Chapter 2

Green Functions and Observables

2.1 Green Functions in Quantum Mechanics

We will be interested in studying the properties of the ground state of a quantum mechanical many particle system. We will also be interested in understanding the physical properties of its low energy excitations. In order to accomplish these goals we will consider the following problem. Let $|G\rangle$ be the ground state of the system. We will imagine that at some time t in the past we have acted on the system with a local perturbation, which we will describe in terms of a local operator $\widehat{O}(\vec{r}, t)^\dagger$, and created a particular initial state $\widehat{O}(\vec{r}, t)^\dagger |G\rangle$. We may want to ask what is the quantum mechanical amplitude to find the system in state $\widehat{O}(\vec{r}\,')^\dagger |G\rangle$ at time $t + T$. In other words, we will prepare the system in some initial state which differs from the ground state by a few local excitations, a disturbance, and we will watch how this disturbance evolves in space and time. Any local measurement done on a quantum many-particle system can be described by a process essentially of this type.

Since we are going to be talking about time dependence it is useful to use the Heisenberg representation of the quantum evolution in which the operators evolve according to the law

$$\widehat{O}_H(t) = e^{i\widehat{H}t/\hbar}\widehat{O}\ e^{-i\widehat{H}t/\hbar} \tag{2.1}$$

Hence, the Heisenberg *operator* $\widehat{O}_H(t)$ obeys the *equation of motion*

$$\frac{\partial \widehat{O}}{\partial t} = \frac{i}{\hbar} \left[H, \widehat{O} \right] \tag{2.2}$$

To simplify the notation we will drop the H label of the Heisenberg operators from now on.

Consider now a measurement in which at some time t we prepare the system in the initial state $\widehat{O}^\dagger(\vec{r}, t)|G\rangle$ and that we wish to ask for the amplitude that at some later time t' the system is in the final state $\widehat{O}^\dagger(\vec{r}, t')|G\rangle$. The quantum mechanical amplitude of interest is:

$$\text{Amplitude } = \langle G|\widehat{O}(\vec{r}', t' \ )\ \widehat{O}^\dagger(\vec{r}, t)|G\rangle \tag{2.3}$$

We will be interested in considering two combinations of amplitudes of this type:

- A time-ordered amplitude
- A causal amplitude

As we shall see, the results of physical measurements is given in terms of a causal amplitude but we will be able to compute more directly the time-ordered amplitude instead. In general these two amplitudes are related by a well defined analytic continuation procedure.

We will define the *time-ordered* product of two Heisenberg operators $\widehat{A}(t_1)$ and $\widehat{B}(t_2)$ to be

$$T(\widehat{A}(t_1)\widehat{B}(t_2)) = \begin{cases} \widehat{A}(t_1)\widehat{B}(t_2), & \text{for } t_1 > t_2 \\ \pm\widehat{B}(t_2)\widehat{A}(t_1), & \text{for } t_2 > t_1 \end{cases} \tag{2.4}$$

where the plus (+) sign applies for *bosons* and the minus (−) sign applies for *fermions*. Note that operators with an *even* number of fermion operators are bosonic. Let us define the Heaviside (or step) function $\theta(t)$,

$$\theta(t) = \begin{cases} 1, & \text{for } t \geq 0 \\ 0, & \text{for } t < 0 \end{cases} \tag{2.5}$$

in terms of which the time-ordered product of two operators is

$$T\left(\widehat{A}(t_1)\widehat{B}(t_2)\right) = \theta(t_1 - t_2)\ \widehat{A}(t_1)\ \widehat{A}(t_2) \pm \theta(t_2 - t_1)\ \widehat{B}(t_2)\ \widehat{A}(t_1) \tag{2.6}$$

In this language, the time-ordered amplitude, or *Feynman propagator* for the operator $\widehat{O}$, is

$$G_F(\vec{r},t;\vec{r}\,',t') = -i\langle G|T(\widehat{O}(\vec{r},t)\widehat{O}^\dagger(\vec{r}\,',t'))|G\rangle \tag{2.7}$$

while the *causal propagator* is

$$G_c(\vec{r},t;\vec{r}\,',t') = -i\theta(t-t')\langle G|\left[\widehat{O}(\vec{r},t),\widehat{O}^\dagger(\vec{r}\,',t')\right]_\pm|G\rangle \tag{2.8}$$

where

$$[A,B]_\pm = AB \mp BA \tag{2.9}$$

where, $-$ applies for bosons and $+$ applies for fermions respectively. In contrast with the time-ordered amplitude, the causal amplitude vanishes unless $t' > t$.

2.2 The Feynman propagator at finite density

Let us consider first the simplest example: the amplitude for a particle of spin σ at $(\vec{r},t)$ to propagate freely to (r',t'). We will assume that the system has a finite density ρ. Let us denote by $\psi^\dagger_\sigma(\vec{r},t)$ and $\psi_\sigma(\vec{r},t)$ the creation and annihilation operators for a particle at $\vec{r}$ at time t. For the moment we will consider both the cases of fermions and bosons on the same footing.

The one-particle Feynman (time-ordered) propagator is

$$G_F(\vec{r},t,\sigma;\vec{r}\,',t',\sigma') = -i\ \langle G|T\psi_\sigma(\vec{r},t)\ \psi^\dagger_{\sigma'}(\vec{r}\,',\ t'))|G\rangle \tag{2.10}$$

and the causal function is

$$G_c(\vec{r},t,\sigma;\vec{r}\,',\ t',\sigma') = -i\ \theta(t-t')\langle G|\left[\psi_\sigma(\vec{r},t),\psi^+_{\sigma'},(r'\ ,t')\right]_{-\zeta}|G\rangle \tag{2.11}$$

where $\theta(t)$ is the Heaviside function, and $\zeta = \pm$, for bosons and fermions respectively, *i.e.* a commutator for bosons and an anticommutator for fermions.

Let us calculate the Feynman propagator G_F for a system of non-interacting particles at finite density ρ. From the definition of a time-ordered product we get

$$\begin{aligned} G_F(\vec{r},t,\sigma;\vec{r}\,',\ t',\sigma') =& -i\theta(t-t')\ \langle G|\psi_\sigma(\vec{r},t)\psi^\dagger_{\sigma'}(\vec{r}\,',t')|G\rangle \\ & - i\ \theta(t'-t)\ \zeta\ \langle G|\psi^\dagger_{\sigma'}(\vec{r}\,',t')\psi_\sigma(\vec{r},t)|G\rangle \end{aligned} \tag{2.12}$$

We now will use the evolution equation for a Heisenberg operator,

$$\psi_\sigma(\vec{r},t) = e^{iHt/\hbar}\psi_\sigma(\vec{r})e^{-iHt/\hbar} \tag{2.13}$$

and plug it back into the expression for the two amplitudes in the Feynman propagator. For the first amplitude in Eq.(2.12), which holds for $t > t'$, we get:

$$\langle G|\psi_\sigma(\vec{r},t)\psi^\dagger_{\sigma'}(\vec{r}\,',t')|G\rangle = \langle G|e^{iHt/\hbar}\psi_\sigma(\vec{r})e^{-iHt/\hbar}\; e^{iHt'/\hbar}\psi^\dagger_\sigma(\vec{r}\,')e^{-iHt'/\hbar}|G\rangle \tag{2.14}$$

Here $|G\rangle$ is the normalized ground state of the system and E_G is the ground state energy

$$H|G\rangle = E_G|G\rangle, \qquad \langle G|G\rangle = 1 \tag{2.15}$$

in terms of which the first amplitude in Eq.(2.12) becomes

$$\langle G|\psi_\sigma(\vec{r},t)\psi^\dagger_{\sigma'}(\vec{r}\,',t')|G\rangle = e^{iE_G(t-t')/\hbar}\langle G|\psi_\sigma(\vec{r})e^{-iH(t-t')/\hbar}\psi^\dagger_{\sigma'}(\vec{r}\,')|G\rangle \tag{2.16}$$

The operator $\psi_\sigma(\vec{r})$ has the mode expansion

$$\psi_\sigma(\vec{r}) = \sum_\alpha c_{\alpha,\sigma}\; \varphi_n(\vec{r}) \tag{2.17}$$

where $\{\varphi_n(\vec{r})\}$ are the wave functions of a complete set of one-particle states $\{|\alpha\rangle\}$, labeled by an index α, and $c_{\alpha,\sigma^\dagger}$ and $c_{\alpha,\sigma}$ are the associated creation and annihilation operators in Fock space, which obey

$$[c_{\alpha,\sigma}, c_{\alpha',\sigma'}]_{-\zeta} = \left[c^\dagger_{\alpha,\sigma}, c^\dagger_{\alpha',\sigma'}\right]_{-\zeta} = 0, \qquad \left[c_{\alpha,\sigma}, c^\dagger_{\alpha',\sigma'}\right]_{-\zeta} = \delta_{\alpha\alpha'}\delta_{\sigma\sigma'} \tag{2.18}$$

To make further progress we will need to specify the ground state. We will restrict ourselves for the moment to the case of *fermions*. We will discuss the case of bosons at finite density later on. The ground state $|G\rangle$ of a system of fermions at finite density is the *filled Fermi sea*

$$|G\rangle = \prod_{\alpha\leq G}\prod_{\sigma=\uparrow,\downarrow} c^\dagger_{\alpha\sigma}\;|0\rangle \tag{2.19}$$

We will now perform a particle-hole transformation for $\alpha \leq G$, and define new creation and annihilation operators such that the annihilation operators destroy the filled Fermi sea $|G\rangle$, *i.e.* we will define new operators which are *normal ordered* with respect to the *filled Fermi sea*:

$$b_{\alpha\sigma} = a^\dagger_{\alpha\sigma}, \quad b^\dagger_{\alpha\sigma} = a_{\alpha\sigma}, \qquad \text{for } \alpha \leq G \tag{2.20}$$

which satisfy

$$\begin{aligned} a_{\alpha\sigma}|G\rangle &= 0, \text{ for } \alpha > G \\ b_{\alpha\sigma}|G\rangle &= 0, \text{ for } \alpha \leq G \end{aligned} \tag{2.21}$$

Thus, we write mode expansion now as

$$\begin{aligned} \psi_\sigma(\vec{r}) &= \sum_\alpha \varphi_\alpha(\vec{r})\, c_{\alpha\sigma} = \sum_{\alpha>G} \varphi_\alpha(\vec{r})\, a_{\alpha\sigma} + \sum_{\alpha\leq G} \varphi_\alpha(\vec{r})\, b^\dagger_{\alpha\sigma} \\ \psi^\dagger_\sigma(\vec{r}) &= \sum_\alpha \varphi^*_\alpha(\vec{r})\, c^\dagger_{\alpha\sigma} = \sum_{\alpha>G} \varphi^*_\alpha(\vec{r})\, a^\dagger_{\alpha\sigma} + \sum_{\alpha\leq G} \varphi^*_\alpha(\vec{r})\, b_{\alpha\sigma} \end{aligned} \tag{2.22}$$

Let us consider the first term in the Feynman propagator, Eq.(2.12). Upon inserting an complete set $\{|n\rangle\}$ of eigenstates of the Hamiltonian H (not just the one-particle states!),

$$H|n\rangle = E_n|n\rangle \tag{2.23}$$

we find that the first amplitude in Eq.(2.12) can be expanded as

$$\langle G|\psi_\sigma(\vec{r})e^{-iH(t-t')/\hbar}\psi^\dagger_{\sigma'}(\vec{r}\,')|G\rangle = \sum_n \langle G|\psi_\sigma(\vec{r})|n\rangle e^{-i(E_n-E_G)(t-t')/\hbar}\langle n|\psi^\dagger_{\sigma'}(\vec{r}\,')|G\rangle \tag{2.24}$$

The matrix element $\langle G|\psi_\sigma(\vec{r})|n\rangle$ has the explicit form

$$\begin{aligned} \langle G|\psi_\sigma(\vec{r})|n\rangle &= \sum_{\alpha>G} \langle G|a_{\alpha\sigma}|n\rangle\varphi_\alpha(\vec{r}) + \sum_{\alpha\leq G} \langle G|b^\dagger_{\alpha\sigma}|n\rangle\varphi_\alpha(\vec{r}) \\ &= \sum_{\alpha>G} \langle G|a_{\alpha\sigma}|n\rangle\varphi_\alpha(\vec{r}) \end{aligned} \tag{2.25}$$

since $b_{\alpha\sigma}|G\rangle = 0$. Similarly we find

$$\begin{aligned} \langle n|\psi^\dagger_{\sigma'}(\vec{r}\,')|G\rangle &= \sum_{\alpha'>G} \langle n|a^\dagger_{\alpha'\sigma'}|G\rangle\, \varphi^*_{\alpha'}(\vec{r}\,') + \sum_{\alpha'\leq G} \langle n|b_{\alpha'\sigma'}|G\rangle\varphi^*_{\alpha'}(\vec{r}\,') \\ &= \sum_{\alpha'>G} \langle n|a^\dagger_{\alpha'\sigma'}|G\rangle\, \varphi^*_{\alpha'}(\vec{r}\,') \end{aligned} \tag{2.26}$$

Thus, we see that only the states with $\alpha > G$, which we shall call *particle* states, contribute to Eq.(2.25) and Eq.(2.26).

It will be convenient to simplify the notation by introducing the symbol

$$\theta(\alpha - G) = \begin{cases} 1 & \alpha > G \\ 0 & \alpha \leq G \end{cases} \tag{2.27}$$

which is analogous to the Heaviside function $\theta(t)$ introduced above. With this notation the mode expansion becomes

$$\psi_\sigma(\vec{r}) = \sum_\alpha \left[\theta(\alpha - G) a_{\alpha\sigma}\ \varphi_\alpha(\vec{r}) + \theta(G - \alpha) b^\dagger_{\alpha\sigma}\varphi_\alpha(\vec{r})\right] \tag{2.28}$$

and the first amplitude in the Feynman propagator, Eq.(2.12), becomes

$$\langle G|\psi_\sigma(\vec{r})e^{-iH(t-t')}\ \psi^\dagger_{\sigma'}(\vec{r}\,')|G\rangle = \sum_n \langle G|\psi_\sigma(\vec{r})|n\rangle\ \langle n|\psi^\dagger_{\sigma'}(\vec{r}\,')|G\rangle e^{-i(E_n-E_G)(t-t')/\hbar}$$

$$\begin{aligned} = \sum_{\alpha\alpha'}\sum_n e^{-i(E_n-E_G)(t-t')/\hbar}\varphi^*_\alpha(\vec{r})\varphi_{\alpha'}(\vec{r}\,') \times \Big\{ & \theta(\alpha - G)\theta(\alpha' - G)\langle G|a_{\alpha\sigma}|n\rangle\langle n|a^\dagger_{\alpha'\sigma'}|G\rangle \\ & + \theta(G-\alpha)\theta(G-\alpha')\langle G|b^\dagger_{\alpha\sigma}|n\rangle\ \langle n|b_{\alpha'\sigma'}|G\rangle \\ & + \theta(\alpha - G)\theta(G-\alpha')\langle G|a_{\alpha\sigma}|n\rangle\langle n|b_{\alpha'\sigma'}|G\rangle \\ & + \theta(G-\alpha)\theta(\alpha' - G)\langle G|b^\dagger_{\alpha\sigma}|n\rangle\langle n|a^\dagger_{\alpha'\sigma'}|G\rangle \Big\} \end{aligned} \tag{2.29}$$

The matrix elements in Eq.(2.29) vanish unless the intermediate states $|n\rangle$ satisfy

$$\begin{aligned} |n\rangle &= a^\dagger_{\alpha\sigma}|G\rangle = a^\dagger_{\alpha'\sigma'}|G\rangle \\ |n\rangle &= b_{\alpha\sigma}|G\rangle \ = \ b_{\alpha'\sigma'}|G\rangle = 0 \end{aligned} \tag{2.30}$$

both of which require that $\alpha = \alpha'$ and $\sigma = \sigma'$, and $\alpha > G$. In other terms, the only intermediate states $|n\rangle$ which contribute to the expansion are states which differ from the ground state $|G\rangle$ by a single *particle* state $|\alpha, \sigma\rangle \equiv |\alpha, \sigma; G\rangle$, of either spin component. We conclude that the first amplitude in the Feynman propagator, Eq.(2.12), is

$$\langle G|\psi_\sigma(\vec{r})e^{-iH(t-t')}\ \psi^\dagger_{\sigma'}(\vec{r}\,')|G\rangle = \delta_{\sigma\sigma'} \sum_\alpha\ e^{-i(E_\alpha-E_G)(t-t')/\hbar}\ \varphi^*_\alpha(r)\ \varphi_\alpha(r')\theta(\alpha - G) \tag{2.31}$$

where $E_\alpha - E_G$ is the excitation energy of the particle-like state $|\alpha,\sigma\rangle = a^\dagger_{\alpha\sigma}|0\rangle$, with $\alpha > G$.

Likewise, the second amplitude in the Feynman propagator Eq.(2.12), which applies for $t < t'$, involves the same operators but acting now in reverse order. The only change is that now the contributing intermediate states are

$$\begin{aligned} |n\rangle &= b^\dagger_{\alpha\sigma}|G\rangle = b^\dagger_{\alpha'\sigma'}|G\rangle \\ |n\rangle &= a_{\alpha\sigma}|G\rangle = a_{\alpha'\sigma'}|G\rangle = 0 \end{aligned} \tag{2.32}$$

which once again require that $\alpha = \alpha'$ and $\sigma = \sigma'$, but now $\alpha \leq G$. Thus, in this case only the *single hole states* (of either spin component) contribute to the amplitude. Therefore, we can write the second amplitude in the Feynman propagator, Eq.(2.12), as

$$\langle G|\psi^\dagger_\sigma(\vec{r}\,')e^{-iH(t-t')/\hbar}\;\psi_{\sigma'}(\vec{r})|G\rangle = \delta_{\sigma\sigma'}\sum_\alpha e^{-i(E_\alpha-E_G)(t-t')/\hbar}\varphi^*_\alpha(\vec{r})\varphi_\alpha(\vec{r}\,')\theta(G-\alpha) \tag{2.33}$$

where $E_\alpha - E_G$ is the excitation energy of the hole-like state $|\alpha,\sigma\rangle = b^\dagger_{\alpha,\sigma}|0\rangle$, with $\alpha \leq G$.

In conclusion, we find that the Feynman propagator, Eq.(2.12), has the explicit form

$$\begin{aligned} G_F(\vec{r},t,\sigma;\vec{r}\,',t',\sigma') &= -i\delta_{\sigma\sigma'}\sum_\alpha \varphi^*_\alpha(\vec{r})\varphi_\alpha(r') \\ &\times\left[\theta(\alpha-G)e^{-i(E_\alpha-E_G)(t-t')/\hbar}\theta(t-t') - \theta(G-\alpha)e^{-i(E_\alpha-E_G)(t-t')/\hbar}\theta(t'-t)\right] \end{aligned} \tag{2.34}$$

We will now perform a Fourier transform in time and define

$$G_F(\vec{r}\,\sigma,\vec{r}\,'\sigma';\Omega) = \int_{-\infty}^{+\infty} dt \;\; G_F(\vec{r},t,\sigma;\vec{r}\,',t',\sigma')e^{i\Omega(t-t')} \tag{2.35}$$

The Heaviside function $\theta(t)$ has the following representation as a contour integral in the complex frequency plane

$$\theta(t) = \lim_{\delta\to 0^+}\oint_\Gamma \frac{d\omega}{2\pi i}\,\frac{e^{i\omega t}}{\omega - i\delta} \tag{2.36}$$

where $\Gamma = \Gamma^+$ is the counter-clockwise oriented contour obtained by closing the contour on the upper half plane as shown in Fig.2.2, while $\Gamma = \Gamma^-$ is the negatively oriented contour obtained by closing the contour on the lower half plane, also shown in Fig.2.2. The integral on the real axis can be extended to the large arc Γ^+ of radius $R \to \infty$ provided that $t > 0$, and to the large arc Γ^- for $t < 0$, as in these cases the integrals over the arcs vanishes. That this is a representation of the function $\theta(t)$ can be seen by noting that the integrand of Eq.(2.36) has a pole only in the upper half plane, located at $\omega = i\delta$ (where $\delta > 0$), which implies that if we choose the contour Γ^+ we pick up the pole but if we choose the contour Γ^- we do not. Using the Theorem of the Residues we get

$$\theta(t) = \lim_{\delta \to 0^+} \begin{cases} \text{Res}\left[\dfrac{e^{i\omega t}}{\omega - i\delta}\ , i\delta\right] \ = \ e^{-\omega\delta} \longrightarrow 1 & \text{(closing upward)} \\ \\ 0 & \text{(closing downward)} \end{cases} \tag{2.37}$$

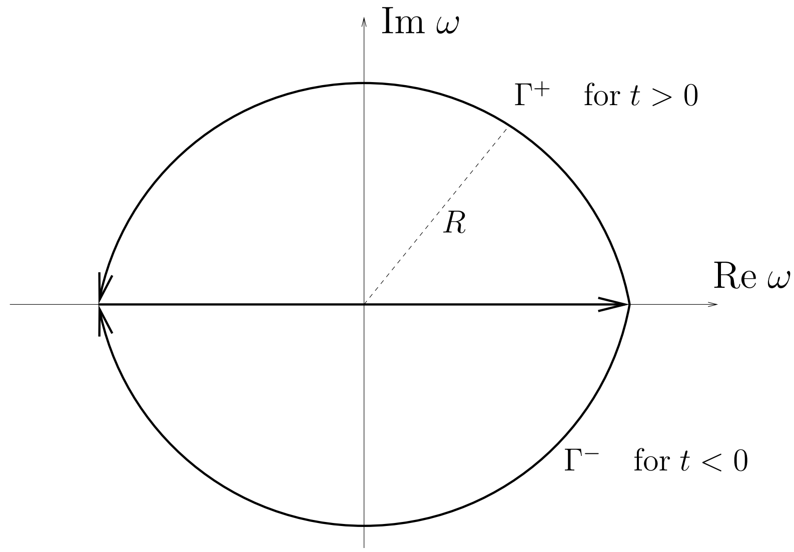

Figure 2.1: Contours on the complex frequency plane used in Eq.(2.36)

We will now use this integral representation to write

$$\begin{aligned}
\int_{-\infty}^{\infty} dt\, e^{i\Omega t}\, \theta(t)\, e^{-i(E_\alpha - E_G)t/\hbar} &= \int_{-\infty}^{\infty} dt\, e^{i\Omega t} \oint_\Gamma \frac{d\omega}{2\pi i}\, e^{-i(E_\alpha - E_G)t/\hbar}\, \frac{e^{i\omega t}}{\omega - i\delta} \\
&= \oint \frac{d\omega}{2\pi i} \frac{1}{\omega - i\delta} \int_{-\infty}^{\infty} dt\, e^{i(\omega + \Omega - (E_\alpha - E_G)/\hbar)t} \\
&\equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{2\pi\delta\left(\omega + \Omega - (E_\alpha - E_G)/\hbar\right)}{\omega - i\delta} \\
&= \frac{i}{\Omega - \left(\frac{E_\alpha - E_G}{\hbar}\right) + i\delta}
\end{aligned} \tag{2.38}$$

On the other hand, a similar line of argument shows that

$$\int_{-\infty}^{\infty} dt\, e^{i\Omega t}\, \theta(-t)\, e^{-i(E_\alpha - E_G)t/\hbar} = \frac{i}{\Omega - \left(\frac{E_\alpha - E_G}{\hbar}\right) - i\delta} \tag{2.39}$$

Hence,

$$\begin{aligned}
&G_F(\vec{r}\sigma, \vec{r}\,'\sigma'; \omega) = \\
&= \delta_{\sigma\sigma'} \sum_\alpha \varphi_\alpha^*(\vec{r})\varphi_\alpha(\vec{r}\,') \left[\underbrace{\frac{\theta(\alpha - G)}{\omega - \left(\frac{E_\alpha - E_G}{\hbar}\right) + i\delta}}_{\substack{\text{particle} \\ \text{contribution}}} + \underbrace{\frac{\theta(G - \alpha)}{\omega - \left(\frac{E_\alpha - E_G}{\hbar}\right) - i\delta}}_{\substack{\text{hole} \\ \text{contribution}}} \right]
\end{aligned} \tag{2.40}$$

Thus, particles contribute with poles in the lower half plane with positive excitation energy, and holes contribute with poles in the upper half plane also with positive excitation energy.

The representation of the Feynman propagator of Eq.(2.40), known as the *Lehmann representation*, is correct for *any* free fermion system. (We will see later on that it also holds for interacting systems provided the physical eigenstates have finite overlap with the states created by free fermion operators.)

For the case of free fermions in free space the one-particle eigenstates are just momentum eigenstates, $|\alpha\rangle \equiv |\vec{p}\rangle$, the excitation energies are

$$\varepsilon(\vec{p}) = E(\vec{p}) - E_G \equiv \frac{\vec{p}^{\,2}}{2m} \tag{2.41}$$

and the wave functions $\varphi_{\vec{p}}(\vec{r})$ are just plane waves,

$$\varphi_{\vec{p}}(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar} \tag{2.42}$$

In this case the label G corresponds to the Fermi momentum p_F

$$G_F(\vec{r}\sigma, \vec{r}\,'\sigma'; \omega) = \hbar\delta_{\sigma\sigma'} \int \frac{d^3p}{(2\pi\hbar)^3} \; e^{i\vec{p}\cdot(\vec{r}-\vec{r}\,')/\hbar} \left[\frac{\theta(|\,\vec{p}\,| - p_F)}{\hbar\omega - \frac{\vec{p}\,^2}{2m} + i\delta} \;+\; \frac{\theta(p_F - |\,\vec{p}\,|)}{\hbar\omega - \frac{\vec{p}\,^2}{2m} - i\delta} \right] \tag{2.43}$$

where the Fermi momentum p_F and the Fermi energy E_F are determined in terms of the density $\rho = N/V$,

$$p_F = \hbar \left(6\pi^2\rho\right)^{1/3}, \qquad E_F = \frac{\hbar^2}{2m}\left(6\pi^2\rho\right)^{2/3} \tag{2.44}$$

We can use these results to write an expression for the Fourier transform $\widetilde{G}_F(\vec{p}, \omega)$

$$\widetilde{G}_F(\vec{p}, \omega) = \frac{\hbar\Theta(|\vec{p}| - p_F)}{\hbar\omega - E(\vec{p}) + i\epsilon} + \frac{\hbar\Theta(p_F - |\vec{p}|)}{\hbar\omega - E(\vec{p}) - i\epsilon} \tag{2.45}$$

where $E(\vec{p}) = \epsilon(\vec{p}) - \mu$. An equivalent (and more compact) expression is

$$\widetilde{G}_F(\vec{p}, \omega) = \frac{\hbar}{\hbar\omega - E(\vec{p}) + i\epsilon\,\mathrm{sign}(|\vec{p}| - p_F)} \tag{2.46}$$

Notice that

$$\begin{aligned} \mathrm{Im}\widetilde{G}_F(\vec{p}, \omega) &= -\hbar\pi\Theta(|\vec{p}| - p_F)\delta(\hbar\omega - \epsilon(\vec{p}) + \mu) + \hbar\pi\Theta(p_F - |\vec{p}|)\delta(\hbar\omega - \epsilon(\vec{p}) + \mu) \\ &= -\hbar\pi\delta(\hbar\omega - \epsilon(\vec{p}) + \mu)\left[\Theta\left(|\vec{p}| - p_F\right) - \Theta(p_F - |\vec{p}|)\right] \end{aligned} \tag{2.47}$$

The last identity shows that

$$\mathrm{sign}\ \mathrm{Im}\widetilde{\mathrm{G}}_{\mathrm{F}}(\tilde{\mathrm{p}}, \omega) = -\mathrm{sign}\ \omega \tag{2.48}$$

Hence, we may also write $\widetilde{G}_F(p, \omega)$ as

$$\widetilde{G}_F(\vec{p}, \omega) = \frac{\hbar}{\hbar\omega - E(\vec{p}) + i\epsilon\ \mathrm{sign}\ \omega} \tag{2.49}$$

With this expression, we see that $\widetilde{G}_F(\vec{p}, \omega)$ has poles at $\omega = E(\vec{p})$ and that all the poles with $\omega > 0$ are infinitesimally shifted downwards to the lower half-plane, while the others are raised upwards to the upper half-plane by the same amount. Since $E(p) = \epsilon(p) - \mu$, all poles with $\epsilon(p) > \mu$ are shifted downwards, while all poles with $\epsilon(p) < \mu$ are shifted upwards.

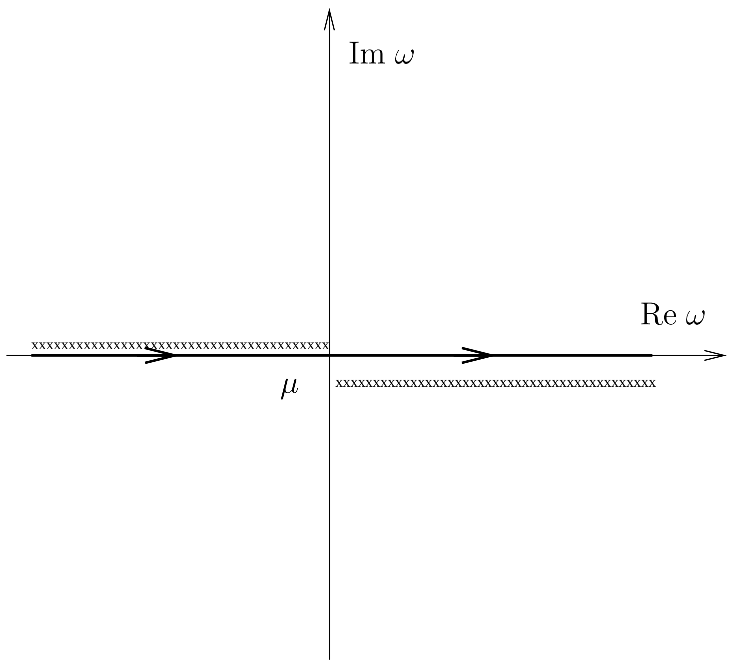

Figure 2.2: Analytic structure of the Green function at finite chemical potential μ in the complex frequency plane.

2.2.1 Propagators and observables

In a non-interacting system, the propagator is known explicitly and it can be used to compute expectation values of physical observables. However the following relations hold for a general system regardless of the interactions. Thus, the ground state expectation value of the density operator $\langle\rho(\vec{r})\rangle$ is

$$\langle\rho(\vec{r})\rangle = -i \lim_{\vec{r}\,'\to\vec{r}} \lim_{t'\to t^-} \sum_{\sigma} G_F(\vec{r}, t, \sigma; \vec{r}\,'t'\sigma') \tag{2.50}$$

while the spin density (or local magnetization) is

$$\langle\vec{S}(\vec{r})\rangle = -i \lim_{\vec{r}\,'\to\vec{r}} \lim_{t'\to t^-} \sum_{\sigma,\sigma'} \vec{S}_{\sigma'\sigma} G_F(\vec{r}, t, \sigma; \vec{r}\,'t'\sigma') \tag{2.51}$$

where

$$\vec{S} = \frac{\hbar}{2}\vec{\tau} \tag{2.52}$$

and τ^a (with $a = 1, 2, 3$) are the three Pauli matrices.

The second quantized local current density operator $J_i(\vec{r})$ is

$$J_i(\vec{r}) = \frac{\hbar}{2mi} \sum_\sigma \left[\psi^\dagger_\sigma(\vec{r}) \nabla_i \psi_\sigma(\vec{r}) - \nabla_i \psi^\dagger_\sigma(\vec{r}) \psi_\sigma(\vec{r})\right] \tag{2.53}$$

$$\equiv \frac{\hbar}{2mi} \sum_\sigma \psi^\dagger_\sigma(\vec{r}) \overleftrightarrow{\nabla}_i \psi_\sigma(\vec{r}) \tag{2.54}$$

$$\equiv \lim_{\vec{r}\,' \to \vec{r}} \frac{\hbar}{2mi} \sum_\sigma \left[\psi^\dagger_\sigma(\vec{r}\,')\ \nabla^i_{\vec{r}} \psi_\sigma(\vec{r}) - \nabla^i_{\vec{r}\,'} \psi^\dagger_\sigma(\vec{r}\,') \psi_\sigma(\vec{r})\right] \tag{2.55}$$

and its ground state expectation value is

$$\langle G|J_i(\vec{r})|G\rangle = \lim_{\vec{r}\,' \to \vec{r}} \frac{\hbar}{2mi} \sum_\sigma \left[\langle G|\psi^\dagger_\sigma(\vec{r}\,')\ \nabla^i_{\vec{r}} \psi_\sigma(\vec{r})|G\rangle - \langle G|\nabla^i_{\vec{r}\,'} \psi^\dagger_\sigma(\vec{r}\,') \psi_\sigma(\vec{r})|G\rangle\right] \tag{2.56}$$

$$= -\frac{\hbar}{2m} \lim_{\vec{r}\,' \to \vec{r}} \lim_{t' \to t^-} \left[\nabla^i_{\vec{r}} G_F(\vec{r}, t, \sigma; \vec{r}\,', t', \sigma') - \nabla^i_{\vec{r}\,'} G_F(\vec{r}, t, \sigma; \vec{r}\,', t', \sigma')\right] \tag{2.57}$$

2.3 Interacting Systems

In the Schrödinger representation, or *Schrödinger Picture*, the states $|\Psi_S(t)\rangle$ are time-dependent functions whose evolution is governed by the Schrödinger's equation

$$i\hbar\, \partial_t |\Psi_S(t)\rangle = H|\Psi_S(t)\rangle \tag{2.58}$$

which can be solved (formally) by

$$|\Psi_S(t)\rangle = e^{-iH(t-t_0)/\hbar}\, |\Psi_S(t_0)\rangle \tag{2.59}$$

where $|\Psi_S(t_0)\rangle$ is the initial state. The problem with this statement is that the (unitary) evolution operator $U(t, t_0)$

$$U(t, t_0) = e^{-iH(t-t_0)/\hbar} \tag{2.60}$$

is very complicated and we don't really know how to construct it in almost all cases.

Alternatively we can use the *Heisenberg Picture* in which the states are fixed and the operators obey equations of motion with

$$\partial_t A_H(t) = \frac{i}{\hbar}\,[H, A_H(t)]\,, \qquad A_H(t) \;=\; e^{iH(t-t_0)/\hbar} A_S(t_0) e^{-iH(t-t_0)} \quad (2.61)$$

where $A_S(t_0)$ is a fixed (initial) operator. Again we need to solve these generally non-linear equations which are also very complex.

However, let us suppose that $H = H_0 + H_1$ and that we know how to solve for H_0. Still we want to include the effects of H_1. This is the standard problem of perturbation theory. This situation motivates the introduction of the *Interaction Picture*, in which the *states* are $|\Psi_I(t)\rangle$

$$|\Psi_I(t)\rangle = e^{iH_0 t/\hbar}\,|\Psi_S(t)\rangle \quad (2.62)$$

and satisfy the evolution equation

$$i\hbar|\Psi_I(t)\rangle = H_1(t)|\psi_I(t)\rangle \quad (2.63)$$

where $H_1(t)$, is

$$H_1(t) = e^{iH_0 t/\hbar} H_1 e^{-H_0 t/\hbar} \quad (2.64)$$

and thus obeys the equation of motion

$$\partial_t H_1(t) = \frac{i}{\hbar}\,[H_0, H_1(t)] \quad (2.65)$$

Thus, in the interaction representation the time evolution of the states is governed by the perturbation $H_1(t)$ while all possible operators $A(t)$, the perturbation H_1 among them, obey the Heisenberg equations of motion associated with H_0

$$A_I(t) = e^{iH_0 t/\hbar} A e^{-iH_0 t/\hbar}, \qquad i\hbar\partial_t A_I(t) = [H_0, A_I(t)] \quad (2.66)$$

Hence the interaction representation is the Heisenberg representation of H_0.

In particular, the time evolution operator $U(t, t_0)$, in the Interaction Representation satisfies

$$|\Psi_I(t)\rangle = U_I(t, t_0)|\Psi_I(t_0)\rangle \quad (2.67)$$

and obeys the evolution equation

$$i\hbar\partial_t U_I(t, t_0) = H_I(t) U_I(t, t_0) \quad (2.68)$$

The evolution operators have the properties

$$\begin{aligned} U(t_1,t_2)U(t_2,t_3) &= U(t_1,t_3) \quad \text{(form a group)} \\ U(t_1,t_2)^{-1} &= U(t_1,t_2)^\dagger \quad \text{(unitarity)} \\ U(t_1,t_2)^{-1} &= U(t_2,t_1) \quad \text{(inverse)} \end{aligned} \tag{2.69}$$

Furthermore, the Heisenberg and Interaction Representations are related as follows

$$|\Psi_H\rangle = e^{iHt/\hbar}e^{-iH_0t/\hbar}|\Psi_I(t)\rangle = U(t,t_0)^\dagger|\Psi_I(t)\rangle \tag{2.70}$$

$$A_H(t) = U(t,t_0)^\dagger A_I(t)U(t,t_0) \tag{2.71}$$

The equation of motion of the evolution operator $U(_I(t,t_0)$, Eq.(2.68) can also be written as an integral equation (we will drop the label "I" from now on):

$$U(t,t_0) = U(t_0,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt' \; H_1(t')U(t',t_0) \tag{2.72}$$

with $U(t_0,t_0)=1$

$$U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt' H_1(t')U(t',t_0) \tag{2.73}$$

We will solve this equation by iteration. For this approach to converge we need to require that $H_1(t)$ be switched on and off very slowly (*adiabatically*). This amounts to making the replacement

$$H_1 \to e^{-\epsilon|t|}\; H_1(t) \tag{2.74}$$

and taking the limit $\epsilon \to 0^+$ afterwords. Hence, we can write a formal iterative solution of the form

$$\Rightarrow U(t,t_0) = 1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} dt' \; H_1(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \; H_1(t')H_1(t'')+\dots \tag{2.75}$$

However it is easy to verify that

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_1(t')H_1(t'') = \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' T\left(H_1(t')H_1(t'')\right) \tag{2.76}$$

where $T\left(H_1(t')H_1(t'')\right)$ is the *time-ordered-product* of the two operators.

Moreover, all terms involving nested time integrations can be written in a more compact form in terms of time-ordered products:

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n \; H_1(t_1)H_1(t_2)\ldots H_1(t_n) = \\ = \frac{1}{n!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_n \; T\left(H_1(t_1)H_1(t_2)\ldots H_1(t_n)\right) \tag{2.77}$$

Thus, the evolution operator can be written as an expansion in terms of time-ordered products:

$$U(t_1 t_0) \;=\; \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{t_0}^{t} dt_1 \ldots \int_{t_0}^{t} dt_n \;\; T\left(H_1(t_1)\ldots H_1(t_n)\right) \tag{2.78}$$

Hence, the evolution operator $U(t, t_0)$ can be represented formally as a time-ordered exponential:

$$U(t, t_0) \equiv T e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt' H_1(t')} \tag{2.79}$$

We should be careful to note that Eq.(2.79) is simply a short-hand notation used to write the formal expression for the evolution operator given in Eq.(2.78) in a more compact form. (In other words we have not shown that the series exponentiates!)

The evolution operator $U(t, t_0)$ will play a central role in much of what we will do. In particular, it can be used to determine the exact (Heisenberg) eigenstates which are given by

$$|\psi_H\rangle \;=\; |\psi_I(0)\rangle \;=\; \hat{U}(0, t_0)|\Psi_I(t_0)\rangle \tag{2.80}$$

Once again, in order to use expressions of this type we must we imagine switching the interaction adiabatically slowly, *i.e.* $H_1 \to e^{-\epsilon|t|}H_1(t)$)

Let us consider now two states, $|\Phi_0\rangle$ which is an exact non-degenerate eigenstate of H_0, and $|\Psi_0\rangle$ which is an exact (also non-degenerate) eigenstate of $H = H_0 + H_1$. We will assume once again that the interaction H_1 was absent in the remote past and that it was turned on adiabatically slowly, and that during this process there is no level crossing involved. Hence, the state remains non-degenerate during the process. Then the following identity, known as the Gell-Mann Low Theorem, holds:

$$\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = \lim_{\epsilon\to 0^+} \frac{U_\epsilon(0,-\infty)|\Phi_0\rangle}{\langle\Phi_0|U_\epsilon(0,-\infty|\Phi_0\rangle} \tag{2.81}$$

where we have $U_\epsilon(t,t')$ is the evolution operator for an adiabatically switched on perturbation $H_1(t)$.

The Gell-Mann Low Theorem, Eq.(2.81), simply states that the eigenstate $|\Phi_0\rangle$ of H_0 evolves smoothly into the exact eigenstate $|\Psi_0\rangle$ of H. In particular it means that the exact expectation value of a Heisenberg operator $A_H(t)$ in the state $|\Psi_0\rangle$, an exact eigenstate of H, in terms of expectation values in the interaction representation is given by

$$\frac{\langle\Psi_0|A_H(t)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \frac{\langle\Phi_0|TA_I(t)\mathcal{S}|\Phi_0\rangle}{\langle\Phi_0|\mathcal{S}|\Phi_0\rangle} \tag{2.82}$$

where the left hand side is an expectation value in the Heisenberg representation while the right hand side involves only expectation values in the interaction representation. In Eq.(2.82) where we introduced the *S-matrix*, $\mathcal{S} = U_\epsilon(\infty,-\infty)$, whose expectation value in the state $|\Phi_0\rangle$ is

$$\langle\Phi_0|\mathcal{S}|\Phi_0\rangle = \langle\Phi_0|Te^{-\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt' H_1(t')}|\Phi_0\rangle \tag{2.83}$$

In particular, these results tell us how to write an expression for the Feynman propagator, which is an expectation value in the *Heisenberg Representation*, in terms of expectation values in the *Interaction Representation*. Thus, (ignoring spin indices) we find that the Feynman propagator has the representation

$$G_F(\vec{x},t;\vec{x}',t') = -i\frac{\langle\Phi_0|T\ \psi_I(\vec{x}t)\psi_I^\dagger(\vec{x}\,'t')\ e^{-\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt'' H_1(t'')}|\Phi_0\rangle}{\langle\Phi_0|T\ e^{-\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt'' H_1(t'')}|\Phi_0\rangle} \tag{2.84}$$

where $|\Phi_0\rangle$ is the ground state of H_0. However, since the evolution operator is a time-ordered exponential, which is defined by a series in powers of the perturbation H_1, Eq.(2.82) and Eq.(2.83) are nothing but a perturbative evaluation of the propagator.

2.4 Perturbation Theory and Feynman Diagrams

Thus we have reduced the calculation of G_F, the Feynman propagator (or Green function) for the electron, to a power series expansion in which each term is an expectation value calculated in the Interaction Representation. This is just perturbation theory. The factor in the denominator, ${}_0\langle G|\mathcal{S}|G\rangle_0$, is simply the consequence of the renormalization of norm of the ground state $|G\rangle_0$ due to the effects of the perturbation H_1.

We have seen that fermion field operator $\psi(\vec{x},t)$ has a mode expansion of the form

$$\psi(x) = \sum_\alpha \left[\theta(\alpha - G)\varphi_\alpha(x)a_\alpha + \theta(G-\alpha)\varphi_\alpha(x)b_\alpha^\dagger\right] \tag{2.85}$$

where $a_\alpha|G\rangle_0 = 0$ and $b_\alpha|G\rangle_0 = 0$, and $\{\varphi_\alpha\}$ are a complete set of single-particle wave functions.

Then, we can split the operator $\psi(\vec{x},t)$ into two pieces, $\psi^{(\pm)}(\vec{x},t)$,

$$\psi(x) = \psi^{(+)}(x) + \psi^{(-)} \tag{2.86}$$

where both $\psi^{(+)}$ and $\psi^{(-)\dagger}$ annihilate the ground state $|G\rangle_0$:

$$\psi^{(+)}|G\rangle_0 = 0, \qquad \text{and} \qquad \psi^{(-)\dagger}|G\rangle_0 = 0 \tag{2.87}$$

We have seen that *inside* a time-ordered product, fermionic operators *anti-commute*,

$$T(AB) = -T(BA) \tag{2.88}$$

which will play a central role in what follows.

We will now define the useful concept of a *normal ordered* product. The normal ordered product of any number of operators is an ordered product in which all annihilation operators appear to the right of all creation operators. Furthermore, inside a normal ordered product operators can be reordered up to a sign determined by the parity of the permutation P used to reorder the operators.

We define the normal ordered product of a set of n *Heisenberg* operators $\{A_j\}$, with $j = 1, \ldots, n$, which we will denote by $:A_1A_2\ldots A_n:$, to satisfy

$$:A_1A_2\ldots A_n:|G\rangle_0 = 0 \tag{2.89}$$

$$:A_1\ldots A_n: = (-1)^P :A_3A_1A_2\ldots A_n: \tag{2.90}$$

where the factor of $(-1)^P$ holds only for fermionic operators.

Furthermore,

$$
\begin{aligned}
:\psi^{(+)}(x)\psi^{(-)}(y): &= -\psi^{(-)}(y)\psi^{(+)}(x) \\
:\psi^{(+)}(x)\psi^{(+)\dagger}(y): &= -\psi^{(+)\dagger}(y)\psi^{(+)}(x)
\end{aligned}
\tag{2.91}
$$

We also note that, by definition, the expectation value of any normal ordered product vanishes:

$$
{}_0\langle G|\,:A_1 \ldots A_n:\,|G\rangle_0 = 0 \tag{2.92}
$$

We will now define the *contraction* of two operators as the difference of their time-ordered and normal-ordered products:

$$
\overbrace{AB} \equiv T(AB) - :AB: \tag{2.93}
$$

Since

$$
T(\psi^{(+)}(x)\psi^{(-)}(x')) = \begin{cases} \psi^{(+)}(x)\psi^{(-)}(x') & \text{for } t_x > t_{x'} \\ -\psi^{(-)}(x)\psi^{(+)}(x') & \text{for } t_{x'} > t_x \end{cases} \tag{2.94}
$$

we see that

$$
T(\psi^{(+)}(x)\psi^{(-)}(x')) = -\psi^{(-)}(x')\psi^{(+)}(x) \tag{2.95}
$$

Similarly, we also get

$$
:\psi^{(+)}(x)\psi^{(-)}(x'):= -\psi^{(-)}(x')\psi^{(+)}(x) \tag{2.96}
$$

Thus the contraction of a $\psi^{(+)}$ operator and a $\psi^{(-)}$ operator vanishes:

$$
\psi^{\overbrace{(+)}(x)\psi^{(-)}}(x') = 0 \tag{2.97}
$$

The only non-vanishing contractions are

$$
\begin{aligned}
\psi^{\overbrace{(+)}(x)\psi^{(+)\dagger}}(x') &= \begin{cases} i\ G_F^0(x,x') & \text{for } t_x > t_{x'} \\ 0 & \text{for } t_x < t_{x'} \end{cases} \\
\psi^{\overbrace{(-)}(x)\psi^{(-)\dagger}}(x') &= \begin{cases} 0 & \text{for } t_x > t_{x'} \\ i\ G_F^0(x,x') & \text{for } t_x < t_{x'} \end{cases}
\end{aligned}
\tag{2.98}
$$

Hence, the ground state expectation value of the time-ordered product of two operators can be related to the expectation value of the contraction of the operators. Indeed,

$$\begin{aligned} {}_0\langle G|T(AB)|G\rangle_0 &= {}_0\langle G|\overbrace{AB}|G\rangle_0 + {}_0\langle G|:AB:|G\rangle_0 \\ &\equiv {}_0\langle G|\overbrace{AB}|G\rangle_0 \equiv \overbrace{AB} \end{aligned} \tag{2.99}$$

Hence,

$$ {}_0\langle G|T(AB)|G\rangle_0 = \overbrace{AB} \tag{2.100}$$

This result allows us to identify the contraction of the field operators with the Feynman propagator:

$$\overbrace{\psi(x)\psi^\dagger}(x') = i\, G_F^0(x,x') \tag{2.101}$$

We will also need to know how to compute normal ordered products with partially contracted operators. For instance it easy to show that

$$:\contraction{}{A}{B}{C}ABCD\ldots:= -:\overbrace{AC}BD\ldots:= -\overbrace{AC}N(BD\ldots) \tag{2.102}$$

These results lead to the following identity, known as *Wick's Theorem*, which relates time-ordered products to normal ordered products and contractions. Let $A_1, \ldots, A_N$ be a set of N operators. Then,

$$\begin{aligned} &T(A_1\ldots A_N) =: A_1\ldots A_N: \\ &+ :\overbrace{A_1A_2}A_3A_4\ldots A_N: + \text{other normal ordered terms with one contraction} \\ &+ :\contraction{}{A_1}{A_2}{A_3}\contraction[2ex]{A_1}{A_2}{A_3}{A_4}A_1A_2A_3A_4\ldots A_N: + \text{other normal ordered terms with two contractions} \\ &+\ldots \\ &+\overbrace{A_1A_2}\,\overbrace{A_3A_4}\ldots\overbrace{A_{N-1}A_N} + \text{all other products of pairs of contractions} \end{aligned} \tag{2.103}$$

It is also easy to verify that

$$\begin{aligned} :A_1\ldots A_N:\ B &= :A_1\ldots \overbrace{A_N B}: + :A_1\ldots \contraction{}{A_{N-1}}{A_N}{B}A_{N-1}A_N B: + \ldots + :\contraction{}{A_1}{\ldots A_N}{B}A_1\ldots A_N B: + \\ &+ :A_1\ldots A_N B: \end{aligned} \tag{2.104}$$

In particular, we find that the ground state expectation value of a time-ordered product of operators is equal to the sum of all possible products of contractions of pairs of operators:

$$\boxed{\langle G|T(A_1 \ldots A_N)|G\rangle = \overbrace{A_1 A_2}\,\overbrace{A_3 A_4} \ldots \overbrace{A_{N-1} A_N} + \ldots} \tag{2.105}$$

where the ellipsis ... represents the sum of all other products of pairs of contractions. Notice that if we are dealing with fermionic operators, each term in this sum will have a sign determined by the number of permutations done in the process of contacting the operators.