t_0) &= -\hat{H}_{\mathbf{s},0}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{U}_{\mathbf{s}}(t,t_0)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t_0} + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\left(i\hbar\frac{\partial}{\partial t}\hat{U}_{\mathbf{s}}(t,t_0)\right)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t_0}, \\
&= -\hat{H}_{\mathbf{s},0}\hat{U}_{\mathbf{i}}(t,t_0) + \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}H_{\mathbf{s}}\hat{U}_{\mathbf{s}}(t,t_0)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t_0}, \\
&= -\left(\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{H}_{\mathbf{s},0}\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\right)\hat{U}_{\mathbf{i}}(t,t_0) + \left(\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}H_{\mathbf{s}}\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\right)\left(\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{U}_{\mathbf{s}}(t,t_0)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t_0}\right), \\
&= \hat{H}_{\mathbf{i},1}(t)\hat{U}_{\mathbf{i}}(t,t_0).
\end{aligned} \tag{1.89}$$

Also, using Eqs. (1.1), (1.44), (1.69), (1.70), and (1.88), the relations between the Heisenberg and interaction representations can be expressed for the state vector and the operator as:

$$|\Psi_{\mathbf{h}}\rangle = \hat{U}_{\mathbf{s}}(0,t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Psi_{\mathbf{i}}(t)\rangle = \hat{U}_{\mathbf{i}}(0,t)|\Psi_{\mathbf{i}}(t)\rangle, \tag{1.90}$$

$$\hat{A}_{\mathbf{h}}(t) = \hat{U}_{\mathbf{i}}(0,t)\hat{A}_{\mathbf{i}}(t)\hat{U}_{\mathbf{i}}(t,0). \tag{1.91}$$

1.5 Formal solution of the time evolution operator

The formal expression is derived for the time evolution operator $\hat{U}_{\mathbf{i}}$ in the interaction representation. Starting from the differential equation Eq. (1.89), we formally integrate the equation as:

$$\begin{aligned}
\int_{\hat{U}_{\mathbf{i}}(t_0,t_0)}^{\hat{U}_{\mathbf{i}}(t,t_0)} d\hat{U}_{\mathbf{i}} &= -\frac{i}{\hbar}\int_{t_0}^{t} dt_1\hat{H}_{\mathbf{i},1}(t_1)\hat{U}_{\mathbf{i}}(t_1,t_0), \\
\hat{U}_{\mathbf{i}}(t,t_0) - \hat{U}_{\mathbf{i}}(t_0,t_0) &= -\frac{i}{\hbar}\int_{t_0}^{t} dt_1\hat{H}_{\mathbf{i},1}(t_1)\hat{U}_{\mathbf{i}}(t_1,t_0),
\end{aligned} \tag{1.92}$$

Noting $\hat{U}_{\mathbf{i}}(t_0,t_0) = 1$ leads to

$$\hat{U}_{\mathbf{i}}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\hat{H}_{\mathbf{i},1}(t_1)\hat{U}_{\mathbf{i}}(t_1,t_0). \tag{1.93}$$

As well, the time evolution operator $\hat{U}_{\mathbf{i}}(t_1,t_0)$ in the right hand side of Eq. (1.93) can also be expressed by

$$\hat{U}_{\mathbf{i}}(t_1,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t_1} dt_2\hat{H}_{\mathbf{i},1}(t_2)\hat{U}_{\mathbf{i}}(t_2,t_0), \tag{1.94}$$

where $t_1 > t_2$. Putting Eq. (1.94) into Eq. (1.93) gives

$$\hat{U}_{\mathbf{i}}(t,t_0) = 1 + \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t} dt_1 \hat{H}_{\mathbf{i},1}(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \hat{H}_{\mathbf{i},1}(t_1)\hat{H}_{\mathbf{i},1}(t_2)\hat{U}_{\mathbf{i}}(t_2,t_0). \tag{1.95}$$

By applying the same procedure repeatedly, we obtain the formal solution of the time evolution operator as:

$$\hat{U}_{\mathbf{i}}(t,t_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \hat{H}_{\mathbf{i},1}(t_1)\hat{H}_{\mathbf{i},1}(t_2)\cdots\hat{H}_{\mathbf{i},1}(t_n), \tag{1.96}$$

where $t_1 > t_2 > \cdots > t_{n-1} > t_n$, and the term for $n = 0$ in the summation means the identity operator. It is noted that $\hat{H}_{\mathbf{i},1}$ with later time are ordered in the left side in the product of $\hat{H}_{\mathbf{i},1}$ being the integrand in the integration. Let us consider to make the integration range unique, i.e., from t_0 to t. When we simply change the integration range into that from t_0 to t for every integration, the time ordering that later time are placed at the left side cannot be preserved. However, by noting that t_1, t_2, $\cdots$, t_n are just arbitrary variables, we can permutate the variables t_1, t_2, $\cdots$, t_n so that the time ordering can be kept. Moreover, considering that the number of permutation for the variables is $n!$, Eq. (1.96) can be eventually rewritten by

$$\hat{U}_{\mathbf{i}}(t,t_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \frac{1}{n!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n T[\hat{H}_{\mathbf{i},1}(t_1)\hat{H}_{\mathbf{i},1}(t_2)\cdots\hat{H}_{\mathbf{i},1}(t_n)], \tag{1.97}$$

where $T[\cdots]$ is a time ordering operator which orders operators in the parenthesis in order of a rule that one with later time is put to the left side. Since the expansion given by Eq. (1.97) can be formally regarded as the Taylor expansion of the exponential funtion, sometimes, Eq. (1.97) is written as

$$\hat{U}_{\mathbf{i}}(t,t_0) = T\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt' \hat{H}_{\mathbf{i},1}(t')]\right)\right]. \tag{1.98}$$

Although the entity of Eq. (1.98) is not so clear at glance, it just means Eq. (1.97).

Time ordering operator

Let us reconsider the time ordering operator $T[\cdots]$ appearing in Eq. (1.97). The precise definition of the time ordering operator is that $T[\cdots]$ orders **field** operators in the parenthesis in order of a rule that one with later time is put to the left side. In addition, if the field operators are for Fermion, a factor $(-1)^P$ is attached, where P is the number of permutation. For example, if $\hat{\Psi}_i(t_i)$ $(i = 1-4)$ are Fermion field operators and $t_3 > t_4 > t_1 > t_2$, then

$$\begin{aligned} T\left[\hat{\Psi}_1(t_1)\hat{\Psi}_2(t_2)\hat{\Psi}_3(t_3)\hat{\Psi}_4(t_4)\right] &= (-1)^4\hat{\Psi}_3(t_3)\hat{\Psi}_4(t_4)\hat{\Psi}_1(t_1)\hat{\Psi}_2(t_2), \\ &= \hat{\Psi}_3(t_3)\hat{\Psi}_4(t_4)\hat{\Psi}_1(t_1)\hat{\Psi}_2(t_2), \end{aligned} \tag{1.99}$$

In Eq. (1.97), we did not consider the factor $(-1)^P$ in the time ordering operator. This is because $\hat{H}_{\mathbf{i},1}$ consists of an even number of field operators. As shown above, for example, it is found that the following permutation $(\hat{\Psi}_1(t_1)\hat{\Psi}_2(t_2))(\hat{\Psi}_3(t_3)\hat{\Psi}_4(t_4)) \rightarrow (\hat{\Psi}_3(t_3)\hat{\Psi}_4(t_4))(\hat{\Psi}_1(t_1)\hat{\Psi}_2(t_2))$ is made by permutating the operators four times. Thus, we find that the factor alway cancels in the time ordering operator in Eq. (1.97). Also, it is noted how the case with $t_1 = t_2$ should be treated. In our treatment, we define for Fermion as

$$T[\hat{A}(t)\hat{B}(t')] = \theta(t-t')\hat{A}(t)\hat{B}(t') - \bar{\theta}(t'-t)\hat{B}(t')\hat{A}(t), \tag{1.100}$$

where two kinds of step functions $\theta(x)$ and $\bar{\theta}(x)$ are defined by

$$\theta(x) = \begin{cases} 1 & \text{for } x \geq 0 \\ 0 & \text{for } 0 > x \end{cases}, \tag{1.101}$$

$$\bar{\theta}(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } 0 \geq x \end{cases}, \tag{1.102}$$

Chapter 2

Equilibrium Green functions (EGF)

2.1 Definition

In this section, we discuss equilibrium Green functions. First, let us define[1] the one particle causal Green function $G^c(\mathbf{r}t, \mathbf{r}'t')$ as:

$$\begin{aligned} G^c(\mathbf{r}t, \mathbf{r}'t') &= -i\left(\theta(t-t')\frac{\langle\Psi_{\mathbf{h}}|\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')|\Psi_{\mathbf{h}}\rangle}{\langle\Psi_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle} \mp \bar{\theta}(t'-t)\frac{\langle\Psi_{\mathbf{h}}|\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)|\Psi_{\mathbf{h}}\rangle}{\langle\Psi_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle}\right), \\ &= -i\frac{\langle\Psi_{\mathbf{h}}|T[\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')]|\Psi_{\mathbf{h}}\rangle}{\langle\Psi_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle} \end{aligned} \tag{2.1}$$

with the definition of $T[\cdots]$, so called the time-ordering operator:

$$T[\hat{A}(t)\hat{B}(t')] = \theta(t-t')\hat{A}(t)\hat{B}(t') \mp \bar{\theta}(t'-t)\hat{B}(t')\hat{A}(t), \tag{2.2}$$

where $\hat{A}$ and $\hat{B}$ are field operators, and the upper and lower signs are for Fermion and Boson, respectively.[2] In Eq. (2.1), $\Psi_{\mathbf{h}}$ is the ground state of an interacting system in the Heisenberg representation, and satisfies the following time independent Schrodinger equation:

$$\hat{H}_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle = E|\Psi_{\mathbf{h}}\rangle. \tag{2.3}$$

Note that the suffix for time is dropped in the notation, because of the time independence of $\Psi_{\mathbf{h}}$. Since the notation of Eq. (2.1) is too weighty, let us introduce a simplified notation as follows:

$$\langle T[\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')]\rangle \equiv \frac{\langle\Psi_{\mathbf{h}}|T[\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')]|\Psi_{\mathbf{h}}\rangle}{\langle\Psi_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle}. \tag{2.4}$$

Then, we can simply write the causal Green function as:

$$G^c(\mathbf{r}t, \mathbf{r}'t') = -i\langle T[\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')]\rangle \tag{2.5}$$

Considering Eq. (1.63), the time derivative of $G^c(\mathbf{r}t, \mathbf{r}'t')$ with respect to the time t becomes:

$$i\hbar\frac{\partial}{\partial t}G^c(\mathbf{r}t, \mathbf{r}'t') = -i\left(i\hbar\delta(t-t')\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle \pm i\hbar\delta(t-t')\langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle\right.$$

[1] Green functions defined in many particle physics are not those defined in a mathematical sense.

[2] The time ordering operator is just same as that discussed in the previous section

$$
\begin{aligned}
& +\langle T\left[\left(i\hbar\frac{\partial}{\partial t}\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\right)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\right]\rangle\Big), \\
= \quad & -i\left(i\hbar\delta(t-t')\langle[\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t),\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t)]_{\pm}\rangle + \langle T[\hat{v}_1(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')]\rangle\right. \\
& \left. +\langle\hat{v}'_2(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\rangle - \langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\hat{v}'_2(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle\right), \\
= \quad & \hbar\delta(t-t')\delta(\mathbf{r}-\mathbf{r}') + \hat{v}_1(\mathbf{r},t)\left(-i\langle T[\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')]\rangle\right) \\
& +\langle\hat{v}'_2(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\rangle - \langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\hat{v}'_2(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle, \\
= \quad & \hbar\delta(t-t')\delta(\mathbf{r}-\mathbf{r}') + \hat{v}_1(\mathbf{r},t)G^c(\mathbf{r}t,\mathbf{r}'t') \\
& +\langle\hat{v}'_2(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\rangle - \langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\hat{v}'_2(\mathbf{r},t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle, \qquad (2.6)
\end{aligned}
$$

where $\hat{v}'_2(\mathbf{r},t)$ is a potential related to the two particle operator in Eq. (1.63), and given by

$$
\hat{v}'_2(\mathbf{r},t) = \int d\mathbf{r}''\hat{v}_2(\mathbf{r},\mathbf{r}'',t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'',t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}'',t). \qquad (2.7)
$$

Putting Eq. (2.7) into the third and fourth terms in the right hand side of the final line of Eq. (2.6), we find

$$
\langle\hat{v}'_2(\mathbf{r}t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\rangle = \int d\mathbf{r}''\hat{v}_2(\mathbf{r},\mathbf{r}'',t)\langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}''t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}''t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\rangle, \qquad (2.8)
$$

$$
\langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\hat{v}'_2(\mathbf{r}t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle, = \int d\mathbf{r}''\hat{v}_2(\mathbf{r},\mathbf{r}'',t)\langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}''t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}''t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle. \qquad (2.9)
$$

The third and fourth terms can be written by a two-particle Green function, although we do not discuss about it here. If the Hamiltonian does not contain the two particle operator, Eq. (2.6) recovers a differential equation determing the Green function in a mathematical sense as follows:

$$
\left(i\hbar\frac{\partial}{\partial t} - \hat{v}_1(\mathbf{r},t)\right)G^c(\mathbf{r}t,\mathbf{r}'t') = \hbar\delta(t-t')\delta(\mathbf{r}-\mathbf{r}'). \qquad (2.10)
$$

The problem is how one can relate the causal Green function with physical quantities. Like the derivation of Eq. (1.52), in general, the one particle operator $\hat{O}_{\mathbf{h}}$ in the second quantized Heisenberg representation is given by

$$
\hat{O}_{\mathbf{h}}(\mathbf{r}t) = \int d\mathbf{r}'\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t)\hat{o}(\mathbf{r}t,\mathbf{r}')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}'t). \qquad (2.11)
$$

The expection value of the one particle operator is evaluated by

$$
\begin{aligned}
\langle\hat{O}_{\mathbf{h}}(\mathbf{r}t)\rangle = \quad & \frac{\langle\Psi_{\mathbf{h}}|\int d\mathbf{r}'\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t)\hat{o}(\mathbf{r}t,\mathbf{r}')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}'t)|\Psi_{\mathbf{h}}\rangle}{\langle\Psi_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle}, \qquad (2.12) \\
= \quad & \int d\mathbf{r}'\langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t)\hat{o}(\mathbf{r}t,\mathbf{r}')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}'t)\rangle, \\
= \quad & \lim_{t'\to t^+}\lim_{r''\to r'}\int d\mathbf{r}'\hat{o}(\mathbf{r}t,\mathbf{r}')\langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}''t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}'t')\rangle, \\
= \quad & \mp i\lim_{t'\to t^+}\lim_{r''\to r'}\int d\mathbf{r}'\hat{o}(\mathbf{r}t,\mathbf{r}')\left(\pm i\langle\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}''t)\hat{\Psi}_{\mathbf{h}}(\mathbf{r}'t')\rangle\right), \\
= \quad & \mp i\lim_{t'\to t^+}\lim_{r''\to r'}\int d\mathbf{r}'\hat{o}(\mathbf{r}t,\mathbf{r}')G^c(\mathbf{r}''t,\mathbf{r}'t'), \\
= \quad & \mp i\lim_{r''\to r'}\int d\mathbf{r}'\hat{o}(\mathbf{r}t,\mathbf{r}')G^c(\mathbf{r}''t,\mathbf{r}'t^+), \qquad (2.13)
\end{aligned}
$$

where t^+ stands for the time positively infinitely later than the time t, and in the final line $\lim_{t' \to t^+}$ is simplified by just putting t^+ into t'. For example, when we consider the number density operator, the operator $\hat{o}(\mathbf{r}t, \mathbf{r}')$ is replaced by $\hat{n}(\mathbf{r})$ defined by

$$\hat{n}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}'). \tag{2.14}$$

Note that this is the definition of the number density operator in the second quantization, since we do not need to consider the summation over the index of particle in this case. Putting Eq. (2.14) into Eq. (2.13), we get the number density as:

$$\langle \hat{n}(\mathbf{r}) \rangle = \mp i G^c(\mathbf{r}t, \mathbf{r}t^+). \tag{2.15}$$

Also, it is convenient for later discussion to define four Green functions:

Retarded Green function:

$$\begin{aligned} G^r(\mathbf{r}t, \mathbf{r}'t') &= -i\theta(t-t')\langle\{\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t), \hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\}\rangle, \\ &= -i\theta(t-t')\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle - i\theta(t-t')\langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle. \end{aligned} \tag{2.16}$$

Advanced Green function:

$$\begin{aligned} G^a(\mathbf{r}t, \mathbf{r}'t') &= i\bar{\theta}(t'-t)\langle\{\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t), \hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\}\rangle, \\ &= i\bar{\theta}(t'-t)\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle + i\bar{\theta}(t'-t)\langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle. \end{aligned} \tag{2.17}$$

Lesser Green function:

$$G^<(\mathbf{r}t, \mathbf{r}'t') = i\langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle \tag{2.18}$$

Greater Green function:

$$G^>(\mathbf{r}t, \mathbf{r}'t') = -i\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle \tag{2.19}$$

They are not independent of each other, including the causal Green function. Several relations can be found as:

$$\begin{aligned} G^r(\mathbf{r}t, \mathbf{r}'t') - G^a(\mathbf{r}t, \mathbf{r}'t') &= -i\left(\theta(t-t') + \bar{\theta}(t'-t)\right)\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle + \langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle, \\ &= G^>(\mathbf{r}t, \mathbf{r}'t') - G^<(\mathbf{r}t, \mathbf{r}'t'). \end{aligned} \tag{2.20}$$

$$\begin{aligned} G^c(\mathbf{r}t, \mathbf{r}'t') &= -i\theta(t-t')\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle \pm i\bar{\theta}(t'-t)\langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle, \\ &= \theta(t-t')G^>(\mathbf{r}t, \mathbf{r}'t') \pm \bar{\theta}(t'-t)G^<(\mathbf{r}t, \mathbf{r}'t'). \end{aligned} \tag{2.21}$$

$$\begin{aligned} G^r(\mathbf{r}t, \mathbf{r}'t') &= -i\theta(t-t')\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle - i\theta(t-t')\langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle, \\ &= \theta(t-t')G^>(\mathbf{r}t, \mathbf{r}'t') - \theta(t-t')G^<(\mathbf{r}t, \mathbf{r}'t'). \end{aligned} \tag{2.22}$$

$$\begin{aligned} G^a(\mathbf{r}t, \mathbf{r}'t') &= i\bar{\theta}(t'-t)\langle\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\rangle + i\bar{\theta}(t'-t)\langle\hat{\Psi}^\dagger_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\rangle, \\ &= -\bar{\theta}(t'-t)G^>(\mathbf{r}t, \mathbf{r}'t') + \bar{\theta}(t'-t)G^<(\mathbf{r}t, \mathbf{r}'t'). \end{aligned} \tag{2.23}$$

In addition, it is possible to express the physical quantities using $G^>$ or $G^<$ such as

$$\langle \hat{n}(\mathbf{r}) \rangle = \mp i G^<(\mathbf{r}t, \mathbf{r}t).$$

2.2 Gell-Mann and Low theorem

2.3 Perturbation expansion

We now consider the perturbation expansion of the causal Green function. The purpose of the perturbation expansion is to develop a way of evaluating the Green function by using the ground state of a *non-interacting* system. Let us start our discussion by expressing the expectation values in the right hand side of the first line of Eq. (2.1) in the interaction represenation. Putting Eqs. (1.90) and (1.91) into the expectation values in Eq. (2.1), we obtain
In case of $t > t'$,

$$
\begin{aligned}
\frac{\langle\Psi_{\mathbf{h}}|\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')|\Psi_{\mathbf{h}}\rangle}{\langle\Psi_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle} &= \frac{\langle\Psi_{\mathbf{i}}(t)|\hat{U}_{\mathbf{i}}(t,0)\hat{U}_{\mathbf{i}}(0,t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,0)\hat{U}_{\mathbf{i}}(0,t')\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',0)\hat{U}_{\mathbf{i}}(0,t')|\Psi_{\mathbf{i}}(t')\rangle}{\langle\Psi_{\mathbf{i}}(t)|\hat{U}_{\mathbf{i}}(t,0)\hat{U}_{\mathbf{i}}(0,t)\Psi_{\mathbf{i}}(t)\rangle}, \\
&= \frac{\langle\Psi_{\mathbf{i}}(t)|\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,t')\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')|\Psi_{\mathbf{i}}(t')\rangle}{\langle\Psi_{\mathbf{i}}(t)|\Psi_{\mathbf{i}}(t)\rangle}, \\
&= \frac{\left(\frac{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)|\Phi_{\mathbf{i}}\rangle}\right)\hat{U}_{\mathbf{i}}(0,t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,t')\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',0)\left(\frac{\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}\right)}{\left(\frac{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)|\Phi_{\mathbf{i}}\rangle}\right)\hat{U}_{\mathbf{i}}(0,t)\hat{U}_{\mathbf{i}}(t,0)\left(\frac{\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}\right)}, \\
&= \frac{\langle\Phi_{\mathbf{i}}|T[\hat{U}_{\mathbf{i}}(+\infty,t)\hat{U}_{\mathbf{i}}(t,t')\hat{U}_{\mathbf{i}}(t',-\infty)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle}, \\
&= \frac{\langle\Phi_{\mathbf{i}}|T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle}, \qquad (2.24)
\end{aligned}
$$

In case of $t' > t$,

$$
\begin{aligned}
\frac{\langle\Psi_{\mathbf{h}}|\hat{\Psi}^{\dagger}_{\mathbf{h}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)|\Psi_{\mathbf{h}}\rangle}{\langle\Psi_{\mathbf{h}}|\Psi_{\mathbf{h}}\rangle} &= \frac{\langle\Psi_{\mathbf{i}}(t')|\hat{U}_{\mathbf{i}}(t',0)\hat{U}_{\mathbf{i}}(0,t')\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',0)\hat{U}_{\mathbf{i}}(0,t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,0)\hat{U}_{\mathbf{i}}(0,t)|\Psi_{\mathbf{i}}(t)\rangle}{\langle\Psi_{\mathbf{i}}(t)|\hat{U}_{\mathbf{i}}(t,0)\hat{U}_{\mathbf{i}}(0,t)\Psi_{\mathbf{i}}(t)\rangle}, \\
&= \frac{\langle\Psi_{\mathbf{i}}(t')|\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)|\Psi_{\mathbf{i}}(t)\rangle}{\langle\Psi_{\mathbf{i}}(t)|\Psi_{\mathbf{i}}(t)\rangle}, \\
&= \frac{\left(\frac{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)|\Phi_{\mathbf{i}}\rangle}\right)\hat{U}_{\mathbf{i}}(0,t')\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,0)\left(\frac{\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}\right)}{\left(\frac{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)|\Phi_{\mathbf{i}}\rangle}\right)\hat{U}_{\mathbf{i}}(0,t)\hat{U}_{\mathbf{i}}(t,0)\left(\frac{\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle}\right)}, \\
&= \frac{\langle\Phi_{\mathbf{i}}|T[\hat{U}_{\mathbf{i}}(+\infty,t')\hat{U}_{\mathbf{i}}(t',t)\hat{U}_{\mathbf{i}}(t,-\infty)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)]|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle}, \\
&= \mp\frac{\langle\Phi_{\mathbf{i}}|T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle}{\langle\Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle}, \qquad (2.25)
\end{aligned}
$$

where S_i is the S-matrix defined by

$$\hat{S}_{\mathbf{i}} = \hat{U}_{\mathbf{i}}(+\infty,-\infty). \qquad (2.26)$$

It should be noted that the permutation on $\hat{U}_{\mathbf{i}}$ does not change the sign, since $\hat{H}_i$, being the component of $\hat{U}_{\mathbf{i}}$, consists of an even number of field operators as mentioned before. As a result, one can see that the both cases, $t > t'$ and $t' > t$, give the same expression, while the sign is different. By inserting these expressions into Eq. (2.1), we can express the causal Green function as

$$G^c(\mathbf{r}t, \mathbf{r}'t') = -i\frac{\langle\Phi_\mathbf{i}|T[\hat{S}_\mathbf{i}\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}'t')]|\Phi_\mathbf{i}\rangle}{\langle\Phi_\mathbf{i}|\hat{S}_\mathbf{i}|\Phi_\mathbf{i}\rangle}. \tag{2.27}$$

Furthermore, as discussed before, $\hat{S}_\mathbf{i}$ can be expanded using Eq. (1.97). So, putting Eq. (1.97) into Eq. (2.27), we obtain the perturbation expansion of the Green function as:

$$G^c(\mathbf{r}t, \mathbf{r}'t') = -i\frac{\sum_{n=0}^\infty\left(-\frac{i}{\hbar}\right)^n\frac{1}{n!}\int_{-\infty}^\infty dt_1\cdots\int_{-\infty}^\infty dt_n\langle\Phi_\mathbf{i}|T[\hat{H}_{\mathbf{i},1}(t_1)\cdots\hat{H}_{\mathbf{i},1}(t_n)\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}'t')]|\Phi_\mathbf{i}\rangle}{\sum_{n=0}^\infty\left(-\frac{i}{\hbar}\right)^n\frac{1}{n!}\int_{-\infty}^\infty dt_1\cdots\int_{-\infty}^\infty dt_n\langle\Phi_\mathbf{i}|T[\hat{H}_{\mathbf{i},1}(t_1)\cdots\hat{H}_{\mathbf{i},1}(t_n)]|\Phi_\mathbf{i}\rangle}. \tag{2.28}$$

If $\hat{H}_{\mathbf{i},1}$ contains just the one-particle interaction in Eq. (1.80) such as

$$\hat{H}_{\mathbf{i},1} = \int d\mathbf{r}\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}t)\hat{v}_{1,1}(\mathbf{r}t)\hat{\Psi}_\mathbf{i}(\mathbf{r}t), \tag{2.29}$$

then the numerator in Eq. (2.28) can be explicitly expanded, by letting it $i\tilde{G}^c$, as

$$\begin{aligned} i\tilde{G}^c(\mathbf{r}t, \mathbf{r}'t') &= iG_0^c(\mathbf{r}t, \mathbf{r}'t') \\ &+ \left(-\frac{i}{\hbar}\right)\int dt_1\int d\mathbf{r}_1\hat{v}_{1,1}(\mathbf{r}_1t_1)\langle\Phi_\mathbf{i}|T[\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}_1t_1)\hat{\Psi}_\mathbf{i}(\mathbf{r}_1t_1)\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}'t')]|\Phi_\mathbf{i}\rangle, \\ &+ \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2\int dt_1\int d\mathbf{r}_1\hat{v}_{1,1}(\mathbf{r}_1t_1)\int dt_2\int d\mathbf{r}_2\hat{v}_{1,1}(\mathbf{r}_2t_2) \\ &\times\langle\Phi_\mathbf{i}|T[\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}_1t_1)\hat{\Psi}_\mathbf{i}(\mathbf{r}_1t_1)\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}_2t_2)\hat{\Psi}_\mathbf{i}(\mathbf{r}_2t_2)\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}'t')]|\Phi_\mathbf{i}\rangle + \cdots, \end{aligned} \tag{2.30}$$

where $G_0^c(\mathbf{r}t, \mathbf{r}'t')$ is the Green function of the non-interacting system given by $\hat{H}_{\mathbf{i},0}$, and defined by

$$iG_0^c(\mathbf{r}t, \mathbf{r}'t') = \langle\Phi_\mathbf{i}|T[\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{\Psi}_\mathbf{i}^\dagger(\mathbf{r}'t')]|\Phi_\mathbf{i}\rangle. \tag{2.31}$$

2.4 The Wick theorem

A systematic way of evaluating the higher order terms in Eq. (2.30) is discussed in this section. The idea is to express the time ordering operator (or T-product) $T[\cdots]$ by using the normal ordering operator (or N-product) $N[\cdots]$, where, for example, $N[\cdots]$ operates such as

$$N[\hat{\Psi}_\mathrm{u}\hat{\Psi}_\mathrm{o}^\dagger\hat{\Psi}_\mathrm{u}] = -\hat{\Psi}_\mathrm{o}^\dagger\hat{\Psi}_\mathrm{u}\hat{\Psi}_\mathrm{u}. \tag{2.32}$$

The operator $N[\cdots]$ permutates the destruction and creation field operators so that all the destruction operators can be arranged to the right hand side of the creation operator, and a factor $(-1)^P$ with the number of permutations P is attached in case of Fermion. The field operators such as $\hat{\Psi}_\mathrm{u}$ and $\hat{\Psi}_\mathrm{o}$ in Eq. (2.32) will be discussed later. The systematic way is based on the Wick theorem which is the subject of this section.

If the reference Hamiltonian given by Eq. (1.80) consists of only the time-independent one-particle contribution, one can write it in the Schrodinger representation as:

$$\hat{H}_{\mathbf{s},0} = \int d\mathbf{r}\hat{\Psi}_\mathbf{s}^\dagger(\mathbf{r})\hat{v}_{1,0}(\mathbf{r})\hat{\Psi}_\mathbf{s}(\mathbf{r}),$$

$$
\begin{aligned}
&= \int d\mathbf{r}\Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r})\hat{v}_{1,0}(\mathbf{r})\Psi_{\mathbf{s},j}(\mathbf{r})\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j}, \\
&= \sum_{i=1}^{\infty}\hbar w_i \hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i},
\end{aligned} \tag{2.33}
$$

where $\Psi_{\mathbf{s},i}(\mathbf{r})$ obeys

$$
\hat{v}_{1,0}(\mathbf{r})\Psi_{\mathbf{s},i}(\mathbf{r}) = \hbar w_i \Psi_{\mathbf{s},i}(\mathbf{r}). \tag{2.34}
$$

It is noted that only the diagonal terms survive due to the orthonormality of $\{\Psi\}$ in Eq. (2.33). Then, the destruction operator $\hat{a}$ can be expressed using Eq. (1.70) in the interaction representation as:

$$
\begin{aligned}
\hat{a}_{\mathbf{i},i} &= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}\hat{a}_{\mathbf{s},i}\mathrm{e}^{-\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}, \\
&= \left(\prod_{k=1}^{\infty}\mathrm{e}^{itw_k\hat{a}^{\dagger}_{\mathbf{s},k}\hat{a}_{\mathbf{s},k}}\right)\hat{a}_{\mathbf{s},i}\left(\prod_{k'=1}^{\infty}\mathrm{e}^{-itw_{k'}\hat{a}^{\dagger}_{\mathbf{s},k'}\hat{a}_{\mathbf{s},k'}}\right), \\
&= \left(\mathrm{e}^{itw_i\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}}\right)\hat{a}_{\mathbf{s},i}\left(\mathrm{e}^{-itw_i\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}}\right), \\
&= \mathrm{e}^{-itw_i}\hat{a}_{\mathbf{s},i}.
\end{aligned} \tag{2.35}
$$

where we used the following relations for $i \neq j$, being the consequence of the anticommutation relations, Eqs. (1.34) and (1.35):

$$
\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}\hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}_{\mathbf{s},j} = -\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j} = \hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j} = -\hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j}\hat{a}_{\mathbf{s},i} = \hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}_{\mathbf{s},j}\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}, \tag{2.36}
$$

$$
\hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}_{\mathbf{s},j}\hat{a}_{\mathbf{s},i} = -\hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j} = \hat{a}_{\mathbf{s},i}\hat{a}^{\dagger}_{\mathbf{s},j}\hat{a}_{\mathbf{s},j}. \tag{2.37}
$$

The equivalence of the two expressions given in the third and fourth lines of Eq. (2.35) can be confirmed by applying those to arbitrary abstarct state[3] The similar analysis leads to

$$
\hat{a}^{\dagger}_{\mathbf{i},i} = \mathrm{e}^{itw_i}\hat{a}^{\dagger}_{\mathbf{s},i}. \tag{2.38}
$$

Using Eqs. (2.35) and (2.38), the Fermion field operators can be written in the interaction representation as:

$$
\hat{\Psi}_{\mathbf{i}} = \hat{\Psi}_{\mathrm{u}} + \hat{\Psi}^{\dagger}_{\mathrm{o}} \tag{2.39}
$$

with the definitions:

$$
\hat{\Psi}_{\mathrm{u}} = \sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\hat{a}_{\mathbf{i},i}, \tag{2.40}
$$

$$
\hat{\Psi}^{\dagger}_{\mathrm{o}} = \sum_{i\in\mathrm{occ}}\Psi_{\mathbf{s},i}(\mathbf{r})\hat{a}_{\mathbf{i},i}. \tag{2.41}
$$

---

[3] By applying $\hat{a}_{\mathbf{i},i}$ to $|\Phi_{\mathbf{i}}\rangle$ step by step, one can confirm Eq. (2.35) as follows: $\hat{a}_{\mathbf{i},i}|\Phi_{\mathbf{i}}\rangle = \hat{a}_{\mathbf{i},i}\mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Phi_{\mathbf{s}}\rangle = \hat{a}_{\mathbf{i},i}\left(\prod_{k=1}^{\infty}\mathrm{e}^{itw_k\hat{a}^{\dagger}_{\mathbf{s},k}\hat{a}_{\mathbf{s},k}}\right)|\Phi_{\mathbf{s}}\rangle = \left(\prod_{k=1}^{\infty}\mathrm{e}^{itw_kn_k}\right)\left(\mathrm{e}^{itw_i\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}}\right)\hat{a}_{\mathbf{s},i}\left(\mathrm{e}^{-itw_i\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}}\right)|\Phi_{\mathbf{s}}\rangle = \mathrm{e}^{-itw_in_i}\left(\prod_{k=1}^{\infty}\mathrm{e}^{itw_kn_k}\right)\left(\mathrm{e}^{itw_i\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i}}\right)\hat{a}_{\mathbf{s},i}|\Phi_{\mathbf{s}}\rangle = \mathrm{e}^{-itw_in_i}\left(\prod_{k=1}^{\infty}\mathrm{e}^{itw_kn_k}\right)\left(1 + itw_i\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},i} + \cdots\right)\hat{a}_{\mathbf{s},i}|\Phi_{\mathbf{s}}\rangle = \left(\prod_{k=1}^{\infty}\mathrm{e}^{itw_kn_k}\right)\mathrm{e}^{-itw_in_i}\hat{a}_{\mathbf{s},i}|\Phi_{\mathbf{s}}\rangle$, where $|\Phi_{\mathbf{s}}\rangle$ is the abstract state vector in the Schrodinger representation, and n_k is the occupation number of the one-particle state k in $|\Phi_{\mathbf{s}}\rangle$. The factor $\left(\prod_{k=1}^{\infty}\mathrm{e}^{itw_kn_k}\right)$ in the final expression is implicitly ignored since the factor cancels out when the expectation value $\langle\Phi_{\mathbf{i}}|\hat{A}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle$ is considered. Also, n_i is 0 or 1 for Fermion, which allows us to write Eq. (2.35).

satisfying

$$\hat{\Psi}_{\mathrm{u}}\Phi_{\mathbf{i}} = 0, \qquad \hat{\Psi}_{\mathrm{o}}\Phi_{\mathbf{i}} = 0. \tag{2.42}$$

where $i \in$ unocc and $i \in$ occ stand for the summations over unoccupied and occupied states, respectively, and $\Phi_{\mathbf{i}}$ is the abstract representation of the ground state for the Hamiltonian given by Eq. (2.33). Since one cannot destruct (create) the unoccuied (occupied) states in $\Phi_{\mathbf{i}}$ anymore, Eq. (2.42) can be confirmed.

Using Eq. (2.39), the Green function of the non-interacting system Eq. (2.31) can be evaluated explicitly.

$$\begin{aligned} iG_0^c(\mathbf{r}t,\mathbf{r}'t') &= \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle, \\ &= \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{u}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{u}}^\dagger(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle + \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{u}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{o}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle \\ &\quad + \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{o}}^\dagger(\mathbf{r}t)\hat{\Psi}_{\mathbf{u}}^\dagger(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle + \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{o}}^\dagger(\mathbf{r}t)\hat{\Psi}_{\mathbf{o}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle, \\ &= \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{u}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{u}}^\dagger(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle + \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{o}}^\dagger(\mathbf{r}t)\hat{\Psi}_{\mathbf{o}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle, \end{aligned} \tag{2.43}$$

where the first and fourth terms in the second lind of the right hand side only survive due to Eq. (2.42) and the absence of a couple of a destruction and the same kind of creation operators. By noting that[4]

$$\begin{aligned} \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{u}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{u}}^\dagger(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle &= \langle\Phi_{\mathbf{i}}|T\left[\left(\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\hat{a}_{\mathbf{i},i}\right)\left(\sum_{j\in\mathrm{unocc}}\Psi_{\mathbf{s},j}^\dagger(\mathbf{r}')\hat{a}_{\mathbf{i},j}^\dagger\right)\right]|\Phi_{\mathbf{i}}\rangle, \\ &= \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}^\dagger(\mathbf{r}')\langle\Phi_{\mathbf{i}}|T[\hat{a}_{\mathbf{i},i}(t)\hat{a}_{\mathbf{i},j}^\dagger(t')]|\Phi_{\mathbf{i}}\rangle, \\ &= \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}^\dagger(\mathbf{r}')\mathrm{e}^{-itw_i}\mathrm{e}^{it'w_j}\langle\Phi_{\mathbf{i}}|T[\hat{a}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j}^\dagger]|\Phi_{\mathbf{i}}\rangle, \\ &= \begin{cases} \displaystyle\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},i}^\dagger(\mathbf{r}')\mathrm{e}^{-i(t-t')w_i} & \text{for } t \geq t' \\ 0 & \text{for } t' > t \end{cases} \end{aligned} \tag{2.44}$$

and

$$\begin{aligned} \langle\Phi_{\mathbf{i}}|T[\hat{\Psi}_{\mathbf{o}}^\dagger(\mathbf{r}t)\hat{\Psi}_{\mathbf{o}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle &= \langle\Phi_{\mathbf{i}}|T\left[\left(\sum_{i\in\mathrm{occ}}\Psi_{\mathbf{s},i}(\mathbf{r})\hat{a}_{\mathbf{i},i}\right)\left(\sum_{j\in\mathrm{occ}}\Psi_{\mathbf{s},j}^\dagger(\mathbf{r}')\hat{a}_{\mathbf{i},j}^\dagger\right)\right]|\Phi_{\mathbf{i}}\rangle, \\ &= \sum_{i,j\in\mathrm{occ}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}^\dagger(\mathbf{r}')\mathrm{e}^{-itw_i}\mathrm{e}^{it'w_j}\langle\Phi_{\mathbf{i}}|T[\hat{a}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j}^\dagger]|\Phi_{\mathbf{i}}\rangle, \\ &= \begin{cases} 0 & \text{for } t \geq t' \\ \displaystyle -\sum_{i\in\mathrm{occ}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},i}^\dagger(\mathbf{r}')\mathrm{e}^{-i(t-t')w_i} & \text{for } t' > t \end{cases}, \end{aligned} \tag{2.45}$$

$iG_0^c(\mathbf{r}t,\mathbf{r}'t')$ is explicitly written by

$$iG_0^c(\mathbf{r}t,\mathbf{r}'t') = \begin{cases} \displaystyle\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},i}^\dagger(\mathbf{r}')\mathrm{e}^{-i(t-t')w_i} & \text{for } t \geq t' \\ \displaystyle -\sum_{i\in\mathrm{occ}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},i}^\dagger(\mathbf{r}')\mathrm{e}^{-i(t-t')w_i} & \text{for } t' > t \end{cases}. \tag{2.46}$$

[4] Since $|\Phi_{\mathbf{i}}\rangle = \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Phi_{\mathbf{s}}\rangle = \prod_{k=1}^{\infty}\mathrm{e}^{itw_k\hat{a}_{\mathbf{s},k}^\dagger\hat{a}_{\mathbf{s},k}}|\Phi_{\mathbf{s}}\rangle = \prod_{k=1}^{\infty}\mathrm{e}^{itw_kn_k}|\Phi_{\mathbf{s}}\rangle$, where Eq. (2.33) is used for $\hat{H}_{\mathbf{s},0}$, $|\Phi_{\mathbf{s}}\rangle$ is the abstract state vector in the Schrodinger representation, and n_k is the occupation number of the one-particle state k in $|\Phi_{\mathbf{s}}\rangle$, the expectation value $\langle\Phi_{\mathbf{i}}|T[\hat{a}_{\mathbf{i},i}(t)\hat{a}_{\mathbf{i},j}^\dagger(t')]|\Phi_{\mathbf{i}}\rangle$ can be evaluated as $\langle\Phi_{\mathbf{s}}|T[\hat{a}_{\mathbf{i},i}(t)\hat{a}_{\mathbf{i},j}^\dagger(t')]|\Phi_{\mathbf{s}}\rangle$.

When we transform $T[\cdots]$ into $N[\cdots]$, it is important to know the difference between them. Thus, we now define the contraction defined by

$$\hat{A}^{\cdot}\hat{B}^{\cdot} = T[AB] - N[AB]. \tag{2.47}$$

The contraction has the following properties:

$$\begin{aligned}
\hat{A}^{\cdot}\hat{B}^{\cdot} &= -\hat{B}^{\cdot}\hat{A}^{\cdot}, && (2.48)\\
(\hat{A}^{\cdot}+\hat{B}^{\cdot})\hat{C}^{\cdot} &= \hat{A}^{\cdot}\hat{B}^{\cdot}+\hat{A}^{\cdot}\hat{C}^{\cdot}, && (2.49)\\
\hat{A}^{\cdot}\hat{B}^{\cdot} &= 0 \qquad \text{if } \hat{\mathrm{A}} \text{ and } \hat{\mathrm{B}} \text{ are anticommutable.} && (2.50)
\end{aligned}$$

Eqs. (2.48) and (2.49) are trivial from the definition, and Eq. (2.50) can be confirmed by noting that $T[\hat{A}\hat{B}] = \theta(t_A - t_B)\hat{A}\hat{B} - \bar{\theta}(t_B - t_A)\hat{B}\hat{A} = \hat{A}\hat{B}$ and $N[\hat{A}\hat{B}] = \hat{A}\hat{B}$ or $-\hat{B}\hat{A} = \hat{A}\hat{B}$. Due to Eq. (2.50), the following contractions become zero:

$$\begin{aligned}
\hat{\Psi}^{\cdot}_{\mathrm{u}}\hat{\Psi}^{\cdot}_{\mathrm{u}} &= 0, \qquad \hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}} = 0,\\
\hat{\Psi}^{\cdot}_{\mathrm{o}}\hat{\Psi}^{\cdot}_{\mathrm{o}} &= 0, \qquad \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}\hat{\Psi}^{\dagger\cdot}_{\mathrm{o}} = 0,\\
\hat{\Psi}^{\cdot}_{\mathrm{u}}\hat{\Psi}^{\dagger\cdot}_{\mathrm{o}} &= 0, \qquad \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}\hat{\Psi}^{\cdot}_{\mathrm{u}} = 0,\\
\hat{\Psi}^{\cdot}_{\mathrm{o}}\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}} &= 0, \qquad \hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}\hat{\Psi}^{\cdot}_{\mathrm{o}} = 0,\\
\hat{\Psi}^{\cdot}_{\mathrm{o}}\hat{\Psi}^{\cdot}_{\mathrm{u}} &= 0, \qquad \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}} = 0,\\
\hat{\Psi}^{\cdot}_{\mathrm{u}}\hat{\Psi}^{\cdot}_{\mathrm{o}} &= 0, \qquad \hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}\hat{\Psi}^{\dagger\cdot}_{\mathrm{o}} = 0.
\end{aligned} \tag{2.51}$$

For example $\hat{\Psi}^{\cdot}_{\mathrm{u}}\hat{\Psi}^{\cdot}_{\mathrm{u}} = 0$ is confirmed using the distributive properties of the time and normal ordering operators and Eq. (2.50) as follows:

$$\begin{aligned}
&\hat{\Psi}^{\cdot}_{\mathrm{u}}(t_1)\hat{\Psi}^{\cdot}_{\mathrm{u}}(t_2) =\\
&T\left[\left(\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\hat{a}_{\mathbf{i},i}\right)\left(\sum_{j\in\mathrm{unocc}}\Psi_{\mathbf{s},j}(\mathbf{r})\hat{a}_{\mathbf{i},j}\right)\right] - N\left[\left(\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\hat{a}_{\mathbf{i},i}\right)\left(\sum_{j\in\mathrm{unocc}}\Psi_{\mathbf{s},j}(\mathbf{r})\hat{a}_{\mathbf{i},j}\right)\right],\\
=\;& \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}(\mathbf{r})T[\hat{a}_{\mathbf{i},i}(t_1)\hat{a}_{\mathbf{i},j}(t_2)] - \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}(\mathbf{r})N[\hat{a}_{\mathbf{i},i}(t_1)\hat{a}_{\mathbf{i},j}(t_2)],\\
=\;& \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}(\mathbf{r})\mathrm{e}^{-it_1w_i}\mathrm{e}^{-it_2w_j}T[\hat{a}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j}] - \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}(\mathbf{r})\mathrm{e}^{-it_1w_i}\mathrm{e}^{-it_2w_j}N[\hat{a}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j}],\\
=\;& \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi_{\mathbf{s},j}(\mathbf{r})\mathrm{e}^{-it_1w_i}\mathrm{e}^{-it_2w_j}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\cdot}_{\mathbf{s},j},\\
=\;& 0.
\end{aligned} \tag{2.52}$$

As well, the other relations can be easily confirmed. A little contractions are not zero, and we find the non-zero ones as follows:

$$\begin{aligned}
\hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}_2t_2) &= \sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{-it_1w_i}\mathrm{e}^{it_2w_j}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},j},\\
&= \sum_{i\neq j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{-it_1w_i}\mathrm{e}^{it_2w_j}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},j}\\
&\quad + \sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_1-t_2)w_i}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},i},\\
&= \sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_1-t_2)w_i}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},i},
\end{aligned}$$

$$
\begin{aligned}
&= \begin{cases} \sum\limits_{i\in\mathrm{unocc}} \Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_1-t_2)w_i} & \text{for } t_1 \geq t_2 \\ 0 & \text{for } t_2 > t_1 \end{cases}, \\
&= \begin{cases} iG^c_0(\mathbf{r}_1t_1,\mathbf{r}_2t_2) & \text{for } t_1 \geq t_2 \\ 0 & \text{for } t_2 > t_1 \end{cases}, \qquad (2.53)
\end{aligned}
$$

$$
\begin{aligned}
\hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}_2t_2) &= \sum_{i,j\in\mathrm{occ}} \Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{-it_1w_i}\mathrm{e}^{it_2w_j}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},j}, \\
&= \sum_{i\neq j\in\mathrm{occ}} \Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{-it_1w_i}\mathrm{e}^{it_2w_j}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},j} \\
&\quad + \sum_{i\in\mathrm{occ}} \Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_1-t_2)w_i}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},i}, \\
&= \sum_{i\in\mathrm{occ}} \Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_1-t_2)w_i}\hat{a}^{\cdot}_{\mathbf{s},i}\hat{a}^{\dagger\cdot}_{\mathbf{s},i}, \\
&= \begin{cases} 0 & \text{for } t_1 \geq t_2 \\ -\sum\limits_{i\in\mathrm{occ}} \Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_1-t_2)w_i} & \text{for } t_2 > t_1 \end{cases}, \\
&= \begin{cases} 0 & \text{for } t_1 \geq t_2 \\ iG^c_0(\mathbf{r}_1t_1,\mathbf{r}_2t_2) & \text{for } t_2 > t_1 \end{cases}, \qquad (2.54)
\end{aligned}
$$

It should be noted that the normal ordering operator in the derivation of Eqs. (2.53) and (2.54) operates on not $\hat{a}$, but the field operators. Also, it is important that the resultant contractions are not the operator anymore, and they are just a c-number. Now we can evaluate the contractions of the field operators itself using Eqs. (2.51), (2.53), and (2.54) as follows:

$$
\begin{aligned}
\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'t') &= (\hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}t) + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}t))(\hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}'t')), \\
&= \hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= 0, \qquad (2.55)
\end{aligned}
$$

$$
\begin{aligned}
\hat{\Psi}^{\dagger\cdot}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathbf{i}}(\mathbf{r}'t') &= (\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}t) + \hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}t))(\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}'t')), \\
&= \hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}'t') + \hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= 0, \qquad (2.56)
\end{aligned}
$$

$$
\begin{aligned}
\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathbf{i}}(\mathbf{r}'t') &= (\hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}t) + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}t))(\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}'t')), \\
&= \hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= \hat{\Psi}^{\cdot}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger\cdot}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\cdot}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= iG^c_0(\mathbf{r}t,\mathbf{r}'t'). \qquad (2.57)
\end{aligned}
$$

Based on the above discussion, we proceed to the Wick theorem.

The Wick theorem

The Wick theorem transforms the T-product of field operators $\hat{A}_1 \cdots \hat{A}_n$ into the sum of N-products of those as follows:

$$
\begin{aligned}
T[\hat{A}_1 \cdots \hat{A}_n] \;=\; & N[\hat{A}_1 \cdots \hat{A}_n] \\
& + \sum_{i,j} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_n] \\
& + \sum_{i,j,k,l} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l N[\hat{A}_1 \cdots (ijkl) \cdots \hat{A}_n] \\
& + \cdots \\
& + \sum (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l \cdots,
\end{aligned}
\tag{2.58}
$$

where $N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_n]$ is the N-product of the remaining field operators after elimination of $\hat{A}_i$ and $\hat{A}_j$, and P is the number of permutations from $\hat{A}_1 \cdots \hat{A}_1$ to $\hat{A}_i \hat{A}_j \hat{A}_1 \cdots (ij) \cdots \hat{A}_1$. Also, the last term means the product of paired contractions of which number is $n/2$ when n is even, and the product of paired contractions of which number is $(n-1)/2$ and a remaining operator when n is odd.

To prove Eq. (2.58), first let us prove the following lemma:

Lemma 1

If the time associated with $\hat{B}$ is earliest compared to all the times associated with $\hat{A}_1, \cdots, \hat{A}_n$, then

$$
\begin{aligned}
N[\hat{A}_1 \cdots \hat{A}_n]\hat{B} \;=\; & N[\hat{A}_1 \cdots \hat{A}_{n-1}]\hat{A}^{\cdot}_n \hat{B}^{\cdot} + (-1) N[\hat{A}_1 \cdots \hat{A}_{n-2}\hat{A}_n]\hat{A}^{\cdot}_{n-1}\hat{B}^{\cdot} + \cdots \\
& + (-1)^{n-k} N[\hat{A}_1 \cdots \hat{A}_{n-(k+1)}\hat{A}_{n-(k-1)} \cdots \hat{A}_n]\hat{A}^{\cdot}_k \hat{B}^{\cdot} + \cdots \\
& + (-1)^{n-1} N[\hat{A}_2 \cdots \hat{A}_n]\hat{A}^{\cdot}_1 \hat{B}^{\cdot} + N[\hat{A}_1 \cdots \hat{A}_n \hat{B}]
\end{aligned}
\tag{2.59}
$$

Proof of the lemma 1

(i) *If $\hat{B}$ is the destruction operator*, then $\hat{A}^{\cdot}_k B^{\cdot} = 0$. Also, indeed $N[\hat{A}_1 \cdots \hat{A}_n]\hat{B} = N[\hat{A}_1 \cdots \hat{A}_n \hat{B}]$ due to the definition of the N-product. Thus, the lemma is accepted.

(ii) *If $\hat{B}$ is the creation operator*, it is possible to assume that $\hat{A}_1, \cdots,$ and $\hat{A}_n$ are all the destruction operators. Arbitrary case can be generated by multiplying the both sides by a creation operator $\hat{A}$ from the left side repeatedly and by permutating the order of field operators in the N-product, since $\hat{A}N[\hat{A}_1 \cdots] = N[\hat{A}\hat{A}_1 \cdots]$ and the changes of sign due to the permutation of the field operators to get the case in the N-product cancel out.

In this case that $\hat{B}$ is the creation operator and that $\hat{A}_1, \cdots, \hat{A}_n$ are all the destruction operators, the lemma can be proved by the principle of induction. For $n = 1$, we obtain $\hat{A}_1 \hat{B} = T[\hat{A}_1 \hat{B}] = A^{\cdot}_1 \hat{B}^{\cdot} + N[A_1 \hat{B}]$. This is the definition of the contaction. Thus, the lemma is accepted. Next, let us assume that the lemma is accepted for $n = m$. Letting $\hat{A}$ be a destruction operator, we have

$$
\begin{aligned}
N[\hat{A}\hat{A}_1 \cdots \hat{A}_m]\hat{B} \;=\; & \hat{A}N[\hat{A}_1 \cdots \hat{A}_m]\hat{B}, \\
=\; & \hat{A}\Big(N[\hat{A}_1 \cdots \hat{A}_{m-1}]\hat{A}^{\cdot}_m \hat{B}^{\cdot} + (-1) N[\hat{A}_1 \cdots \hat{A}_{m-2}\hat{A}_m]\hat{A}^{\cdot}_{m-1}\hat{B}^{\cdot} + \cdots \\
& + (-1)^{m-k} N[\hat{A}_1 \cdots \hat{A}_{m-(k+1)}\hat{A}_{m-(k-1)} \cdots \hat{A}_m]\hat{A}^{\cdot}_k \hat{B}^{\cdot} + \cdots \\
& + (-1)^{m-1} N[\hat{A}_2 \cdots \hat{A}_m]\hat{A}^{\cdot}_1 \hat{B}^{\cdot} + N[\hat{A}_1 \cdots \hat{A}_m \hat{B}] \Big),
\end{aligned}
$$

$$
\begin{aligned}
&= N[\hat{A}\hat{A}_1\cdots\hat{A}_{m-1}]\hat{A}^{\cdot}_m\hat{B}^{\cdot} + (-1)N[\hat{A}\hat{A}_1\cdots\hat{A}_{m-2}\hat{A}_m]\hat{A}^{\cdot}_{m-1}\hat{B}^{\cdot} + \cdots \\
&\quad +(-1)^{m-k}N[\hat{A}\hat{A}_1\cdots\hat{A}_{m-(k+1)}\hat{A}_{m-(k-1)}\cdots\hat{A}_m]\hat{A}^{\cdot}_k\hat{B}^{\cdot} + \cdots \\
&\quad +(-1)^{m-1}N[\hat{A}\hat{A}_2\cdots\hat{A}_m]\hat{A}^{\cdot}_1\hat{B}^{\cdot} + \hat{A}N[\hat{A}_1\cdots\hat{A}_m\hat{B}],
\end{aligned}
\tag{2.60}
$$

where the last term of the final line in the right hand side is evaluated as:

$$
\begin{aligned}
\hat{A}N[\hat{A}_1\cdots\hat{A}_m\hat{B}] &= (-1)^m\hat{A}\hat{B}\hat{A}_1\cdots\hat{A}_m, \\
&= (-1)^m\tilde{T}[\hat{A}\hat{B}]\hat{A}_1\cdots\hat{A}_m, \\
&= (-1)^m(\hat{A}^{\cdot}\hat{B}^{\cdot} + N[\hat{A}\hat{B}])\hat{A}_1\cdots\hat{A}_m, \\
&= (-1)^m N[\hat{A}_1\cdots\hat{A}_m]\hat{A}^{\cdot}\hat{B}^{\cdot} + (-1)^{m+1}\hat{B}\hat{A}\hat{A}_1\cdots\hat{A}_m, \\
&= (-1)^m N[\hat{A}_1\cdots\hat{A}_m]\hat{A}^{\cdot}\hat{B}^{\cdot} + N[\hat{A}\hat{A}_1\cdots\hat{A}_m\hat{B}].
\end{aligned}
\tag{2.61}
$$

By putting Eq. (2.61) into Eq. (2.57), we can get the lemma for $n = m+1$. Thus, the lemma is proven.

Proof of the Wick theorem

The theorem is proven by the principle of induction. For $n = 1$, we obtain $T[\hat{A}_1\hat{A}_2] = N[\hat{A}_1\hat{A}_2] + \hat{A}^{\cdot}_1\hat{A}^{\cdot}_2$. This is the definition of the contaction. Thus, the theorem is accepted. Next, let us assume that the theorem is accepted for $n = m$. Letting $\hat{A}_{m+1}$ be a field operator at the earliest time among $\hat{A}_1, \cdots, \hat{A}_{m+1}$, then

$$
\begin{aligned}
T[\hat{A}_1\cdots\hat{A}_m\hat{A}_{m+1}] &= T[\hat{A}_1\cdots\hat{A}_m]\hat{A}_{m+1} \\
&= \Big(N[\hat{A}_1\cdots\hat{A}_m] \\
&\quad +\sum_{i,j}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j N[\hat{A}_1\cdots(ij)\cdots\hat{A}_m] \\
&\quad +\sum_{i,j,k,l}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l N[\hat{A}_1\cdots(ijkl)\cdots\hat{A}_m] \\
&\quad +\cdots \\
&\quad +\sum(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l\cdots\Big)\hat{A}_{m+1}, \\
&= N[\hat{A}_1\cdots\hat{A}_m]\hat{A}_{m+1} \\
&\quad +\sum_{i,j}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j N[\hat{A}_1\cdots(ij)\cdots\hat{A}_m]\hat{A}_{m+1} \\
&\quad +\sum_{i,j,k,l}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l N[\hat{A}_1\cdots(ijkl)\cdots\hat{A}_m]\hat{A}_{m+1} \\
&\quad +\cdots \\
&\quad +\sum(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l\cdots\hat{A}_{m+1}, \\
&= \sum_{i}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_{m+1}N[\hat{A}_1\cdots(im+1)\cdots\hat{A}_{m+1}] + N[\hat{A}_1\cdots\hat{A}_{m+1}] \\
&\quad +\sum_{i,j,k,l}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_{m+1}N[\hat{A}_1\cdots(ijk(m+1))\cdots\hat{A}_{m+1}] \\
&\quad +\sum_{i,j}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j N[\hat{A}_1\cdots(ij)\cdots\hat{A}_{m+1}]
\end{aligned}
$$

$$
\begin{aligned}
& +\sum_{i,j,k,l}(-1)^P \hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l N[\hat{A}_1\cdots(ijkl)\cdots\hat{A}_{m+1}] \\
& +\cdots \\
& +\sum(-1)^P \hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l\cdots\hat{A}_{m+1} \\
= \; & N[\hat{A}_1\cdots\hat{A}_{m+1}] \\
& +\sum_{i,j}(-1)^P \hat{A}^{\cdot}_i\hat{A}^{\cdot}_j N[\hat{A}_1\cdots(ij)\cdots\hat{A}_{m+1}] \\
& +\sum_{i,j,k,l}(-1)^P \hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l N[\hat{A}_1\cdots(ijkl)\cdots\hat{A}_{m+1}] \\
& +\cdots \\
& +\sum(-1)^P \hat{A}^{\cdot}_i\hat{A}^{\cdot}_j\hat{A}^{\cdot}_k\hat{A}^{\cdot}_l\cdots,
\end{aligned}
\tag{2.62}
$$

where the lemma 1 is used for the derivation. So, we can reproduce the theorem for $n = m + 1$. The assumption that $\hat{A}_{m+1}$ is a field operator associated with the earliest time among $\hat{A}_1, \cdots, \hat{A}_{m+1}$ can be eliminated by permutating the field operators in the T- and N-products for arbitrary case of Eq. (2.63) so that the operator associated with the earliest time can be located at the most right side. The changes of sign due to the permutation for both the sides in Eq. (2.63) cancel each other. Thus, the theorem is proven. It is also noted that the Wick theorem can be applied to the field operator $\hat{\Psi}_{\mathbf{i}}$ itself as a consequence of the distributive properties of the T- and N-products.[5] Although we have proved the Wick theorem, the meaning of the summations in Eq. (2.58) is not so clear. Let us see the formulas upto $n = 4$ below:

For $n = 2$

$$
T[\hat{A}_1\hat{A}_2] = \hat{A}^{\cdot}_1\hat{A}^{\cdot}_2 + N[\hat{A}_1\hat{A}_2], \tag{2.63}
$$

For $n = 3$

$$
\begin{aligned}
T[\hat{A}_1\hat{A}_2\hat{A}_3] &= T[\hat{A}_1\hat{A}_2]\hat{A}_3, \\
&= (\hat{A}^{\cdot}_1\hat{A}^{\cdot}_2 + N[\hat{A}_1\hat{A}_2])\hat{A}_3, \\
&= N[\hat{A}_1\hat{A}_2]\hat{A}_3 + N[\hat{A}_3]\hat{A}^{\cdot}_1\hat{A}^{\cdot}_2, \\
&= N[\hat{A}_1]\hat{A}^{\cdot}_2\hat{A}^{\cdot}_3 - N[\hat{A}_2]\hat{A}^{\cdot}_1\hat{A}^{\cdot}_3 + N[\hat{A}_3]\hat{A}^{\cdot}_1\hat{A}^{\cdot}_2 + N[\hat{A}_1\hat{A}_2\hat{A}_3],
\end{aligned}
\tag{2.64}
$$

For $n = 4$

$$
\begin{aligned}
T[\hat{A}_1\hat{A}_2\hat{A}_3\hat{A}_4] &= T[\hat{A}_1\hat{A}_2\hat{A}_3]\hat{A}_4, \\
&= (N[\hat{A}_1]\hat{A}^{\cdot}_2\hat{A}^{\cdot}_3 - N[\hat{A}_2]\hat{A}^{\cdot}_1\hat{A}^{\cdot}_3 + N[\hat{A}_3]\hat{A}^{\cdot}_1\hat{A}^{\cdot}_2 + N[\hat{A}_1\hat{A}_2\hat{A}_3])\hat{A}_4, \\
&= N[\hat{A}_1]\hat{A}_4\hat{A}^{\cdot}_2\hat{A}^{\cdot}_3 - N[\hat{A}_2]\hat{A}_4\hat{A}^{\cdot}_1\hat{A}^{\cdot}_3 + N[\hat{A}_3]\hat{A}_4\hat{A}^{\cdot}_1\hat{A}^{\cdot}_2 + N[\hat{A}_1\hat{A}_2\hat{A}_3]\hat{A}_4, \\
&= (\hat{A}^{\cdot}_1\hat{A}^{\cdot}_4 + N[\hat{A}_1\hat{A}_4])\hat{A}^{\cdot}_2\hat{A}^{\cdot}_3 - (\hat{A}^{\cdot}_2\hat{A}^{\cdot}_4 + N[\hat{A}_2\hat{A}_4])\hat{A}^{\cdot}_1\hat{A}^{\cdot}_3 + (\hat{A}^{\cdot}_3\hat{A}^{\cdot}_4 + N[\hat{A}_3\hat{A}_4])\hat{A}^{\cdot}_1\hat{A}^{\cdot}_2 \\
&\quad + N[\hat{A}_1\hat{A}_2]\hat{A}^{\cdot}_3\hat{A}^{\cdot}_4 - N[\hat{A}_1\hat{A}_3]\hat{A}^{\cdot}_2\hat{A}^{\cdot}_4 + N[\hat{A}_2\hat{A}_3]\hat{A}^{\cdot}_1\hat{A}^{\cdot}_4 + N[\hat{A}_1\hat{A}_2\hat{A}_3\hat{A}_4],
\end{aligned}
$$

[5] This statement tends to cause a misunderstanding for the treatment of the N-product. Although the Wick theorem is valid for the field operator $\hat{\Psi}_{\mathbf{i}}$ itself, it should be noted that $N[\hat{\Psi}_i\hat{\Psi}_i^{\dagger}] \neq \hat{\Psi}_i^{\dagger}\hat{\Psi}_i$. This can be easily confirmed as: $N[\hat{\Psi}_i\hat{\Psi}_i^{\dagger}] = N[\hat{\Psi}_u\hat{\Psi}_u^{\dagger}] + N[\hat{\Psi}_u\hat{\Psi}_o] + N[\hat{\Psi}_o^{\dagger}\hat{\Psi}_u^{\dagger}] + N[\hat{\Psi}_o^{\dagger}\hat{\Psi}_o] = \hat{\Psi}_u^{\dagger}\hat{\Psi}_u + \hat{\Psi}_u\hat{\Psi}_o + \hat{\Psi}_o^{\dagger}\hat{\Psi}_u^{\dagger} + \hat{\Psi}_o^{\dagger}\hat{\Psi}_o$, on the other hand, $\hat{\Psi}_i^{\dagger}\hat{\Psi}_i = \hat{\Psi}_u^{\dagger}\hat{\Psi}_u + \hat{\Psi}_o\hat{\Psi}_u + \hat{\Psi}_u^{\dagger}\hat{\Psi}_o^{\dagger} + \hat{\Psi}_o\hat{\Psi}_o^{\dagger}$. Therefore, after transforming the T-product using the Wick theorem, the resultant N-products have to be evaluated based on the field operators $\hat{\Psi}_o$ and $\hat{\Psi}_u$.

$$
\begin{aligned}
= \quad & N[\hat{A}_1\hat{A}_2\hat{A}_3\hat{A}_4] + \hat{A}^{\cdot}_1\hat{A}^{\cdot}_2 N[\hat{A}_3\hat{A}_4] - \hat{A}^{\cdot}_1\hat{A}^{\cdot}_3 N[\hat{A}_2\hat{A}_4] + \hat{A}^{\cdot}_1\hat{A}^{\cdot}_4 N[\hat{A}_2\hat{A}_3] \\
& + \hat{A}^{\cdot}_2\hat{A}^{\cdot}_3 N[\hat{A}_1\hat{A}_4] - \hat{A}^{\cdot}_2\hat{A}^{\cdot}_4 N[\hat{A}_1\hat{A}_3] + \hat{A}^{\cdot}_3\hat{A}^{\cdot}_4 N[\hat{A}_1\hat{A}_2] \\
& + \hat{A}^{\cdot}_1\hat{A}^{\cdot\cdot}_2\hat{A}^{\cdot\cdot}_3\hat{A}^{\cdot}_4 - \hat{A}^{\cdot}_1\hat{A}^{\cdot\cdot}_3\hat{A}^{\cdot\cdot}_2\hat{A}^{\cdot}_4 + \hat{A}^{\cdot\cdot}_2\hat{A}^{\cdot}_3\hat{A}^{\cdot}_1\hat{A}^{\cdot\cdot}_4 .
\end{aligned}
\tag{2.65}
$$

As shown above, the T-product of field oprators can be transformed into the sum of the N-products and a term consisting of the product of contranctions. The expectation values of the N-products for the ground state $\Psi_{\mathbf{i}}$ are all zero due to Eq. (2.42). Thus, the last term in Eq. (2.58) only contributes to the expecation value of the T-product. This is the usefulness of the Wick theorem.

2.5 Dyson's equation

As discussed in the previous section, by making use of the Wick theorem one can evaluate the expectation value in the second term of Eq. (2.42) as:

$$
\begin{aligned}
\langle\Phi_{\mathbf{i}}|T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle &= (\hat{\Psi}^{\dagger\cdot}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}^{\cdot}_{\mathbf{i}}(\mathbf{r}_1t_1))(\hat{\Psi}^{\cdot}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger\cdot}_{\mathbf{i}}(\mathbf{r}'t')) \\
&\quad -(\hat{\Psi}^{\dagger\cdot}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}^{\cdot}_{\mathbf{i}}(\mathbf{r}t))(\hat{\Psi}^{\cdot}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger\cdot}_{\mathbf{i}}(\mathbf{r}'t')) \\
&= -i^2G^c_0(\mathbf{r}_1t_1,\mathbf{r}_1t_1)G^c_0(\mathbf{r}t,\mathbf{r}'t') + i^2G^c_0(\mathbf{r}t,\mathbf{r}_1t_1)G^c_0(\mathbf{r}_1t_1,\mathbf{r}'t').
\end{aligned}
\tag{2.66}
$$

Putting Eq. (2.66) into Eq. (2.30) yields

$$
\begin{aligned}
i\tilde{G}^c(\mathbf{r}t,\mathbf{r}'t') &= iG^c_0(\mathbf{r}t,\mathbf{r}'t') \\
&\quad -\left(-\frac{i}{\hbar}\right) iG^c_0(\mathbf{r}t,\mathbf{r}'t')\int dt_1\int d\mathbf{r}_1\hat{v}_{1,1}(\mathbf{r}_1t_1)iG^c_0(\mathbf{r}_1t_1,\mathbf{r}_1t_1) \\
&\quad +\left(-\frac{i}{\hbar}\right)\int dt_1\int d\mathbf{r}_1 iG^c_0(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG^c_0(\mathbf{r}_1t_1,\mathbf{r}'t') + \cdots, \\
&= \left(1-\left(-\frac{i}{\hbar}\right)\int dt_1\int d\mathbf{r}_1\hat{v}_{1,1}(\mathbf{r}_1t_1)iG^c_0(\mathbf{r}_1t_1,\mathbf{r}_1t_1)+\cdots\right) \\
&\quad \times\left(iG^c_0(\mathbf{r}t,\mathbf{r}'t') + \left(-\frac{i}{\hbar}\right)\int dt_1\int d\mathbf{r}_1 iG^c_0(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG^c_0(\mathbf{r}_1t_1,\mathbf{r}'t')+\cdots\right),
\end{aligned}
\tag{2.67}
$$

where the factorized final form can be practically confirmed by expanding higher order terms. Also, the denominator of Eq. (2.28) can be evaluated using the Wick theorem as:

$$
\begin{aligned}
&\sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n\frac{1}{n!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}dt_n\langle\Phi_{\mathbf{i}}|T[\hat{H}_{\mathbf{i},1}(t_1)\cdots\hat{H}_{\mathbf{i},1}(t_n)]|\Phi_{\mathbf{i}}\rangle \\
&\quad = \left(1-\left(-\frac{i}{\hbar}\right)\int dt_1\int d\mathbf{r}_1\hat{v}_{1,1}(\mathbf{r}_1t_1)iG^c_0(\mathbf{r}_1t_1,\mathbf{r}_1t_1)+\cdots\right).
\end{aligned}
\tag{2.68}
$$

Thus, we find that the terms in the first parenthesis in Eq. (2.67) cancel by the denominator. Noting $-i(\frac{-i}{\hbar})^n i^{n+1} = \frac{1}{\hbar^n}$, finally Eq. (2.28) can be written by

$$
\begin{aligned}
G^c(\mathbf{r}t,\mathbf{r}'t') &= G^c_0(\mathbf{r}t,\mathbf{r}'t') + \frac{1}{\hbar}\int dt_1\int d\mathbf{r}_1 G^c_0(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)G^c_0(\mathbf{r}_1t_1,\mathbf{r}'t') \\
&\quad +\frac{1}{\hbar^2}\int dt_1\int d\mathbf{r}_1\int dt_2\int d\mathbf{r}_2 G^c_0(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)G^c_0(\mathbf{r}_1t_1,\mathbf{r}_2t_2)\hat{v}_{1,1}(\mathbf{r}_2t_2)G^c_0(\mathbf{r}_2t_2,\mathbf{r}'t') \\
&\quad +\text{higher order terms},
\end{aligned}
$$

$$
\begin{aligned}
&= G_0^c(\mathbf{r}t,\mathbf{r}'t') + \frac{1}{\hbar}\int dt_1 \int d\mathbf{r}_1 G_0^c(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1) \\
&\quad \times \left(G_0^c(\mathbf{r}_1t_1,\mathbf{r}'t') + \frac{1}{\hbar}\int dt_2 \int d\mathbf{r}_2 G_0^c(\mathbf{r}_1t_1,\mathbf{r}_2t_2)\hat{v}_{1,1}(\mathbf{r}_2t_2) G_0^c(\mathbf{r}_2t_2,\mathbf{r}'t') + \cdots \right) \\
&= G_0^c(\mathbf{r}t,\mathbf{r}'t') + \frac{1}{\hbar}\int dt_1 \int d\mathbf{r}_1 G_0^c(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1) G^c(\mathbf{r}_1t_1,\mathbf{r}'t'). \qquad (2.69)
\end{aligned}
$$

The final result of Eq. (2.69) is called Dyson's equation for the case that Eq. (2.29) is assumed.

Chapter 3

Non-equilibrium Green functions (NEGF)

3.1 Definition

For the equilibrium Green function, the perturbation expansion of the Green function is made through the Gell-Mann-Low theorem by using the ground state of the non-interacting system. On the other hand, for the non-equilibrium Green function, the reference state used for the expansion can be arbitrary state as long as the state is given by the one-particle Hamiltonian. For example, starting from a state that a conductor is disconnected from infinite leads, where each part is at thermal equilibrium with each chemical potential, and switching on the interaction between the conductor and the leads on adiabatically, then the evolving state cannot return to the starting state even if the interaction is adiabatically switched off. This can be understood by a fact that the state, initially associated with the conductor, disappear somewhere in the lead at the time when the connection is fully switched on. In other words, one cannot specify the final state, while one can specify the initial state. Thus, we expand the non-equilibrium Green function perturbatively using only the initial state. The Green function defined by Eq. (2.1) in the Heisenberg representation is transformed by an initial state Φ_i, which can be related a mixed ensemble, in the interaction representation as:

In case of $t > t'$,

$$\begin{aligned}
\frac{\langle\Psi_\mathbf{h}|\hat{\Psi}_\mathbf{h}(\mathbf{r}t)\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}'t')|\Psi_\mathbf{h}\rangle}{\langle\Psi_\mathbf{h}|\Psi_\mathbf{h}\rangle} &= \frac{\langle\Phi_\mathbf{i}|\hat{U}_\mathbf{i}(-\infty,0)\hat{U}_\mathbf{i}(0,t)\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{U}_\mathbf{i}(t,t')\hat{\Psi}^\dagger_\mathbf{i}(\mathbf{r}'t')\hat{U}_\mathbf{i}(t',0)\hat{U}_\mathbf{i}(0,-\infty)|\Phi_\mathbf{i}\rangle}{\langle\Phi_\mathbf{i}|\hat{U}_\mathbf{i}(-\infty,0)\hat{U}_\mathbf{i}(0,t)\hat{U}_\mathbf{i}(t,0)\hat{U}_\mathbf{i}(0,-\infty)|\Phi_\mathbf{i}\rangle}, \\
&= \frac{\langle\Phi_\mathbf{i}|\hat{U}_\mathbf{i}(-\infty,t)\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{U}_\mathbf{i}(t,t')\hat{\Psi}^\dagger_\mathbf{i}(\mathbf{r}'t')\hat{U}_\mathbf{i}(t',-\infty)|\Phi_\mathbf{i}\rangle}{\langle\Phi_\mathbf{i}|\Phi_\mathbf{i}\rangle}, \\
&= \langle\Phi_\mathbf{i}|\hat{U}_\mathbf{i}(-\infty,+\infty)\hat{U}_\mathbf{i}(+\infty,t)\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{U}_\mathbf{i}(t,t')\hat{\Psi}^\dagger_\mathbf{i}(\mathbf{r}'t')\hat{U}_\mathbf{i}(t',-\infty)|\Phi_\mathbf{i}\rangle, \\
&= \langle\Phi_\mathbf{i}|\hat{U}_\mathbf{i}(-\infty,+\infty)T[\hat{U}_\mathbf{i}(+\infty,t)\hat{U}_\mathbf{i}(t,t')\hat{U}_\mathbf{i}(t',-\infty)\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{\Psi}^\dagger_\mathbf{i}(\mathbf{r}'t')]|\Phi_\mathbf{i}\rangle, \\
&= \langle\Phi_\mathbf{i}|\hat{S}^\dagger_\mathbf{i}T[\hat{S}_\mathbf{i}\hat{\Psi}_\mathbf{i}(\mathbf{r}t)\hat{\Psi}^\dagger_\mathbf{i}(\mathbf{r}'t')]|\Phi_\mathbf{i}\rangle. \qquad (3.1)
\end{aligned}$$

In case of $t' > t$,

$$\frac{\langle\Psi_\mathbf{h}|\hat{\Psi}^\dagger_\mathbf{h}(\mathbf{r}'t')\hat{\Psi}_\mathbf{h}(\mathbf{r}t)|\Psi_\mathbf{h}\rangle}{\langle\Psi_\mathbf{h}|\Psi_\mathbf{h}\rangle} = \frac{\langle\Phi_\mathbf{i}|\hat{U}_\mathbf{i}(-\infty,0)\hat{U}_\mathbf{i}(0,t')\hat{\Psi}_\mathbf{i}(\mathbf{r}'t')\hat{U}_\mathbf{i}(t',t)\hat{\Psi}^\dagger_\mathbf{i}(\mathbf{r}t)\hat{U}_\mathbf{i}(t,0)\hat{U}_\mathbf{i}(0,-\infty)|\Phi_\mathbf{i}\rangle}{\langle\Phi_\mathbf{i}|\hat{U}_\mathbf{i}(-\infty,0)\hat{U}_\mathbf{i}(0,t)\hat{U}_\mathbf{i}(t,0)\hat{U}_\mathbf{i}(0,-\infty)|\Phi_\mathbf{i}\rangle},$$

$$
\begin{aligned}
&= \frac{\langle \Phi_{\mathbf{i}} | \hat{U}_{\mathbf{i}}(-\infty, t') \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}'t') \hat{U}_{\mathbf{i}}(t', t) \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t) \hat{U}_{\mathbf{i}}(t, -\infty) | \Phi_{\mathbf{i}} \rangle}{\langle \Phi_{\mathbf{i}} | \Phi_{\mathbf{i}} \rangle}, \\
&= \langle \Phi_{\mathbf{i}} | \hat{U}_{\mathbf{i}}(-\infty, +\infty) \hat{U}_{\mathbf{i}}(+\infty, t') \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}'t') \hat{U}_{\mathbf{i}}(t', t) \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t) \hat{U}_{\mathbf{i}}(t, -\infty) | \Phi_{\mathbf{i}} \rangle, \\
&= \langle \Phi_{\mathbf{i}} | \hat{U}_{\mathbf{i}}(-\infty, +\infty) T[\hat{U}_{\mathbf{i}}(+\infty, t') \hat{U}_{\mathbf{i}}(t', t) \hat{U}_{\mathbf{i}}(t, -\infty) \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}'t') \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)] | \Phi_{\mathbf{i}} \rangle, \\
&= \mp \langle \Phi_{\mathbf{i}} | \hat{S}^\dagger_{\mathbf{i}} T[\hat{S}_{\mathbf{i}} \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t) \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle. \qquad (3.2)
\end{aligned}
$$

As a result, one can see that the both cases, $t > t'$ and $t' > t$, give the same expression, while the sign is different. By inserting these expressions into Eq. (2.1), we can express the causal Green function as

$$
G^c(\mathbf{r}t, \mathbf{r}'t') = -i \langle \Phi_{\mathbf{i}} | \hat{S}^\dagger_{\mathbf{i}} T[\hat{S}_{\mathbf{i}} \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t) \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle. \qquad (3.3)
$$

It can be seen that the expression is different from the Green function for the equilibrium state Eq. (2.27). Henceforth, the Green function given by Eq. (3.3) is refered to as the *non-equilibrium* Green function. Let us consider the perturbation expansion of Eq. (3.3) by expanding both the $\hat{S}^\dagger_{\mathbf{i}}$ and $\hat{S}_{\mathbf{i}}$. Considering Eqs. (1.97) and (2.26), $\hat{S}^\dagger_{\mathbf{i}}$ is given by

$$
\begin{aligned}
\hat{S}^\dagger_{\mathbf{i}} &= \sum_{n=0}^{\infty} \left(\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \cdots \int_{-\infty}^{\infty} dt_n \left\{ T[\hat{H}_{\mathbf{i},1}(t_1) \hat{H}_{\mathbf{i},1}(t_2) \cdots \hat{H}_{\mathbf{i},1}(t_n)] \right\}^\dagger, \\
&= \sum_{n=0}^{\infty} \left(\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \cdots \int_{-\infty}^{\infty} dt_n \tilde{T}[\hat{H}_{\mathbf{i},1}(t_1) \hat{H}_{\mathbf{i},1}(t_2) \cdots \hat{H}_{\mathbf{i},1}(t_n)], \qquad (3.4)
\end{aligned}
$$

where it is assumed that $\hat{H}_{\mathbf{i},1}$ is Helmitian, and $\tilde{T}$ is the anti-time ordering operator which orders field operators in the parenthesis in order of a rule that one with early time is put to the left side. Considering the definition of the time ordering operator by Eq. (1.100), it should be noted that the step functions in the anti-time ordering operator appear in a different way compared to the time ordering operator as shown below:

$$
\begin{aligned}
\tilde{T}[\hat{H}_{\mathbf{i},1}(t_1) \hat{H}_{\mathbf{i},1}(t_2)] &= \left\{ T[\hat{H}_{\mathbf{i},1}(t_1) \hat{H}_{\mathbf{i},1}(t_2)] \right\}^\dagger, \qquad (3.5) \\
&= \left\{ \theta(t_1 - t_2) \hat{H}_{\mathbf{i},1}(t_1) \hat{H}_{\mathbf{i},1}(t_2) + \bar{\theta}(t_2 - t_1) \hat{H}_{\mathbf{i},1}(t_2) \hat{H}_{\mathbf{i},1}(t_1) \right\}^\dagger, \\
&= \bar{\theta}(t_2 - t_1) \hat{H}_{\mathbf{i},1}(t_1) \hat{H}_{\mathbf{i},1}(t_2) + \theta(t_1 - t_2) \hat{H}_{\mathbf{i},1}(t_2) \hat{H}_{\mathbf{i},1}(t_1).
\end{aligned}
$$

One can find the anti-time ordering operator permutates the field operators for the case with $t_1 = t_2$, while the time ordering operator does not.

In this section, the Hamiltonian is supporsed to be

$$
\hat{H}_{\mathbf{i}} = \hat{H}_{\mathbf{i},0} + \hat{H}_{\mathbf{i},1}(t) \qquad (3.6)
$$

with

$$
\begin{aligned}
\hat{H}_{\mathbf{i},0} &= \int d\mathbf{r} \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}t) \hat{v}_{1,0}(\mathbf{r}) \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t), \\
\hat{H}_{\mathbf{i},1}(t) &= \int d\mathbf{r} \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}t) \hat{v}_{1,1}(\mathbf{r}t) \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t). \qquad (3.7)
\end{aligned}
$$

From above expressions, it is found that the two-particle operator is excluded. Then, one can write $\hat{S}^\dagger_{\mathbf{i}}$ and $T[\hat{S}_{\mathbf{i}} \hat{\Psi}_{\mathbf{i}}(\mathbf{r}t) \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}'t')]$, which are the constitutents in Eq. (3.3), as

$$
\begin{aligned}
\hat{S}^\dagger_{\mathbf{i}} = 1 \quad &+ \left(\frac{i}{\hbar}\right) \int dt_1 \int \mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \tilde{T}[\hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}_1 t_1) \hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)] \\
&+ \frac{1}{2} \left(\frac{i}{\hbar}\right)^2 \int dt_1 \int \mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \int dt_2 \int \mathbf{r}_2 \hat{v}_{1,1}(\mathbf{r}_2 t_2) \tilde{T}[\hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}_1 t_1) \hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1) \hat{\Psi}^\dagger_{\mathbf{i}}(\mathbf{r}_2 t_2) \hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2 t_2)] + \cdots, \\
&\qquad (3.8)
\end{aligned}
$$

$$
\begin{aligned}
T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] &= T[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] \\
&+ \left(\frac{-i}{\hbar}\right)\int dt_1 \int \mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] \\
&+ \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \int dt_1 \int d\mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \int dt_2 \int d\mathbf{r}_2 \hat{v}_{1,1}(\mathbf{r}_2 t_2) \\
&\quad \times \langle \Phi_{\mathbf{i}} | T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_2 t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2 t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle \\
&\quad + \cdots .
\end{aligned} \tag{3.9}
$$

By multiplying Eq. (3.8) by Eq. (3.9), we can obtain its expectation value as:

$$
\begin{aligned}
\langle \Phi_{\mathbf{i}} | \hat{S}^{\dagger}_{\mathbf{i}} T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle &= \langle \Phi_{\mathbf{i}} | T[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle \\
&+ \left(\frac{-i}{\hbar}\right)\int dt_1 \int \mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \langle \Phi_{\mathbf{i}} | T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle \\
&+ \left(\frac{i}{\hbar}\right)\int dt_1 \int \mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \langle \Phi_{\mathbf{i}} | \tilde{T}[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)] T[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle \\
&+ \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \int dt_1 \int d\mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \int dt_2 \int d\mathbf{r}_2 \hat{v}_{1,1}(\mathbf{r}_2 t_2) \\
&\quad \times \langle \Phi_{\mathbf{i}} | T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_2 t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2 t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] | \Phi_{\mathbf{i}} \rangle \\
&+ \left(\frac{i}{\hbar}\right)\left(\frac{-i}{\hbar}\right)\int dt_1 \int \mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \int dt'_1 \int \mathbf{r}'_1 \hat{v}_{1,1}(\mathbf{r}'_1 t'_1) \\
&\quad \times \tilde{T}[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)] T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'_1 t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'_1 t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] \\
&+ \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 \int dt_1 \int \mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1 t_1) \int dt_2 \int \mathbf{r}_2 \hat{v}_{1,1}(\mathbf{r}_2 t_2) \\
&\quad \times \tilde{T}[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1 t_1)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_2 t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2 t_2)] T[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] \\
&+ \cdots
\end{aligned} \tag{3.10}
$$

The first, second, and fourth terms have been already discussed in the chapter for the equilibrium Green function. After investigating the properties of the second Wick theorem, we will analyze the third, fifth, sixth terms in Eq. (3.10) in later section.

3.2 The second Wick theorem

We define $\hat{A}^{\cdot}\hat{B}^{\cdot}$ as an analog of the contraction defined by Eq. (2.47) as follows:

$$
\hat{A}^{\cdot}\hat{B}^{\cdot} = \tilde{T}[\hat{A}\hat{B}] - N[\hat{A}\hat{B}]. \tag{3.11}
$$

Hereafter the contractions defined by Eqs. (2.47) and (3.11) will be refered to as *first* and *second* contractions, respectively. The second contraction has the following properties:

$$
\begin{aligned}
\hat{A}^{\cdot}\hat{B}^{\cdot} &= -\hat{B}^{\cdot}\hat{A}^{\cdot}, && (3.12) \\
(\hat{A}^{\cdot} + \hat{B}^{\cdot})\hat{C}^{\cdot} &= \hat{A}^{\cdot}\hat{B}^{\cdot} + \hat{A}^{\cdot}\hat{C}^{\cdot}, && (3.13) \\
\hat{A}^{\cdot}\hat{B}^{\cdot} &= 0 \qquad \text{if } \hat{A} \text{ and } \hat{B} \text{ are anticommutable.} && (3.14)
\end{aligned}
$$

Eqs. (3.12) and (3.13) are trivial from the definition, and Eq. (3.14) can be confirmed by noting that $\tilde{T}[\hat{A}\hat{B}] = \theta(t_B - t_A)\hat{A}\hat{B} - \bar{\theta}(t_A - t_B)\hat{B}\hat{A} = \hat{A}\hat{B}$ and $N[\hat{A}\hat{B}] = \hat{A}\hat{B}$ or $-\hat{B}\hat{A} = \hat{A}\hat{B}$. Due to Eq. (3.14), the following contractions become zero:

$$\begin{aligned}
\hat{\Psi}^{;}_{\rm u}\hat{\Psi}^{;}_{\rm u} &= 0, \qquad \hat{\Psi}^{\dagger;}_{\rm u}\hat{\Psi}^{\dagger;}_{\rm u} = 0,\\
\hat{\Psi}^{;}_{\rm o}\hat{\Psi}^{;}_{\rm o} &= 0, \qquad \hat{\Psi}^{\dagger;}_{\rm o}\hat{\Psi}^{\dagger;}_{\rm o} = 0,\\
\hat{\Psi}^{;}_{\rm u}\hat{\Psi}^{\dagger;}_{\rm o} &= 0, \qquad \hat{\Psi}^{\dagger;}_{\rm o}\hat{\Psi}^{;}_{\rm u} = 0,\\
\hat{\Psi}^{;}_{\rm o}\hat{\Psi}^{\dagger;}_{\rm u} &= 0, \qquad \hat{\Psi}^{\dagger;}_{\rm u}\hat{\Psi}^{;}_{\rm o} = 0,\\
\hat{\Psi}^{;}_{\rm o}\hat{\Psi}^{;}_{\rm u} &= 0, \qquad \hat{\Psi}^{\dagger;}_{\rm o}\hat{\Psi}^{\dagger;}_{\rm u} = 0,\\
\hat{\Psi}^{;}_{\rm u}\hat{\Psi}^{;}_{\rm o} &= 0, \qquad \hat{\Psi}^{\dagger;}_{\rm u}\hat{\Psi}^{\dagger;}_{\rm o} = 0.
\end{aligned} \tag{3.15}$$

The proof for above relations is same as for the first contraction. A little contractions are not zero, and they are given by

$$\begin{aligned}
\hat{\Psi}^{\dagger;}_{\rm u}(\mathbf{r}_1t_1)\hat{\Psi}^{;}_{\rm u}(\mathbf{r}_2t_2) &= \sum_{i,j\in\text{unocc}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{it_1w_i}\mathrm{e}^{-it_2w_j}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},j},\\
&= \sum_{i\neq j\in\text{unocc}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{it_1w_i}\mathrm{e}^{-it_2w_j}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},j}\\
&\quad + \sum_{i\in\text{unocc}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_2-t_1)w_i}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},i},\\
&= \sum_{i\in\text{unocc}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_2-t_1)w_i}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},i},\\
&= \begin{cases} -\sum_{i\in\text{unocc}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_2-t_1)w_i} & \text{for } t_1\geq t_2\\ 0 & \text{for } t_2>t_1\end{cases},\\
&= \begin{cases} iG^{c,*}_0(\mathbf{r}_1t_1,\mathbf{r}_2t_2) & \text{for } t_1\geq t_2\\ 0 & \text{for } t_2>t_1\end{cases},
\end{aligned} \tag{3.16}$$

$$\begin{aligned}
\hat{\Psi}^{;}_{\rm o}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger;}_{\rm o}(\mathbf{r}_2t_2) &= \sum_{i,j\in\text{occ}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{it_1w_i}\mathrm{e}^{-it_2w_j}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},j},\\
&= \sum_{i\neq j\in\text{occ}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},j}(\mathbf{r}_2)\mathrm{e}^{it_1w_i}\mathrm{e}^{-it_2w_j}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},j}\\
&\quad + \sum_{i\in\text{occ}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_2-t_1)w_i}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},i},\\
&= \sum_{i\in\text{occ}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_2-t_1)w_i}\hat{a}^{\dagger;}_{\mathbf{s},i}\hat{a}^{;}_{\mathbf{s},i},\\
&= \begin{cases} 0 & \text{for } t_1\geq t_2\\ \sum_{i\in\text{occ}} \Psi^{\dagger}_{\mathbf{s},i}(\mathbf{r}_1)\Psi_{\mathbf{s},i}(\mathbf{r}_2)\mathrm{e}^{-i(t_2-t_1)w_i} & \text{for } t_2>t_1\end{cases},\\
&= \begin{cases} 0 & \text{for } t_1\geq t_2\\ iG^{c,*}_0(\mathbf{r}_1t_1,\mathbf{r}_2t_2) & \text{for } t_2>t_1\end{cases},
\end{aligned} \tag{3.17}$$

where $G^{c,*}_0(\mathbf{r}_1t_1,\mathbf{r}_2t_2)$ is the conjugate complex of $G^{c}_0(\mathbf{r}_1t_1,\mathbf{r}_2t_2)$. As mentioned in the chapter for the equilibrium Green function, note that the normal ordering operator in the derivation of Eqs. (3.16) and (3.17) operates on not $\hat{a}$, but the field operators. Using Eqs. (3.15), (3.16), and (3.17), the second contraction can be obtained as follows:

$$\hat{\Psi}^{;}_{\rm i}(\mathbf{r}t)\hat{\Psi}^{;}_{\rm i}(\mathbf{r}'t') = (\hat{\Psi}^{;}_{\rm u}(\mathbf{r}t)+\hat{\Psi}^{\dagger;}_{\rm o}(\mathbf{r}t))(\hat{\Psi}^{;}_{\rm u}(\mathbf{r}'t')+\hat{\Psi}^{\dagger;}_{\rm o}(\mathbf{r}'t')),$$

$$
\begin{aligned}
&= \hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= 0,
\end{aligned} \tag{3.18}
$$

$$
\begin{aligned}
\hat{\Psi}^{\dagger;}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathbf{i}}(\mathbf{r}'t') &= (\hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}t) + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}t))(\hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}'t')), \\
&= \hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= 0,
\end{aligned} \tag{3.19}
$$

$$
\begin{aligned}
\hat{\Psi}^{\dagger;}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathbf{i}}(\mathbf{r}'t') &= (\hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}'t'))(\hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}t) + \hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}t)), \\
&= \hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= \hat{\Psi}^{\dagger;}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}^{;}_{\mathrm{u}}(\mathbf{r}'t') + \hat{\Psi}^{;}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger;}_{\mathrm{o}}(\mathbf{r}'t'), \\
&= iG^{c,*}_{0}(\mathbf{r}t, \mathbf{r}'t').
\end{aligned} \tag{3.20}
$$

The second Wick theorem

The second Wick theorem transforms the $\tilde{T}$-product of field operators $\hat{A}_1 \cdots \hat{A}_n$ into the sum of N-products of those plus a product of the second contraction as follows:

$$
\begin{aligned}
\tilde{T}[\hat{A}_1 \cdots \hat{A}_n] &= N[\hat{A}_1 \cdots \hat{A}_n] \\
&\quad + \sum_{i,j} (-1)^P \hat{A}^{;}_i \hat{A}^{;}_j N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_n] \\
&\quad + \sum_{i,j,k,l} (-1)^P \hat{A}^{;}_i \hat{A}^{;}_j \hat{A}^{;}_k \hat{A}^{;}_l N[\hat{A}_1 \cdots (ijkl) \cdots \hat{A}_n] \\
&\quad + \cdots \\
&\quad + \sum (-1)^P \hat{A}^{;}_i \hat{A}^{;}_j \hat{A}^{;}_k \hat{A}^{;}_l \cdots,
\end{aligned} \tag{3.21}
$$

where $N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_n]$ is the N-product of the remaining field operators after elimination of $\hat{A}_i$ and $\hat{A}_j$, and P is the number of permutations from $\hat{A}_1 \cdots \hat{A}_1$ to $\hat{A}_i \hat{A}_j \hat{A}_1 \cdots (ij) \cdots \hat{A}_1$. Also, the last term means the product of paired second contractions of which number is $n/2$ when n is even, and the product of paired contractions of which number is $(n-1)/2$ and a remaining operator when n is odd.

Although the proof of the theorem is very similar to that of the first Wick theorem, for completeness the proof is shown below. To prove Eq. (3.21), first let us prove the following lemma:

Lemma 2

If the time associated with $\hat{B}$ is latest compared to all the times associated with $\hat{A}_1, \cdots, \hat{A}_n$, then

$$
\begin{aligned}
N[\hat{A}_1 \cdots \hat{A}_n]\hat{B} &= N[\hat{A}_1 \cdots \hat{A}_{n-1}]\hat{A}^{;}_n \hat{B}^{;} + (-1)N[\hat{A}_1 \cdots \hat{A}_{n-2}\hat{A}_n]\hat{A}^{;}_{n-1}\hat{B}^{;} + \cdots \\
&\quad + (-1)^{n-k} N[\hat{A}_1 \cdots \hat{A}_{n-(k+1)}\hat{A}_{n-(k-1)} \cdots \hat{A}_n]\hat{A}^{;}_k \hat{B}^{;} + \cdots \\
&\quad + (-1)^{n-1} N[\hat{A}_2 \cdots \hat{A}_n]\hat{A}^{;}_1 \hat{B}^{;} + N[\hat{A}_1 \cdots \hat{A}_n \hat{B}]
\end{aligned} \tag{3.22}
$$

This proof is similar to that of the lemma 1 which is discussed in the chapter for the equilibrium Green function.

Proof of the lemma 2

(i) *If $\hat{B}$ is the destruction operator*, then $\hat{A}^{\cdot}_k\hat{B}^{\cdot} = 0$. Also, indeed $N[\hat{A}_1 \cdots \hat{A}_n]\hat{B} = N[\hat{A}_1 \cdots \hat{A}_n\hat{B}]$ due to the definition of the N-product. Thus, the lemma is accepted.

(ii) *If $\hat{B}$ is the creation operator*, it is possible to assume that $\hat{A}_1, \cdots$, and $\hat{A}_n$ are all the destruction operators. Arbitrary case can be generated by multiplying the both sides by a creation operator $\hat{A}$ from the left side repeatedly and by permutating the order of field operators in the N-product, since $\hat{A}N[\hat{A}_1 \cdots] = N[\hat{A}\hat{A}_1 \cdots]$ and the changes of sign due to the permutation of the field operators to get the case in the N-product cancel out.

In this case that $\hat{B}$ is the creation operator and that $\hat{A}_1, \cdots, \hat{A}_n$ are all the destruction operators, the lemma can be proved by the principle of induction. For $n = 1$, we obtain $\hat{A}_1\hat{B} = \tilde{T}[\hat{A}_1\hat{B}] = A^{\cdot}_1\hat{B}^{\cdot} + N[A_1\hat{B}]$. This is the definition of the contaction. Thus, the lemma is accepted. Next, let us assume that the lemma is accepted for $n = m$. Letting $\hat{A}$ be a destruction operator, we have

$$
\begin{aligned}
N[\hat{A}\hat{A}_1 \cdots \hat{A}_m]\hat{B} &= \hat{A}N[\hat{A}_1 \cdots \hat{A}_m]\hat{B}, \\
&= \hat{A}\Big(N[\hat{A}_1 \cdots \hat{A}_{m-1}]\hat{A}^{\cdot}_m\hat{B}^{\cdot} + (-1)N[\hat{A}_1 \cdots \hat{A}_{m-2}\hat{A}_m]\hat{A}^{\cdot}_{m-1}\hat{B}^{\cdot} + \cdots \\
&\quad + (-1)^{m-k}N[\hat{A}_1 \cdots \hat{A}_{m-(k+1)}\hat{A}_{m-(k-1)} \cdots \hat{A}_m]\hat{A}^{\cdot}_k\hat{B}^{\cdot} + \cdots \\
&\quad + (-1)^{m-1}N[\hat{A}_2 \cdots \hat{A}_m]\hat{A}^{\cdot}_1\hat{B}^{\cdot} + N[\hat{A}_1 \cdots \hat{A}_m\hat{B}]\Big), \\
&= N[\hat{A}\hat{A}_1 \cdots \hat{A}_{m-1}]\hat{A}^{\cdot}_m\hat{B}^{\cdot} + (-1)N[\hat{A}\hat{A}_1 \cdots \hat{A}_{m-2}\hat{A}_m]\hat{A}^{\cdot}_{m-1}\hat{B}^{\cdot} + \cdots \\
&\quad + (-1)^{m-k}N[\hat{A}\hat{A}_1 \cdots \hat{A}_{m-(k+1)}\hat{A}_{m-(k-1)} \cdots \hat{A}_m]\hat{A}^{\cdot}_k\hat{B}^{\cdot} + \cdots \\
&\quad + (-1)^{m-1}N[\hat{A}\hat{A}_2 \cdots \hat{A}_m]\hat{A}^{\cdot}_1\hat{B}^{\cdot} + \hat{A}N[\hat{A}_1 \cdots \hat{A}_m\hat{B}],
\end{aligned} \tag{3.23}
$$

where the last term of the final line in the right hand side is evaluated as:

$$
\begin{aligned}
\hat{A}N[\hat{A}_1 \cdots \hat{A}_m\hat{B}] &= (-1)^m\hat{A}\hat{B}\hat{A}_1 \cdots \hat{A}_m, \\
&= (-1)^m\tilde{T}[\hat{A}\hat{B}]\hat{A}_1 \cdots \hat{A}_m, \\
&= (-1)^m(\hat{A}^{\cdot}\hat{B}^{\cdot} + N[\hat{A}\hat{B}])\hat{A}_1 \cdots \hat{A}_m, \\
&= (-1)^m N[\hat{A}_1 \cdots \hat{A}_m]\hat{A}^{\cdot}\hat{B}^{\cdot} + (-1)^{m+1}\hat{B}\hat{A}\hat{A}_1 \cdots \hat{A}_m, \\
&= (-1)^m N[\hat{A}_1 \cdots \hat{A}_m]\hat{A}^{\cdot}\hat{B}^{\cdot} + N[\hat{A}\hat{A}_1 \cdots \hat{A}_m\hat{B}].
\end{aligned} \tag{3.24}
$$

By putting Eq. (3.24) into Eq. (3.23), we can get the lemma for $n = m + 1$. Thus, the lemma is proven.

Proof of the second Wick theorem

The theorem is proven by the principle of induction. For $n = 1$, we obtain $\tilde{T}[\hat{A}_1\hat{A}_2] = N[\hat{A}_1\hat{A}_2] + \hat{A}^{\cdot}_1\hat{A}^{\cdot}_2$. This is the definition of the second contaction. Thus, the theorem is accepted. Next, let us assume that the theorem is accepted for $n = m$. Letting $\hat{A}_{m+1}$ be a field operator at the latest time among $\hat{A}_1, \cdots, \hat{A}_{m+1}$, then

$$
\begin{aligned}
\tilde{T}[\hat{A}_1 \cdots \hat{A}_m\hat{A}_{m+1}] &= \tilde{T}[\hat{A}_1 \cdots \hat{A}_m]\hat{A}_{m+1} \\
&= \Big(N[\hat{A}_1 \cdots \hat{A}_m] \\
&\quad + \sum_{i,j}(-1)^P\hat{A}^{\cdot}_i\hat{A}^{\cdot}_j N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_m]
\end{aligned}
$$

$$
\begin{aligned}
& + \sum_{i,j,k,l} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l N[\hat{A}_1 \cdots (ijkl) \cdots \hat{A}_m] \\
& + \cdots \\
& + \sum (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l \cdots \Big) \hat{A}_{m+1}, \\
= \; & N[\hat{A}_1 \cdots \hat{A}_m] \hat{A}_{m+1} \\
& + \sum_{i,j} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_m] \hat{A}_{m+1} \\
& + \sum_{i,j,k,l} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l N[\hat{A}_1 \cdots (ijkl) \cdots \hat{A}_m] \hat{A}_{m+1} \\
& + \cdots \\
& + \sum (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l \cdots \hat{A}_{m+1}, \\
= \; & \sum_i (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_{m+1} N[\hat{A}_1 \cdots (i(m+1)) \cdots \hat{A}_{m+1}] + N[\hat{A}_1 \cdots \hat{A}_{m+1}] \\
& + \sum_{i,j,k,l} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_{m+1} N[\hat{A}_1 \cdots (ijk(m+1)) \cdots \hat{A}_{m+1}] \\
& + \sum_{i,j} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_{m+1}] \\
& + \sum_{i,j,k,l} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l N[\hat{A}_1 \cdots (ijkl) \cdots \hat{A}_{m+1}] \\
& + \cdots \\
& + \sum (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l \cdots \hat{A}_{m+1} \\
= \; & N[\hat{A}_1 \cdots \hat{A}_{m+1}] \\
& + \sum_{i,j} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j N[\hat{A}_1 \cdots (ij) \cdots \hat{A}_{m+1}] \\
& + \sum_{i,j,k,l} (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l N[\hat{A}_1 \cdots (ijkl) \cdots \hat{A}_{m+1}] \\
& + \cdots \\
& + \sum (-1)^P \hat{A}^{\cdot}_i \hat{A}^{\cdot}_j \hat{A}^{\cdot}_k \hat{A}^{\cdot}_l \cdots,
\end{aligned}
\tag{3.25}
$$

where the lemma 2 is used for the derivation. So, we can reproduce the theorem for $n = m + 1$. The assumption that $\hat{A}_{m+1}$ is a field operator associated with the latest time among $\hat{A}_1, \cdots, \hat{A}_{m+1}$ can be eliminated by permutating the field operators in the T- and N-products for arbitrary case of Eq. (3.25) so that the operator associated with the latest time can be located at the most right side. The changes of sign due to the permutation for both the sides in Eq. (3.25) cancel each other. Thus, the theorem is proven. It is also noted that the second Wick theorem can be applied to the field operator $\hat{\Psi}_{\mathbf{i}}$ itself as a consequence of the distributive properties of the T- and N-products.[1]

Although we have proved the second Wick theorem, the meaning of the summations in Eq. (3.21) is not so clear. Let us see the formulas upto $n = 4$ below:

For $n = 2$

$$
\tilde{T}[\hat{A}_1 \hat{A}_2] = \hat{A}^{\cdot}_1 \hat{A}^{\cdot}_2 + N[\hat{A}_1 \hat{A}_2], \tag{3.26}
$$

For $n = 3$

[1] See the footnote for the Wick theorem.

$$
\begin{aligned}
\tilde{T}[\hat{A}_1\hat{A}_2\hat{A}_3] &= \tilde{T}[\hat{A}_1\hat{A}_2]\hat{A}_3, \\
&= (\hat{A}_1^{\cdot}\hat{A}_2^{\cdot} + N[\hat{A}_1\hat{A}_2])\hat{A}_3, \\
&= N[\hat{A}_1\hat{A}_2]\hat{A}_3 + N[\hat{A}_3]\hat{A}_1^{\cdot}\hat{A}_2^{\cdot}, \\
&= N[\hat{A}_1]\hat{A}_2^{\cdot}\hat{A}_3^{\cdot} - N[\hat{A}_2]\hat{A}_1^{\cdot}\hat{A}_3^{\cdot} + N[\hat{A}_3]\hat{A}_1^{\cdot}\hat{A}_2^{\cdot} + N[\hat{A}_1\hat{A}_2\hat{A}_3], \qquad (3.27)
\end{aligned}
$$

For $n = 4$

$$
\begin{aligned}
\tilde{T}[\hat{A}_1\hat{A}_2\hat{A}_3\hat{A}_4] &= \tilde{T}[\hat{A}_1\hat{A}_2\hat{A}_3]\hat{A}_4, \\
&= (N[\hat{A}_1]\hat{A}_2^{\cdot}\hat{A}_3^{\cdot} - N[\hat{A}_2]\hat{A}_1^{\cdot}\hat{A}_3^{\cdot} + N[\hat{A}_3]\hat{A}_1^{\cdot}\hat{A}_2^{\cdot} + N[\hat{A}_1\hat{A}_2\hat{A}_3])\hat{A}_4, \\
&= N[\hat{A}_1]\hat{A}_4\hat{A}_2^{\cdot}\hat{A}_3^{\cdot} - N[\hat{A}_2]\hat{A}_4\hat{A}_1^{\cdot}\hat{A}_3^{\cdot} + N[\hat{A}_3]\hat{A}_4\hat{A}_1^{\cdot}\hat{A}_2^{\cdot} + N[\hat{A}_1\hat{A}_2\hat{A}_3]\hat{A}_4, \\
&= (\hat{A}_1^{\cdot}\hat{A}_4^{\cdot} + N[\hat{A}_1\hat{A}_4])\hat{A}_2^{\cdot}\hat{A}_3^{\cdot} - (\hat{A}_2^{\cdot}\hat{A}_4^{\cdot} + N[\hat{A}_2\hat{A}_4])\hat{A}_1^{\cdot}\hat{A}_3^{\cdot} + (\hat{A}_3^{\cdot}\hat{A}_4^{\cdot} + N[\hat{A}_3\hat{A}_4])\hat{A}_1^{\cdot}\hat{A}_2^{\cdot} \\
&\quad + N[\hat{A}_1\hat{A}_2]\hat{A}_3^{\cdot}\hat{A}_4^{\cdot} - N[\hat{A}_1\hat{A}_3]\hat{A}_2^{\cdot}\hat{A}_4^{\cdot} + N[\hat{A}_2\hat{A}_3]\hat{A}_1^{\cdot}\hat{A}_4^{\cdot} + N[\hat{A}_1\hat{A}_2\hat{A}_3\hat{A}_4], \\
&= N[\hat{A}_1\hat{A}_2\hat{A}_3\hat{A}_4] + \hat{A}_1^{\cdot}\hat{A}_2^{\cdot}N[\hat{A}_3\hat{A}_4] - \hat{A}_1^{\cdot}\hat{A}_3^{\cdot}N[\hat{A}_2\hat{A}_4] + \hat{A}_1^{\cdot}\hat{A}_4^{\cdot}N[\hat{A}_2\hat{A}_3] \\
&\quad + \hat{A}_2^{\cdot}\hat{A}_3^{\cdot}N[\hat{A}_1\hat{A}_4] - \hat{A}_2^{\cdot}\hat{A}_4^{\cdot}N[\hat{A}_1\hat{A}_3] + \hat{A}_3^{\cdot}\hat{A}_4^{\cdot}N[\hat{A}_1\hat{A}_2] \\
&\quad + \hat{A}_1^{\cdot}\hat{A}_2^{\cdot}\hat{A}_3^{\cdot}\hat{A}_4^{\cdot} - \hat{A}_1^{\cdot}\hat{A}_3^{\cdot}\hat{A}_2^{\cdot}\hat{A}_4^{\cdot} + \hat{A}_2^{\cdot}\hat{A}_3^{\cdot}\hat{A}_1^{\cdot}\hat{A}_4^{\cdot}. \qquad (3.28)
\end{aligned}
$$

3.3 Structure of the NEGF

The first contractions arising from the T-product, $T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')]$, in Eq. (3.3) are equivalent to those of the numerator of Eq. (2.27) for the equilibrium Green funtion, and by using Eqs. (2.67) and Eqs. (2.68) and they are given by

First contractions in $T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')]$

$$
\begin{aligned}
&= \left(1 - \left(-\frac{i}{\hbar}\right)\int dt_1 \int d\mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1t_1) iG_0^c(\mathbf{r}_1t_1, \mathbf{r}_1t_1) + \cdots\right) \\
&\quad \times \left(iG_0^c(\mathbf{r}t, \mathbf{r}'t') + \left(-\frac{i}{\hbar}\right)\int dt_1 \int d\mathbf{r}_1 iG_0^c(\mathbf{r}t, \mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1) iG_0^c(\mathbf{r}_1t_1, \mathbf{r}'t') + \cdots\right), \\
&= \langle\Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle \left(iG_0^c(\mathbf{r}t, \mathbf{r}'t') + \left(-\frac{i}{\hbar}\right)\int dt_1 \int d\mathbf{r}_1 iG_0^c(\mathbf{r}t, \mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1) iG_0^c(\mathbf{r}_1t_1, \mathbf{r}'t') + \cdots\right). \qquad (3.29)
\end{aligned}
$$

Also, the second contractions of $\hat{S}^{\dagger}_{\mathbf{i}}$ can be found using Eqs. (3.8), (3.20), and (3.28) as

Second contractions in $\hat{S}^{\dagger}_{\mathbf{i}}$

$$
\begin{aligned}
&= 1 + \left(\frac{i}{\hbar}\right)\int dt_1 \int d\mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1t_1) iG_0^{c,*}(\mathbf{r}_1t_1, \mathbf{r}_1t_1) \\
&\quad + \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 \int dt_1 \int d\mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1t_1) \int dt_2 \int d\mathbf{r}_2 \hat{v}_{1,1}(\mathbf{r}_2t_2) iG_0^{c,*}(\mathbf{r}_1t_1, \mathbf{r}_1t_1) iG_0^{c,*}(\mathbf{r}_2t_2, \mathbf{r}_2t_2) \\
&\quad - \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 \int dt_1 \int d\mathbf{r}_1 \hat{v}_{1,1}(\mathbf{r}_1t_1) \int dt_2 \int d\mathbf{r}_2 \hat{v}_{1,1}(\mathbf{r}_2t_2) iG_0^{c,*}(\mathbf{r}_2t_2, \mathbf{r}_1t_1) iG_0^{c,*}(\mathbf{r}_1t_1, \mathbf{r}_2t_2) + \cdots, \\
&= \langle\Phi_{\mathbf{i}}|\hat{S}^{\dagger}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle. \qquad (3.30)
\end{aligned}
$$

The term $\langle\Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle$ in the Eq. (3.29) can be explictly evaluated by assuming the following special form of $\hat{H}_{\mathbf{i},1}(t)$:

$$
\hat{H}_{\mathbf{i},1}(-t) = \hat{H}_{\mathbf{i},1}(t).
$$

At least, if $\hat{H}_{\mathbf{i},1}(t)$ is the coupling between leads and the conductor, the assumption is presumably acceptable. With the assumption, $\hat{U}_{\mathbf{i}}(0,-\infty)$ can be written as:

$$\begin{aligned}
\hat{U}_{\mathbf{i}}(0,-\infty) &= T\left[\exp\left(-\frac{i}{\hbar}\int_{-\infty}^{0} dt\hat{H}_{\mathbf{i},1}(t)]\right)\right], \\
&= T\left[\exp\left(-\frac{i}{\hbar}\int_{+\infty}^{0} (-dt')\hat{H}_{\mathbf{i},1}(-t')]\right)\right], \\
&= -T\left[\exp\left(-\frac{i}{\hbar}\int_{+\infty}^{0} dt'\hat{H}_{\mathbf{i},1}(t')]\right)\right], \\
&= -\hat{U}_{\mathbf{i}}(0,+\infty),
\end{aligned} \tag{3.31}$$

where the variable change of $t' = -t$ is made. Then, it turns out that

$$\begin{aligned}
\langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle &= \langle \Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)\hat{U}_{\mathbf{i}}(0,-\infty)|\Phi_{\mathbf{i}}\rangle, \\
&= \langle \Phi_{\mathbf{i}}|\hat{U}_{\mathbf{i}}(+\infty,0)(-\hat{U}_{\mathbf{i}}(0,+\infty))|\Phi_{\mathbf{i}}\rangle, \\
&= -1.
\end{aligned} \tag{3.32}$$

Moreover, noting that $\left(\langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle\right)^{\dagger} = \langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}^{\dagger}|\Phi_{\mathbf{i}}\rangle$, it is found to be $\langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}^{\dagger}|\Phi_{\mathbf{i}}\rangle\langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle = 1$. Therefore, Eq. (3.10) can be rewritten by the sum of two contributions. One of them consists of the terms in the parenthesis in Eq. (3.29), and the other is a characteristic contribution which appears in the NEGF not in the EGF, and will be discussed later on. Temporarily, letting the second contribution be η, one can write Eq. (3.10) as:

$$\begin{aligned}
&\langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}^{\dagger}T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^{\dagger}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle \\
&\quad = \left(iG_0^c(\mathbf{r}t,\mathbf{r}'t') + \left(-\frac{i}{\hbar}\right)\int dt_1 \int d\mathbf{r}_1 iG_0^c(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG_0^c(\mathbf{r}_1t_1,\mathbf{r}'t') + \cdots\right) + \eta.
\end{aligned} \tag{3.33}$$

The first contribution is equivalent to the connected diagrams appearing in the EGF.

To investigate the second contributin η, first let us see the third term in Eq. (3.10) which is the first order term in η. The product of the $\tilde{T}$- and T-products being the constituent in the third term of Eq. (3.10) can be expanded using Eq. (2.39) as

$$\begin{aligned}
&\tilde{T}[\hat{\Psi}_{\mathbf{i}}^{\dagger}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)]T[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^{\dagger}(\mathbf{r}'t')] \\
&\quad = \tilde{T}[(\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}_1t_1) + \hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1))(\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1) + \hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}_1t_1))] \times T[(\hat{\Psi}_{\mathrm{u}}(\mathbf{r}t) + \hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}t))(\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}'t') + \hat{\Psi}_{\mathrm{o}}(\mathbf{r}'t'))], \\
&\quad = \left(\tilde{T}[\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)] + \tilde{T}[\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}_1t_1)] + \tilde{T}[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)] + \tilde{T}[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}_1t_1)]\right) \\
&\qquad \times \left(T[\hat{\Psi}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}'t')] + T[\hat{\Psi}_{\mathrm{u}}(\mathbf{r}t)\hat{\Psi}_{\mathrm{o}}(\mathbf{r}'t')] + T[\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}'t')] + T[\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}t)\hat{\Psi}_{\mathrm{o}}(\mathbf{r}'t')]\right).
\end{aligned} \tag{3.34}$$

When the expectation value of Eq. (3.34) is considered with respect to $\Phi_{\mathbf{i}}$, it is found that the sum of the first and second terms in the first parenthesis gives $iG_0^{c,*}(\mathbf{r}_1t_1,\mathbf{r}_1t_1)$, and that the sum of the first and second terms in the second parenthesis gives $iG_0^c(\mathbf{r}t,\mathbf{r}'t')$. They are parts of $\langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}^{\dagger}|\Phi_{\mathbf{i}}\rangle\langle \Phi_{\mathbf{i}}|\hat{S}_{\mathbf{i}}|\Phi_{\mathbf{i}}\rangle$, and cancel as discussed above. The other surving term is $\langle \Phi_{\mathbf{i}}|\tilde{T}[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)]T[\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle$. Although the contribution from the contractions in the expectation value is zero, it is found using Eqs. (2.51), (2.63), (3.15), and (3.26) that the contribution from the N-products survives as:

$$\begin{aligned}
\langle \Phi_{\mathbf{i}}|\tilde{T}[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)]T[\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle &= \langle \Phi_{\mathbf{i}}|N[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)]N[\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle, \\
&= \langle \Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{o}}^{\dagger}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}^{\dagger}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle.
\end{aligned} \tag{3.35}$$

Noting that

$$
\begin{aligned}
|\Phi_{\mathbf{i}}\rangle &= \mathrm{e}^{\frac{i}{\hbar}\hat{H}_{\mathbf{s},0}t}|\Phi_{\mathbf{s}}\rangle, \\
&= \prod_{k=1}^{\infty} \mathrm{e}^{itw_k n_k}|\Phi_{\mathbf{s}}\rangle,
\end{aligned} \tag{3.36}
$$

one can explicitly evaluate Eq. (3.35) as

$$
\begin{aligned}
&\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle \\
&\quad= -\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle \\
&\quad= -\langle\Phi_{\mathbf{s}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{*}_{\mathbf{s},i}(\mathbf{r}')\mathrm{e}^{-i(t_1-t')w_i}|\Phi_{\mathbf{s}}\rangle, \\
&\quad= -\left(\sum_{j\in\mathrm{occ}}\Psi_{\mathbf{s},j}(\mathbf{r})\Psi^{*}_{\mathbf{s},j}(\mathbf{r}_1)\mathrm{e}^{-i(t-t_1)w_j}\right)\left(\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r}_1)\Psi^{*}_{\mathbf{s},i}(\mathbf{r}')\mathrm{e}^{-i(t_1-t')w_i}\right).
\end{aligned} \tag{3.37}
$$

As defined in the chapter of the EGF, we now define the lesser and greater Green functions $G_0^<$ and $G_0^>$ for the NEGF by

$$
\begin{aligned}
G_0^<(\mathbf{r}t,\mathbf{r}'t') &= i\langle\Phi_{\mathbf{i}}|\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)|\Phi_{\mathbf{i}}\rangle, \\
&= i\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathbf{o}}(\mathbf{r}'t')\hat{\Psi}^{\dagger}_{\mathbf{o}}(\mathbf{r}t)|\Phi_{\mathbf{i}}\rangle, \\
&= i\langle\Phi_{\mathbf{i}}|\left(\sum_{i\in\mathrm{occ}}\Psi^{*}_{\mathbf{s},i}(\mathbf{r}')\hat{a}^{\dagger}_{\mathbf{i},i}(t')\right)\left(\sum_{j\in\mathrm{occ}}\Psi_{\mathbf{s},j}(\mathbf{r})\hat{a}_{\mathbf{i},j}(t)\right)|\Phi_{\mathbf{i}}\rangle, \\
&= i\sum_{i,j\in\mathrm{occ}}\Psi_{\mathbf{s},j}(\mathbf{r})\Psi^{*}_{\mathbf{s},i}(\mathbf{r}')\mathrm{e}^{-itw_j}\mathrm{e}^{it'w_i}\langle\Phi_{\mathbf{s}}|\hat{a}^{\dagger}_{\mathbf{s},i}\hat{a}_{\mathbf{s},j}|\Phi_{\mathbf{s}}\rangle, \\
&= i\sum_{i\in\mathrm{occ}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi^{*}_{\mathbf{s},i}(\mathbf{r}')\mathrm{e}^{-i(t-t')w_i}
\end{aligned} \tag{3.38}
$$

and

$$
\begin{aligned}
G_0^>(\mathbf{r}t,\mathbf{r}'t') &= -i\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle, \\
&= -i\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathbf{u}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{u}}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle, \\
&= -i\langle\Phi_{\mathbf{i}}|\left(\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\hat{a}_{\mathbf{i},i}(t)\right)\left(\sum_{j\in\mathrm{unocc}}\Psi^{*}_{\mathbf{s},j}(\mathbf{r}')\hat{a}^{\dagger}_{\mathbf{i},j}(t')\right)|\Phi_{\mathbf{i}}\rangle, \\
&= -i\sum_{i,j\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi^{*}_{\mathbf{s},j}(\mathbf{r}')\mathrm{e}^{-itw_i}\mathrm{e}^{it'w_j}\langle\Phi_{\mathbf{s}}|\hat{a}_{\mathbf{s},i}\hat{a}^{\dagger}_{\mathbf{s},j}|\Phi_{\mathbf{s}}\rangle, \\
&= -i\sum_{i\in\mathrm{unocc}}\Psi_{\mathbf{s},i}(\mathbf{r})\Psi^{*}_{\mathbf{s},j}(\mathbf{r}')\mathrm{e}^{-i(t-t')w_i}.
\end{aligned} \tag{3.39}
$$

Using the lesser and greater Green functions, one can write Eq. (3.37) as:

$$
\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle = iG_0^<(\mathbf{r}t,\mathbf{r}_1t_1)iG_0^>(\mathbf{r}_1t,\mathbf{r}'t'). \tag{3.40}
$$

Thus, considering Eqs. (3.10) and (3.33), the first order term (F.O.T) of η is give by

$$
\text{F.O.T in } \eta = \left(\frac{i}{\hbar}\right)\int dt_1\int \mathbf{r}_1 iG_0^<(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG_0^>(\mathbf{r}_1t_1,\mathbf{r}'t'). \tag{3.41}
$$

The fifth and sixth terms in Eq. (3.10) give rise to the second order terms (S.O.T) in η. First, let us analyze the fifth term. In the fifth term, the $\tilde{T}$-, and T-products can be expressed by using the Wick theorems as follows:

$$\tilde{T}[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)] = iG^{c,*}_0(\mathbf{r}_1t_1,\mathbf{r}_1t_1) + N[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)]. \tag{3.42}$$

$$\begin{aligned}
&T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] \\
&\quad = N[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] \\
&\quad -iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'_1t'_1)N[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] + iG^c_0(\mathbf{r}t,\mathbf{r}'_1t'_1)N[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')] \\
&\quad -iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'t')N[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)] + iG^c_0(\mathbf{r}t,\mathbf{r}'t')N[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'_1t'_1)] \\
&\quad -iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'_1t'_1)iG^c_0(\mathbf{r}t,\mathbf{r}'t') + iG^c_0(\mathbf{r}t,\mathbf{r}'_1t'_1)iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'t').
\end{aligned} \tag{3.43}$$

Noting that

$$\begin{aligned}
\hat{\Psi}^{\dagger}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}} &= \hat{\Psi}^{\dagger}_{\mathrm{u}}\hat{\Psi}_{\mathrm{u}} + \hat{\Psi}^{\dagger}_{\mathrm{u}}\hat{\Psi}^{\dagger}_{\mathrm{o}} + \hat{\Psi}_{\mathrm{o}}\hat{\Psi}_{\mathrm{u}} + \hat{\Psi}_{\mathrm{o}}\hat{\Psi}^{\dagger}_{\mathrm{o}}, \\
\hat{\Psi}_{\mathbf{i}}\hat{\Psi}^{\dagger}_{\mathbf{i}} &= \hat{\Psi}_{\mathrm{u}}\hat{\Psi}^{\dagger}_{\mathrm{u}} + \hat{\Psi}_{\mathrm{u}}\hat{\Psi}_{\mathrm{o}} + \hat{\Psi}^{\dagger}_{\mathrm{o}}\hat{\Psi}^{\dagger}_{\mathrm{u}} + \hat{\Psi}^{\dagger}_{\mathrm{o}}\hat{\Psi}_{\mathrm{o}},
\end{aligned} \tag{3.44}$$

In the expectation value for the product of the $\tilde{T}$-, and T-products, the surving terms contributing to η are given by

$$\begin{aligned}
&\text{The terms contributing to } \eta \text{ in } \langle\Phi_{\mathbf{i}}|\tilde{T}[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)]T[\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathbf{i}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle \\
&= -iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'_1t'_1)\langle\Phi_{\mathbf{i}}|N[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)]N[\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle \\
&\quad +iG^c_0(\mathbf{r}t,\mathbf{r}'_1t'_1)\langle\Phi_{\mathbf{i}}|N[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)]N[\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}'_1t'_1)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'t')]|\Phi_{\mathbf{i}}\rangle \\
&\quad -iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'t')\langle\Phi_{\mathbf{i}}|N[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)]N[\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'_1t'_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)]|\Phi_{\mathbf{i}}\rangle \\
&\quad +iG^c_0(\mathbf{r}t,\mathbf{r}'t')\langle\Phi_{\mathbf{i}}|N[\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)]N[\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'_1t'_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}'_1t'_1)]|\Phi_{\mathbf{i}}\rangle, \\
&= +iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'_1t'_1)\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle \\
&\quad -iG^c_0(\mathbf{r}t,\mathbf{r}'_1t'_1)\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'t')|\Phi_{\mathbf{i}}\rangle \\
&\quad -iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'t')\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}t)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'_1t'_1)|\Phi_{\mathbf{i}}\rangle \\
&\quad +iG^c_0(\mathbf{r}t,\mathbf{r}'t')\langle\Phi_{\mathbf{i}}|\hat{\Psi}_{\mathrm{o}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{o}}(\mathbf{r}'_1t'_1)\hat{\Psi}_{\mathrm{u}}(\mathbf{r}_1t_1)\hat{\Psi}^{\dagger}_{\mathrm{u}}(\mathbf{r}'_1t'_1)|\Phi_{\mathbf{i}}\rangle, \\
&= +iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'_1t'_1)(-i)G^<_0(\mathbf{r}t,\mathbf{r}_1t_1)iG^>_0(\mathbf{r}_1t_1,\mathbf{r}'t') \\
&\quad -iG^c_0(\mathbf{r}t,\mathbf{r}'_1t'_1)(-i)G^<_0(\mathbf{r}'_1t'_1,\mathbf{r}_1t_1)iG^>_0(\mathbf{r}_1t_1,\mathbf{r}'t') \\
&\quad -iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'t')(-i)G^<_0(\mathbf{r}t,\mathbf{r}_1t_1)iG^>_0(\mathbf{r}_1t_1,\mathbf{r}'_1t'_1) \\
&\quad +iG^c_0(\mathbf{r}t,\mathbf{r}'t')(-i)G^<_0(\mathbf{r}'_1t'_1,\mathbf{r}_1t_1)iG^>_0(\mathbf{r}_1t_1,\mathbf{r}'_1t'_1),
\end{aligned} \tag{3.45}$$

where the final expression is derived by the same procedure as for Eq. (3.37). By putting Eq. (3.45) into Eq. (3.10), one can explicitly express the terms contributing to η in the fifth term of Eq. (3.10) as follows:

$$\begin{aligned}
&\text{The terms contributing to } \eta \text{ in the fifth term of Eq. (3.10)} \\
&= \left(\frac{i}{\hbar}\right)\left(\frac{-i}{\hbar}\right)\int dt'_1\int \mathbf{r}'_1\hat{v}_{1,1}(\mathbf{r}'_1t'_1)iG^c_0(\mathbf{r}'_1t'_1,\mathbf{r}'_1t'_1)\int dt_1\int \mathbf{r}_1(-i)G^<_0(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG^>_0(\mathbf{r}_1t_1,\mathbf{r}'t')
\end{aligned}$$

$$+\left(\frac{i}{\hbar}\right)\left(\frac{-i}{\hbar}\right)\int dt_1\int \mathbf{r}_1\int dt_1'\int \mathbf{r}_1'(-i)G_0^c(\mathbf{r}t,\mathbf{r}_1't_1')\hat{v}_{1,1}(\mathbf{r}_1't_1')(-i)G_0^<(\mathbf{r}_1't_1',\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG_0^>(\mathbf{r}_1t_1,\mathbf{r}'t')$$
$$+\left(\frac{i}{\hbar}\right)\left(\frac{-i}{\hbar}\right)\int dt_1\int \mathbf{r}_1\int dt_1'\int \mathbf{r}_1'(-i)G_0^<(\mathbf{r}t,\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG_0^>(\mathbf{r}_1t_1,\mathbf{r}_1't_1')\hat{v}_{1,1}(\mathbf{r}_1't_1')(-i)G_0^c(\mathbf{r}_1't_1',\mathbf{r}'t')$$
$$+\left(\frac{i}{\hbar}\right)\left(\frac{-i}{\hbar}\right)iG_0^c(\mathbf{r}t,\mathbf{r}'t')\int dt_1\int \mathbf{r}_1\int dt_1'\int \mathbf{r}_1'(-i)G_0^<(\mathbf{r}_1't_1',\mathbf{r}_1t_1)\hat{v}_{1,1}(\mathbf{r}_1t_1)iG_0^>(\mathbf{r}_1t_1,\mathbf{r}_1't_1')\hat{v}_{1,1}(\mathbf{r}_1't_1'). \tag{3.46}$$

$$\begin{aligned}
&\tilde{T}[\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_2t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2t_2)]\\
=\quad & N[\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_2t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2t_2)]\\
&+iG_0^{c,*}(\mathbf{r}_1t_1,\mathbf{r}_1t_1)N[\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_2t_2)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2t_2)]+iG_0^{c,*}(\mathbf{r}_1t_1,\mathbf{r}_2t_2)N[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_2t_2)]\\
&-iG_0^{c,*}(\mathbf{r}_2t_2,\mathbf{r}_1t_1)N[\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_2t_2)]+iG_0^{c,*}(\mathbf{r}_2t_2,\mathbf{r}_2t_2)N[\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}_1t_1)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}_1t_1)]\\
&+iG_0^{c,*}(\mathbf{r}_1t_1,\mathbf{r}_1t_1)iG_0^{c,*}(\mathbf{r}_2t_2,\mathbf{r}_2t_2)-iG_0^{c,*}(\mathbf{r}_2t_2,\mathbf{r}_1t_1)iG_0^{c,*}(\mathbf{r}_1t_1,\mathbf{r}_2t_2).
\end{aligned}\tag{3.47}$$

$$T[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')]=iG_0^c(\mathbf{r}t,\mathbf{r}'t')+N[\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')]. \tag{3.48}$$

3.4 Finite temperature formalism

In case of $t>t'$,

$$\begin{aligned}
[\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{h}}^\dagger(\mathbf{r}'t')] &= \sum_k w_k\langle\Psi_{\mathbf{h},k}|\hat{\Psi}_{\mathbf{h}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{h}}^\dagger(\mathbf{r}'t')|\Psi_{\mathbf{h},k}\rangle,\\
&= \sum_k w_k\langle\Psi_{\mathbf{i},k}(t)|\hat{U}_{\mathbf{i}}(t,0)\hat{U}_{\mathbf{i}}(0,t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,0)\hat{U}_{\mathbf{i}}(0,t')\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',0)\hat{U}_{\mathbf{i}}(0,t')|\Psi_{\mathbf{i},k}(t')\rangle,\\
&= \sum_k w_k\langle\Psi_{\mathbf{i},k}(t)|\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,t')\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')|\Psi_{\mathbf{i},k}(t')\rangle,\\
&= \sum_k w_k\langle\Phi_{\mathbf{i},k}|\hat{U}_{\mathbf{i}}(-\infty,t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,t')\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',-\infty)|\Phi_{\mathbf{i},k}\rangle,\\
&= \sum_k w_k\langle\Phi_{\mathbf{i},k}|\hat{U}_{\mathbf{i}}(-\infty,+\infty)\hat{U}_{\mathbf{i}}(+\infty,t)\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{U}_{\mathbf{i}}(t,t')\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')\hat{U}_{\mathbf{i}}(t',-\infty)|\Phi_{\mathbf{i},k}\rangle,\\
&= \sum_k w_k\langle\Phi_{\mathbf{i},k}|\hat{S}_{\mathbf{i}}^\dagger T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')]|\Phi_{\mathbf{i},k}\rangle,\\
&= \sum_{i,j}\langle\chi_j|\left[\sum_k w_k|\Phi_{\mathbf{i},k}\rangle\langle\Phi_{\mathbf{i},k}|\right]|\chi_i\rangle\langle\chi_i|\hat{S}_{\mathbf{i}}^\dagger T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')]|\chi_j\rangle,\\
&= \operatorname{tr}\left(\hat{\rho}_0\hat{S}_{\mathbf{i}}^\dagger T[\hat{S}_{\mathbf{i}}\hat{\Psi}_{\mathbf{i}}(\mathbf{r}t)\hat{\Psi}_{\mathbf{i}}^\dagger(\mathbf{r}'t')]\right),
\end{aligned}$$

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