Many body theory

Janos Polonyi
Louis Pasteur University, Strasbourg, France
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I. INTRODUCTION

These notes represent a brief introduction to the quantum treatment of nonrelativistic many body systems. The details are kept minimal, students planning to continue in theoretical directions should work through a more exhaustive presentation of the subject.

The there are three main topics covered, the general description of the second quantized electron-phonon system, the introduction of Green functions and finally, the theory of perturbation for causal and for retarded Green functions.

II. SECOND QUANTIZATION

The formalism of the usual Quantum Mechanics is not sufficient to consider realistic systems composed of a large number of particles. The reason is the equivalence of particles, a genuine quantum effect, which requires the (anti)symmetrization of the wave functions. The resulting wave functions are too complicated for any useful calculation. Another representation of the many particle system, based on the occupation number offers a simple mathematical setup where the complications created by the (anti)symmetrization simply disappear.

But there is another, less technical reason of seeking an extension of the usual Quantum Mechanical framework, related to the fact that energy can be converted into the creation of particles. This phenomenon is well known in high energy physics where the available kinetic energy can be far higher than the rest mass energy of the particles in the system. But this does no exhaust the examples of converting energy and particles into each other. Small fluctuations of a crystalline structure, the phonons which are the normal modes of the leading order, quadratic approximation for the displacement of the constituents of the ionic crystal can be viewed as the law energy 'elementary particles' of the ionic degrees of freedom. They can be created by energies available in the solids and the treatment of such processes requires the use of some ideas borrowed from high energy physics.

The extension of Quantum Mechanics to treat many body system and processes with changing number of degrees of freedom is traditionally called 'second quantization', leaving the name 'first quantization' for the usual Quantum Mechanical formalism. These names are misleading as we shall see below but are kept for historical reason.

A. Harmonic oscillators

Let us now imagine a system of free, equivalent particles characterized by the dispersion relation, the relation between their energy and momentum, $E(\hbar \boldsymbol{q})$, $\boldsymbol{q}$ being the wave vector of the particle. Due to the lack of interactions the total energy is additive,

$$E_{\rm tot} = \sum_j E(\hbar \boldsymbol{q}_j)$$

where $\boldsymbol{q}_j$ stands for the wave vector of the j-th particle. A better way to write this energy is to regroup particles with the same momentum by introducing the occupational number, $n_{\boldsymbol{q}}$ giving the number of particles with wave vector $\boldsymbol{q}$, and writing

$$\begin{aligned} E_{\rm tot} &= \sum_{\boldsymbol{q}} E(\hbar \boldsymbol{q}) n_{\boldsymbol{q}} \\ &= \int \frac{d^3q}{(2\pi)^3} E(\hbar \boldsymbol{q}) n(\boldsymbol{q}). \end{aligned}$$

where the thermodynamical limit has been taken, $V = L^3 \to \infty$, $\Delta q = \frac{2\pi}{L}$, in arriving at the second equation where the notation

$$n(\boldsymbol{q}) = V n_{\boldsymbol{q}}$$

is introduced for the occupation number, considered as a function of continuous variable.

To simplify the search for the representation of systems where the number of equivalent particles is not fixed let us suppose that all particle of our system have the same momentum $\hbar \boldsymbol{q}$. The energy spectrum of such a system is equidistant,

$$E_{\rm tot} = E(\hbar \boldsymbol{q}) n_{\boldsymbol{q}}.$$

The only quantum mechanical system whose spectrum is an arithmetic series is the harmonic oscillator. Therefore, we introduce a formal harmonic oscillator for each possible value of the wave vector $\boldsymbol{q}$, together with its Hilbert space $\mathcal{H}_{\boldsymbol{q}}$ and canonical operator pair, $\Pi_{\boldsymbol{q}}$ and $Q_{\boldsymbol{q}}$, satisfying

$$[Q_{\boldsymbol{q}_j}, \Pi_{\boldsymbol{q}_k}]_\xi = i\hbar \delta_{j,k}$$

for finite volume and

$$[Q(\boldsymbol{q}), \Pi(\boldsymbol{r})]_\xi = i\hbar (2\pi)^3 \delta(\boldsymbol{q} - \boldsymbol{r})$$

in the thermodynamical limit where

$$[A,B]_\xi = A\cdot B - \xi B\cdot A, \tag{1}$$

choosing $\xi = 1$ at the time being

$$Q(\boldsymbol{q}) = \sqrt{V}Q_{\boldsymbol{q}}, \qquad \Pi(\boldsymbol{r}) = \sqrt{V}\Pi_{\boldsymbol{r}}$$

and

$$\delta(\boldsymbol{q}-\boldsymbol{r}) = \frac{V}{(2\pi)^3}\delta_{j,k}.$$

The Hamilton operator of the oscillator corresponding to the wave vector $\boldsymbol{q}$ is

$$H_{\boldsymbol{q}} = \frac{\Pi_{\boldsymbol{q}}^2}{2m_{\boldsymbol{q}}} + \frac{m_{\boldsymbol{q}}\omega_{\boldsymbol{q}}^2}{2}Q_{\boldsymbol{q}}^2 = \frac{1}{V}\left[\frac{\Pi^2(\boldsymbol{q})}{2m(\boldsymbol{q})} + \frac{m(\boldsymbol{q})\omega^2(\boldsymbol{q})}{2}Q^2(\boldsymbol{q})\right] = \frac{1}{V}H(\boldsymbol{q})$$

with $m_{\boldsymbol{q}} = m(\boldsymbol{q})$ and $\omega_{\boldsymbol{q}} = \omega(\boldsymbol{q})$.

One introduces the creation and destruction operators for particles corresponding to a given wave vector,

$$\begin{aligned} a_{\boldsymbol{q}}^\dagger &= \frac{m_{\boldsymbol{q}}\omega_{\boldsymbol{q}}Q_{\boldsymbol{q}} - i\Pi_{\boldsymbol{q}}}{\sqrt{2m_{\boldsymbol{q}}\omega_{\boldsymbol{q}}\hbar}}, \qquad a_{\boldsymbol{q}} = \frac{m_{\boldsymbol{q}}\omega_{\boldsymbol{q}}Q_{\boldsymbol{q}} + i\Pi_{\boldsymbol{q}}}{\sqrt{2m_{\boldsymbol{q}}\omega_{\boldsymbol{q}}\hbar}}, \\ a^\dagger(\boldsymbol{q}) &= \frac{m(\boldsymbol{q})\omega(\boldsymbol{q})Q(\boldsymbol{q}) - i\Pi(\boldsymbol{q})}{\sqrt{2m(\boldsymbol{q})\omega(\boldsymbol{q})\hbar}}, \qquad a(\boldsymbol{q}) = \frac{m(\boldsymbol{q})\omega(\boldsymbol{q})Q(\boldsymbol{q}) + i\Pi(\boldsymbol{q})}{\sqrt{2m(\boldsymbol{q})\omega(\boldsymbol{q})\hbar}}, \end{aligned} \tag{2}$$

satisfying the canonical commutation relation

$$[a(\boldsymbol{q}_j), a^\dagger(\boldsymbol{q}_k)]_\xi = \delta_{j,k}, \qquad [a(\boldsymbol{q}_j), a(\boldsymbol{q}_k)]_\xi = 0,$$

for finite system and

$$[a(\boldsymbol{q}), a^\dagger(\boldsymbol{r})]_\xi = (2\pi)^3\delta(\boldsymbol{q}-\boldsymbol{r}), \qquad [a(\boldsymbol{q}), a(\boldsymbol{r})]_\xi = 0 \tag{3}$$

in the thermodynamical limit. The number operator,

$$N(\boldsymbol{q}) = a^\dagger(\boldsymbol{q})a(\boldsymbol{q}),$$

can be used to express the Hamiltonian as

$$H(\boldsymbol{q}) = \hbar\omega(\boldsymbol{q})\left(N(\boldsymbol{q}) + \frac{1}{2}\right).$$

The energy of the n-th excited state $|n\rangle_{\boldsymbol{q}}$,

$$N(\boldsymbol{q})|n\rangle_{\boldsymbol{q}} = n|n\rangle_{\boldsymbol{q}},$$

is

$$E_n(\boldsymbol{q}) = \hbar\omega(\boldsymbol{q})\left(n + \frac{1}{2}\right)$$

which leads to the condition $\hbar\omega(\boldsymbol{q}) = E(\hbar\boldsymbol{q})$, leaving $m(\boldsymbol{q})$ arbitrary. The relations

$$\begin{aligned} a^\dagger(\boldsymbol{q})|n\rangle_{\boldsymbol{q}} &= \sqrt{n+1}|n+1\rangle_{\boldsymbol{q}} \\ a(\boldsymbol{q})|n\rangle_{\boldsymbol{q}} &= \sqrt{n}|n-1\rangle_{\boldsymbol{q}} \\ |n\rangle_{\boldsymbol{q}} &= \frac{(a^\dagger(\boldsymbol{q}))^n}{\sqrt{n!}}|0\rangle_{\boldsymbol{q}}, \quad a(\boldsymbol{q})|0\rangle_{\boldsymbol{q}} = 0 \end{aligned}$$

will be useful later.

The Hilbert space of the system of all harmonic oscillator, $\mathcal{H}_F$, called Fock-space is $\mathcal{H}_F = \otimes \prod_{\boldsymbol{k}} \mathcal{H}_{\boldsymbol{k}}$ and the Hamilton operator acting on it is

$$H_{\rm tot} = \int \frac{d^3q}{(2\pi)^3} \left[\frac{\Pi^2(\boldsymbol{q})}{2m(\boldsymbol{q})} + \frac{m(\boldsymbol{q})\omega^2(\boldsymbol{q})}{2} Q^2(\boldsymbol{q}) \right].$$

The total number of particles is represented by the operator

$$N_{\rm tot} = \int \frac{d^3\boldsymbol{q}}{(2\pi)^3} a^\dagger(\boldsymbol{q}) a(\boldsymbol{q})$$

Let us consider some simple states for bosons. The ground state is clearly that of with no particles,

$$|0\rangle = \otimes \prod_{\boldsymbol{q}} |0\rangle_{\boldsymbol{q}}. \tag{4}$$

Let us denote the state with a single particle of wave vector $\boldsymbol{q}$ by

$$|\boldsymbol{q}\rangle = a^\dagger(\boldsymbol{q})|0\rangle. \tag{5}$$

The one particle state whose wave function is $\Psi_1(\hbar\boldsymbol{q})$ in the momentum representation is

$$|\Psi_1\rangle = \int \frac{d^3\boldsymbol{q}}{(2\pi)^3} \Psi_1(\hbar\boldsymbol{q}) a^\dagger(\boldsymbol{q})|0\rangle. \tag{6}$$

The state with two particles of wave vectors $\boldsymbol{q}_j$, $j = 1, 2$ is

$$|\boldsymbol{q}_1, \boldsymbol{q}_2\rangle = a^\dagger(\boldsymbol{q}_1) a^\dagger(\boldsymbol{q}_2)|0\rangle. \tag{7}$$

Notice that due to the second commutation relation in (3) the two particle state is symmetrical with respect to the exchange of the particles,

$$|\boldsymbol{q}_1, \boldsymbol{q}_2\rangle = |\boldsymbol{q}_2, \boldsymbol{q}_1\rangle \tag{8}$$

which requires the choice $\xi = 1$ for bosons. The two particle state characterized by the wave function $\Psi_2(\hbar\boldsymbol{q}_1, \hbar\boldsymbol{q}_2)$ in momentum representation is

$$|\Psi_2\rangle = \frac{1}{2} \int \frac{d^3\boldsymbol{q}_1 d^3\boldsymbol{q}_2}{(2\pi)^6} \Psi_2(\hbar\boldsymbol{q}_1, \hbar\boldsymbol{q}_2) a^\dagger(\boldsymbol{q}_1) a^\dagger(\boldsymbol{q}_2)|0\rangle. \tag{9}$$

Finally, a general state of the Fock-space has an ill defined particle number and can be written as

$$|\Psi\rangle = \left[\Psi_0 + \int \frac{d^3\boldsymbol{q}}{(2\pi)^3} \Psi_1(\hbar\boldsymbol{q}) a^\dagger(\boldsymbol{q}) + \frac{1}{2} \int \frac{d^3\boldsymbol{q}_1 d^3\boldsymbol{q}_2}{(2\pi)^6} \Psi_2(\hbar\boldsymbol{q}_1, \hbar\boldsymbol{q}_2) a^\dagger(\boldsymbol{q}_1) a^\dagger(\boldsymbol{q}_2)|0\rangle + \cdots \right] |0\rangle. \tag{10}$$

Ground states with ill defined particle number are the hallmark of the Bose-Einstein condensates and broken symmetries.

The relation

$$N|\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\rangle = n|\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\rangle \tag{11}$$

is a simple result of applying the commutation relation (3).

One expects some complications for fermions due to the Pauli exclusion principle. The impossibility of placing two fermions in the same state can be expressed by the equation

$$(a^\dagger(\boldsymbol{q}))^2 = \frac{1}{2}[a^\dagger(\boldsymbol{q}), a^\dagger(\boldsymbol{q})]_- = 0.$$

In fact, applying both sides of this equation on an arbitrary state $\Psi\rangle$ on has $a^\dagger(\boldsymbol{q}) a^\dagger(\boldsymbol{q})|\Psi\rangle = 0$, indicating the absence of vectors in the Fock-space with two fermions in the same state. The Pauli principle restricts the dimensions of $\mathcal{H}_{\boldsymbol{q}} = \{c_0|0\rangle_{\boldsymbol{q}} + c_1|1\rangle_{\boldsymbol{q}}\}$ to 2. This suggest that the canonical commutation relations will be imposed with $\xi = -1$ for fermions.

The relations (4)-(11) can be re-derived for fermions except the modification of Eq. (8),

$$|\boldsymbol{q}_1, \boldsymbol{q}_2\rangle = -|\boldsymbol{q}_2, \boldsymbol{q}_1\rangle \tag{12}$$

which results from Eq. (3) applied with $\xi = -1$. As a simple example let us consider

$$\begin{aligned} N|\Psi_1\rangle &= \int \frac{d^3\boldsymbol{q}}{(2\pi)^3} a^\dagger(\boldsymbol{q})a(\boldsymbol{q}) \int \frac{d^3\boldsymbol{r}}{(2\pi)^3} \Psi_1(\boldsymbol{r})a^\dagger(\boldsymbol{r})|0\rangle \\ &= \int \frac{d^3\boldsymbol{q}d^3\boldsymbol{r}}{(2\pi)^6} \Psi_1(\boldsymbol{r})a^\dagger(\boldsymbol{q})[\xi a^\dagger(\boldsymbol{r})a(\boldsymbol{q}) + (2\pi)^3\delta(\boldsymbol{q}-\boldsymbol{r})]|0\rangle = |\Psi_1\rangle. \end{aligned}$$

The spin can be taken into account in a trivial manner, by the introduction of a harmonic oscillator for each pair $(\boldsymbol{q}, \sigma)$ which amounts to the replacements $a(\boldsymbol{q}) \to a_\sigma(\boldsymbol{q})$, $[a_\sigma(\boldsymbol{q}), a^\dagger_\kappa(\boldsymbol{r})]_- = (2\pi)^3\delta(\boldsymbol{q}-\boldsymbol{r})\delta_{\sigma,\kappa}$.

B. Quantum field

It is well known that the operator algebra of a harmonic oscillator is the simplest in terms of the creation and destruction operators. This observation gives the idea of considering

$$a(\boldsymbol{p}) = \frac{m(\boldsymbol{p})\omega(\boldsymbol{p})X(\boldsymbol{p}) + i\pi(\boldsymbol{p})}{\sqrt{2m(\boldsymbol{p})\omega(\boldsymbol{p})\hbar}},$$

(an operator valued function, acting on the Fock-space and defined in the space of wave vectors) as the fundamental variable for the description of the system of infinitely many harmonic oscillators. Our intuition is better developed in real (coordinate) space due to a very restrictive constrain on physical laws, the locality. Thus we seek the corresponding variable constructed in real space what can formally be defined by means of a Fourier transformation,

$$\psi_\sigma(\boldsymbol{x}) = \int \frac{d^3q}{(2\pi)^3} e^{i\boldsymbol{q}\boldsymbol{x}} a_\sigma(\boldsymbol{q}), \tag{13}$$

whose hermitian conjugate is

$$\psi^\dagger_\sigma(\boldsymbol{x}) = \int \frac{d^3\boldsymbol{q}}{(2\pi)^3} e^{-i\boldsymbol{q}\boldsymbol{x}} a^\dagger_\sigma(\boldsymbol{q}).$$

The inverse Fourier transformations are given by

$$\begin{aligned} a_\sigma(\boldsymbol{q}) &= \int d^3x e^{-i\boldsymbol{q}\boldsymbol{x}} \psi_\sigma(\boldsymbol{x}), \\ a^\dagger_\sigma(\boldsymbol{q}) &= \int d^3x e^{i\boldsymbol{q}\boldsymbol{x}} \psi^\dagger_\sigma(\boldsymbol{x}). \end{aligned}$$

Since $a^\dagger(\boldsymbol{q})$ and $a(\boldsymbol{q})$ are the creation and destruction operators for a given momentum one expects their linear combination $\psi^\dagger(\boldsymbol{x})$ and $\psi(\boldsymbol{x})$ playing the role of creation and destruction operators at a given space location. This guess is confirmed by the canonical commutation relations

$$\begin{aligned} \big[\psi(\boldsymbol{x}), \psi^\dagger(\boldsymbol{y})\big]_\xi &= \int\int \frac{d^3\boldsymbol{q}d^3\boldsymbol{r}}{(2\pi)^6} e^{i\boldsymbol{q}\boldsymbol{x} - i\boldsymbol{r}\boldsymbol{y}} [a(\boldsymbol{q}), a^\dagger(\boldsymbol{r})]_\xi = \delta(\boldsymbol{x}-\boldsymbol{y}) \\ [\psi(\boldsymbol{x}), \psi(\boldsymbol{y})]_\xi &= \int\int \frac{d^3\boldsymbol{q}d^3\boldsymbol{r}}{(2\pi)^6} e^{i\boldsymbol{q}\boldsymbol{x} + i\boldsymbol{r}\boldsymbol{y}} [a(\boldsymbol{q}), a(\boldsymbol{r})]_\xi = 0 \\ \big[\psi^\dagger(\boldsymbol{x}), \psi^\dagger(\boldsymbol{y})\big]_\xi &= \int\int \frac{d^3\boldsymbol{q}d^3\boldsymbol{r}}{(2\pi)^6} e^{-i\boldsymbol{q}\boldsymbol{x} - i\boldsymbol{r}\boldsymbol{y}} [a^\dagger(\boldsymbol{q}), a^\dagger(\boldsymbol{r})]_\xi = 0 \end{aligned}$$

As a little exercise, one can construct simple one particle states, such as

$$|\boldsymbol{x}\rangle = \psi^\dagger(\boldsymbol{x})|0\rangle$$

which is localized at $\boldsymbol{x}$ and

$$|\Psi_1\rangle = \int d^3x \Psi_1(\boldsymbol{x})\psi^\dagger(\boldsymbol{x})|0\rangle$$

whose Schrödinger wave function is $\Psi_1(\boldsymbol{x})$. The removal of a particle from the state $|\boldsymbol{x}\rangle$ at the location $\boldsymbol{y}$ yields

$$\psi(\boldsymbol{y})|\boldsymbol{x}\rangle = \psi(\boldsymbol{y})\psi^\dagger(\boldsymbol{x})|0\rangle = [\xi\psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{y}) + \delta(\boldsymbol{x}-\boldsymbol{y})]|0\rangle = \delta(\boldsymbol{x}-\boldsymbol{y})|0\rangle,$$

the null vector when $\boldsymbol{y} \neq \boldsymbol{x}$ and the no-particle ground state for $\boldsymbol{y} = \boldsymbol{x}$.

Another simple exercise is to check the exchange statistics. Let us define the localized two particle state as

$$|\boldsymbol{y}, \boldsymbol{x}\rangle = \psi^\dagger(\boldsymbol{y})|\boldsymbol{x}\rangle.$$

The removal of a particle at $\boldsymbol{z}$ leads to the state

$$\begin{aligned}\psi(\boldsymbol{z})|\boldsymbol{y},\boldsymbol{x}\rangle &= \psi(\boldsymbol{z})\psi^\dagger(\boldsymbol{y})\psi^\dagger(\boldsymbol{x})|0\rangle \\ &= [\xi\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{z}) + \delta(\boldsymbol{y}-\boldsymbol{z})]\psi^\dagger(\boldsymbol{x})|0\rangle = \xi\delta(\boldsymbol{z}-\boldsymbol{x})|\boldsymbol{y}\rangle + \delta(\boldsymbol{z}-\boldsymbol{y})|\boldsymbol{x}\rangle\end{aligned}$$

The exchange statistical factor ξ appears in the first term because the first placed particle is removed first which necessitate the exchange of the two particles in the state.

It is easy to verify that

$$n(\boldsymbol{x}) = \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x})$$

plays the role of particle density operator and the states $|\boldsymbol{x}\rangle$ and $|\boldsymbol{x},\boldsymbol{y}\rangle$ are eigenstates of the total particle number operator

$$N_{\rm tot} = \int d^3x n(\boldsymbol{x})$$

with eigenvalues 1 and 2, respectively.

C. Observables

1. *One-body operators*

Let us now consider the simplest observables which are constructed from one particle observables in an additive manner. The operator $F_S(\boldsymbol{p}) = F_S\left(\frac{\hbar}{i}\boldsymbol{\nabla}_x\right)$, the function of the momentum operator of the usual Schrödinger picture defines a one-particle operator. Its additive extension for many body system acts on the Fock-space,

$$\begin{aligned}F_S(\boldsymbol{p}) \;\rightarrow\; F_F &\equiv \int \frac{d^3k}{(2\pi)^3} a^\dagger(\boldsymbol{k})a(\boldsymbol{k})F_S(\hbar\boldsymbol{k}) \\ &= \int \frac{d^3k}{(2\pi)^3} d^3x d^3y \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{y})e^{i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{y})}F_S(\hbar\boldsymbol{k}) \\ &= \int \frac{d^3k}{(2\pi)^3} d^3x d^3y \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{y})F_S\left(-\frac{\hbar}{i}\boldsymbol{\nabla}_y\right)e^{i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{y})} \\ &= \int d^3x d^3y \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{y})F_S\left(-\frac{\hbar}{i}\boldsymbol{\nabla}_y\right)\delta(\boldsymbol{x}-\boldsymbol{y}) \\ &= \int d^3x d^3y \psi^\dagger(\boldsymbol{x})\delta(\boldsymbol{x}-\boldsymbol{y})\left[F_S\left(\frac{\hbar}{i}\boldsymbol{\nabla}_y\right)\psi(\boldsymbol{y})\right] \\ &= \int d^3x \psi^\dagger(\boldsymbol{x})F_S\left(\frac{\hbar}{i}\boldsymbol{\nabla}_x\right)\psi(\boldsymbol{x}) \qquad (14)\end{aligned}$$

where a partial integration was performed in arriving at the fifth equation, looks formally as an expectation value in first quantized Quantum Mechanics for the state described by the wave function $\psi(\boldsymbol{x})$. But this 'wave function' is now operator valued because we need the quantum version of the harmonic oscillators due to the discreteness of the

FIG. 1: Symbolic representation of one-particle operators. $f_S(\boldsymbol{p})$ is diagonal in momentum space but $f_S(\boldsymbol{x})$ changes the momentum.

particle number. It is as if the 'wave function' $\psi(\boldsymbol{x})$ appearing in the naive interpretation of Eq. (14) would have to be quantized again, the second time. In another way arriving at similar conclusion is to interpret the Fourier mode in the Fourier integral of Eq. (13) as the wave function of a particle with momentum $\boldsymbol{p} = \hbar\boldsymbol{q}$. This is the historical source of the name 'second quantization'. But it is misleading for it holds for non-interactive particles only. When interactions are present one can not isolate one-particle states anymore due to the entanglement and this analogy is completely lost.

Similar construction for first quantized operator $F_S(\boldsymbol{x})$ which is diagonal in the coordinate representation is

$$\begin{aligned} F_S(\boldsymbol{x}) \to F_F &\equiv \int d^3x \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x}) f_S(\boldsymbol{x}) \\ &= \int \frac{d^3q d^3r}{(2\pi)^6} d^3\boldsymbol{x} a^\dagger(\boldsymbol{q}) a(\boldsymbol{r}) e^{i\boldsymbol{x}(\boldsymbol{r}-\boldsymbol{q})} F_S(\boldsymbol{x}) \\ &= \int \frac{d^3q d^3r}{(2\pi)^6} a^\dagger(\boldsymbol{q}) a(\boldsymbol{r}) \tilde{F}_S(\boldsymbol{q}-\boldsymbol{r}), \end{aligned}$$

where

$$\tilde{F}_S(\boldsymbol{q}) = \int d^3x e^{-i\boldsymbol{q}\boldsymbol{x}} F_S(\boldsymbol{x})$$

Examples:

1. Kinetic energy:

$$\begin{aligned} H_S(\hbar\boldsymbol{k}) &= \frac{\hbar^2\boldsymbol{k}^2}{2m} \\ H_F &= \int \frac{d^3k}{(2\pi)^3} a^\dagger(\boldsymbol{k}) a(\boldsymbol{k}) H_S(\hbar\boldsymbol{k}) = \int d^3x \psi^\dagger(\boldsymbol{x}) H_S\left(\frac{\hbar}{i}\partial\right)\psi(\boldsymbol{x}) \end{aligned}$$

2. Potential energy:

$$U_S \to U_F = \int d^3x \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x}) U_S(\boldsymbol{x}) = \int \frac{d^3q d^3r}{(2\pi)^6} a^\dagger(\boldsymbol{q}) a(\boldsymbol{r}) \tilde{U}_S(\boldsymbol{q}-\boldsymbol{r})$$

3. Particle density:

$$\begin{aligned} n_F(\boldsymbol{x}) &= \int d^3x' \psi^\dagger(\boldsymbol{x}') \underbrace{\delta(\boldsymbol{x}'-\boldsymbol{x})}_{n_S(\boldsymbol{x}')} \psi(\boldsymbol{x}') = \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x}) \\ \tilde{n}_F(\boldsymbol{s}) &= \int \frac{d^3q d^3r}{(2\pi)^6} d^3\boldsymbol{x} a^\dagger(\boldsymbol{q}) a(\boldsymbol{r}) e^{-i(\boldsymbol{q}-\boldsymbol{r}+\boldsymbol{s})\boldsymbol{x}} \\ &= \int \frac{d^3q d^3r}{(2\pi)^6} a^\dagger(\boldsymbol{q}) a(\boldsymbol{r}) \delta(\boldsymbol{q}-\boldsymbol{r}+\boldsymbol{s}) \\ &= \int \frac{d^3q}{(2\pi)^3} a^\dagger(\boldsymbol{q}) a(\boldsymbol{q}+\boldsymbol{s}) \end{aligned}$$

4. Current density:

$$\begin{aligned}
\boldsymbol{J}_F(\boldsymbol{x}) &= \frac{\hbar}{2mi}[\psi^\dagger(\boldsymbol{x})\boldsymbol{\nabla}\psi(\boldsymbol{x}) - \boldsymbol{\nabla}\psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x})] \\
\tilde{\boldsymbol{J}}_F(\boldsymbol{s}) &= \frac{\hbar}{2mi}\int \frac{d^3q d^3r}{(2\pi)^6} d^3\boldsymbol{x} a^\dagger(\boldsymbol{q})a(\boldsymbol{r})e^{-i(\boldsymbol{q}-\boldsymbol{r}+\boldsymbol{s})\boldsymbol{x}} i(\boldsymbol{q}+\boldsymbol{r}) \\
&= \frac{\hbar}{2m}\int \frac{d^3q d^3r}{(2\pi)^6} a^\dagger(\boldsymbol{q})a(\boldsymbol{r})\delta(\boldsymbol{q}-\boldsymbol{r}+\boldsymbol{s})(\boldsymbol{q}+\boldsymbol{r}) \\
&= \frac{\hbar}{m}\int \frac{d^3q}{(2\pi)^3} a^\dagger(\boldsymbol{q})a(\boldsymbol{q}+\boldsymbol{s})\left(\boldsymbol{q}+\frac{\boldsymbol{s}}{2}\right)
\end{aligned}$$

2. Two-body operators

The most important two-body operator represents the interactions among pairs of particles,

$$U_S = \frac{1}{2}\sum_{i,j} U(\boldsymbol{x}_i - \boldsymbol{x}_j) = \frac{1}{2}\sum_{i\neq j} U(\boldsymbol{x}_i - \boldsymbol{x}_j) + \frac{N}{2}U(0).$$

A characteristic difference between classical and quantum physics is that the last term is usually not considered in the classical theory but is necessarily present in the quantum case where the particles are indistinguishable and is not possible to separate $i = j$ from $i \neq j$. It clearly plays entirely different role in the dynamics than 'real' interactions, taking place between different particles. To separate them in an automatic manner one introduces the normal ordered product, $A \cdot B \rightarrow : A \cdot B :$, for operators composed of creation and destruction operators. The rule is to order all destruction operators right to the creation operators and inserting the statical phase factor ξ for each exchange, eg.

$$\begin{aligned}
:\psi(\boldsymbol{x})\psi(\boldsymbol{y}): &= \psi(\boldsymbol{x})\psi(\boldsymbol{y}) \\
:\psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{y}): &= \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{y}) \\
:\psi(\boldsymbol{x})\psi^\dagger(\boldsymbol{y}): &= \xi\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{x}),
\end{aligned}$$

according to the canonical commutation relations (14) and neglecting their right hand side of the first equation. The additive potential energy acting on the Fock-space can then be written as

$$\begin{aligned}
U_F &= \frac{1}{2}\int d^3x d^3y \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x})U(\boldsymbol{x}-\boldsymbol{y})\psi^\dagger(\boldsymbol{y})\psi(\boldsymbol{y}) \\
&= \frac{1}{2}\int d^3x d^3y \psi^\dagger(\boldsymbol{x})\psi^\dagger(\boldsymbol{y})U(\boldsymbol{x}-\boldsymbol{y})\psi(\boldsymbol{y})\psi(\boldsymbol{x}) + \frac{1}{2}\int d^3x \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x})U(0) \\
&= :U: + \frac{N}{2}U(0),
\end{aligned}$$

the normal order prescription identifying the 'real' interaction.

As an application of this formalism let us now calculate the matrix element of the potential energy, $\langle\Psi| : U : |\Phi\rangle$, between two-particle states

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\int d^3x d^3y \Psi(\boldsymbol{x},\boldsymbol{y})\psi^\dagger(\boldsymbol{x})\psi^\dagger(\boldsymbol{y})|0\rangle, \qquad |\Phi\rangle = \frac{1}{\sqrt{2}}\int d^3x d^3y \Phi(\boldsymbol{x},\boldsymbol{y})\psi^\dagger(\boldsymbol{x})\psi^\dagger(\boldsymbol{y})|0\rangle.$$

By means of the relation

$$\begin{aligned}
\psi(\boldsymbol{u})\psi(\boldsymbol{v})\psi^\dagger(\boldsymbol{x})\psi^\dagger(\boldsymbol{y})|0\rangle &= \psi(\boldsymbol{u})\left[\delta(\boldsymbol{v}-\boldsymbol{x}) + \xi\psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{v})\right]\psi^\dagger(\boldsymbol{y})|0\rangle \\
&= \left[\delta(\boldsymbol{v}-\boldsymbol{x})\delta(\boldsymbol{u}-\boldsymbol{y}) + \xi\delta(\boldsymbol{v}-\boldsymbol{y})\delta(\boldsymbol{u}-\boldsymbol{x})\right]|0\rangle
\end{aligned}$$

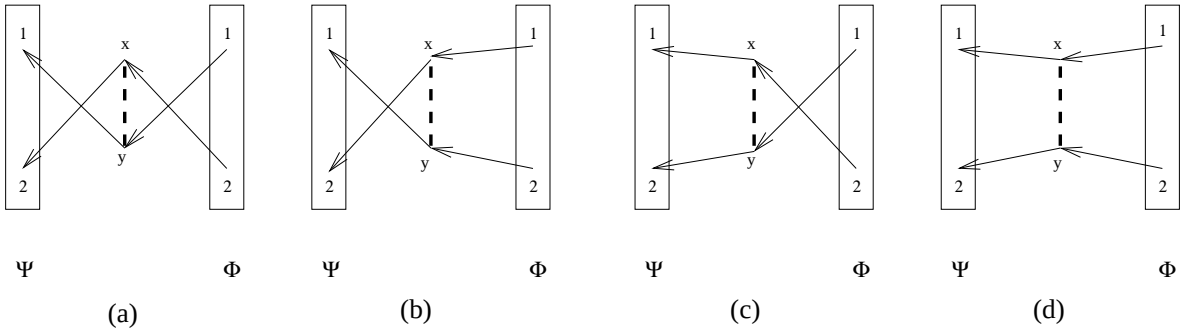

FIG. 2: Symbolic representation of the four contributions of the second equation of Eq. (15), (a): $B \cdot Z$, (b): $A \cdot Z$, (c): $B \cdot W$, (d): $A \cdot W$.

we have

$$\begin{aligned}
\langle\Psi| : U : |\Phi\rangle &= \frac{1}{2}\int d^3x_v d^3y_v d^3x_1 d^3y_1 d^3x_2 d^3y_2 \Psi^*(\boldsymbol{x}_1,\boldsymbol{y}_1) U(\boldsymbol{x}_v-\boldsymbol{y}_v)\Phi(\boldsymbol{x}_2,\boldsymbol{y}_2) \\
&\quad \times\langle 0|\psi(\boldsymbol{y}_1)\psi(\boldsymbol{x}_1)\psi^\dagger(\boldsymbol{x}_v)\psi^\dagger(\boldsymbol{y}_v)\psi(\boldsymbol{y}_v)\psi(\boldsymbol{x}_v)\psi^\dagger(\boldsymbol{x}_2)\psi^\dagger(\boldsymbol{y}_2)|0\rangle \\
&= \frac{1}{2}\int d^3x_v d^3y_v d^3x_1 d^3y_1 d^3x_2 d^3y_2 \Psi^*(\boldsymbol{x}_1,\boldsymbol{y}_1) U(\boldsymbol{x}_v-\boldsymbol{y}_v)\Phi(\boldsymbol{x}_2,\boldsymbol{y}_2) \\
&\quad \times[\overbrace{\delta(\boldsymbol{x}_1-\boldsymbol{x}_v)\delta(\boldsymbol{y}_1-\boldsymbol{y}_v)}^{A} + \xi\overbrace{\delta(\boldsymbol{x}_1-\boldsymbol{y}_v)\delta(\boldsymbol{y}_1-\boldsymbol{x}_v)}^{B}] \\
&\quad \times[\underbrace{\delta(\boldsymbol{x}_v-\boldsymbol{x}_2)\delta(\boldsymbol{y}_v-\boldsymbol{y}_2)}_{W} + \xi\underbrace{\delta(\boldsymbol{x}_v-\boldsymbol{y}_2)\delta(\boldsymbol{y}_v-\boldsymbol{x}_2)}_{Z}] \\
&= \int d^3x d^3y U(\boldsymbol{x}-\boldsymbol{y})\left[\Psi^*(\boldsymbol{x},\boldsymbol{y})\Phi(\boldsymbol{x},\boldsymbol{y}) + \xi\Psi^*(\boldsymbol{x},\boldsymbol{y})\Phi(\boldsymbol{y},\boldsymbol{x})\right] \qquad (15)
\end{aligned}$$

for $U(\boldsymbol{x}-\boldsymbol{y}) = U(\boldsymbol{y}-\boldsymbol{x})$.

The analogous calculation in the first quantized formalism gives identical result,

$$\begin{aligned}
\langle \boldsymbol{x},\boldsymbol{y}|\Psi\rangle &= \frac{1}{\sqrt{2}}\left[\Psi(\boldsymbol{x},\boldsymbol{y}) + \xi\Psi(\boldsymbol{y},\boldsymbol{x})\right] \\
\langle\Psi| : U : |\Phi\rangle &= \frac{1}{2}\int d^3x_1 d^3y_1 d^3x_2 d^3y_2 \langle\Psi|\boldsymbol{x}_1,\boldsymbol{y}_1\rangle\langle\boldsymbol{x}_1,\boldsymbol{y}_1|U|\boldsymbol{x}_2,\boldsymbol{y}_2\rangle\langle\boldsymbol{x}_2,\boldsymbol{y}_2|\Phi\rangle \\
&= \frac{1}{2}\int d^3x_1 d^3y_1 d^3x_2 d^3y_2 \left[\Psi^*(\boldsymbol{y}_1,\boldsymbol{x}_1) + \xi\Psi^*(\boldsymbol{x}_1,\boldsymbol{y}_1)\right] \\
&\quad \times\delta(\boldsymbol{x}_1-\boldsymbol{y}_2)\delta(\boldsymbol{y}_1-\boldsymbol{x}_2)U(\boldsymbol{x}_1-\boldsymbol{y}_1)\left[\Phi(\boldsymbol{x}_2,\boldsymbol{y}_2) + \xi\Phi(\boldsymbol{y}_2,\boldsymbol{x}_2)\right] \\
&= \int d^3x d^3y U(\boldsymbol{x}-\boldsymbol{y})[\Psi^*(\boldsymbol{y},\boldsymbol{x})\Phi(\boldsymbol{y},\boldsymbol{x}) + \xi\Psi^*(\boldsymbol{y},\boldsymbol{x})\Phi(\boldsymbol{x},\boldsymbol{y})]
\end{aligned}$$

In particular, for the Slater-determinant

$$\langle \boldsymbol{x},\boldsymbol{y}|\Psi\rangle = \frac{1}{\sqrt{2}}\left[\psi_1(\boldsymbol{x})\psi_2(\boldsymbol{y}) - \psi_2(\boldsymbol{x})\psi_1(\boldsymbol{y})\right]$$

we have

$$\begin{aligned}
\langle\Psi| : U : |\Psi\rangle &= \int d^3x d^3y U(\boldsymbol{x}-\boldsymbol{y})[\psi_1^*(\boldsymbol{y})\psi_1(\boldsymbol{y})\psi_2^*(\boldsymbol{x})\psi_2(\boldsymbol{x}) - \psi_1^*(\boldsymbol{y})\psi_2(\boldsymbol{y})\psi_2^*(\boldsymbol{x})\psi_1(\boldsymbol{x})] \\
&= \int d^3x d^3y \frac{1}{\sqrt{2}}\begin{vmatrix}\psi_1(\boldsymbol{x}) & \psi_1(\boldsymbol{y}) \\ \psi_2(\boldsymbol{x}) & \psi_2(\boldsymbol{y})\end{vmatrix}^* U(\boldsymbol{x}-\boldsymbol{y})\frac{1}{\sqrt{2}}\begin{vmatrix}\psi_1(\boldsymbol{x}) & \psi_1(\boldsymbol{y}) \\ \psi_2(\boldsymbol{x}) & \psi_2(\boldsymbol{y})\end{vmatrix}.
\end{aligned}$$

The matrix element in momentum space reads

$$\langle\Psi| : U : |\Phi\rangle = \int d^3x d^3y \frac{d^3q d^3r d^3s d^3t}{(2\pi)^{12}} U(\boldsymbol{x}-\boldsymbol{y})\tilde{\Psi}^*(\boldsymbol{q},\boldsymbol{r})\tilde{\Phi}(\boldsymbol{s},\boldsymbol{t})\left[e^{i(\boldsymbol{s}-\boldsymbol{q})\boldsymbol{x}+i(\boldsymbol{t}-\boldsymbol{r})\boldsymbol{y}} + \xi e^{i(\boldsymbol{t}-\boldsymbol{q})\boldsymbol{x}+i(\boldsymbol{s}-\boldsymbol{r})\boldsymbol{y}}\right]$$

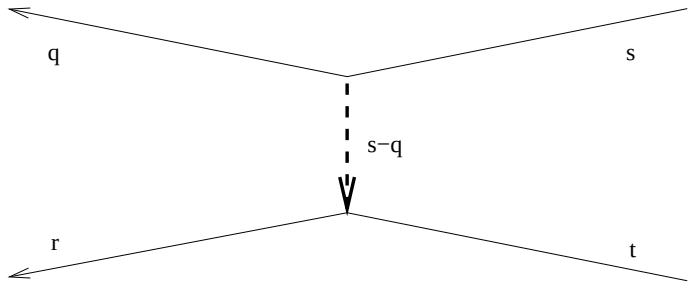

FIG. 3: Graphical representation of the first, direct term in the two-particle interaction energy, Eq. (16), in momentum space.

where

$$\tilde{\Phi}(\boldsymbol{q},\boldsymbol{r}) = \int d^3x d^3y e^{-i\boldsymbol{q}\boldsymbol{x}-i\boldsymbol{r}\boldsymbol{y}}\Phi(\boldsymbol{x},\boldsymbol{y})$$

The introduction of the center of mass and relative coordinates, $\boldsymbol{r}_r = \boldsymbol{x}-\boldsymbol{y}$ and $\boldsymbol{R} = (\boldsymbol{x}+\boldsymbol{y})/2$, respectively, factorizes the Fourier transform of the potential,

$$\begin{aligned}
\langle\Psi|:U:|\Phi\rangle &= \int d^3Rd^3r_r \frac{d^3qd^3rd^3sd^3t}{(2\pi)^{12}} U(\boldsymbol{r}_r)\Psi^*(\boldsymbol{q},\boldsymbol{r})\Phi(\boldsymbol{s},\boldsymbol{t}) \\
&\quad\times\left[e^{i(\boldsymbol{s}-\boldsymbol{q})(\boldsymbol{R}+\frac{\boldsymbol{r}_r}{2})+i(\boldsymbol{t}-\boldsymbol{r})(\boldsymbol{R}-\frac{\boldsymbol{r}_r}{2})} + \xi e^{i(\boldsymbol{t}-\boldsymbol{q})(\boldsymbol{R}+\frac{\boldsymbol{r}_r}{2})+i(\boldsymbol{s}-\boldsymbol{r})(\boldsymbol{R}-\frac{\boldsymbol{r}_r}{2})}\right] \\
&= \int d^3r_r \frac{d^3qd^3rd^3sd^3t}{(2\pi)^{12}} U(\boldsymbol{r}_r)\Psi^*(\boldsymbol{q},\boldsymbol{r})\Phi(\boldsymbol{s},\boldsymbol{t})(2\pi)^3\delta(\boldsymbol{t}+\boldsymbol{s}-\boldsymbol{q}-\boldsymbol{r})\left[e^{i(\boldsymbol{s}-\boldsymbol{q}-\boldsymbol{t}+\boldsymbol{r})\frac{\boldsymbol{r}_r}{2}} + \xi e^{i(\boldsymbol{t}-\boldsymbol{q}-\boldsymbol{s}+\boldsymbol{r})\frac{\boldsymbol{r}_r}{2}}\right] \\
&= \int \frac{d^3qd^3rd^3sd^3t}{(2\pi)^{12}}(2\pi)^3\delta(\boldsymbol{t}+\boldsymbol{s}-\boldsymbol{q}-\boldsymbol{r})\Psi^*(\boldsymbol{q},\boldsymbol{r})\Phi(\boldsymbol{s},\boldsymbol{t})\left[\tilde{U}\left(\frac{\boldsymbol{q}-\boldsymbol{s}-\boldsymbol{r}+\boldsymbol{t}}{2}\right) + \xi\tilde{U}\left(\frac{\boldsymbol{q}-\boldsymbol{t}-\boldsymbol{r}+\boldsymbol{s}}{2}\right)\right] \\
&= \int \frac{d^3qd^3rd^3sd^3t}{(2\pi)^{12}}(2\pi)^3\delta(\boldsymbol{t}+\boldsymbol{s}-\boldsymbol{q}-\boldsymbol{r})\Psi^*(\boldsymbol{q},\boldsymbol{r})\Phi(\boldsymbol{s},\boldsymbol{t})[\tilde{U}(\boldsymbol{q}-\boldsymbol{s}) + \xi\tilde{U}(\boldsymbol{q}-\boldsymbol{t})]. \qquad (16)
\end{aligned}$$

3. Electron gas

For point like charges interacting vie the Coulomb potential,

$$U(\boldsymbol{x}) = \frac{e^2}{|\boldsymbol{x}|}$$

the Hamiltonian

$$H = H_0 + H_1 = \sum_\sigma \int d^3\boldsymbol{x}\psi^\dagger_\sigma(\boldsymbol{x})\left(-\frac{\hbar^2}{2m}\Delta\right)\psi_\sigma(\boldsymbol{x}) + \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d^3xd^3y\psi^\dagger_{\sigma_1}(\boldsymbol{x})\psi^\dagger_{\sigma_2}(\boldsymbol{y})U(\boldsymbol{x}-\boldsymbol{y})\psi_{\sigma_2}(\boldsymbol{y})\psi_{\sigma_1}(\boldsymbol{x})$$

gives in momentum space the kinetic energy

$$H_0 = \sum_\sigma \int \frac{d^3k}{(2\pi)^3} a^\dagger_\sigma(\boldsymbol{k})\frac{\hbar^2\boldsymbol{k}^2}{2m}a_\sigma(\boldsymbol{k})$$

and interaction term

$$\begin{aligned}
H_1 &= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3xd^3y\frac{d^3qd^3rd^3sd^3t}{(2\pi)^{12}}e^{i\boldsymbol{x}(\boldsymbol{s}-\boldsymbol{q})+i\boldsymbol{y}(\boldsymbol{t}-\boldsymbol{r})}U(\boldsymbol{x}-\boldsymbol{y})a^\dagger_\sigma(\boldsymbol{q})a^\dagger_{\sigma'}(\boldsymbol{r})a_{\sigma'}(\boldsymbol{t})a_\sigma(\boldsymbol{s}) \\
&= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3Rd^3r_r\frac{d^3qd^3rd^3sd^3t}{(2\pi)^{12}}e^{i(\boldsymbol{R}+\frac{1}{2}\boldsymbol{r}_r)(\boldsymbol{s}-\boldsymbol{q})+i(\boldsymbol{R}-\frac{1}{2}\boldsymbol{r}_r)(\boldsymbol{t}-\boldsymbol{r})}U(\boldsymbol{r}_r)a^\dagger_\sigma(\boldsymbol{q})a^\dagger_{\sigma'}(\boldsymbol{r})a_{\sigma'}(\boldsymbol{t})a_\sigma(\boldsymbol{s}) \\
&= \frac{1}{2}\sum_{\sigma,\sigma'}\int \frac{d^3qd^3rd^3sd^3t}{(2\pi)^{12}}(2\pi)^3\delta(\boldsymbol{q}+\boldsymbol{r}-\boldsymbol{s}-\boldsymbol{t})\tilde{U}(\boldsymbol{t}-\boldsymbol{r})a^\dagger_\sigma(\boldsymbol{q})a^\dagger_{\sigma'}(\boldsymbol{r})a_{\sigma'}(\boldsymbol{t})a_\sigma(\boldsymbol{s}) \qquad (17)
\end{aligned}$$

with

$$\tilde{U}(\boldsymbol{p}) = \frac{4\pi e^2}{p^2}.$$

It is known from classical electrodynamics that an infinite, homogeneous charge distribution electrostatic energy density is infinite in the vacuum due to the long range nature of the unscreened Coulomb potential. This infrared divergence appears in our expressions as well and it is removed by evoking that the solids are electrically neutral, the charge of the electrons is always compensated for by that of the ion core. This ion charge distribution is inhomogeneous and polarizes the electron states. In order to separate the two problems, the infrared problem due to the non-vanishing electron charge, considered now, and the polarization effect of the ion core, addressed in the band structure theory, we assume here the presence of classical positive charges distributed by a homogeneous, static density $n = N/V$ (N is the number of electron and V is the volume) which neutralizes the electron gas. The homogeneity assures that no polarization effects arises due to the presence of this artificial device introduce to eliminate the infrared divergence only. The Hamiltonian is now

$$H = H_{nn} + H_{ne} + : H_{ee} : \tag{18}$$

where the self interaction of the classical background charge is given by

$$H_{nn} = \frac{n^2}{2} \int d^3x d^3y U(\boldsymbol{x} - \boldsymbol{y}) = \frac{n^2}{2} \int d^3R d^3r U(\boldsymbol{r}) = \frac{n^2}{2} V \tilde{U}(0)$$

and the interaction energy between the electrons and the background charges is

$$H_{ne} = -n \sum_{i=1}^{N} \int d^3y U(\boldsymbol{y} - \boldsymbol{x}_i) = -nN\tilde{U}(0) = -n^2 V \tilde{U}(0)$$

The Hamiltonian in the normal ordered expression of the right hand side of Eq. (18), H_{ee}, stands for the self interaction of the electrons, given by Eq. (17) and its infrared contribution is

$$\langle 0| : H_{ee} :_{I.R.} |0\rangle = \frac{1}{2} \int_{|\boldsymbol{x}-\boldsymbol{y}|\to\infty} d^3x d^3y \psi^\dagger(\boldsymbol{x}) \psi^\dagger(\boldsymbol{y}) U(\boldsymbol{x} - \boldsymbol{y}) \psi(\boldsymbol{y}) \psi(\boldsymbol{x}) \approx \frac{n^2}{2} V \tilde{U}(0)$$

and the vacuum expectation value of the Hamiltonian (18) is infrared finite, $\mathcal{O}\left(V^0\right)$.

D. Representations of the time evolution

Once the basic observables have been identified and the Hamiltonian is known Schrödinger equation, describes the time dependence of the state vector $|\Psi(t)\rangle$. By analogy with classical field theory one expects that our quantum fields become time dependent as well in order to reproduce the usual time dependent averages known from classical field theory. How can we place the time dependence, generated in the state vector by the Schrödinger equation, into the field operator? The answer is given by recognizing that the time dependence can freely be distributed between the state vector and the observables and our expectation corresponds to one particular choice in this question.

1. Schrödinger representation

The time is a classical, external parameter in non-relativistic Quantum Mechanics. In the usual representation of the time dependence the observables are considered time independent functions of the canonical pairs of coordinates and momenta,

$$\partial_t A_S = 0$$

and the time evolution is entirely placed on the state vector, by the Schrödinger equation

$$i\hbar \partial_t |\Psi(t)\rangle_S = H |\Psi(t)\rangle_S$$

whose solution is

$$|\Psi(t)\rangle_S = U(t,t_0)|\Psi(t_0)\rangle_S$$

where $U(t,t_0)$ satisfies the equation of motion

$$i\hbar\partial_t U(t,t_0) = HU(t,t_0)$$

together with the initial condition $U(t_0,t_0) = \mathbb{1}$. The solution of these equations is

$$U(t,t_0) = e^{-\frac{i}{\hbar}(t-t_0)H}.$$

2. Heisenberg representation

Another extremity is to place all time dependence in the observables and leave the state vector time independent. This can be achieved by performing a time dependent unitary transformation,

$$|\Psi(t)\rangle_H = e^{\frac{i}{\hbar}(t-t_0)H}|\Psi(t)\rangle_S = |\Psi(t_0)\rangle_S$$

where the two representations agree for $t = t_0$. This transformation does not affect the expectation values,

$$A_H = e^{\frac{i}{\hbar}(t-t_0)H}A_S e^{-\frac{i}{\hbar}(t-t_0)H},$$

but stops the state vector,

$$i\hbar\partial_t|\Psi(t)\rangle_H = 0.$$

The equation of motion for the time dependent observables is the Heisenberg equation,

$$i\hbar\partial_t A_H = [A_H, H].$$

Let us consider as a simples exercise non-interacting, spinless particles whose Hamiltonian density is

$$H = \int \frac{d^3k}{(2\pi)^3} a^\dagger(t,\boldsymbol{k})E(\hbar\boldsymbol{k})a(t,\boldsymbol{k}). \tag{19}$$

It is the conservation of the particle number what allows the replacement of the operators by their time dependent version in this expression and the value of the time is left arbitrary. Note that the canonical commutation relations (3) are valid for arbitrary time,

$$[a(t,\boldsymbol{q}), a^\dagger(t,\boldsymbol{r})]_\xi = (2\pi)^3\delta(\boldsymbol{q}-\boldsymbol{r}), \qquad [a(t,\boldsymbol{q}), a(t,\boldsymbol{r})]_\xi = 0. \tag{20}$$

The Heisenberg equation becomes

$$\begin{aligned} i\hbar\partial_t\psi(t,\boldsymbol{x}) &= [\psi(t,\boldsymbol{x}), H] \\ &= \int \frac{d^3k d^3q}{(2\pi)^6} e^{i\boldsymbol{q}\boldsymbol{x}}E(\hbar\boldsymbol{k})[a(t,\boldsymbol{q}), a^\dagger(t,\boldsymbol{k})a(t,\boldsymbol{k})]. \end{aligned}$$

The use of the identity $[A,BC] = B[A,C]+[A,B]C$ and the canonical commutation relation (20) leads to the equations of motion

$$\begin{aligned} i\hbar\partial_t\psi(t,\boldsymbol{x}) &= \int \frac{d^3q}{(2\pi)^3} e^{i\boldsymbol{q}\boldsymbol{x}} i\hbar\partial_t a(t,\boldsymbol{q}) \\ &= \int \frac{d^3q}{(2\pi)^3} e^{i\boldsymbol{q}\boldsymbol{x}} E(\hbar\boldsymbol{q})a(t,\boldsymbol{q}) \end{aligned} \tag{21}$$

or

$$i\hbar\partial_t a(t,\boldsymbol{q}) = E(\hbar\boldsymbol{q})a(t,\boldsymbol{q})$$

whose solution is satisfying the initial condition

$$a(t_0, \boldsymbol{q}) = a(\boldsymbol{q})$$

is

$$a(t, \boldsymbol{q}) = e^{-\frac{i}{\hbar}E(\hbar\boldsymbol{q})(t-t_0)}a(\boldsymbol{q}).$$

Therefore, the time dependence of the quantum field is

$$\psi(t, \boldsymbol{x}) = \int \frac{d^3q}{(2\pi)^3} e^{-\frac{i}{\hbar}E(\hbar\boldsymbol{q})t + i\boldsymbol{q}\boldsymbol{x}} a(\boldsymbol{q}) \tag{22}$$

for $t_0 = 0$.

The time dependence obtained above make spossible to achieve a formally similar treatment for the trivial vacuum and the Fermi-sphere. Fermions with finite density are described in the grand canonical ensemble where the Hamiltonian is modified by the chemical potential,

$$H \to H - \mu \sum_\sigma \int d^3x \psi^\dagger_\sigma(t, \boldsymbol{x})\psi_\sigma(t, \boldsymbol{x}).$$

The Fermi-sphere

$$|\mu\rangle = \otimes \prod_{\hbar|\boldsymbol{k}| \le p_F} a^\dagger(\boldsymbol{k})|0\rangle$$

of the electron gas with Fermi energy μ is defined by the properties

$$a_\sigma(\boldsymbol{k})|\mu\rangle = 0 \quad \text{for } E(\hbar\boldsymbol{k}) > \mu, \qquad \text{and} \qquad a^\dagger_\sigma(\boldsymbol{k})|\mu\rangle = 0 \quad \text{for } E(\hbar\boldsymbol{k}) < \mu.$$

It is advantageous to perform a canonical transformation $a_\sigma(\boldsymbol{k}) \to b_\sigma(\boldsymbol{k})$ of the creation and destruction operators (canonical transformations preserves the canonical commutation relations) where

$$b_\sigma(\boldsymbol{k}) = \begin{cases} a^\dagger_\sigma(\boldsymbol{k}) & |\boldsymbol{k}| \le k_F \\ a_\sigma(\boldsymbol{k}) & |\boldsymbol{k}| > k_F \end{cases}.$$

We have a more homogeneous notation in this manner because $b^\dagger_\sigma(\boldsymbol{k})$ and $b_\sigma(\boldsymbol{k})$ are the creation and destruction operators, respectively, as can be seen from the canonical commutation relation,

$$[b_\sigma(\boldsymbol{k}), b^\dagger_\sigma(\boldsymbol{k'})]_- = (2\pi)^3\delta(\boldsymbol{k} - \boldsymbol{k'})$$

and from

$$b_\sigma(\boldsymbol{k})|\mu\rangle = 0.$$

The fermion field operator is then written as

$$\psi_\sigma(t, \boldsymbol{x}) = \int_{\boldsymbol{k}} e^{-i\omega_{\boldsymbol{k}}t + \boldsymbol{k}\boldsymbol{x}} a_\sigma(\boldsymbol{k}) = \psi^{(-)} + \psi^{(+)}$$

where

$$\begin{aligned} \psi^{(+)} &= \int_{\boldsymbol{k} > k_F} e^{-i\omega_{\boldsymbol{k}}t + \boldsymbol{k}\boldsymbol{x}} b_\sigma(\boldsymbol{k}) \\ \psi^{(-)} &= \int_{\boldsymbol{k} \le k_F} e^{i|\omega_{\boldsymbol{k}}|t + \boldsymbol{k}\boldsymbol{x}} b^\dagger_\sigma(\boldsymbol{k}) \end{aligned}$$

denote the positive and negative energy part of the field, defined by the condition

$$\psi^{(+)}|\mu\rangle = \psi^{(-)\dagger}|\mu\rangle = 0$$

3. Interaction representation

We considered non-interacting particles so far. When interactions are introduced, $H = H_0 + H_1$, the Hamiltonian (19) which is identified with the non-perturbed part, H_0, is completed by some higher than quadratic order terms in the quantum field, H_1. In this case the algebraic manipulation leading to Eq. (21) give nonlinear differential equation whose solution is not easy to find. One may turn to perturbation expansion by assuming that the non-quadratic part of the Hamiltonian is small compared to the quadratic part. Though the usual perturbation expansion of the Schrödinger for the state vector allows us to make some progress in this direction the perturbative solution of the Heisenberg operator equation generates a perturbation series which is too involved to work with. Thus one looks for a compromise to save the perturbation expansion by leaving the time dependence coming from the non-interacting part of the Hamiltonian in the operators and putting the more complicated but weak time dependence, generated by the interaction Hamiltonian into the state vector for which the perturbation expansion is manageable.

The removal of the time dependence due to the on-interacting dynamics is achieved by the unitary transformation

$$|\Psi(t)\rangle_i = e^{\frac{i}{\hbar}(t-t_0)H_0}|\Psi(t)\rangle_S \tag{23}$$

which transforms the operators transform as

$$A_i = e^{\frac{i}{\hbar}(t-t_0)H_0}A_S e^{-\frac{i}{\hbar}(t-t_0)H_0}.$$

The equation of motion for the state vector and the operators read

$$\begin{aligned} i\hbar\partial_t|\Psi(t)\rangle_i &= e^{\frac{i}{\hbar}(t-t_0)H_0}(-H_0+H_0+H_1)|\Psi(t)\rangle_S \\ &= H_{1i}(t)|\Psi(t)\rangle_i, \end{aligned} \tag{24}$$

and

$$i\hbar\partial_t A_i = [A_i, H_0]$$

respectively. We have thus proven that the unitary transformation (23) indeed leads to a Schrödinger equation involving the interaction Hamiltonian (taken in the interaction representation) and the free Heisenberg equation.

Notice that the free and the interaction part of the Hamiltonian do not commute and $H_{1i}(t)$ is time dependent. The formal solution of the Schrödinger equation with time-dependent Hamiltonian can be given easier in terms of chronological products. We have already introduced a modified multiplication for operators build up from the creation and destruction operators, the normal ordering. Now we introduce a third multiplication for operators which depend on the time,

$$T[A(t_1)B(t_2)] = \Theta(t_1-t_2)A(t_1)B(t_2) + \xi\Theta(t_2-t_1)B(t_2)A(t_1)$$

Such a multiplication law allows us to write the general solution of time evolution operator $U_i(t,t_0)$ which satisfies the equation of motion

$$i\hbar\partial_t U_i(t,t_0) = H_{1i}(t)U_i(t,t_0) \tag{25}$$

and expresses the solution of the Schrödinger equation (24) as

$$|\Psi(t)\rangle_i = U_i(t,t_0)|\Psi(t_0)\rangle$$

in a simple form,

$$U_i(t,t_0) = T\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t}dt' H_{1i}(t')}\right].$$

The definition of the chronological product of a function of the operators is given by means of the Taylor expanded form,

$$\begin{aligned} T\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t}dt' H_{1i}(t')}\right] &= \sum_{n=0}^{\infty}\frac{(-\frac{i}{\hbar})^n}{n!}T\left[\left(\int_{t_0}^{t}dt' H_{1i}(t')\right)^n\right] \\ &= \sum_{n=0}^{\infty}\frac{(-\frac{i}{\hbar})^n}{n!}\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_n T[H_{1i}(t_1)\cdots H_{1i}(t_n)] \end{aligned} \tag{26}$$

which leads to Eq. (25),

$$\begin{aligned}\partial_t U_i(t,t_0) &= \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar})^n}{n!} n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_{n-1} T[H_{1i}(t_1)\cdots H_{1i}(t_{n-1})H_{1i}(t)] \\ &= -\frac{i}{\hbar} H_{1i}(t) \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar})^n}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n T[H_{1i}(t_1)\cdots H_{1i}(t_n)] \\ &= -\frac{i}{\hbar} H_{1i}(t) U_i(t,t_0).\end{aligned}$$

The chronological product is a simple device to place always the Hamiltonian taken at the time t at the very left of the expressions and thereby avoiding the ambiguities arising from the non-commutativity of $H_{1i}(t)$ taken at different time.

4. Finite temperature

Finally, let us mention here another issue of time dependence, the relation between the averages of a canonical ensemble and the analytically continued Quantum Mechanics for imaginary time. The average of an observable A in the canonical ensemble described by the density matrix

$$\rho = \frac{e^{-\beta H}}{Z}$$

is

$$\ll A \gg = \mathrm{Tr}[\rho A] = \frac{1}{Z}\mathrm{Tr}[e^{-\beta H} A]$$

where $\beta = \frac{1}{k_B T}$ and

$$Z = \mathrm{Tr} e^{-\beta H}.$$

These expressions can be obtained by performing the analytic continuation for imaginary time, Wick rotation,

$$E_R = iE_I, \qquad t_R = -it_I\hbar$$

of the time evolution operator $U(t-t_0) = U(t,t_0)$ for time independent Hamiltonian as

$$\begin{aligned} U_R(t) &= e^{-\frac{i}{\hbar}tH} \to U_I(\tau) = U_R(-i\hbar\tau) = e^{-\tau H} \\ Z &= \mathrm{Tr} U_I(\beta) \\ \ll A \gg &= \frac{1}{Z}\mathrm{Tr}[U_I(\beta)A] \end{aligned}$$

The lesson is that static or equal time quantum statistical averages can be obtained by means of the Wick-rotated time evolution operator. Perturbation expansion and the interaction representation can be worked out for imaginary time with no difficulty.

E. Phonons

The part of the dynamics of solid state crystal where the particle number is not conserved is related to the ion core where the fluctuations around the equilibrium position of the ions are represented as 'elementary particles'. The elementary excitations of the ions are either internal excitations or spatial motion of the ions. Internal excitations tend to be more energetic than the spatial motion therefore, we shall consider the latter.

Let us consider a perfect crystalline structure with lattice spacing a where the equilibrium position of the α-th atom in the cluster labeled by $\boldsymbol{j}$ is

$$\boldsymbol{r}^0_{\boldsymbol{j}\alpha} = \boldsymbol{j}a + \boldsymbol{r}^0_\alpha.$$

The dynamics of the spatial motion of non-excited ions is described by the atom coordinates $\boldsymbol{r}_{\boldsymbol{j}\alpha}$. We shall assume that the temperature range and the forces acting between the ions are such that the fluctuations

$$\boldsymbol{\chi}^0_{\boldsymbol{j}\alpha} = \boldsymbol{r}_{\boldsymbol{j}\alpha} - \boldsymbol{r}^0_{\boldsymbol{j}\alpha}$$

are small compared to the lattice spacing. The classical Hamiltonian of the ion positions is taken to be

$$H = \sum_{\boldsymbol{j},\alpha} \frac{\boldsymbol{p}^2_{\boldsymbol{j}\alpha}}{2m_\alpha} + \sum_{\boldsymbol{j},\boldsymbol{j}',\alpha,\alpha'} V(\boldsymbol{r}_{\boldsymbol{j}\alpha} - \boldsymbol{r}_{\boldsymbol{j}'\alpha'})$$

where $V(\boldsymbol{r})$ is some pair potential energy for the ions and is assumed to be independent of α for simplicity. By assuming that the potential changes slowly within the range of the typical ion displacements we have

$$\begin{aligned} H \;\approx\; & \sum_{\boldsymbol{j},\alpha} \frac{\boldsymbol{p}^2_{\boldsymbol{j}\alpha}}{2m_\alpha} + \sum_{\boldsymbol{j},\boldsymbol{j}',\alpha,\alpha'} \Big[V(\boldsymbol{r}^0_{\boldsymbol{j}\alpha} - \boldsymbol{r}^0_{\boldsymbol{j}\alpha}) + (\boldsymbol{\chi}_{\boldsymbol{j}\alpha} - \boldsymbol{\chi}_{\boldsymbol{j}'\alpha'}) \cdot \boldsymbol{\nabla} V(\boldsymbol{r}^0_{\boldsymbol{j}\alpha} - \boldsymbol{r}^0_{\boldsymbol{j}\alpha}) \\ & + \frac{1}{2} (\chi_{\boldsymbol{j}\alpha} - \chi_{\boldsymbol{j}'\alpha'})^a (\chi_{\boldsymbol{j}\alpha} - \chi_{\boldsymbol{j}'\alpha'})^b \nabla_a \nabla_b V(\boldsymbol{r}^0_{\boldsymbol{j}\alpha} - \boldsymbol{r}^0_{\boldsymbol{j}\alpha}) + \mathcal{O}\left((\chi_{\boldsymbol{j}\alpha} - \chi_{\boldsymbol{j}'\alpha'})^3\right) \Big]. \end{aligned}$$

The second and the third terms on the right hand side can be dropped, the former being an irrelevant constant and the latter is vanishing in the equilibrium position around which the expansion is made. The two quadratic forms, the kinetic and the potential energies can be diagonalized simultaneously because the kinetic energy is $\boldsymbol{j}$-independent for each fixed α. The basis where both are diagonal gives the normal modes, the phonon degrees of freedom. The change to the diagonal basis is written as

$$\begin{aligned} \boldsymbol{\chi}_{\boldsymbol{j}\alpha} &= \sum_\lambda \int \frac{d^3k}{(2\pi)^3} \chi_\lambda(\boldsymbol{k}) \boldsymbol{e}^\lambda_\alpha(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{j}a} \\ \boldsymbol{p}_{\boldsymbol{j}\alpha} &= \sum_\lambda \int \frac{d^3k}{(2\pi)^3} \pi_\lambda(\boldsymbol{k}) \boldsymbol{e}^\lambda_\alpha(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{j}a} \end{aligned}$$

leading to $\chi_\lambda(\boldsymbol{k})$ and $\pi_\lambda(\boldsymbol{k})$ as phonon coordinates and momenta, respectively. The continuous, wave number quantum number $\boldsymbol{k}$ appears in the diagonal basis because the phonons provides a representation of the discrete translation symmetry of the crystal. The quantum number λ takes care of the remaining discrete labels and called band quantum number. The value of the wave vector $\boldsymbol{k}$ is then restricted to the first Brillouin zone in this manner. The phonon quantum field, the coordinate expressed in terms of creation and destruction operators by inverting the relations (2), is written

$$\boldsymbol{\chi}(t,\boldsymbol{x}) = \sum_\lambda \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{\hbar}{2m_\lambda \omega_\lambda(\boldsymbol{k})}} [\boldsymbol{e}^\lambda_\alpha(\boldsymbol{k}) e^{-i\omega_\lambda(\boldsymbol{k})t + i\boldsymbol{x}\boldsymbol{k}} c_\lambda(\boldsymbol{k}) + \boldsymbol{e}^{\lambda *}_\alpha(\boldsymbol{k}) e^{i\omega_\lambda(\boldsymbol{k})t + i\boldsymbol{x}\boldsymbol{k}} c^\dagger_\lambda(-\boldsymbol{k})]$$

in the continuum limit. The minus sign in the argument of $c^\dagger$ on the right hand side is needed to make the phonon field hermitian, $\boldsymbol{\chi}^\dagger(t,\boldsymbol{x}) = \boldsymbol{\chi}(t,\boldsymbol{x})$.

The quadratic part of the Hamiltonian defines the noninteracting phonon dynamics,

$$H_{ph} = \sum_\lambda \int \frac{d^3k}{(2\pi)^3} \left[\frac{\pi^2_\lambda(\boldsymbol{k})}{2m_\lambda} + \frac{m_\lambda \omega^2_\lambda}{2} \chi^2_\lambda(\boldsymbol{k}) \right]$$

and the remaining terms

$$H_i = \frac{1}{3!} \sum_{\boldsymbol{j},\boldsymbol{j}',\alpha,\alpha'} (\chi_{\boldsymbol{j}\alpha} - \chi_{\boldsymbol{j}'\alpha'})^a (\chi_{\boldsymbol{j}\alpha} - \chi_{\boldsymbol{j}'\alpha'})^b (\chi_{\boldsymbol{j}\alpha} - \chi_{\boldsymbol{j}'\alpha'})^c \nabla_a \nabla_b \nabla_c V(\boldsymbol{r}^0_{\boldsymbol{j}\alpha} - \boldsymbol{r}^0_{\boldsymbol{j}\alpha}) + \cdots$$

stand for the interactions among the photons can be taken into account in the framework of the perturbation expansion but will be ignored in what follows.

The change to the normal mode basis introduces automatically the system of harmonic oscillators which was evoked in the case of electrons in an indirect manner. The quantum treatment of the oscillators is achieved by introducing

the creation and destruction operators, $c^\dagger_\lambda(\boldsymbol{k})$ and $c_\lambda(\boldsymbol{k})$, respectively for phonons with the non-vanishing commutator relations being

$$[c_\lambda(\boldsymbol{k}), c^\dagger_{\lambda'}(\boldsymbol{k'})]_+ = (2\pi)^3\delta(\boldsymbol{k}-\boldsymbol{k'})\delta_{\lambda,\lambda'}.$$

The Hamiltonian for non-interacting phonons is

$$H_{ph} = \sum_\lambda \int \frac{d^3k}{(2\pi)^3}\hbar\omega_\lambda(\boldsymbol{k})c^\dagger_\lambda(\boldsymbol{k})c_\lambda(\boldsymbol{k})$$

after dropping an unimportant constant, coming from the zero point fluctuations.

The quantum field for electrons propagating in the presence of the periodic core potential is

$$\psi_\sigma(\boldsymbol{x}) = \int \frac{d^3q}{(2\pi)^3}a_\sigma(\boldsymbol{q})\phi_{\sigma\boldsymbol{q}}(\boldsymbol{x})$$

where $\phi_{\sigma\boldsymbol{q}}(\boldsymbol{x})$ is the Bloch wave function and the Hamiltonian containing their kinetic and the potential energy reads

$$H = \sum_\sigma \int d^3x\psi^\dagger_\sigma(\boldsymbol{x})\left(-\frac{\hbar^2}{2m}\Delta\right)\psi_\sigma(\boldsymbol{x}) + \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d^3xd^3y\psi^\dagger_{\sigma_1}(\boldsymbol{x})\psi^\dagger_{\sigma_2}(\boldsymbol{y})U_{ee}(\boldsymbol{x}-\boldsymbol{y})\psi_{\sigma_2}(\boldsymbol{y})\psi_{\sigma_1}(\boldsymbol{x}).$$

The interaction energy between electrons and the ion core,

$$H_i = \sum_{\boldsymbol{j},\alpha}\int d^3xU_{en}(\boldsymbol{x}-\boldsymbol{r}_{\boldsymbol{j}\alpha}),$$

with $n(\boldsymbol{x}) = \psi^\dagger_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})$ being the density, is rewritten by expanding in the fluctuations of the ions around the equilibrium positions,

$$H_i = \sum_{\boldsymbol{j},\alpha}\int d^3xn(\boldsymbol{x})U_{en}(\boldsymbol{x}-\boldsymbol{r}^0_{\boldsymbol{j}\alpha}) - \sum_{\boldsymbol{j},\alpha}\int d^3xn(\boldsymbol{x})\boldsymbol{\chi}_{\boldsymbol{j}\alpha}\boldsymbol{\nabla}U_{en}(\boldsymbol{x}-\boldsymbol{r}^0_{\boldsymbol{j}\alpha}) + \mathcal{O}\left(\boldsymbol{\chi}^2\right).$$

The first term on the right hand side is responsible for the formation of the band structure and can be ignored when the Bloch wave functions are used for the one-particle states. In fact the Bloch wavefunctions already take into account the preiodic ion core potential. The ignored $\mathcal{O}\left(\boldsymbol{\chi}^2\right)$ terms renormalize the phonon dispersion relation $\omega_\lambda(\boldsymbol{k})$ and introduce further phonon-electron interactions. They will be ignored. Therefore, we are lead to

$$H_i = -\sum_{\boldsymbol{j},\alpha}\int d^3xn(\boldsymbol{x})\boldsymbol{\chi}_{\boldsymbol{j}\alpha}\boldsymbol{\nabla}U_{en}(\boldsymbol{x}-\boldsymbol{r}^0_{\boldsymbol{j}\alpha})$$

what is rewritten by inserting the electron field in terms of the creation and destruction operators,

$$H_i = -\sum_{\boldsymbol{j},\alpha,\sigma}\int d^3x\frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3}\phi^*_{\sigma\boldsymbol{p}}(\boldsymbol{x})\phi_{\sigma\boldsymbol{p}'}(\boldsymbol{x})a^\dagger_\sigma(\boldsymbol{p})a_\sigma(\boldsymbol{p'})\boldsymbol{\chi}_{\boldsymbol{j}\alpha}\boldsymbol{\nabla}U_{en}(\boldsymbol{x}-\boldsymbol{r}^0_{\boldsymbol{j}\alpha}).$$

In the next step we perform the shift $\boldsymbol{x}\to\boldsymbol{x}+\boldsymbol{j}a$ of the integral variable,

$$H_i = -\sum_\sigma\int\frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3}a^\dagger_\sigma(\boldsymbol{p})a_\sigma(\boldsymbol{p'})\sum_{\boldsymbol{j},\alpha}\int d^3x\phi^*_{\sigma\boldsymbol{p}}(\boldsymbol{x}+\boldsymbol{j}a)\phi_{\sigma\boldsymbol{p}'}(\boldsymbol{x}+\boldsymbol{j}a)\boldsymbol{\nabla}U_{en}(\boldsymbol{x}-\boldsymbol{r}^0_\alpha)\boldsymbol{\chi}_{\boldsymbol{j}\alpha}.$$

By means of the periodicity of the Bloch functions,

$$\phi_{\sigma\boldsymbol{p}}(\boldsymbol{x}+\boldsymbol{j}a) = \phi_{\sigma\boldsymbol{p}}(\boldsymbol{x})e^{i\boldsymbol{p}\boldsymbol{j}a},$$

we have

$$H_i = \sum_\sigma\int\frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3}a^\dagger_\sigma(\boldsymbol{p})a_\sigma(\boldsymbol{p'})\sum_{\boldsymbol{j},\alpha}e^{i(\boldsymbol{p'}-\boldsymbol{p})\boldsymbol{j}a}\boldsymbol{W}_\alpha(\boldsymbol{p},\boldsymbol{p'})\boldsymbol{\chi}_{\boldsymbol{j}\alpha}$$

with

$$\boldsymbol{W}_\alpha(\boldsymbol{p},\boldsymbol{p}') = -\int d^3x \phi^*_{\sigma\boldsymbol{p}}(\boldsymbol{x})\phi_{\sigma\boldsymbol{p}'}(\boldsymbol{x})\boldsymbol{\nabla}U_{en}(\boldsymbol{x}-\boldsymbol{r}^0_\alpha).$$

The insertion of the phonon coordinate in terms of the creation and destruction operators,

$$\chi_\lambda(\boldsymbol{k}) = \sqrt{\frac{\hbar}{2m_\lambda\omega_\lambda(\boldsymbol{k})}}[c_\lambda(\boldsymbol{k}) + c^\dagger_\lambda(-\boldsymbol{k})],$$

produces

$$\begin{aligned} H_i &= \sum_\sigma \int \frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3} a^\dagger_\sigma(\boldsymbol{p})a_\sigma(\boldsymbol{p}') \sum_{\boldsymbol{j},\alpha} e^{i(\boldsymbol{p}'-\boldsymbol{p})\boldsymbol{j}a}\boldsymbol{W}_\alpha(\boldsymbol{p},\boldsymbol{p}') \sum_\lambda \int \frac{d^3k}{(2\pi)^3}\chi_\lambda(\boldsymbol{k})\boldsymbol{e}^\lambda_\alpha(\boldsymbol{k})e^{i\boldsymbol{k}\boldsymbol{j}a} \\ &= \sum_\sigma \int \frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3} a^\dagger_\sigma(\boldsymbol{p})a_\sigma(\boldsymbol{p}') \sum_{\alpha,\lambda} \boldsymbol{W}_\alpha(\boldsymbol{p},\boldsymbol{p}')\chi_\lambda(\boldsymbol{p}-\boldsymbol{p}'+\boldsymbol{K})\boldsymbol{e}^\lambda_\alpha(\boldsymbol{p}-\boldsymbol{p}'+\boldsymbol{K}), \end{aligned}$$

$\boldsymbol{K}$ being such a vector in the reciprocal lattice for which $\boldsymbol{p}-\boldsymbol{p}'+\boldsymbol{K}$ falls into the first Brillouin zone. Finally, on introduces the form factor

$$g_\lambda(\boldsymbol{p},\boldsymbol{p}') = \sum_\alpha \boldsymbol{W}_\alpha(\boldsymbol{p},\boldsymbol{p}')\boldsymbol{e}^\lambda_\alpha(\boldsymbol{p}-\boldsymbol{p}'+\boldsymbol{K})\sqrt{\frac{\hbar}{2m_\lambda\omega_\lambda(\boldsymbol{p}-\boldsymbol{p}'+\boldsymbol{K})}}$$

what allows us to write

$$H_i = \sum_{\sigma,\lambda}\int \frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3} g_\lambda(\boldsymbol{p},\boldsymbol{p}')a^\dagger_\sigma(\boldsymbol{p})a_\sigma(\boldsymbol{p}')[c_\lambda(\boldsymbol{p}-\boldsymbol{p}'+\boldsymbol{K}) + c^\dagger_\lambda(-\boldsymbol{p}+\boldsymbol{p}'-\boldsymbol{K})]$$

where the second term in the square bracket is to assure the hermicity of the Hamiltonian.

III. GREEN FUNCTIONS

The construction of observables in terms of canonical conjugate coordinates and momenta or the creation and destruction operators, together with the canonical commutation relations define the algebraic structure in which any usual quantum mechanical calculation can in principle be carried out. But even a modest goal leads to enormous complications as soon as interactions are introduced. Therefore, one needs some new elements to render the perturbation expansion easier. Such a help will come from the introduction of Green functions.

The need of considering transition amplitudes rather than quantum states and observables in a separated manner actually comes from Relativistic Quantum Mechanics. An unexpected obstacle is encountered when the causal structure of Special Relativity is imposed on Quantum Mechanics: the state vector of the system is not relativistic covariant and even worst, not always well defined during the time the system evolves. Despite this complication the transition amplitudes between states observed at certain times preserve the expected relativistical structure. Therefore, one expresses the expectation values of observables in terms of well defined transition amplitudes, called Green functions. Apart of such a conceptual need, this change in the formalism responds to the need mentioned in the preceding paragraph and makes the calculation of expectation values simpler.

A related advantage arising from the use of Green functions is the decoupling of the spectator particles from the active ones. Let us suppose that we are interested in the expectation value of an n-body operator. In a many body system where the elementary interactions are supposed to be simple, pair interactions one expects that at low order of the perturbation expansion few particles participate only in the interactions with our n particles. These few particles are called active ones and the particles in the rest of the system are the spectators. The perturbation expansion should be organized in such a manner that the increased accuracy, the increased order of the expansion should increase gradually the number of active particles, the amount of work to obtain the result. We shall see that the introduction of Green functions which correspond to transition amplitudes for a given number of particles seems to be just the right object to achieve this goal.

We shall introduce first the Green functions for non-interacting particles in this chapter. The spectral representation, discussed in Appendix B, offers an insight into the structure of the interacting propagators. The explicit form of the interactive Green functions will be given by means of perturbation expansion in the Chapter IV.

A. Electrons

1. Definition

Let us consider two states of an electron,

$$|\Psi_i^{(e)}\rangle = \psi^\dagger_{\alpha_i}(t_i,\boldsymbol{p}_i)|\mu\rangle, \qquad |\Psi_f^{(e)}\rangle = \psi^\dagger_{\alpha_f}(t_f,\boldsymbol{p}_f)|\mu\rangle,$$

and for a hole,

$$|\Psi_i^{(h)}\rangle = \psi_{\alpha_i}(t_i,\boldsymbol{p}_i)|\mu\rangle, \qquad |\Psi_f^{(h)}\rangle = \psi_{\alpha_f}(t_f,\boldsymbol{p}_f)|\mu\rangle,$$

for $t_f > t_i$. Their overlaps,

$$\mathcal{A}^{(e)} = \langle\mu|\psi_{\alpha_f}(t_f,\boldsymbol{p}_f)\psi^\dagger_{\alpha_i}(t_i,\boldsymbol{p}_i)|\mu\rangle, \qquad \mathcal{A}^{(h)} = \langle\mu|\psi^\dagger_{\alpha_f}(t_f,\boldsymbol{p}_f)\psi_{\alpha_i}(t_i,\boldsymbol{p}_i)|\mu\rangle$$

are the transition amplitudes of the initial state into the final one. In fact, these amplitudes, written in the Schrödinger representation,

$$\begin{aligned}
\mathcal{A}^{(e)} &= \langle\mu|e^{\frac{i}{\hbar}(t_f-t_0)H}\psi_{\alpha_f}(\boldsymbol{p}_f)e^{-\frac{i}{\hbar}(t_f-t_0)H}e^{\frac{i}{\hbar}(t_i-t_0)H}\psi^\dagger_{\alpha_i}(\boldsymbol{p}_i)e^{-\frac{i}{\hbar}(t_i-t_0)H}|\mu\rangle \\
&= \langle\mu|\psi_{\alpha_f}(\boldsymbol{p}_f)e^{-\frac{i}{\hbar}(t_f-t_i)H}\psi^\dagger_{\alpha_i}(\boldsymbol{p}_i)|\mu\rangle, \\
\mathcal{A}^{(h)} &= \langle\mu|\psi^\dagger_{\alpha_f}(\boldsymbol{p}_f)e^{-\frac{i}{\hbar}(t_f-t_i)H}\psi_{\alpha_i}(\boldsymbol{p}_i)|\mu\rangle,
\end{aligned}$$

give the amplitude of propagation of an electron or hole. Naturally these amplitudes are non-vanishing for $\boldsymbol{p}_i \neq \boldsymbol{p}_f$ in the presence of an external potential only. Both amplitudes are defined for $t_i < t_f$ which allows to pack then together into a single function, called the causal or Feynman propagator,

$$i\hbar G_{\alpha\beta}((t,\boldsymbol{p}),(t'\boldsymbol{p}')) = \langle\mu|T[\psi_\alpha(t,\boldsymbol{p})\psi^\dagger_\beta(t',\boldsymbol{p}')]|\mu\rangle = \Theta(t-t')\langle\mu|\psi_\alpha(t,\boldsymbol{p})\psi^\dagger_\beta(t',\boldsymbol{p}')|\mu\rangle + \xi\Theta(t'-t)\langle\mu|\psi^\dagger_\beta(t',\boldsymbol{p}')\psi_\alpha(t,\boldsymbol{p})|\mu\rangle$$

whose real-space version is

$$i\hbar G_{\alpha\beta}(x,x') = \langle 0|T[\psi_\alpha(x)\psi^\dagger_\beta(x')]|0\rangle = \langle 0|\Theta(t-t')\psi_\alpha(x)\psi^\dagger_\beta(x') + \xi\Theta(t'-t)\psi^\dagger_\beta(x')\psi_\alpha(x)|0\rangle \tag{27}$$

will be used in the perturbation expansion therefore, it is defined in terms of the chronological product, cf. Eq. (26), the starting point for this expansion. The vacuum state $|0\rangle$ should naturally be replaced by the Fermi sphere $|\mu\rangle$ at finite density, $\mu \neq 0$. The chronological product allows us to keep both the particle and the hole propagation amplitude in the same, common function. But there is a price for this convenience. The causal propagator $i\hbar G_{\alpha\beta}(x,x')$ gives the transition amplitude of a particle created at time t' and captured at time t. In case of holes the process of creation is at time t and the hole is captured at time t'. This remark, without regarding into Eq. (27) gives the impression that holes propagate in an opposite direction in time than particles. Such a formal point of view is further supported by noting that the hole excitations must have positive energies. Thus the phase factor $e^{-\frac{i}{\hbar}Et}$ corresponding to the time evolution of an energy eigenstate requires the change $t \to -t$ in order to produce the expected time evolution for a state with $E = E(\hbar\boldsymbol{k}) - \mu < 0$. But there is no well-defined meaning in the word 'direction of time' as used in the preceding sentences. This is simply another problem which is settled by the second quantized formalism in a consistent manner.

The numerical value of the causal propagator is a transition amplitude. But most many body system problem aims at expectation values of observables. To obtain an expectation value the retarded and advanced propagators,

$$\begin{aligned}
i\hbar G^R_{\alpha\beta}(x,x') &= \langle 0|[\psi_\alpha(x),\psi^\dagger_\beta(x')]_-0\rangle\Theta(t-t') \\
i\hbar G^A_{\alpha\beta}(x,x') &= -\langle 0|[\psi_\alpha(x),\psi^\dagger_\beta(x')]_-0\rangle\Theta(t'-t)
\end{aligned}$$

prove to be useful. Naturally, the knowledge of the causal propagator is sufficient in principle but the resulting expressions for the expectation values are simpler when written in terms of retarded or advanced Green functions.

Finally, thermal averages in equilibrium can easily be expressed in terms of the imaginary time propagator,

$$\hbar G^E_{\alpha\beta}(x,x') = -\langle 0|T[\psi_\alpha(x)\psi^\dagger_\beta(x')]|0\rangle,$$

where the time argument parameterizes the imaginary time axis and the chronological product is defined according to this parameter.

Green functions can be introduced for more particles, in particular the two-particle causal Green function is

$$-\hbar^2 G_{\alpha_1\alpha_2\beta_1\beta_2}(x_1,x_2,x_1',x_2') = \langle 0|T[\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\psi^\dagger_{\beta_1}(x_1')\psi^\dagger_{\beta_2}(x_2')]|0\rangle,$$

etc.

2. Relation to expectation values

Vacuum expectation values of one-body operators can be expressed in terms of one-particle causal functions, eg. the expectation value of the density

$$n(x) = \sum_\alpha \psi_\alpha^\dagger(x)\psi_\alpha(x)$$

is

$$\langle 0|n(x)|0\rangle = -i\hbar \mathrm{tr} G((t,\boldsymbol{x}),(t+\eta,\boldsymbol{x}))$$

with $\eta = 0^+$. The expectation value of the kinetic energy

$$T = \int d^3x \psi_\alpha^\dagger(\boldsymbol{x}) E\left(\frac{\hbar}{i}\boldsymbol{\nabla}\right)\psi_\alpha(\boldsymbol{x})$$

can be written as

$$\langle 0|T|0\rangle = -i\hbar \int d^3x d^3y \delta(\boldsymbol{x}-\boldsymbol{y}) \mathrm{tr} E\left(\frac{\hbar}{i}\boldsymbol{\nabla}_{\boldsymbol{x}}\right) G((\boldsymbol{x},t),(\boldsymbol{y},t+\eta))$$

The vacuum expectation values of two-body operators are expressed by means of two-particle Green function, eg. the interaction energy

$$:U(t) := \frac{1}{2}\int d^3\boldsymbol{x} d^3\boldsymbol{y} \psi_\alpha^\dagger(\boldsymbol{x},t)\psi_\beta^\dagger(\boldsymbol{y},t)U(\boldsymbol{x}-\boldsymbol{y})\psi_\beta(\boldsymbol{y},t)\psi_\alpha(\boldsymbol{x},t)$$

gives the leading order energy shift

$$\langle 0|:U(t):|0\rangle = \frac{\hbar^2}{2}\int d^3\boldsymbol{x} d^3\boldsymbol{y} G_{\beta\alpha\alpha\beta}((\boldsymbol{y},t),(\boldsymbol{x},t),(\boldsymbol{x},t+2\eta),(\boldsymbol{y},t+\eta))U(\boldsymbol{x}-\boldsymbol{y}).$$

in the vacuum.

The retarded and advanced propagators are useful to express expectation values of observables in excited states. The imaginary time Green functions facilitate the calculation of expectation values in thermal equilibrium.

3. Equation of motion

An explicit expression for the causal propagator can be obtained by means of the equation of motion

$$\left[i\hbar\partial_t - E\left(\frac{\hbar}{i}\boldsymbol{\nabla}\right)\right]\psi(x) = 0$$

for the field $\psi(x)$, the equation which governs the time evolution of the transition amplitudes. Let us start with the relation

$$\begin{aligned}
\left[i\hbar\partial_t - E\left(\frac{\hbar}{i}\boldsymbol{\nabla}_x\right)\right] T[\psi(x)\psi^\dagger(x')] &= \left[i\hbar\partial_t - E\left(\frac{\hbar}{i}\boldsymbol{\nabla}_x\right)\right][\Theta(t-t')\psi(x)\psi^\dagger(x') + \xi\Theta(t'-t)\psi^\dagger(x')\psi(x)] \\
&= T\left[\left[i\hbar\partial_t - E\left(\frac{\hbar}{i}\boldsymbol{\nabla}_x\right)\right]\psi(x)\psi^\dagger(x')\right] + i\hbar\delta(t-t')\underbrace{[\psi(x),\psi^\dagger(x')]_\xi}_{\delta(\boldsymbol{x}-\boldsymbol{x'})\mathbb{1}} \\
&= i\hbar\delta(x-x')\mathbb{1} \qquad (28)
\end{aligned}$$

where the canonical commutation relation was used in the second equation. The vacuum expectation value of this equation,

$$\left[i\hbar\partial_t - E\left(\frac{\hbar}{i}\boldsymbol{\nabla}\right)\right] G_{\alpha\beta}(x,x') = \delta(x-x') \qquad (29)$$

follows for the causal propagator, justifying the name Green function, borrowed from the theory of linear differential equations. One can actually extract more information from Eq. (28). The null-space of the equation of motion operator, $i\hbar\partial_t - E\left(\frac{\hbar}{i}\boldsymbol{\nabla}_x\right)$, consists of the time dependent one-particle wave functions which solve the Schrödinger equation and this equation shows that the Fock-space operator $T[\psi(x)\psi^\dagger(x')]$ is a c-number times the identity operator of the Fock-space for wave function outside of the null-space.

The formal solution of Eq. (29), given in terms of the Fourier integral

$$i\hbar G(x,x') = i\int \frac{d^3k d\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})} \tag{30}$$

with $\hbar\omega(\boldsymbol{k}) = E(\hbar\boldsymbol{k})$, is not well defined due to the zero modes of the differential operator $i\hbar\partial_t - E(\frac{\hbar}{i}\boldsymbol{\nabla})$. In fact, one can add the expression,

$$i\hbar G(x,x') \to i\hbar G(x,x') + \int \frac{d^3k}{(2\pi)^3} f(\boldsymbol{k}) e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} \tag{31}$$

to the propagator with an arbitrary $f(\boldsymbol{k})$ without affecting the defining relation (29). The zero modes where the propagator is not yet well defined are just the free one-particle wave functions, the most important type of functions as far as the physical relevance is concerned.

The way out from this dilemma and the actual form of $f(\boldsymbol{k})$ comes from the boundary conditions in time on the propagator, just as Green functions are uniquely defined in the theory of linear differential equations. Our goal is to develop a formalism to deal with, among other problems, the interactions of atoms and photons. We know in this case that the atoms should be found in their ground state after being exposed to the interaction with electromagnetic field for long enough time. In fact, let us suppose that an atom is in its excited state at the initial time. With some probability it will be de-excited and one or several photons will be emitted. The probability of capturing these photons by the same or another atom is vanishing in the thermodynamical limit, where the volume available for the photons tends to infinity. Thus the final boundary condition in time is that all excited state must decay and we recover the ground state. Holes or negative energy states appear as propagating backward in time therefore, the should be no holes, or anti-particles in the language of high energy physics, in the initial state. The form of the function $f(\boldsymbol{k})$ should be chosen in such a manner that these boundary condition are satisfied.

From the point of view of mathematics the extra additive contribution, parameterized by the function $f(\boldsymbol{k})$, can be build into the Fourier integral (30) by adding Dirac-delta contributions. This latter can be obtained by certain prescription about avoiding the poles of the integrand of the Fourier integral appearing at the zero modes. The simplest, heuristic way of finding this prescription is to note that the slow, adiabatic decay of excited states can be achieved by assigning an infinitesimally small, negative imaginary part of the one-particle energies, $\omega(\boldsymbol{k}) \to \omega(\boldsymbol{k}) - i\epsilon$ for $\omega(\boldsymbol{k}) > 0$ with $\epsilon = 0^+$. In fact, the time dependence of the state vector of the excited state, $e^{-it(\omega(\boldsymbol{k})-i\epsilon)}|\Psi\rangle$ introduced by this imaginary part makes the state slowly disappearing, $e^{-it(\omega(\boldsymbol{k})-i\epsilon)}|\Psi\rangle \to 0$, as $t \to \infty$. For negative energy states the modification of the energy level is $\omega(\boldsymbol{k}) \to \omega(\boldsymbol{k}) + i\epsilon$, leading to $e^{-it(\omega(\boldsymbol{k})+i\epsilon)}|\Psi\rangle \to 0$ for $t \to -\infty$.

A more systematical way to arrive to the same result is to calculate directly (27) by means of the Fourier representation

$$\Theta(t) = i\int \frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{\omega+i\epsilon}$$

of the Heavyside-function. We use the Fourier integral

$$\psi(x) = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{k}\boldsymbol{x}} a(\boldsymbol{k})$$

for the quantum field and

$$\hbar\omega(\boldsymbol{k}) = \frac{\hbar^2\boldsymbol{k}^2}{2m} - \mu$$

which yield spin-independent propagators,

$$\begin{aligned}
G_{\alpha\beta}(x,x') &= \delta_{\alpha\beta}G(x,x') \\
G^R_{\alpha\beta}(x,x') &= \delta_{\alpha\beta}G^R(x,x') \\
G^A_{\alpha\beta}(x,x') &= \delta_{\alpha\beta}G^A(x,x') \\
G^E_{\alpha\beta}(x,x') &= \delta_{\alpha\beta}G^E(x,x').
\end{aligned}$$

The causal propagators reads

$$\begin{aligned}
i\hbar G(x,x') &= \langle 0|\Theta(t-t')\psi(x)\psi^\dagger(x') - \Theta(t'-t)\psi^\dagger(x')\psi(x)|0\rangle \\
&= i\int_{|\boldsymbol{k}|>k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')}}{\omega+i\epsilon}e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} - i\int_{|\boldsymbol{k}|<k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t'-t)}}{\omega+i\epsilon}e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} \\
&= i\int_{|\boldsymbol{k}|>k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon} - i\int_{|\boldsymbol{k}|<k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(\omega(\boldsymbol{k})-\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon} \\
&= i\int_{|\boldsymbol{k}|>k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})+i\epsilon} - i\int_{|\boldsymbol{k}|<k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+\omega(\boldsymbol{k})+i\epsilon} \\
&= i\int_{|\boldsymbol{k}|>k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})+i\epsilon} + i\int_{|\boldsymbol{k}|<k_F} \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')-i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})-i\epsilon} \\
&= i\int_{\boldsymbol{k}} \frac{d^3k}{(2\pi)^3}\int\frac{d\omega}{2\pi}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})+i\mathrm{sign}(\omega(\boldsymbol{k}))\epsilon}.
\end{aligned}$$

We find in the energy-momentum variables $(E,\boldsymbol{p})$

$$\begin{aligned}
\hbar G(E,\boldsymbol{p}) &= \int dtd^3x e^{\frac{i}{\hbar}\omega t-\frac{i}{\hbar}\boldsymbol{px}}\hbar G((t,\boldsymbol{x}),0) \\
&= \frac{\hbar}{E-E(\boldsymbol{p})+i\mathrm{sign}(E(\boldsymbol{k}))\epsilon}
\end{aligned}$$

where $E(\boldsymbol{k})=\hbar\omega(\boldsymbol{k})$ is the one particle energy and $\boldsymbol{p}=\hbar\boldsymbol{k}$.

Few remarks are in order at this point.

1. The propagator $\hbar G(x,x')$, a measure of quantum fluctuations, is $\mathcal{O}(\hbar)$ because $\hbar G(x,x')$ was obtained by applying the canonical commutation relations whose non-vanishing part is $\mathcal{O}(\hbar)$.

2. The order of the integration is written explicitely in the last equation because Fubini theorem does not hold for this multiple integral without uniform convergence. One has always to perform the frequency integration first in dealing with propagators, followed by the integration of the spatial quantum numbers.

3. The relation

$$\frac{1}{x\pm i\epsilon} = P\frac{1}{x}\mp i\pi\delta(x) \tag{32}$$

where P denotes the principal value integral allows as to write

$$i\hbar G(x,x') = i\int_{\boldsymbol{k}}\frac{d^3k}{(2\pi)^3}P\int\frac{d\omega}{2\pi}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})} + \mathrm{sign}(\omega(\boldsymbol{k}))\pi\int_{\boldsymbol{k}}\frac{d^3k}{(2\pi)^3}e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})},$$

cf. Eq. (31).

4. The systematic derivation, based on the Fourier-integral representation of the Heavyside-function does not contain any consideration on the boundary conditions in time. But gives no clue about the direction of the flow of the physical time, neither. What the $i\epsilon$ term does is an infinitesimally weak breakdown of the time inversion symmetry. Such a symmetry breaking renders the differential operator $i\hbar\partial_t - E(\frac{\hbar}{i}\boldsymbol{\nabla})$ invertible and the propagator well defined. Had we broken the time inversion symmetry in the opposite way (suppression of excited and negative energy states for $t\to\infty$ and $t\to\infty$, respectively) the experimentally observed time evolution would have been reproduced after a time inversion transformation, $t\to -t$.

5. The infinitesimally weak explicit symmetry breaking leaving finite trace in the dynamics is the hallmark of spontaneous symmetry breaking. This suggests that the breakdown of the time inversion symmetry is spontaneous in Quantum Field Theory. This idea seems to be further supported by the need of the thermodynamical limit mentioned in the heuristic argument, to break the symmetry. (No spontaneous symmetry breaking in finite systems!) This scenario is confirmed by more detailed calculations.

The calculation of the retarded and advanced propagators,

$$\begin{aligned} i\hbar G^R(x,x') &= i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')}}{\omega+i\epsilon}e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} \\ &= i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon} \\ &= i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})+i\epsilon}, \end{aligned}$$

and

$$\begin{aligned} i\hbar G^A(x,x') &= -i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t'-t)}}{\omega+i\epsilon}e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} \\ &= -i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(\omega(\boldsymbol{k})-\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon} \\ &= -i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{-\omega+i\epsilon} \\ &= i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-i\epsilon} \\ &= i\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})-i\epsilon}, \end{aligned}$$

proceeds in similar manner,

The imaginary time propagator and be obtained with no difficulty,

$$\begin{aligned} \hbar G(x,x') &= -i\int_{|\boldsymbol{k}|>k_F}\frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')}}{\omega+i\epsilon}e^{-\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} - i\int_{|\boldsymbol{k}|<k_F}\frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t'-t)}}{\omega+i\epsilon}e^{-\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} \\ &= -i\int_{|\boldsymbol{k}|>k_F}\frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(-i\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon} - i\int_{|\boldsymbol{k}|<k_F}\frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i(-i\omega(\boldsymbol{k})-\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon} \\ &= -i\underbrace{\int_{|\boldsymbol{k}|>k_F}\frac{d^3kd\omega}{(2\pi)^4}}_{\omega\to\omega+i\omega(\boldsymbol{k})}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\omega(\boldsymbol{k})+i\epsilon} - i\underbrace{\int_{|\boldsymbol{k}|<k_F}\frac{d^3kd\omega}{(2\pi)^4}}_{\omega\to\omega-i\omega(\boldsymbol{k})}\frac{e^{i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-i\omega(\boldsymbol{k})+i\epsilon} \\ &= -i\int_{|\boldsymbol{k}|>k_F}\frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\omega(\boldsymbol{k})+i\epsilon} + i\underbrace{\int_{|\boldsymbol{k}|<k_F}\frac{d^3kd\omega}{(2\pi)^4}}_{\omega\to-\omega}\frac{e^{-i\omega(t-t')-i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\omega(\boldsymbol{k})-i\epsilon} \\ &= \int\frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{i\omega-\omega(\boldsymbol{k})} \end{aligned}$$

The poles of the causal propagators is shown on Fig. 4 together with the analytical continuation, called Wick rotation $t_R = -it_I$ and $\omega_R = i\omega_I - \omega(\boldsymbol{k})$, yielding the imaginary time Green functions. All poles of the retarded and advanced Green functions are on the lower and upper half of the complex frequency plane, respectively.

It is interesting to observe that the propagator, considered on the complex frequency plane, displays (anti)periodicity in the imaginary direction with (anti)period length $\beta = 1/k_BT$. Let us consider the purely imaginary time difference for simplicity,

$$\hbar G^E((t,\boldsymbol{x}),(0,\boldsymbol{x'})) = -Tre^{-\beta H}T[\psi(t,\boldsymbol{x})\psi^\dagger(0,\boldsymbol{x'})]$$

for $0 \le t \le \beta$ what we write as

$$\hbar G^E((t,\boldsymbol{x}),(0,\boldsymbol{x'})) = -Tre^{-\beta H}\psi(t,\boldsymbol{x})\psi^\dagger(0,\boldsymbol{x'}).$$

We can shift the imaginary time argument,

$$\begin{aligned} \hbar G^E((t-\beta,\boldsymbol{x}),(0,\boldsymbol{x'})) &= -\xi Tre^{-\beta H}\psi^\dagger(0,\boldsymbol{x'})\psi(t-\beta,\boldsymbol{x}) \\ &= -\xi Tre^{-\beta H}\psi^\dagger(0,\boldsymbol{x'})e^{-\beta H}\psi(t,\boldsymbol{x})e^{\beta H} \\ &= -\xi Tre^{-\beta H}\psi(t,\boldsymbol{x})\psi^\dagger(0,\boldsymbol{x'}), \end{aligned}$$

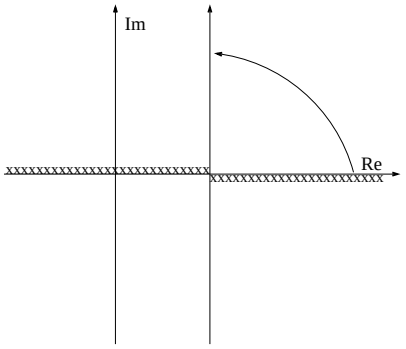

FIG. 4: Wick rotation.

and the result yields the the Kubo-Martin-Schwinger condition,

$$G^E((t-\beta,\boldsymbol{x}),(0,\boldsymbol{x'})) = \xi G^E((t,\boldsymbol{x}),(0,\boldsymbol{x'})).$$

The Fourier series over the frequency for imaginary time is carried out with the Matsubara spectrum, $\omega_n = 2\pi k_B T n$ or $\omega_n = 2\pi k_B T(n+\frac{1}{2})$ for bosons or fermions, respectively. Therefore, the imaginary time propagator can be written

$$\hbar G^E_{\alpha\beta}(x,x') = -\frac{1}{\beta}\sum_n \int_{\boldsymbol{k}} \frac{e^{-i\omega_n(\tau-\tau')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{i\omega_n - \omega(\boldsymbol{k})}$$

IV. PERTURBATION EXPANSION

The expectation values of observables can be expressed in terms of Green functions. Therefore, the perturbation expansion will be presented for Green functions only.

A. Interactive Green functions

Let us consider an n-point function

$$i\hbar G(t_1,\ldots,t_n) = \langle 0|T[A_1(t_1)\cdots A_n(t_n)]|0\rangle$$

where $|0\rangle$ is the ground state. Let us assume for simplicity that $t_n \geq t_{n-1} \geq \cdots \geq t_2 \geq t_1 \geq t_0$, when one finds in the Heisenberg representation

$$i\hbar G(t_1,\ldots,t_n) = \langle 0|T[A_n(t_n)\cdots A_1(t_1)]|0\rangle$$

what can be written as

$$\begin{aligned} i\hbar G(t_1,\ldots,t_n) &= \langle 0|e^{\frac{i}{\hbar}(t_n-t_0)H}A_{nS}e^{-\frac{i}{\hbar}(t_n-t_0)H}\cdots e^{\frac{i}{\hbar}(t_1-t_0)H}A_{1S}e^{-\frac{i}{\hbar}(t_1-t_0)H}|0\rangle \\ &= \langle 0|e^{\frac{i}{\hbar}(t_n-t_0)H}A_{nS}e^{-\frac{i}{\hbar}(t_n-t_{n-1})H}\cdots e^{-\frac{i}{\hbar}(t_2-t_1)H}A_{1S}e^{-\frac{i}{\hbar}(t_1-t_0)H}|0\rangle \end{aligned} \quad (33)$$

by means of the operators of the Schrödinger representation. The interaction representation gives

$$i\hbar G(t_1,\ldots,t_n) = \langle 0|(T[e^{-\frac{i}{\hbar}\int_{t_0}^{t_n}dt' H_1(t')}])^\dagger A_n(t_n)T[e^{-\frac{i}{\hbar}\int_{t_{n-1}}^{t_n}dt' H_1(t')}]\cdots T[e^{-\frac{i}{\hbar}\int_{t_1}^{t_2}dt' H_1(t')}]A_1(t_1)T[e^{-\frac{i}{\hbar}\int_{t_0}^{t_1}dt' H_1(t')}]|0\rangle.$$

In order to have a simple perturbation series one would need a single time ordered product between the vacuum state, ie. the first operator in the second line of (33) should be replaced by $e^{-\frac{i}{\hbar}(t_f-t_n)H}$ where $t_f > t_n$.

Luckily this can be made easily since the vacuum is an eigenstate of the Hamiltonian with vanishing eigenvalue, $e^{-\frac{i}{\hbar}(t_f-t_n)H}|0\rangle = |0\rangle$ and we find

$$\begin{aligned} i\hbar G(t_1,\ldots,t_n) &= \langle 0|T[e^{-\frac{i}{\hbar}\int_{t_n}^{t_f}dt' H_1(t')}]A_n(t_n)T[e^{-\frac{i}{\hbar}\int_{t_{n-1}}^{t_n}dt' H_1(t')}]\cdots T[e^{-\frac{i}{\hbar}\int_{t_1}^{t_2}dt' H_1(t')}]A_1(t_1)T[e^{-\frac{i}{\hbar}\int_{t_0}^{t_1}dt' H_1(t')}]|0\rangle \\ &= \langle 0|T[e^{-\frac{i}{\hbar}\int_{t_n}^{t_f}dt' H_1(t')}A_n(t_n)e^{-\frac{i}{\hbar}\int_{t_{n-1}}^{t_n}dt' H_1(t')}\cdots e^{-\frac{i}{\hbar}\int_{t_1}^{t_2}dt' H_1(t')}A_1(t_1)e^{-\frac{i}{\hbar}\int_{t_0}^{t_1}dt' H_1(t')}]|0\rangle \\ &= \langle 0|T[e^{-\frac{i}{\hbar}\int_{t_0}^{t_f}dt' H_1(t')}A_1(t_1)\cdots A_n(t_n)]|0\rangle \end{aligned} \quad (34)$$

in the interaction representation. In the more realistic cases our initial state contains a large number of excitations and the reduction of the expectation value of the chronological product (33) does not agree with the transition amplitude (34). These cases requires the use of the Heisenberg representation and the resulting Schwinger-Keldysh formalism leads in a natural manner to the linear response formulae derived later. We continue here with the simpler porblems where the reduction (33) $\rightarrow$ (34) applies.

The expansion in the interaction Hamiltonian yields for $t_0 = -\infty$, $t_f = \infty$

$$\begin{aligned} i\hbar G(t_1,\dots,t_n) &= \langle 0|T[e^{-\frac{i}{\hbar}\int_{-\infty}^{\infty} dt' H_1(t')} A_1(t_1)\cdots A_n(t_n)]|0\rangle \\ &= \sum_{m=0}^{\infty} \frac{(-\frac{i}{\hbar})^m}{m!} \int_{-\infty}^{\infty} dt'_1\cdots dt'_m \langle 0|T[H_1(t'_1)\cdots H_1(t'_m)A_1(t_1)\cdots A_n(t_n)]|0\rangle. \end{aligned} \tag{35}$$

The interaction Hamiltonian and the operators A_1,...,A_n can always be written as sum or integral of product of local field operators for a local theory and the vacuum expectation value in the last line is a Green function. The crucial observation is that this Green function corresponds to a free model because the time dependence of the operators is generated by the free part of the Hamiltonian, in other words the field operators are constructed by means of non-interacting fields. The perturbation series obtains the interactive Green function as an infinite sum of free Green functions.

Let us consider as simple example the electron propagator in a system of electrons interacting with a potential $U(\boldsymbol{x})$,

$$\begin{aligned} \langle 0|T[\psi_\alpha(x)\psi^\dagger_\beta(y)]|0\rangle &= \langle 0|T[e^{-\frac{i}{2\hbar}\sum_{\sigma,\sigma'}\int dtd^3vd^3z\psi^\dagger_\sigma(t,\boldsymbol{v})\psi^\dagger_{\sigma'}(t,\boldsymbol{z})U(\boldsymbol{v}-\boldsymbol{z})\psi_{\sigma'}(t,\boldsymbol{z})\psi_\sigma(t,\boldsymbol{v})}\psi(x)\psi^\dagger(y)]|0\rangle \\ &= \sum_{m=0}^{\infty}\frac{(-\frac{i}{2\hbar})^m}{m!}\sum_{\sigma_1,\sigma'_1}\int dtd^3v_1d^3z_1\cdots\sum_{\sigma_m,\sigma'_m}\int dtd^3v_md^3z_mU(\boldsymbol{v}_1-\boldsymbol{z}_1)\cdots U(\boldsymbol{v}_m-\boldsymbol{z}_m) \\ &\times\langle 0|T\big[\psi^\dagger_{\sigma_1}(t_1,\boldsymbol{v}_1)\psi^\dagger_{\sigma'_1}(t_1,\boldsymbol{z}_1)\psi_{\sigma'_1}(t_1,\boldsymbol{z}_1)\psi_{\sigma_1}(t_1,\boldsymbol{v}_1)\cdots \\ &\times\psi^\dagger_{\sigma_m}(t_m,\boldsymbol{v}_m)\psi^\dagger_{\sigma'_m}(t_m,\boldsymbol{z}_m)\psi_{\sigma'_m}(t_m,\boldsymbol{z}_m)\psi_{\sigma_m}(t_m,\boldsymbol{v}_m)\psi(x)\psi^\dagger(y)\big]|0\rangle. \end{aligned} \tag{36}$$

B. Wick theorem

Let us ignore first any other degrees of freedom than electrons for the sake of simplicity. Then the interacting Green functions are given in (35) in terms of the noninteracting $m+n$-point functions

$$G_{\alpha_1,\dots,\alpha_n,\alpha'_1,\dots,\alpha'_n}(x_1,\cdots,x_m,x'_1,\cdots,x'_n) = \langle 0|T[\psi_{\alpha_1}(x_1)\cdots\psi_{\alpha_m}(x_m)\psi^\dagger_{\alpha'_1}(x'_1)\cdots\psi^\dagger_{\alpha'_n}(x'_n)]|0\rangle.$$

It is easy to see that the Green function is vanishing for $m \neq n$. In fact, each field operator creates or removes an excitation. One starts at the right and ends at the left with the vacuum, the state of no excitation. Therefore, each excitation created by a field operator must be removed by another operator. Excitations created by ψ ($\psi^\dagger$) are removed by $\psi^\dagger$ (ψ). Thus we have non-vanishing number of excitation in the state

$$T[\psi_{\alpha_1}(x_1)\cdots\psi_{\alpha_m}(x_m)\psi^\dagger_{\alpha'_1}(x'_1)\cdots\psi^\dagger_{\alpha'_n}(x'_n)]|0\rangle \tag{37}$$

for $m \neq n$ and its overlap with $|0\rangle$ will be vanishing. The $2n$-point function can be interpreted as the propagator, the transition amplitude, for k electrons and $n-k$ holes with $k = 0,\dots,n$, where k depends on the order of the time argument of the space-time vectors, the variables of the Green function.

The Wick theorem expresses the general noninteracting Green functions by means of free causal propagators. The essence of the theorem is the observation that the free Green functions express the transition amplitude for a system of electrons and holes and this factorizes for individual particles or holes in the absence of interactions. Let us consider the field operator with the earliest time argument in the state (37). It acts on the vacuum and the excitation, created by it must be removed by one of n other field operators. The operators which create or removes the same excitation are called pairs. Thus the earliest operator will be paired up with another operator of the chronological product of (37). Once this pair is identified, the excitation corresponding to them can be factorized off from the rest of the Green functions because this is a non-interactive system. The factorization leads to the product of a propagator for an excitation and a $2n-2$-point function. The iterative application of this argument yields the product of n propagators at the end. Since there are several operators which should remove of a given excitation we have to sum over all possibility. This is due to the linear superposition principle of Quantum Mechanics which gives the transition amplitudes as sums over the transition amplitudes of possible processes.

The actual realization of this plan with the construction of the pairing or contraction, $\overbrace{AB}$, of two field operators, A and B. This contraction should satisfy two conditions. First, its vacuum expectation value should be that of the time ordered product $T[AB]$, the quantity we try to factorize. Second, it should be proportional to the identity operator acting on the Fock-space in order to be able to factorize it outside of the expectation value. The choice $\overbrace{AB} = T[AB]$ is not good because the $T[\psi(x)\psi^\dagger(y)]$ is not the identity matrix for the space-time locations outside of the null-space of the equation of motion, as remarked at Eq. (28). To correct this feature without modifying the vacuum expectation value we define

$$\overbrace{AB} = T[AB] - :AB: \tag{38}$$

for elementary field operators. The normal ordering does not change the fact that the space-time dependence of the operators belong to the null-space of the equation of motion, thus the time ordered product is indeed modified in this null-space only. This expression is vanishing if the operators A and B commute, $[A,B]_\xi = 0$ and is a c-number times the identity operator outside of the null-space of the equation of-motion. Among the different pairing a fermion field the only non-vanishing is

$$\begin{aligned}\overbrace{\psi(x)\psi^\dagger(x')} &= \overbrace{[\psi^{(+)}(x)+\psi^{(-)}(x)][\psi^{(+)\dagger}(x')+\psi^{(-)\dagger}(x')]} \\ &= \overbrace{\psi^{(+)}(x)\psi^{(+)\dagger}(x')} + \overbrace{\psi^{(-)}(x)\psi^{(-)\dagger}(x')}\,.\end{aligned}$$

These non-vanishing contributions contain a commutator which is a c-number times the identity operator. In fact, for $t > t'$

$$\begin{aligned}\overbrace{\psi^{(+)}(x)\psi^{(+)\dagger}(x')} &= \psi^{(+)}(x)\psi^{(+)\dagger}(x') - \xi\psi^{(+)\dagger}(x')\psi^{(+)}(x) = [\psi^{(+)}(x),\psi^{(+)\dagger}(x')]_\xi \\ \overbrace{\psi^{(-)}(x)\psi^{(-)\dagger}(x')} &= \psi^{(-)}(x)\psi^{(-)\dagger}(x') - \psi^{(-)}(x)\psi^{(-)\dagger}(x) = 0,\end{aligned}$$

and for $t' > t$

$$\begin{aligned}\overbrace{\psi^{(+)}(x)\psi^{(+)\dagger}(x')} &= \xi\psi^{(+)\dagger}(x')\psi^{(+)}(x) - \xi\psi^{(+)\dagger}(x')\psi^{(+)}(x) = 0, \\ \overbrace{\psi^{(-)}(x)\psi^{(-)\dagger}(x')} &= \xi\psi^{(-)\dagger}(x')\psi^{(-)}(x) - \psi^{(-)}(x)\psi^{(-)\dagger}(x') = [\psi^{(-)}(x),\psi^{(-)\dagger}(x')]_\xi.\end{aligned}$$

The more detailed calculation gives

$$\overbrace{\psi(t,\boldsymbol{x})\psi^\dagger(t',\boldsymbol{x'})} = i\hbar G((t,\boldsymbol{x}),(t',\boldsymbol{x'}))\mathbb{1}$$

The Wick theorem states that the free $2n$-point function can be written as sum of the product of contractions,

$$\langle 0|T[\phi_1\cdots\phi_{2n}]|0\rangle = {\sum_{\pi\in S_{2n}}}' \xi^{\sigma(\pi)} \overbrace{\phi_{\pi(1)}\phi_{\pi(2)}}\cdots\overbrace{\phi_{\pi(2n-1)}\phi_{\pi(2n)}} \tag{39}$$

where the summation is over those permutations of $2n$ objects which yield different pairing structure, eg. the exchange of the two points in a contraction, $\overbrace{\phi_1\phi_2} \to \overbrace{\phi_2\phi_1}$, or the permutation of the contractions themselves, $\overbrace{\phi_1\phi_2}\overbrace{\phi_3\phi_4} \to \overbrace{\phi_3\phi_4}\overbrace{\phi_2\phi_1}$, do not lead to a new pairing. The order of the permutation $\sigma(\pi)$ is 0 or 1, and is determined in the following manner. Any permutation $\pi = \binom{\pi(1),\ldots,\pi(k)}{1,\ldots,k}$ can be written as the product of exchanges of pairs, eg. $\binom{231}{123} = (12)(13)$ and $\binom{213}{123} = (12)$, where (ℓ,m) denotes the permutation changing ℓ and m, leaving other object unchanged. Such a decomposition of permutations is not unique but the number of pair exchanges needed to obtain a given permutation has a unique value modulo 2. This unique value is its order, $\sigma(\pi)$, eg. $\sigma[\binom{231}{123}] = 0$ and $\sigma[\binom{213}{123}] = 1$.

Eq. (39) is the realization of the heuristic argument mentioned above that the contributions of the noninteracting elementary excitations to the propagator factorizes.

Let us check the theorem in a simple case of a four-point function. We assume $t_1 > t_2 > t_3 > t_4$ for the sake of simplicity and consider the Green function

$$i\hbar G(1,2,3,4) = \langle 0|T[\psi_1\psi_2\psi_3^\dagger\psi_4^\dagger]|0\rangle = \langle 0|\psi_1\psi_2\psi_3^\dagger\psi_4^\dagger|0\rangle$$

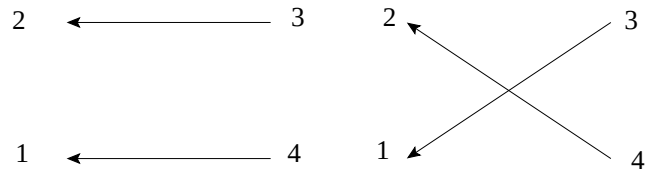

FIG. 5: Graphical representation of the free two-electron propagator (40).

describing the propagation of two electrons. The repeated application of the rule $\overbrace{AB} = T[AB] - :AB:$ gives

$$\begin{aligned}
\langle 0|\psi_1\psi_2\psi_3^\dagger\psi_4^\dagger|0\rangle &= \langle 0|(\psi_1^{(+)}+\psi_1^{(-)})(\psi_2^{(+)}+\psi_2^{(-)})(\psi_3^{(+)\dagger}+\psi_3^{(-)\dagger})(\psi_4^{(+)\dagger}+\psi_4^{(-)\dagger})|0\rangle \\
&= \langle 0|\psi_1^{(-)}\psi_2^{(-)}\psi_3^{(+)\dagger}\psi_4^{(+)\dagger}|0\rangle \\
&= \langle 0|\psi_1^{(-)}(\overbrace{\psi_2^{(-)}\psi_3^{(+)\dagger}}+:\psi_2^{(-)}\psi_3^{(+)\dagger}:)\psi_4^{(+)\dagger}|0\rangle \\
&= \overbrace{\psi_2^{(-)}\psi_3^{(+)\dagger}}\langle 0|\psi_1^{(-)}\psi_4^{(+)\dagger}|0\rangle + \xi\langle 0|\psi_1^{(-)}\psi_3^{(+)\dagger}\psi_2^{(-)}\psi_4^{(+)\dagger}|0\rangle \\
&= \overbrace{\psi_2^{(-)}\psi_3^{(+)\dagger}}\langle 0|\overbrace{\psi_1^{(-)}\psi_4^{(+)\dagger}}+:\psi_1^{(-)}\psi_4^{(+)\dagger}:|0\rangle + \xi\langle 0|\psi_1^{(-)}\psi_3^{(+)\dagger}(\overbrace{\psi_2^{(-)}\psi_4^{(+)\dagger}}+:\psi_2^{(-)}\psi_4^{(+)\dagger}:)|0\rangle \\
&= \overbrace{\psi_2^{(-)}\psi_3^{(+)\dagger}}\overbrace{\psi_1^{(-)}\psi_4^{(+)\dagger}} + \xi\overbrace{\psi_1^{(-)}\psi_3^{(+)\dagger}}\overbrace{\psi_2^{(-)}\psi_4^{(+)\dagger}}. \qquad (40)
\end{aligned}$$

This exercises shows the strategy followed in the more complicated cases, too. For each creation and destruction operator pair appearing beside each other in the wrong order in the time ordered product ie. creation operator right of the destruction operator, Eq. (38) is used. The normal ordered product appearing on the right hand side of Eq. (38) puts the operators in the right order and the price of this exchange of order is the contraction. This latter can be factorized as a c-number and then the procedure is repeated until all destruction (creation) operator are at right (left) between the vacuum.

The Feynman graphs corresponding to this expression, shown in Fig. 5, represent the direct and the exchange contributions, the latter involving the exchange statistical factor ξ. The lines stand for the contractions. The single particle propagator is not a symmetric function, $\langle 0|T[\psi(x)\psi^\dagger(y)]|0\rangle \neq \langle 0|T[\psi(y)\psi^\dagger(x)]|0\rangle$, thus the line is oriented and the arrow point from the space-time position where an electron was created to the point where it is removed.

As an application of the Wick theorem we consider the two-electron propagator,

$$\mathcal{A} = \langle 0|T[\psi(x_1)\psi(x_2)\psi^\dagger(y_2)\psi^\dagger(y_1)]|0\rangle$$

with spin ignored. The perturbation series is

$$\begin{aligned}
\mathcal{A} &= \langle 0|T[e^{-\frac{i}{2\hbar}\int dtd^3vd^3z\psi^\dagger(t,\boldsymbol{v})\psi^\dagger(t,\boldsymbol{z})U(\boldsymbol{v}-\boldsymbol{z})\psi(t,\boldsymbol{z})\psi(t,\boldsymbol{v})}\psi(x_1)\psi(x_2)\psi^\dagger(y_2)\psi^\dagger(y_1)]|0\rangle \\
&= \sum_{m=0}^{\infty}\frac{(-\frac{i}{2\hbar})^m}{m!}\int dtd^3v_1d^3z_1\cdots\int dtd^3v_md^3z_mU(\boldsymbol{v}_1-\boldsymbol{z}_1)\cdots U(\boldsymbol{v}_m-\boldsymbol{z}_m) \\
&\quad\times\langle 0|T\big[\psi^\dagger(t_1,\boldsymbol{v}_1)\psi^\dagger(t_1,\boldsymbol{z}_1)\psi(t_1,\boldsymbol{z}_1)\psi(t_1,\boldsymbol{v}_1)\cdots \\
&\quad\times\psi^\dagger(t_m,\boldsymbol{v}_m)\psi^\dagger(t_m,\boldsymbol{z}_m)\psi(t_m,\boldsymbol{z}_m)\psi(t_m,\boldsymbol{v}_m)\psi(x_1)\psi(x_2)\psi^\dagger(y_2)\psi^\dagger(y_1)\big]|0\rangle \\
&= \langle 0|T[\psi(x_1)\psi(x_2)\psi^\dagger(y_2)\psi^\dagger(y_1)]|0\rangle \\
&\quad -\frac{i}{2\hbar}\int dtd^3vd^3zU(\boldsymbol{v}-\boldsymbol{z})\langle 0|T[\psi^\dagger(t,\boldsymbol{v})\psi^\dagger(t,\boldsymbol{z})\psi(t,\boldsymbol{z})\psi(t,\boldsymbol{v})\psi(x_1)\psi(x_2)\psi^\dagger(y_2)\psi^\dagger(y_1)]|0\rangle+\cdots .
\end{aligned}$$

Zeroth order contribution, depicted in Fig. 5, is just the non-interactive Green function,

$$\mathcal{A}^{(0)} = \langle 0|T[\psi(x_1)\psi(x_2)\psi^\dagger(y_2)\psi^\dagger(y_1)]|0\rangle.$$

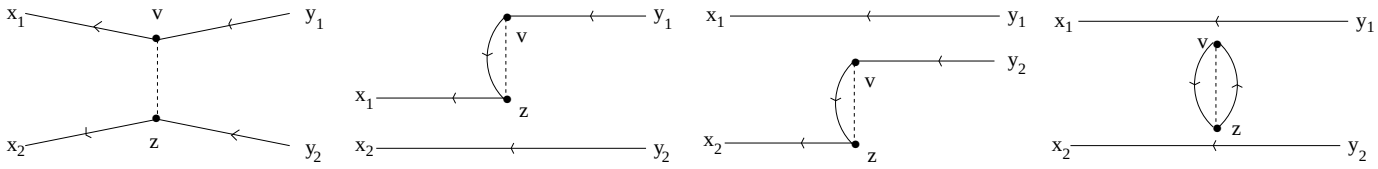

FIG. 6: First order contributions to the two-electron propagator of Eq. (41).

The first order contributions are

$$\begin{aligned}
\mathcal{A}^{(1)} &= -\frac{i}{2\hbar}\int dtd^3vd^3zU(\boldsymbol{v}-\boldsymbol{z})\langle 0|T[\psi^\dagger(t,\boldsymbol{v})\psi^\dagger(t,\boldsymbol{z})\psi(t,\boldsymbol{z})\psi(t,\boldsymbol{v})\psi(x_1)\psi(x_2)\psi^\dagger(y_2)\psi^\dagger(y_1)]|0\rangle \\
&= -\frac{i}{2\hbar}\int dtd^3vd^3zU(\boldsymbol{v}-\boldsymbol{z})\Big[2\overbrace{\psi^\dagger(t,\boldsymbol{v})\psi(x_1)}\overbrace{\psi^\dagger(t,\boldsymbol{z})\psi(x_2)}\overbrace{\psi(t,\boldsymbol{z})\psi^\dagger(y_2)}\overbrace{\psi(t,\boldsymbol{v})\psi^\dagger(y_1)} \\
&\quad +2\overbrace{\psi^\dagger(t,\boldsymbol{z})\psi(x_1)}\overbrace{\psi^\dagger(t,\boldsymbol{z})\psi(t,\boldsymbol{v})}\overbrace{\psi(x_2)\psi^\dagger(y_2)}\overbrace{\psi(t,\boldsymbol{v})\psi^\dagger(y_1)} \\
&\quad +2\overbrace{\psi^\dagger(t,\boldsymbol{v})\psi(x_2)}\overbrace{\psi^\dagger(t,\boldsymbol{z})\psi(t,\boldsymbol{v})}\overbrace{\psi(x_1)\psi^\dagger(y_1)}\overbrace{\psi(t,\boldsymbol{z})\psi^\dagger(y_2)} \\
&\quad +\xi\overbrace{\psi^\dagger(t,\boldsymbol{v})\psi(t,\boldsymbol{z})}\overbrace{\psi^\dagger(t,\boldsymbol{z})\psi(t,\boldsymbol{v})}\overbrace{\psi(x_2)\psi^\dagger(y_2)}\overbrace{\psi(x_1)\psi^\dagger(y_1)}\Big]+\xi(y_1\longleftrightarrow y_2),
\end{aligned} \tag{41}$$

the corresponding Feynman graphs are shown in Fig. 6. The factors 2 in the square bracket stand for the exchange terms $\boldsymbol{v}\leftrightarrow\boldsymbol{z}$.

C. Feynman rules

The calculation presented above can be generalized. The resulting procedure can be summarized in the following manner. Suppose that we are calculating the k-th order contribution to the fermion Green function $\langle 0|T[\psi(x_1)\cdots\psi(x_n)\psi^\dagger(y_1)\cdots\psi^\dagger(y_n)]|0\rangle$.

1. Place $2n$ points, one for each space-time variable in the Green function, external legs and k pairs of points, vertices, on the plane. Add a short line running out,$\longleftarrow\!\bullet$, to n external legs which will stand for $\psi^\dagger(y_i)$ and draw short lines running in to the remaining n external legs,$\longrightarrow\!\bullet$, to represent $\psi(x_j)$. For each vertex point draw a short line in and line out in addition to a dashed line, $-\,-\,-\,-\,-\,-\,-$, representing the potential connecting the pair of points.

2. Distribute the contractions between ψ and $\psi^\dagger$ ie. the connections of the external leg and vertex points in such a manner that every point is connected to another one with the opposite type of short line. There is a unique correspondence between the such contraction distributions and contributions to the Green function. Each oriented line between the points represents a free electron propagator $i\hbar G$ and the line $-\,-\,-\,-\,-\,-\,-$ stands for $-iU/\hbar$.

3. Insert a -1 factor for each fermionic closed loop, eg.
$$T[\psi_3^\dagger\psi_1\psi_1^\dagger\psi_2\psi_2^\dagger\psi_3]=\xi T[\psi_1\psi_1^\dagger\psi_2\psi_2^\dagger\psi_3\psi_3^\dagger]$$

4. Make the replacement $G(x,y)\to G(x,y+\eta\hat{t})$, $\eta=0^+$ in each fermion line which is closed or connects the same potential $U(x-y)=\delta(x^0-y^0)U(\boldsymbol{x}-\boldsymbol{y})$ taken at identical time.

5. Divide the contribution with the order of the symmetry group of the graph, the number of permutations of the points which leave the graph invariant.

Let us consider, as examples, the leading order contributions to the electron propagator, shown in Fig. 7 and 8, respectively. The Hamiltonian is

$$H=\sum_\sigma\int_{\boldsymbol{x}}\psi_\sigma^\dagger(\boldsymbol{x})\left(-\frac{\hbar^2}{2m}\Delta-\mu\right)\psi_\sigma(\boldsymbol{x})+\frac{1}{2}\sum_{\sigma_1,\sigma_2}\int_{\boldsymbol{x},\boldsymbol{y}}:\overbrace{\underbrace{\psi_{\sigma_1}^\dagger(\boldsymbol{x})\psi_{\sigma_2}(\boldsymbol{x})}_{\longleftarrow\!\bullet\!\longleftarrow}}^{\text{vertex}}U(\boldsymbol{x}-\boldsymbol{y})\overbrace{\underbrace{\psi_{\sigma_2}^\dagger(\boldsymbol{y})\psi_{\sigma_1}(\boldsymbol{y})}_{\longleftarrow\!\bullet\!\longleftarrow}}^{\text{vertex}}:$$

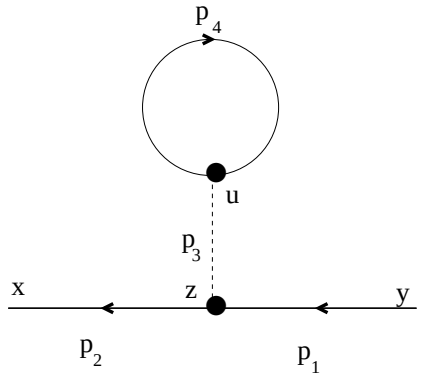

FIG. 7: Hartree contribution to the electron propagator.

The $\mathcal{O}(U)$ Hartree and Fock contributions are

$$\begin{aligned} i\hbar G^H_{\alpha\beta}(x,y) &= -\frac{i}{\hbar}\int dzdu(-i\hbar)G_{\lambda'\lambda}(u,u+\eta\hat{t})U^{\lambda\lambda'}_{\gamma\gamma'}(z,u)i\hbar G_{\alpha\gamma}(x,z)i\hbar G_{\gamma'\beta}(z,y) \\ i\hbar G^F_{\alpha\beta}(x,y) &= -\frac{i}{\hbar}\int dzdui\hbar G_{\alpha\lambda}(x,z)U^{\lambda\lambda'}_{\gamma\gamma'}(z,u)i\hbar G_{\lambda'\gamma}(z,u+\eta\hat{t})i\hbar G_{\gamma'\beta}(u,y). \end{aligned}$$

In the next step we go over energy-momentum space by the the Fourier transformation

$$G(x,y)=\int\frac{dk}{(2\pi)^4}e^{-ik(x-y)}\tilde{G}(k)$$

and we find

$$\begin{aligned} i\hbar G^H_{\alpha\beta}(x,y) &= -\frac{i}{\hbar}\int dzdu(-i\hbar)\underbrace{G_{\lambda'\lambda}(u,u+\eta\hat{t})}_{p_4}\underbrace{U^{\lambda\lambda'}_{\gamma\gamma'}(z,u)}_{p_3}i\hbar\underbrace{G_{\alpha\gamma}(x,z)}_{p_2}i\hbar\underbrace{G_{\gamma'\beta}(z,y)}_{p_1} \\ &= -\frac{i}{\hbar}\int dzdu\frac{dp_1dp_2dp_3dp_4}{(2\pi)^{16}}e^{i\eta p^0_4}(-i\hbar)\tilde{G}_{\lambda'\lambda}(p_4)e^{-ip_3(z-u)}\tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(p_3) \\ &\quad\times e^{-ip_2(x-z)}i\hbar\tilde{G}_{\alpha\gamma}(p_2)e^{-ip_1(z-y)}i\hbar\tilde{G}_{\gamma'\beta}(p_1). \end{aligned}$$

The integration over the vertex positions z and u generates the energy-momentum conservation,

$$\begin{aligned} i\hbar G^H_{\alpha\beta}(x,y) &= -\frac{i}{\hbar}\int\frac{dp_1dp_2dp_3dp_4}{(2\pi)^{16}}(2\pi)^4\delta(p_3-p_2+p_1)(2\pi)^4\delta(p_3)e^{ip_1y-ip_2x}e^{i\eta p^0_4} \\ &\quad\times(-i\hbar)\tilde{G}_{\lambda'\lambda}(p_4)\tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(p_3)i\hbar\tilde{G}_{\alpha\gamma}(p_2)i\hbar\tilde{G}_{\gamma'\beta}(p_1) \\ &= -\frac{i}{\hbar}\int\frac{dp_1dp_4}{(2\pi)^8}(-i\hbar)e^{-ip_1(x-y)+i\eta p^0_4}\tilde{G}_{\lambda'\lambda}(p_4)\tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(0)i\hbar\tilde{G}_{\alpha\gamma}(p_1)i\hbar\tilde{G}_{\gamma'\beta}(p_1) \end{aligned}$$

and we find

$$i\hbar\tilde{G}^H_{\alpha\beta}(p)=-\frac{i}{\hbar}i\hbar\tilde{G}_{\beta\gamma}(p)i\hbar\tilde{G}_{\gamma'\alpha}(p)\tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(0)\int\frac{dq}{(2\pi)^4}(-i\hbar)\tilde{G}_{\lambda'\lambda}(q)$$

.

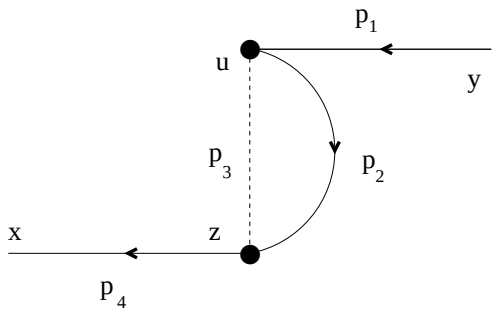

FIG. 8: Fock contribution to the electron propagator.

We find in a similar manner for the Fock contribution

$$\begin{aligned}
i\hbar G^F_{\alpha\beta}(x,y) &= -\frac{i}{\hbar}\int_{z,u} i\hbar \underbrace{G_{\lambda'\lambda}(x,z)}_{p_4}\underbrace{U^{\lambda\lambda'}_{\gamma\gamma'}(z,u)}_{p_3} i\hbar \underbrace{G_{\alpha\gamma}(z,u+\eta\hat{t})}_{p_2} i\hbar \underbrace{G_{\gamma'\beta}(u,y)}_{p_1} \\
&= -\frac{i}{\hbar}\int dzdu \frac{dp_1dp_2dp_3dp_4}{(2\pi)^{16}} e^{-ip_4(x-z)} i\hbar\tilde{G}_{\alpha\lambda}(p_4) e^{-ip_3(z-u)} \tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(p_3) e^{-ip_2(z-u-\eta\hat{t})} i\hbar\tilde{G}_{\lambda'\gamma}(p_2) \\
&\quad \times e^{-ip_1(u-y)} i\hbar\tilde{G}_{\gamma'\beta}(p_1) \\
&= -\frac{i}{\hbar}\int \frac{dp_1dp_2dp_3dp_4}{(2\pi)^{16}} (2\pi)^4\delta(p_2+p_3-p_4)(2\pi)^4\delta(p_1-p_2-p_3) e^{ip_1y-ip_4x+ip_2^0\eta} \\
&\quad \times i\hbar\tilde{G}_{\alpha\lambda}(p_4)\tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(p_3) i\hbar\tilde{G}_{\lambda'\gamma}(p_2) i\hbar\tilde{G}_{\gamma'\beta}(p_1) \\
&= -\frac{i}{\hbar}\int \frac{dp_1dp_2}{(2\pi)^8} e^{-ip_1(x-y)} e^{ip_2^0\eta} i\hbar\tilde{G}_{\alpha\lambda}(p_1)\tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(p_1-p_2) i\hbar\tilde{G}_{\lambda'\gamma}(p_2) i\hbar\tilde{G}_{\gamma'\beta}(p_1)
\end{aligned}$$

and

$$i\hbar G^F_{\alpha\beta}(p) = -\frac{i}{\hbar}\int \frac{dq}{(2\pi)^4} e^{iq^0\eta} i\hbar\tilde{G}_{\alpha\lambda}(p)\tilde{U}^{\lambda\lambda'}_{\gamma\gamma'}(p-q) i\hbar\tilde{G}_{\lambda'\gamma}(q) i\hbar\tilde{G}_{\gamma'\beta}(p).$$

It is instructive to check explicitely the emergence of the energy-momentum conserving Dirac-deltas which arise from the integration of a vertex position. The three-point function generated by the vertex in the space-time,

$$\begin{aligned}
V(x,y,v) &= \int_z G(x-z)G(z-y)U(z-v) \\
&= \int_{z,p,q,r} G_p e^{ip(x-z)} G_q e^{iq(z-y)} U_r e^{ir(z-v)} \\
&= \int_{p,q,r} G(p)e^{ipx} G(q) e^{-iqy} U(r) e^{-irv} (2\pi)^4\delta(q+r-p)
\end{aligned}$$

gives

$$V(p,q,r) = \int_{x,y,v} V(x,y,v) e^{-ipx+iqy+irv} = G(p)G(q)U(r)(2\pi)^4\delta(q+r-p)$$

after Fourier transformation.

This exercise explains the following modification of the Feynman rules in momentum space compared to the rules given above:

1. The external legs are given the energy-momentum carried by the particle in question
2. Insert an energy-momentum conserving Dirac-delta at each vertex.
3. Each propagator or potential is replaced by its Fourier transform.
4. Integrate over the energy-momentum variables corresponding to the internal lines.

D. Schwinger-Dyson equation

The structure of the Feynman graph allows a partial resummation of the perturbation series for the propagator. Let us imagine the infinitely many graphs contributing to the propagator $G(p)$ in momentum space. We shall regroup the series in the following manner. The zeroth order group contains free propagator. The first group contains all graphs which do not fall into two disconnected parts after cutting an internal electron or potential line. After having separated of these contributions the remaining graphs fall into two parts by the cutting of internal lines. The second group contains graphs which fall into two disconnected parts by cutting an internal line. In general, the n-th group contains graphs which fall into n disconnected parts by cutting $n-1$ internal lines.

Consider now the sum of graphs of the first class and divide by $G^2(p)$, remove its two external legs. What is left behind are called one-particle irreducible graphs whose sum is the self energy $-\Sigma(p)$, eg. the sum of graph if Figs. 7 and 8 after the removal of the external legs. A little exercising with examples shows that the full propagator is a geometrical series,

$$\begin{aligned} G(p) &= G_0(p) + G_0(p)\Sigma(p)G_0(p) + G_0(p)\Sigma(p)G_0(p)\Sigma(p)G_0(p) + \cdots \\ &= \frac{G_0(p)}{1-\Sigma(p)G_0(p)} \\ &= \frac{1}{G_0^{-1}(p)-\Sigma(p)} \end{aligned}$$

and we have the Schwinger-Dyson equation

$$G^{-1} = G_0^{-1} - \Sigma.$$

The advantage of this equation is that any approximation to the self-energy together with the solution of this equation for the propagator generates a partial resummation of the perturbation series.

E. Propagation in a disorded medium

Let us consider the propagation of a charge interacting with randomly placed static impurities with the potential $u(\boldsymbol{x}-\boldsymbol{x}')$. We add a constant to this potential to ensure the relation

$$\int d^3x u(\boldsymbol{x}) = 0$$

which will suppresses the interactions with vanishing momentum transfer. The total potential acting on the charge is

$$U(\boldsymbol{x}) = \sum_a u(\boldsymbol{x}-\boldsymbol{x}_a)$$

where x_a denotes the position of the impurities. We shall need the Fourier representation

$$U(\boldsymbol{x}) = \sum_a \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x}_a)} \tilde{U}(\boldsymbol{k})$$

for the potential. The second quantized one-body operator, acting in the Fock-space is

$$U = \int d^3x \psi^\dagger(\boldsymbol{x}) U(\boldsymbol{x}) \psi(\boldsymbol{x}).$$

One can construct the interaction representation by considering the impurity potential as perturbation. The propagator of a charge for a given impurity configuration $\{\boldsymbol{x}_a\}$ is

$$\begin{aligned} G(x,y) &= \langle 0|T[\psi(x)\psi^\dagger(y)]|0\rangle \\ &= \sum_{n=0}^{\infty} \int dz_1 \cdots dz_n G_0(x,z_1)U(z_1)G_0(z_1,z_2)\cdots G_0(z_{n-1},z_n)U(z_n)G_0(z_n,y), \end{aligned} \tag{42}$$

where $G_0(x,y)$ denotes the free propagator.This perturbation series is shown in Fig. 9.

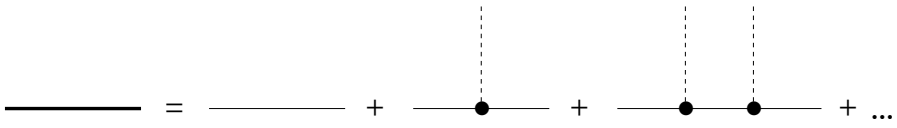

FIG. 9: The propagator in the presence of a given impurity configuration.

In order to include the impurities we compare the characteristic time scales of the motion of the charges and the impurities, $t_{\rm ch}$ and $t_{\rm imp}$, respectively. We can safely assume that the impurities are slower degrees of freedom than the charges, $t_{\rm ch} < t_{\rm imp}$. When $t_{\rm ch}$ and $t_{\rm imp}$ are not too far from each others then we have to include the impurity dynamics in the description as usual, ie. by writing the total Hamiltonian as the sum of the kinetic energy for the impurities, the charges and the interaction energy. Such an averaging over the impurities is called annealed average.

In the other extremity, $t_{\rm ch} \ll t_{\rm imp}$, which is usually realized in real samples we assume that the quantum coherent scatterings among the charges take place much more frequently than the noticeable motion of the impurities. Therefore, it makes sense to calculate the desired Green functions for the charges first for a given static impurity configuration and then averaging this quantum expectation value over static impurity configurations. This is called the quenched averaging over the impurities.

What is left to discuss is the choice of the impurity distribution. We have no knowledge about it thus we try to reproduce the average over a large number of samples, each of which comes with its own static impurity configuration. In order to relate the averaging over the impurity configuration with other, more physical averaging we rely on the assumption of self averaging. This requires that the quenched average of our observable over the impurities is the same as the spatial average carried out in one given large system. One is interested in general in bulk, extensive quantities and the self averaging assumption assures that the measurement of a bulk quantity characterizing a large sample with a given impurity configuration can be reproduced by the quenched averaging method. The Green functions are not self averaging but their combinations making up a bulk quantity usually has this property.

Let us now return to the propagator (42) whose quenched average is

$$\overline{G(x,y)} = \sum_{n=0}^{\infty} \int dz_1 \cdots dz_n G_0(x,z_1) \cdots G_0(z_n,y) \overline{U(z_1) \cdots U(z_n)},$$

where the over-line denotes the average over the impurity configuration $\{\boldsymbol{x}_a\}$,

$$\overline{U(\boldsymbol{x})} = \sum_a \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\boldsymbol{x}} \tilde{U}(\boldsymbol{k}) \overline{e^{-i\boldsymbol{k}\boldsymbol{x}_a}}.$$

We use uniform distribution in space, $p(\boldsymbol{x}_a) = 1/V$, for simplicity yielding

$$\overline{U(\boldsymbol{x})} = \frac{N_i}{V} \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\boldsymbol{x}} \tilde{U}(\boldsymbol{k}) (2\pi)^3 \delta(\boldsymbol{k}) = n\tilde{U}(\boldsymbol{0}) = 0$$

where N_i denotes the number of impurities and $n = N_i/V$. Thus the average of the second graph on the right hand side of Fig. 9 is vanishing.

The second order term in the perturbation series (42) contains the average

$$\overline{U(\boldsymbol{x_1})U(\boldsymbol{x_2})} = \sum_{a_1,a_2} \int \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} e^{i\boldsymbol{k}_1\boldsymbol{x}_1 + i\boldsymbol{k}_2\boldsymbol{x}_2} \tilde{U}(\boldsymbol{k}_1) \tilde{U}(\boldsymbol{k}_2) \overline{e^{-i\boldsymbol{k}_1\boldsymbol{x}_{a_1} - i\boldsymbol{k}_2\boldsymbol{x}_{a_2}}}$$

and is shown in Fig. 10. The averaged Fourier modes

$$\overline{e^{-i\boldsymbol{k}_1\boldsymbol{x}_{a_1} - i\boldsymbol{k}_2\boldsymbol{x}_{a_2}}} = \frac{1}{V} (2\pi)^3 \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2)$$

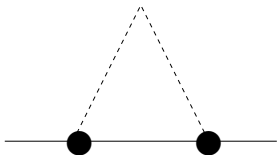

FIG. 10: The $\mathcal{O}\left(U^2\right)$ contribution to the propagator.

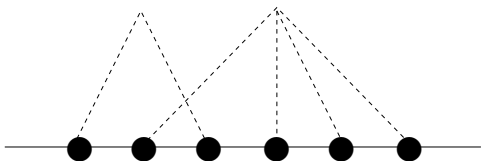

FIG. 11: The $\mathcal{O}\left(n^2U^6\right)$ contribution to the propagator.

give

$$\overline{U(\boldsymbol{x_1})U(\boldsymbol{x_2})} = n\overline{U(\boldsymbol{x_1})U(\boldsymbol{x_2})}_0$$

where

$$\overline{U(\boldsymbol{x_1})U(\boldsymbol{x_2})}_0 = \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}(\boldsymbol{x}_1-\boldsymbol{x}_2)}\tilde{U}(\boldsymbol{k})\tilde{U}(-\boldsymbol{k}).$$

The interaction vertices are connected by a dashed line with the point representing the space-time location of the impurity on the graphs.

The systematics should now be clear: The number of blobs of the graph, such as in Fig. 11, gives the order of the contribution. The number of impurity points gives the power of the density because each independent averaging over an impurity location generates the factor N/V,

$$\begin{aligned}
\overline{U(\boldsymbol{x_1})\cdots U(\boldsymbol{x_m})} &= n\int_{\boldsymbol{k}_1,\ldots,\boldsymbol{k}_m} e^{i\boldsymbol{k}_1\boldsymbol{x}_1+\cdots+i\boldsymbol{k}_m\boldsymbol{x}_m}\tilde{U}(\boldsymbol{k}_1)\cdots\tilde{U}(\boldsymbol{k}_m) + \mathcal{O}\left(n^2\right) \\
&= n\overline{U(\boldsymbol{x_1})\cdots U(\boldsymbol{x_m})}_0 \\
&\quad +n^2\sum_{a\neq b}\overline{U(\boldsymbol{x_a})U(\boldsymbol{x_b})}_0\ \overline{U(\boldsymbol{x_1})\cdots\hat{U}(\boldsymbol{x_a})\cdots\hat{U}(\boldsymbol{x_b})\cdots U(\boldsymbol{x_m})}_0\mathcal{O}\left(n^3\right)
\end{aligned}$$

It is instructive to carry out the partial resummation of the perturbation series by solving the Schwinger-Dyson equation. The leading order contribution to the self energy whose first few graphs are shown in Fig. 12 is

$$\begin{aligned}
\Sigma(\omega,\boldsymbol{k}) &\approx n\int\frac{d^3k}{(2\pi)^3}|\tilde{U}(\boldsymbol{q})|^2G_0(\omega,\boldsymbol{k}-\boldsymbol{q}) + \mathcal{O}\left(U^3\right) \\
&= n\int\frac{d^3k}{(2\pi)^3}|\tilde{U}(\boldsymbol{q}+\boldsymbol{k})|^2G_0(\omega,\boldsymbol{q}) \\
&= n\int\frac{d^3k}{(2\pi)^3}|\tilde{U}(\boldsymbol{q}+\boldsymbol{k})|^2\frac{i}{\omega-\omega(\boldsymbol{q})+i\epsilon\mathrm{sign}(\omega(\boldsymbol{k}))}.
\end{aligned}$$

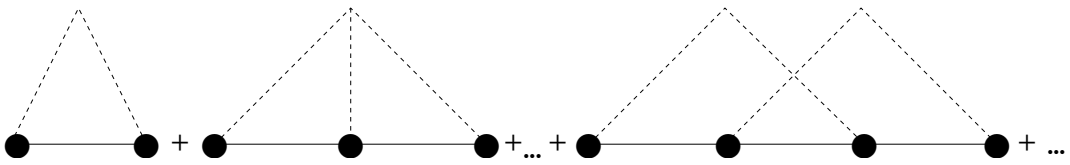

FIG. 12: The first three graphs of the self energy.

The identity

$$\frac{1}{x \pm i\epsilon} = P\frac{1}{x} \mp i\pi\delta(x)$$

gives

$$\begin{aligned}
\Re\Sigma(\omega, \boldsymbol{k}) &= -n \int \frac{d^3q}{(2\pi)^3} P \frac{|\tilde{U}(\boldsymbol{q}+\boldsymbol{k})|^2}{\omega - \omega(\boldsymbol{q})} \\
\Im\Sigma(\omega, \boldsymbol{k}) &= -\mathrm{sign}(\omega) n\pi \int \frac{d^3q}{(2\pi)^3} |\tilde{U}(\boldsymbol{q}+\boldsymbol{k})|^2 \delta(\omega - \omega(\boldsymbol{q})).
\end{aligned}$$

The partially resumed propagator

$$G(\omega, \boldsymbol{k}) = \frac{i}{\omega - \omega(\boldsymbol{q}) - \Sigma(\omega, \boldsymbol{k}) + i\epsilon \mathrm{sign}(\omega(\boldsymbol{k}))}$$

suggests to interpret the real part of the self energy at the Fermi level, $-\delta\mu = \Re\Sigma(0, \boldsymbol{k}_F)$, as the renormalization of the chemical potential up to a sign and the imaginary part evaluated at the Fermi level as the inverse life-time of the charged particle,

$$\begin{aligned}
\tau^{-1} &= -\mathrm{Im}\Sigma(0^+, \boldsymbol{k}_F) \\
&= n\pi \int \frac{d^3q}{(2\pi)^3} |\tilde{U}(\boldsymbol{q}+\boldsymbol{k}_F)|^2 \delta(\omega(\boldsymbol{q})) \\
&= \frac{n\pi}{\hbar} \int d E \nu(E) \frac{1}{4\pi} \int d\Omega |\tilde{U}(k_F \boldsymbol{\Omega} + \boldsymbol{k}_F)|^2 \delta(E - E_F) \\
&= \frac{n\pi}{\hbar} \nu(E_F) |\tilde{U}_F|^2
\end{aligned}$$

with

$$|\tilde{U}_F|^2 = \frac{1}{4\pi} \int d\Omega |\tilde{U}(k_F \boldsymbol{\Omega} + \boldsymbol{k}_F)|^2.$$

How on the earth can it happen that a charged particle, propagating in a random static impurity potential acquires finite life-time despite the charge conservation? The point is that the quenched averaging technique achieves something highly non-trivial and subtle. The core of the random impurity problem is the non-homogeneity created by the randomly distributed scattering centers. The loss of translation invariance changes the physics in a considerable manner. The averaging over the impurity locations formally restores translation invariance. But the reminder of formal nature of this restoration is is betrayed by the finite life-time. In fact, the the lowest lying state of a charge, propagating in a given random impurity configuration has no well-defined momentum. The quenched average of the propagator at a given momentum and energy represent the mixture of the transition amplitudes of different, usually excited states of the inhomogeneous problems which is unstable.

F. Linear response formula for the electric conductivity

The calculation of the current generated by a weak external electric field will be carried out the interaction representation where the external field effect represents the perturbation. We write the Hamiltonian as the sum $H(t) = H_0 + H_1(t)$ and the expectation value of an observable

$$O_i(t) = e^{\frac{i}{\hbar}H_0} O_S e^{-\frac{i}{\hbar}H_0},$$

defined in the interaction representation where $H_1(t)$ is treated as perturbation is

$$\langle\langle O(t)\rangle\rangle = \mathrm{Tr}\rho_i(t)O_i(t)$$

where

$$\rho_i(t) = U_i(t,t_i)\rho(t_i)U^\dagger(t,t_i)$$

is the density matrix. The time evolution operator satisfies the equation of motion

$$i\hbar\partial_t U(t,t_i) = H_{1i}(t)U(t,t_i)$$

according to the Schrödinger equation (24) and the corresponding equation of motion for the density matrix is

$$i\hbar\partial_t\rho_i(t) = [H_{1i}(t), \rho_i(t)].$$

The iterative integration of this equation generates the perturbation expansion whose first order piece,

$$\rho_i(t) = \rho_0 - \frac{i}{\hbar}\int_{t_i}^{t} dt'[H_{1i}(t'), \rho_0]dt' + \mathcal{O}\left(H_{1i}^2\right),$$

gives

$$\begin{aligned}
\delta\langle\langle O(t)\rangle\rangle &= \langle\langle O(t)\rangle\rangle - \mathrm{Tr}\rho_0 O(t) \\
&= -\frac{i}{\hbar}\int_0^t dt'\mathrm{Tr}[H_{1i}(t'), \rho_0]O_i(t)dt' \\
&= \frac{i}{\hbar}\int_0^t dt'\mathrm{Tr}\rho_0[H_{1i}(t'), O_i(t)]dt'
\end{aligned}$$

One can usually separate the time dependence of the perturbation, $H_1(t) = h(t)B_i$, and write

$$\begin{aligned}
\delta\langle\langle A\rangle\rangle &= \frac{i}{\hbar}\int_{t_0}^{t} dt' h(t')\mathrm{Tr}[B_i(t'), O_i(t)]\rho \\
&= \int_{t_0}^{t_f} G^R(t,t')h(t')dt'
\end{aligned}$$

where the retarded Green-function is defined by

$$i\hbar G^R_{O,B}(t,t') = \Theta(t-t')\langle\langle[O_i(t), B_i(t')]\rangle\rangle.$$

Let us apply this formalism for the electric conductivity defined by the proportionality of a weak external electric field and the current induced by it,

$$j_k = \sigma_{k,\ell}E_\ell.$$

The external electric field is written as

$$\boldsymbol{E} = -\partial_t \boldsymbol{A},$$

which leads to the perturbation

$$H_1 = -\int d^3x \boldsymbol{j}(\boldsymbol{x})\boldsymbol{A}(\boldsymbol{x}).$$

The minimal coupling prescription,

$$\boldsymbol{p} \to \boldsymbol{p} - e\boldsymbol{A}$$

in taking into account the electromagnetic field gives the current operator

$$\begin{aligned}
\boldsymbol{j} &= \frac{e\hbar}{2mi}(\psi^\dagger \boldsymbol{\nabla}\psi - \boldsymbol{\nabla}\psi^\dagger\psi) \\
&\to \frac{e\hbar}{2mi}\left[\psi^\dagger\left(\boldsymbol{\nabla} - \frac{ie}{\hbar}\boldsymbol{A}\right)\psi - \left(\boldsymbol{\nabla} - \frac{ie}{\hbar}\boldsymbol{A}\right)\psi^\dagger\psi\right] \\
&= \boldsymbol{j} - \frac{e^2}{m}\boldsymbol{A}\psi^\dagger\psi
\end{aligned}$$

whose expectation value is given by the Kubo-formula,

$$\langle\langle j_k(t,\boldsymbol{x})\rangle\rangle = -\frac{e^2}{m}\boldsymbol{A}\langle\langle\psi^\dagger\psi\rangle\rangle - \int dt' d^3y G^R_{k,\ell}((t,\boldsymbol{x}),(t',\boldsymbol{y}))A_\ell(t',\boldsymbol{y}).$$

This expression identifies the conductivity,

$$\sigma_{k,\ell}(\omega,\boldsymbol{k}) = -\frac{e^2 n}{m\omega} - \frac{1}{\omega}G^R(\omega,\boldsymbol{k}).$$

APPENDIX A: PHONONS

This Appendix contains the details of calculating the non-interactive phonon Green functions. We write the quantum field controlling the phonon excitations in a given band λ as

$$\chi_\lambda(\boldsymbol{x},t) = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\sqrt{\frac{\hbar}{2m_\lambda\omega_\lambda(\boldsymbol{k})}}[e^{-i\omega_\lambda(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c_\lambda(\boldsymbol{k}) + e^{i\omega_\lambda(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c^\dagger_\lambda(-\boldsymbol{k})].$$

It allows us to introduce the propagators

$$\begin{aligned}
i\hbar G(x,x') &= \langle 0|T[\chi(x)\chi(x')]|0\rangle \\
i\hbar G^R(x,x') &= \langle 0|[\chi(x),\chi(x')]_+|0\rangle\Theta(t-t') \\
i\hbar G^A(x,x') &= -\langle 0|[\chi(x),\chi(x')]_+|0\rangle\Theta(t'-t) \\
\hbar G^E(x,x') &= -\langle 0|T[\chi(x)\chi(x')]|0\rangle.
\end{aligned}$$

The steps, analogous to the fermionic case yield the causal propagator

$$
\begin{aligned}
i\hbar G(x,x') &= \int \frac{d^3k d^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}} \\
&\quad \times\langle 0|\Theta(t-t')[e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c(\boldsymbol{k})+e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c^\dagger(-\boldsymbol{k})][e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c(\boldsymbol{k'})+e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c^\dagger(-\boldsymbol{k'})] \\
&\quad +\Theta(t'-t)[e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c(\boldsymbol{k'})+e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c^\dagger(-\boldsymbol{k'})][e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c(\boldsymbol{k})+e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c^\dagger(-\boldsymbol{k})]|0\rangle \\
&= \int \frac{d^3k d^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}}\langle 0|\Theta(t-t')e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c(\boldsymbol{k})e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c^\dagger(-\boldsymbol{k'}) \\
&\quad +\Theta(t'-t)e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c(\boldsymbol{k'})e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c^\dagger(-\boldsymbol{k})|0\rangle \\
&= \int \frac{d^3k d^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}}(2\pi)^3\delta(\boldsymbol{k}+\boldsymbol{k'}) \\
&\quad \times[\Theta(t-t')e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}+\Theta(t'-t)e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}] \\
&= \int \frac{d^3k d\omega}{(2\pi)^4}\frac{\hbar i}{2m}\left(\frac{e^{-i(\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega(\boldsymbol{k})(\omega+i\epsilon)}+\frac{e^{-i(\omega(-\boldsymbol{k})+\omega)(t'-t)+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega(-\boldsymbol{k})(\omega+i\epsilon)}\right) \\
&= \int \frac{d^3k d\omega}{(2\pi)^4}\frac{\hbar i}{2m\omega(\boldsymbol{k})}\left(\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})+i\epsilon}+\frac{e^{-i\omega(t'-t)+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-\omega(\boldsymbol{k})+i\epsilon}\right) \\
&= \int \frac{d^3k d\omega}{(2\pi)^4}\frac{\hbar i}{2m\omega(\boldsymbol{k})}e^{-i\omega(t'-t)+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}\left(\frac{1}{\omega-\omega(\boldsymbol{k})+i\epsilon}-\frac{1}{\omega+\omega(\boldsymbol{k})-i\epsilon}\right) \\
&= \frac{\hbar i}{m}\int \frac{d^3k d\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega^2-\omega^2(\boldsymbol{k})+i\epsilon}
\end{aligned}
$$

The retarded propagators is

$$
\begin{aligned}
i\hbar G^R(x,x') &= \int \frac{d^3k d^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}} \\
&\quad \times\Theta(t-t')\langle 0|[e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c(\boldsymbol{k})+e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c^\dagger(-\boldsymbol{k})][e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c(\boldsymbol{k'})+e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c^\dagger(-\boldsymbol{k'})] \\
&\quad -[e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c(\boldsymbol{k'})+e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c^\dagger(-\boldsymbol{k'})][e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c(\boldsymbol{k})+e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c^\dagger(-\boldsymbol{k})]|0\rangle \\
&= \int \frac{d^3k d^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}}\Theta(t-t')\langle 0|e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c(\boldsymbol{k})e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c^\dagger(-\boldsymbol{k'}) \\
&\quad -e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}c(\boldsymbol{k'})e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}c^\dagger(-\boldsymbol{k})|0\rangle \\
&= \int \frac{d^3k d^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}}(2\pi)^3\delta(\boldsymbol{k}+\boldsymbol{k'}) \\
&\quad \times\Theta(t-t')[e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}-e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'}\boldsymbol{k'}}e^{i\omega(\boldsymbol{k})t+i\boldsymbol{x}\boldsymbol{k}}] \\
&= \int \frac{d^3k}{(2\pi)^3}{}_{\boldsymbol{k}}\frac{\hbar}{2m\omega(\boldsymbol{k})}\Theta(t-t')[e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}-e^{-i\omega(\boldsymbol{k})(t'-t)+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}] \\
&= \int \frac{d^3k d\omega}{(2\pi)^4}\frac{\hbar i}{2m\omega(\boldsymbol{k})}\left(\frac{e^{-i(\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon}-\frac{e^{-i(\omega-\omega(\boldsymbol{k}))(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon}\right) \\
&= \int \frac{d^3k d\omega}{(2\pi)^4}\frac{\hbar i}{2m}\left(\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega(\boldsymbol{k})(\omega-\omega(\boldsymbol{k})+i\epsilon)}-\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega(-\boldsymbol{k})(\omega+\omega(-\boldsymbol{k})+i\epsilon)}\right) \\
&= \int \frac{d^3k d\omega}{(2\pi)^4}\frac{\hbar i}{2m\omega(\boldsymbol{k})}e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}\left(\frac{1}{\omega-\omega(\boldsymbol{k})+i\epsilon}-\frac{1}{\omega+\omega(\boldsymbol{k})+i\epsilon}\right) \\
&= \frac{\hbar i}{m}\int \frac{d^3k d\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega^2-\omega^2(\boldsymbol{k})+i\mathrm{sign}(\omega)\epsilon} \\
&= \frac{\hbar i}{m}\int \frac{d^3k d\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega^2-\omega^2(\boldsymbol{k})+i\mathrm{sign}(\omega(\boldsymbol{k}))\epsilon}.
\end{aligned}
$$

The advanced version is obtained in a similar manner,

$$
\begin{aligned}
i\hbar G^A(x,x') &= -\int \frac{d^3kd^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}} \\
&\times\Theta(t'-t)\langle 0|[e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}c(\boldsymbol{k})+e^{i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}c^\dagger(-\boldsymbol{k})][e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}c(\boldsymbol{k'})+e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}c^\dagger(-\boldsymbol{k'})] \\
&-[e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}c(\boldsymbol{k'})+e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}c^\dagger(-\boldsymbol{k'})][e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}c(\boldsymbol{k})+e^{i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}c^\dagger(-\boldsymbol{k})]|0\rangle \\
&= -\int \frac{d^3kd^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}}\Theta(t'-t)\langle 0|e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}c(\boldsymbol{k})e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}c^\dagger(-\boldsymbol{k'}) \\
&-e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}c(\boldsymbol{k'})e^{i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}c^\dagger(-\boldsymbol{k})|0\rangle \\
&= -\int \frac{d^3kd^3k'}{(2\pi)^6}\frac{\hbar}{2m\sqrt{\omega(\boldsymbol{k})\omega(\boldsymbol{k'})}}(2\pi)^3\delta(\boldsymbol{k}+\boldsymbol{k'}) \\
&\times\Theta(t'-t)[e^{-i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}e^{i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}-e^{-i\omega(\boldsymbol{k'})t'+i\boldsymbol{x'k'}}e^{i\omega(\boldsymbol{k})t+i\boldsymbol{xk}}] \\
&= -\int \frac{d^3k}{(2\pi)^3}\frac{\hbar}{2m\omega(\boldsymbol{k})}\Theta(t'-t)[e^{-i\omega(\boldsymbol{k})(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}-e^{-i\omega(\boldsymbol{k})(t'-t)+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}] \\
&= -\int \frac{d^3kd\omega}{(2\pi)^4}\frac{\hbar i}{2m\omega(\boldsymbol{k})}\left(\frac{e^{-i(\omega(\boldsymbol{k})-\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon}-\frac{e^{-i(-\omega-\omega(\boldsymbol{k}))(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega+i\epsilon}\right) \\
&= \int \frac{d^3kd\omega}{(2\pi)^4}\frac{\hbar i}{2m\omega(\boldsymbol{k})}\left(\frac{e^{-i(\omega(\boldsymbol{k})+\omega)(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-i\epsilon}-\frac{e^{-i(\omega-\omega(\boldsymbol{k}))(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega-i\epsilon}\right) \\
&= \int \frac{d^3kd\omega}{(2\pi)^4}\frac{\hbar i}{2m\omega(\boldsymbol{k})}e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}\left(\frac{1}{\omega-\omega(\boldsymbol{k})-i\epsilon}-\frac{1}{\omega+\omega(\boldsymbol{k})-i\epsilon}\right) \\
&= \frac{\hbar i}{m}\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega^2-\omega^2(\boldsymbol{k})-i\mathrm{sign}(\omega)\epsilon} \\
&= \frac{\hbar i}{m}\int \frac{d^3kd\omega}{(2\pi)^4}\frac{e^{-i\omega(t-t')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega^2-\omega^2(\boldsymbol{k})-i\mathrm{sign}(\omega(\boldsymbol{k}))\epsilon}.
\end{aligned}
$$

Finally, the imaginary time propagator is obtained by the Wick-rotation $t_R=-it_I$ and $\omega_R=i\omega_I$ as

$$\hbar G^E_{\alpha\beta}(x,x')=-\frac{1}{\beta}\sum_n\int_{\boldsymbol{k}}\frac{e^{-i\omega_n(\tau-\tau')+i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})}}{\omega_n^2+\omega_{\boldsymbol{k}}^2}$$

where $\omega_n=2\pi k_BTn$ is the bosonic Matsubara frequency.

APPENDIX B: SPECTRAL REPRESENTATION

The calulation of the different propagators presented in Chapter III is valid for non-interacting particles only. It is interesting to realize that there is a simple extension of the free propagators for interacting system which is parameterized by a spectral weight function only with clear physical interpretation. Apart of being an important tool, this representation offers another view of the propagators with or without interactions.

Let us denote the eigenstates of the Hamiltonian by $|\{n\}\rangle$,

$$H|\{n\}\rangle=\hbar\omega_{\{n\}}|\{n\}\rangle$$

and write the matrix elements of the quantum field as

$$\psi_{\{m\},\{n\}}(\boldsymbol{x})=\langle\{m\}|\psi(0,\boldsymbol{x})|\{n\}\rangle,$$

where $\{n\}$ a set of quantum numbers, such as the occupation number configuration $n(\boldsymbol{q})$, identifying a basis element of the Fock-space. The thermal and quantum average of an observable A is then

$$\langle\langle A\rangle\rangle=\sum_{\{n\}}p_{\{n\}}\langle\{n\}|A|\{n\}\rangle$$

where

$$p_{\{n\}} = \frac{e^{-\beta\hbar\omega_{\{n\}}}}{\sum_{\{n\}} e^{-\beta\hbar\omega_{\{n\}}}}.$$

We are first interested in the causal propagator at a given frequency,

$$\begin{aligned} i\hbar G(\boldsymbol{x},\boldsymbol{x'},\omega) &= \int dt e^{i\omega t}\langle\langle T[\psi(t,\boldsymbol{x})\psi^\dagger(0,\boldsymbol{x'})]\rangle\rangle \\ &= \int_0^\infty dt e^{i\omega t}\langle\langle \psi(t,\boldsymbol{x})\psi^\dagger(0,\boldsymbol{x'})\rangle\rangle - \int_{-\infty}^0 dt e^{i\omega t}\langle\langle \psi^\dagger(0,\boldsymbol{x'})\psi(t,\boldsymbol{x})\rangle\rangle. \end{aligned}$$

The desired boundary conditions in time are implemented by the $i\epsilon$ prescription,

$$\begin{aligned} i\hbar G(\boldsymbol{x},\boldsymbol{x'},\omega) &= \int_0^\infty dt e^{i(\omega+i\epsilon)t}\langle\langle \psi(t,\boldsymbol{x})\psi^\dagger(0,\boldsymbol{x'})\rangle\rangle - \int_{-\infty}^0 dt e^{i(\omega-i\epsilon)t}\langle\langle \psi^\dagger(0,\boldsymbol{x'})\psi(t,\boldsymbol{x})\rangle\rangle \\ &= \int_0^\infty dt e^{i(\omega+i\epsilon)t}\sum_{\{m\},\{n\}} p_{\{m\}} e^{i\omega_{\{m\},\{n\}}t}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'}) \\ &\quad - \int_{-\infty}^0 dt e^{i(\omega-i\epsilon)t}\sum_{\{m\},\{n\}} p_{\{m\}}\psi^\dagger_{\{m\},\{n\}}(\boldsymbol{x'})\psi_{\{n\},\{m\}}(\boldsymbol{x}) e^{i\omega_{\{n\},\{m\}}t} \\ &= -\sum_{\{m\},\{n\}} p_{\{m\}}\left(\frac{\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})}{\omega+i\epsilon+\omega_{\{m\},\{n\}}} + \frac{\psi^\dagger_{\{m\},\{n\}}(\boldsymbol{x'})\psi_{\{n\},\{m\}}(\boldsymbol{x})}{\omega-i\epsilon+\omega_{\{n\},\{m\}}}\right) \\ &= i\sum_{\{m\},\{n\}}\left(p_{\{m\}}\frac{\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})}{\omega+i\epsilon+\omega_{\{m\},\{n\}}} + p_{\{n\}}\frac{\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})}{\omega-i\epsilon+\omega_{\{m\},\{n\}}}\right) \\ &= i\int_{-\infty}^\infty d\lambda \sum_{\{m\},\{n\}} p_{\{m\}}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})\delta(\lambda+\omega_{\{m\},\{n\}})\frac{1}{\omega+i\epsilon-\lambda} \\ &\quad + i\int_{-\infty}^\infty d\lambda \sum_{\{m\},\{n\}} p_{\{n\}}\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})\delta(\lambda+\omega_{\{m\},\{n\}})\frac{1}{\omega-i\epsilon-\lambda}, \end{aligned}$$

where $\omega_{\{m\},\{n\}} = \omega_{\{m\}} - \omega_{\{n\}}$. The relation (32) can be used to write

$$\begin{aligned} i\hbar G(\boldsymbol{x},\boldsymbol{x'},\omega) &= i\int_{-\infty}^\infty d\lambda \sum_{\{m\},\{n\}} p_{\{m\}}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})\delta(\lambda+\omega_{\{m\},\{n\}})\left(\frac{P}{\omega-\lambda} - i\pi\delta(\omega-\lambda)\right) \\ &\quad + i\int_{-\infty}^\infty d\lambda \sum_{\{m\},\{n\}} p_{\{n\}}\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})\delta(\lambda+\omega_{\{m\},\{n\}})\left(\frac{P}{\omega-\lambda} + i\pi\delta(\omega-\lambda)\right) \\ &= i\int_{-\infty}^\infty d\lambda\left[A(\boldsymbol{x},\boldsymbol{x'},\lambda)\frac{P}{\omega-\lambda} - i\pi B(\boldsymbol{x},\boldsymbol{x'},\lambda)\delta(\omega-\lambda)\right] \end{aligned}$$

where

$$A(\boldsymbol{x},\boldsymbol{x'},\lambda) = \sum_{\{m\},\{n\}} (p_{\{m\}} + p_{\{n\}})\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})\delta(\lambda+\omega_{\{m\},\{n\}})$$

and

$$B(\boldsymbol{x},\boldsymbol{x'},\lambda) = \sum_{\{m\},\{n\}} (p_{\{m\}} - p_{\{n\}})\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^\dagger_{\{n\},\{m\}}(\boldsymbol{x'})\delta(\lambda+\omega_{\{m\},\{n\}}).$$

The latter can be recasted in the form

$$\begin{aligned} B(\boldsymbol{x},\boldsymbol{x'},\lambda) &= \sum_{\{m\},\{n\}} \frac{p_{\{m\}}-p_{\{n\}}}{p_{\{m\}}+p_{\{n\}}}(p_{\{m\}}+p_{\{n\}})\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x})\delta(\lambda+\omega_{\{m\},\{n\}}) \\ &= A(\boldsymbol{x},\boldsymbol{x'},\lambda)\frac{1-e^{-\beta\lambda}}{1+e^{-\beta\lambda}} \\ &= A(\boldsymbol{x},\boldsymbol{x'},\lambda)\left(1-\frac{2}{1+e^{\beta\lambda}}\right), \end{aligned}$$

leaving the function $A(\boldsymbol{x},\boldsymbol{x'},\lambda)$ as the only unknown piece of the propagator.

The same function $A(\boldsymbol{x},\boldsymbol{x'},\lambda)$ determines other propagators, too. The retarded propagator is

$$\begin{aligned} i\hbar G^{R}(\boldsymbol{x},\boldsymbol{x'},\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t}\langle\langle[\psi(t,\boldsymbol{x}),\psi^{\dagger}(0,\boldsymbol{x'})]_{+}\rangle\rangle\Theta(t) \\ &\to \int_{0}^{\infty} dt e^{i(\omega+i\epsilon)t}\sum_{\{m\},\{n\}} p_{\{m\}} \\ &\quad\times\left[e^{i\omega_{\{m\},\{n\}}t}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})+\psi^{\dagger}_{\{m\},\{n\}}(\boldsymbol{x'})\psi_{\{n\},\{m\}}(\boldsymbol{x})e^{i\omega_{\{n\},\{m\}}t}\right] \\ &= i\sum_{\{m\},\{n\}} p_{\{m\}}\left(\frac{\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})}{\omega+\omega_{\{m\},\{n\}}+i\epsilon}+\frac{\psi^{\dagger}_{\{m\},\{n\}}(\boldsymbol{x'})\psi_{\{n\},\{m\}}(\boldsymbol{x})}{\omega+\omega_{\{n\},\{m\}}+i\epsilon}\right) \\ &= i\sum_{\{m\},\{n\}}\left(p_{\{m\}}\frac{\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})}{\omega+\omega_{\{m\},\{n\}}+i\epsilon}+p_{\{n\}}\frac{\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})}{\omega+\omega_{\{m\},\{n\}}+i\epsilon}\right) \\ &= i\int_{-\infty}^{\infty} d\lambda\frac{A(\boldsymbol{x},\boldsymbol{x'},\lambda)}{\omega+i\epsilon-\lambda}. \end{aligned}$$

The advanced propagator is obtained in a similar manner,

$$\begin{aligned} i\hbar G^{A}(\boldsymbol{x},\boldsymbol{x'},\omega) &= -\int_{-\infty}^{\infty} dt e^{i\omega t}\langle\langle[\psi(t,\boldsymbol{x}),\psi^{\dagger}(0,\boldsymbol{x'})]_{+}\rangle\rangle\Theta(-t) \\ &\to -\int_{-\infty}^{0} dt e^{i(\omega-i\epsilon)t}\sum_{\{m\},\{n\}} p_{\{m\}} \\ &\quad\times\left[e^{i\omega_{\{m\},\{n\}}t}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})+\psi^{\dagger}_{\{m\},\{n\}}(\boldsymbol{x'})\psi_{\{n\},\{m\}}(\boldsymbol{x})e^{i\omega_{\{n\},\{m\}}t}\right] \\ &= i\sum_{\{m\},\{n\}} p_{\{m\}}\left(\frac{\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})}{\omega+\omega_{\{m\},\{n\}}-i\epsilon}+\frac{\psi^{\dagger}_{\{m\},\{n\}}(\boldsymbol{x'})\psi_{\{n\},\{m\}}(\boldsymbol{x})}{\omega+\omega_{\{n\},\{m\}}-i\epsilon}\right) \\ &= i\sum_{\{m\},\{n\}}\left(p_{\{m\}}\frac{\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})}{\omega+\omega_{\{m\},\{n\}}-i\epsilon}+p_{\{n\}}\frac{\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})}{\omega+\omega_{\{m\},\{n\}}-i\epsilon}\right) \\ &= i\int_{-\infty}^{\infty} d\lambda\frac{A(\boldsymbol{x},\boldsymbol{x'},\lambda)}{\omega-i\epsilon-\lambda} \end{aligned}$$

Finally, the imaginary time propagator is

$$\begin{aligned}
\hbar G^E(\boldsymbol{x},\boldsymbol{x'},\omega) &= \frac{1}{2}\int_{-\beta}^{0} dt e^{i\omega t}\sum_{\{m\},\{n\}} p_{\{n\}} e^{(\omega_m-\omega_n)t}\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x}) \\
&\quad -\frac{1}{2}\int_{0}^{\beta} dt e^{i\omega t}\sum_{\{m\},\{n\}} p_{\{m\}} e^{(\omega_m-\omega_n)t}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'}) \\
&= -\frac{1}{2}\sum_{\{m\},\{n\}} p_{\{n\}}\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})\frac{e^{-\beta(i\omega+\omega_{\{m\},\{n\}})}-1}{i\omega+\omega_{\{m\},\{n\}}} \\
&\quad -\frac{1}{2}\sum_{\{m\},\{n\}} p_{\{m\}}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\frac{e^{\beta(i\omega+\omega_{\{m\},\{n\}})}-1}{i\omega+\omega_{\{m\},\{n\}}} \\
&= -\frac{1}{2}\int_{-\infty}^{\infty} d\lambda\sum_{\{m\},\{n\}} p_{\{n\}}\delta(\lambda+\omega_{\{m\},\{n\}})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})\frac{e^{-\beta(i\omega+\omega_{\{m\},\{n\}})}-1}{i\omega-\lambda} \\
&\quad -\frac{1}{2}\int_{-\infty}^{\infty} d\lambda\sum_{\{m\},\{n\}} p_{\{m\}}\delta(\lambda+\omega_{\{m\},\{n\}})\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\frac{e^{\beta(i\omega+\omega_{\{m\},\{n\}})}-1}{i\omega-\lambda} \\
&= \frac{1}{2}\int_{-\infty}^{\infty} d\lambda\sum_{\{m\},\{n\}} \delta(\lambda+\omega_{\{m\},\{n\}})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})\frac{e^{-\beta\omega_n}(e^{-\beta\omega_{\{m\},\{n\}}}+1)}{i\omega-\lambda} \\
&\quad +\frac{1}{2}\int_{-\infty}^{\infty} d\lambda\sum_{\{m\},\{n\}} \delta(\lambda+\omega_{\{m\},\{n\}})\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\frac{e^{-\beta\omega_m}(e^{\beta\omega_{\{m\},\{n\}}}+1)}{i\omega-\lambda} \\
&= \frac{1}{2}\int_{-\infty}^{\infty} d\lambda\sum_{\{m\},\{n\}} \delta(\lambda+\omega_{\{m\},\{n\}})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})\frac{e^{-\beta\omega_m}+e^{-\beta\omega_n}}{i\omega-\lambda} \\
&\quad +\frac{1}{2}\int_{-\infty}^{\infty} d\lambda\sum_{\{m\},\{n\}} \delta(\lambda+\omega_{\{m\},\{n\}})\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\frac{e^{-\beta\omega_n}+e^{-\beta\omega_m}}{i\omega-\lambda} \\
&= \int_{-\infty}^{\infty} d\lambda\frac{A(\boldsymbol{x},\boldsymbol{x'},\lambda)}{i\omega-\lambda}.
\end{aligned}$$

The common function $A(\boldsymbol{x},\boldsymbol{x'},\omega)$, characterizing the different propagators has a simple physical interpretation, it gives the density of states. We have in coordinate space

$$\begin{aligned}
A(\boldsymbol{x},\boldsymbol{x'},\omega) &= \sum_{\{m\},\{n\}}(p_{\{m\}}+p_{\{n\}})\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\delta(\omega+\omega_{\{m\},\{n\}}) \\
&= \sum_{\{m\},\{n\}}[p_{\{m\}}\psi_{\{m\},\{n\}}(\boldsymbol{x})\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})+p_{\{n\}}\psi^{\dagger}_{\{n\},\{m\}}(\boldsymbol{x'})\psi_{\{m\},\{n\}}(\boldsymbol{x})]\delta(\omega+\omega_{\{m\},\{n\}})
\end{aligned}$$

where the first and the second terms in the second line represent the contributions of the positive energy, particle excitations with $\omega=\omega_n-\omega_m$ and the negative energy, hole excitations because $\omega=-\omega_m-(-\omega_n)$, respectively. The density of state at point $\boldsymbol{x}$ and at energy $\hbar\omega$ is obviously

$$N(\boldsymbol{x},\omega)=A(\boldsymbol{x},\boldsymbol{x},\omega).$$

In the case of a translation invariant system the density of state is constant in the coordinate space but its Fourier transform yields the density of state,

$$N(\boldsymbol{k},\omega)=A(\boldsymbol{k},\omega)=\int d^3x e^{-i\boldsymbol{k}\boldsymbol{x}}A(\boldsymbol{x},0,\omega),$$

in momentum space.

The expressions for the different propagators given in terms of the spectral density function $A(\boldsymbol{x},\boldsymbol{x'},\lambda)$ differ in the

infinitesimal imaginary part of the position of the poles on the complex frequency plan. In particular,

$$\begin{aligned} G^R(\boldsymbol{x},\boldsymbol{x'},\omega) - G^A(\boldsymbol{x},\boldsymbol{x'},\omega) &= \int_{-\infty}^{\infty} d\lambda A(\boldsymbol{x},\boldsymbol{x'},\lambda)\left(\frac{1}{\omega+i\epsilon-\lambda} - \frac{1}{\omega-i\epsilon-\lambda}\right) \\ &= -2\pi i \int_{-\infty}^{\infty} d\lambda A(\boldsymbol{x},\boldsymbol{x'},\lambda)\delta(\omega-\lambda) \\ &= -2\pi i A(\boldsymbol{x},\boldsymbol{x'},\omega). \end{aligned}$$

Since $G^R(\boldsymbol{x},\boldsymbol{x'},\omega) = G^{A*}(\boldsymbol{x},\boldsymbol{x'},\omega)$ the imaginary part of the retarded propagator,

$$A(\boldsymbol{x},\boldsymbol{x'},\omega) = A^*(\boldsymbol{x},\boldsymbol{x'},\omega) = -\frac{1}{\pi} ImG^R(\boldsymbol{x},\boldsymbol{x'},\omega),$$

determines the rest,

$$\begin{aligned} N(\boldsymbol{x},\omega) &= A(\boldsymbol{x},\boldsymbol{x},\omega) = -\frac{1}{\pi} ImG^R(\boldsymbol{x},\boldsymbol{x},\omega) \\ N(\boldsymbol{k},\omega) &= A(\boldsymbol{k},\omega) = -\frac{1}{\pi} ImG^R(\boldsymbol{k},\omega). \end{aligned}$$

The limit $T \to 0$ gives

$$\begin{aligned} A(\boldsymbol{x},\boldsymbol{x'},\lambda) &\to \sum_{\{n\}} \langle\mu|\psi(\boldsymbol{x})|\{n\}\rangle\langle\{n\}|\psi^\dagger(\boldsymbol{x'})|\mu\rangle\delta(\lambda-\omega_{\{n\}}) + \sum_{\{m\}} \langle\mu|\psi^\dagger(\boldsymbol{x'})|\{m\}\rangle\langle\{m\}|\psi(\boldsymbol{x})|\mu\rangle\delta(\lambda+\omega_{\{m\}}) \\ A(\boldsymbol{k},\lambda) &= \int d^3x e^{-i\boldsymbol{k}\boldsymbol{x}} A(\boldsymbol{x},0,\lambda) \to \sum_{\{n\}} n|\langle\{n\}|a^\dagger_{\boldsymbol{k}}|\mu\rangle|^2\delta(\lambda-\omega_n) + \sum_{\{n\}} n|\langle\{n\}|a_{-\boldsymbol{k}}|\mu\rangle|^2\delta(\lambda+\omega_n), \end{aligned}$$

where translation invariance was assumed in deriving the second equation. The first equation gives

$$B(\boldsymbol{x},\boldsymbol{x'},\lambda) = A(\boldsymbol{x},\boldsymbol{x'},\lambda)\frac{1-e^{-\beta\lambda}}{1+e^{-\beta\lambda}} \to \mathrm{sign}(\lambda)A(\boldsymbol{x},\boldsymbol{x'},\lambda)$$

and

$$G(\boldsymbol{x},\boldsymbol{x'},\omega) = \int_{-\infty}^{\infty} d\lambda A(\boldsymbol{x},\boldsymbol{x'},\lambda)\left[\frac{P}{\omega-\lambda} - i\pi\mathrm{sign}(\lambda)\delta(\omega-\lambda)\right] \to \int_{-\infty}^{\infty} d\lambda \frac{A(\boldsymbol{x},\boldsymbol{x'},\lambda)}{\omega-\lambda+i\mathrm{sign}(\omega)\epsilon}.$$

For non-interacting particles we have

$$\begin{aligned} N(\boldsymbol{k},\omega) &= \sum_{\boldsymbol{k}} \sum_{\{m\},\{n\}} (p_{\{m\}} + p_{\{n\}})(a_{\boldsymbol{k}})_{\{m\},\{n\}}(a^\dagger_{\boldsymbol{q}})_{\{n\},\{m\}}\delta(\omega+\omega_{\{m\},\{n\}}) \\ &= \sum_{\boldsymbol{k}} \sum_{m,n} (p_m + p_n)\langle m|a|n\rangle\langle n|a^\dagger|m\rangle\delta_{\boldsymbol{k},\boldsymbol{q}}\delta(\omega+\omega_{m,n}) \\ &= \sum_{m,n} (p_m + p_n)\langle m|a|n\rangle\langle n|a^\dagger|m\rangle\delta(\omega+(m-n)\omega(\boldsymbol{k})) \\ &= \sum_{m} (p_m + p_{m+1})(m+1)\delta(\omega-\omega(\boldsymbol{k})) \end{aligned}$$

which becomes

$$A(\boldsymbol{k},\lambda) = \delta(\lambda-\omega(\boldsymbol{k}))$$

at vanishing temperature.

The decays due to the coupling of radiation fields or to reservoirs introduce a 'leaking' of the excited states into the environment which appears as a gradual decrease of the norm of the state, projected into the system's Fock-space, ignoring the environment. Such a 'leak' generates a finite lint-time for the excited states. Exponential decays in time with life-time $\tau = 1/\gamma$ can phenomenologically be reproduced by means of the spectral density

$$A(\boldsymbol{k},\lambda) = Z\delta_\gamma(\lambda-\omega(\boldsymbol{k})),$$

where the Lorentzian spectral function

$$\delta_\gamma(\lambda) = \frac{\gamma}{\pi}\frac{1}{\lambda^2+\gamma^2}$$

is introduced. In fact, the retarded and advanced propagators,

$$\begin{aligned}
\hbar\overset{R}{G^A}(\boldsymbol{k},\omega) &= \int d^3x e^{-i\boldsymbol{kx}}\hbar\overset{R}{G^A}(\boldsymbol{x},0,\omega) \\
&= \int_{-\infty}^{\infty} d\lambda \frac{A(\boldsymbol{k},\lambda)}{\omega-\lambda\pm i\epsilon} \\
&= Z\frac{\gamma}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{[(\lambda-\omega(\boldsymbol{k}))^2+\gamma^2](\omega-\lambda\pm i\epsilon)} \\
&= -Z\frac{\gamma}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{(\lambda-\omega(\boldsymbol{k})+i\gamma)(\lambda-\omega(\boldsymbol{k})-i\gamma)(\lambda-\omega\mp i\epsilon)} \\
&= \begin{cases} 2iZ\gamma\frac{1}{-2i\gamma(\omega(\boldsymbol{k})-i\gamma-\omega)} \\ -2iZ\gamma\frac{1}{2i\gamma(\omega(\boldsymbol{k})+i\gamma-\omega)} \end{cases} \\
&= \frac{Z}{\omega-\omega(\boldsymbol{k})\pm i\gamma},
\end{aligned}$$

give exponential decay in time,

$$\begin{aligned}
i\hbar\overset{R}{G^A}(\boldsymbol{k},t) &= \int\frac{d\omega}{2\pi}e^{-i\omega t}i\hbar\overset{R}{G^A}(\boldsymbol{k},\omega) \\
&= Ze^{-i(\omega(\boldsymbol{k})\mp i\gamma)t},
\end{aligned}$$

Note that the Lorentzian tends to the Dirac-delta for stable excitations, $\lim_{\gamma\to 0}\delta_\gamma(\lambda)=\delta(\lambda)$.

APPENDIX C: CONTRACTIONS

The explicit calculation of the contractions is shown in this Appendix for the electron field

$$\psi_\sigma(t,\boldsymbol{x}) = \int_{\boldsymbol{k}} e^{-i\omega_{\boldsymbol{k}}t+\boldsymbol{kx}}a_\sigma(\boldsymbol{k}) = \psi^{(-)}+\psi^{(+)}$$

where the positive and negative frequency parts are

$$\begin{aligned}
\psi^{(+)} &= \int_{\boldsymbol{k}>k_F} e^{-i\omega_{\boldsymbol{k}}t+\boldsymbol{kx}}b_\sigma(\boldsymbol{k}) \\
\psi^{(-)} &= \int_{\boldsymbol{k}\le k_F} e^{i|\omega_{\boldsymbol{k}}|t+\boldsymbol{kx}}b^\dagger_\sigma(\boldsymbol{k}),
\end{aligned}$$

respectively. There are altogether 16 different contractions for the fields $\psi^{(+)}$, $\psi^{(-)}$, $\psi^{(+)\dagger}$ and $\psi^{(-)\dagger}$. For a nonrelativistic field with boson exchange statistics one should set $k_F=0$ and $\psi^{(-)}=0$.

Let us consider first two (anti)commuting operators $[A,B]_\xi=0$ with the contraction

$$\overbrace{A(t,\boldsymbol{x})B(t',\boldsymbol{x'})} = T[A(t,\boldsymbol{x})B(t',\boldsymbol{x'})] - :A(t,\boldsymbol{x})B(t',\boldsymbol{x'}):.$$

Note that the time-ordered product

$$T[A(t,\boldsymbol{x})B(t',\boldsymbol{x'})] = \begin{cases} A(t,\boldsymbol{x})B(t',\boldsymbol{x'}) & t<t' \\ \xi B(t',\boldsymbol{x'})A(t,\boldsymbol{x}) & t'<t \end{cases}$$

is independent of the order of the time arguments due to the assumption $[A,B]_\xi=0$. The normal ordered product,

$$:A(t,\boldsymbol{x})B(t',\boldsymbol{x'}): = \begin{cases} A(t,\boldsymbol{x})B(t',\boldsymbol{x'}) \\ \xi B(t',\boldsymbol{x'})A(t,\boldsymbol{x}) \end{cases}$$

formally depends on the order of the operators but the vanishing anti commutator renders the two cases identical. At the end the difference of the time and the normal ordered product is identically vanishing.

The remaining cases are $\overbrace{\psi^{(\pm)}(t,\boldsymbol{x})\psi^{(\pm)\dagger}(t',\boldsymbol{x'})}$. Direct calculation yields for $t > t'$

$$\begin{aligned}
\overbrace{\psi^{(+)}(t,\boldsymbol{x})\psi^{(+)\dagger}(t',\boldsymbol{x'})} &= T[\psi^{(+)}(t,\boldsymbol{x})\psi^{(+)\dagger}(t',\boldsymbol{x'})] - :\psi^{(+)}(t,\boldsymbol{x})\psi^{(+)\dagger}(t',\boldsymbol{x'}): \\
&= \psi^{(+)}(t,\boldsymbol{x})\psi^{(+)\dagger}(t',\boldsymbol{x'}) - \xi\psi^{(+)\dagger}(t',\boldsymbol{x'})\psi^{(+)}(t,\boldsymbol{x}) \\
&= \int_{\boldsymbol{k},\boldsymbol{k'}>k_F} \frac{d^3k d^3k'}{(2\pi)^6} e^{-i\omega(\boldsymbol{k})t+\boldsymbol{kx}+i\omega_{\boldsymbol{k'}}t'-\boldsymbol{k'x'}}[b(\boldsymbol{k}),b^\dagger(\boldsymbol{k'})]_\xi \\
&= \int_{\boldsymbol{k},\boldsymbol{k'}>k_F} \frac{d^3k d^3k'}{(2\pi)^6} e^{-i\omega(\boldsymbol{k})t+\boldsymbol{kx}+i\omega_{\boldsymbol{k'}}t'-\boldsymbol{k'x'}}[a(\boldsymbol{k}),a^\dagger(\boldsymbol{k'})]_\xi \\
&= \int_{\boldsymbol{k}>k_F} \frac{d^3k}{(2\pi)^3} e^{-i\omega(\boldsymbol{k})(t-t')+\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} \\
&= \langle 0|T[\psi^{(+)}(t,\boldsymbol{x})\psi^{(+)\dagger}(t',\boldsymbol{x'})]|0\rangle \\
&= \langle 0|T[(\psi^{(+)}(t,\boldsymbol{x})+\psi^{(-)}(t,\boldsymbol{x}))(\psi^{(+)\dagger}(t',\boldsymbol{x'})+\psi^{(-)\dagger}(t',\boldsymbol{x'}))]|0\rangle \\
&= i\hbar G((t,\boldsymbol{x}),(t',\boldsymbol{x'}))
\end{aligned}$$

and for $t' > t$

$$\overbrace{\psi^{(+)}(t,\boldsymbol{x})\psi^{(+)\dagger}(t',\boldsymbol{x'})} = \xi\psi^{(+)\dagger}(t',\boldsymbol{x'})\psi^{(+)}(t,\boldsymbol{x}) - \xi\psi^{(+)\dagger}(t',\boldsymbol{x'})\psi^{(+)}(t,\boldsymbol{x}) = 0.$$

We have finally

$$\overbrace{\psi^{(+)}(t,\boldsymbol{x})\psi^{(+)\dagger}(t',\boldsymbol{x'})} = \Theta(t-t')i\hbar G((t,\boldsymbol{x}),(t',\boldsymbol{x'})).$$

One finds in a similar manner the fermionic contributions for $t' > t$

$$\begin{aligned}
\overbrace{\psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'})} &= T[\psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'})] - :\psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'}): \\
&= \xi\psi^{(-)\dagger}(t',\boldsymbol{x'})\psi^{(-)}(t,\boldsymbol{x}) - \psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'}) \\
&= -\int_{\boldsymbol{k},\boldsymbol{k'}<k_F} \frac{d^3k d^3k'}{(2\pi)^6} e^{-i\omega(\boldsymbol{k})t+\boldsymbol{kx}+i\omega_{\boldsymbol{k'}}t'-\boldsymbol{k'x'}}[b(\boldsymbol{k}),b^\dagger(\boldsymbol{k'})]_\xi \\
&= -\int_{\boldsymbol{k},\boldsymbol{k'}<k_F} \frac{d^3k d^3k'}{(2\pi)^6} e^{-i\omega(\boldsymbol{k})t+\boldsymbol{kx}+i\omega_{\boldsymbol{k'}}t'-\boldsymbol{k'x'}}(-\xi[a(\boldsymbol{k'}),a^\dagger(\boldsymbol{k})]_\xi) \\
&= \xi\int_{\boldsymbol{k}<k_F} \frac{d^3k}{(2\pi)^3} e^{-i\omega(\boldsymbol{k})(t-t')+\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{x'})} \\
&= \langle 0|T[\psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'})]|0\rangle \\
&= \langle 0|T[(\psi^{(+)}(t,\boldsymbol{x})+\psi^{(-)}(t,\boldsymbol{x}))(\psi^{(+)\dagger}(t',\boldsymbol{x'})+\psi^{(-)\dagger}(t',\boldsymbol{x'}))]|0\rangle \\
&= i\hbar G((t,\boldsymbol{x}),(t',\boldsymbol{x'}))
\end{aligned}$$

and for $t > t'$

$$\overbrace{\psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'})} = \psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'}) - \psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'}) = 0.$$

The last two equations give

$$\overbrace{\psi^{(-)}(t,\boldsymbol{x})\psi^{(-)\dagger}(t',\boldsymbol{x'})} = \Theta(t'-t)i\hbar G((t,\boldsymbol{x}),(t',\boldsymbol{x'})).$$

The contractions for the complete field operator $\psi = \psi^{(-)} + \psi^{(+)}$ are

$$\begin{aligned}
\overbrace{\psi(t,\boldsymbol{x})\psi^\dagger(t',\boldsymbol{x'})} &= \overbrace{(\psi^{(+)}(t,\boldsymbol{x})+\psi^{(-)}(t,\boldsymbol{x}))(\psi^{(+)\dagger}(t',\boldsymbol{x'})+\psi^{(-)\dagger}(t',\boldsymbol{x'}))} \\
&= i\hbar G((t,\boldsymbol{x}),(t',\boldsymbol{x'})) \\
\overbrace{\psi(t,\boldsymbol{x})\psi(t',\boldsymbol{x'})} &= \overbrace{\psi^\dagger(t,\boldsymbol{x})\psi^\dagger(t',\boldsymbol{x'})} = 0
\end{aligned}$$