Chapter 4

Interacting electrons

4.1 Quantum mechanical identical particles

In this chapter we will discuss interacting electrons, i.e. systems of many quantum mechanical identical particles. The fact that they are indentical (in the sense that all intrinsic properties like mass, spin, charge, etc, are identical) imposes a symmetry on the system, namely that its physical properties are invariant upon a permutation of the particles. Such a symmetry has radically different consequences for systems with classical or quantum mechanical particles.

In the case of classical particles, we can describe the state of the system by the instantaneous coordinates and momenta of the particles. Let us consider as an example two classical particles. They will have positions and momenta given by

$$
\begin{aligned}
q_1(t) &= q(t), & q_2(t) = q'(t) \\
p_1(t) &= p(t), & p_2(t) = p'(t)
\end{aligned}
\tag{4.1}
$$

The functions $q(t)$, $p(t)$, $q'(t)$, and $p'(t)$ describe the trajectory of the particles. Since the particles are *indistinguishable*, we could exchange the functions in (4.1).

$$
\begin{aligned}
q_1(t) &= q'(t), & q_2(t) = q(t) \\
p_1(t) &= p'(t), & p_2(t) = p(t)
\end{aligned}
\tag{4.2}
$$

The description of the system is completetly equivalent in both cases. Therefore, it suffices to take one of the possibilities. This means, that we can actually consider them as *distinguishable* particles, since we could distinguish between both possibilities on the basis of the initial conditions.

In the quantum mechanical case, we cannot any more speak about trajectories. Let us consider again two particles that are initially far away from each other, and that they collide after some time. We denote their wavefunctions as follows:

$$
\psi_0\left(\boldsymbol{x}_1, t_0\right), \qquad \psi_0'\left(\boldsymbol{x}_2, t_0\right),
\tag{4.3}
$$

where t_0 is the initial time. We can think of these wavefunctions as wave-packets well separated from each other. The wavefunction of the whole system is

$$
\psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t = t_0\right) = \psi_0\left(\boldsymbol{x}_1, t_0\right) \psi_0'\left(\boldsymbol{x}_2, t_0\right).
\tag{4.4}
$$

Since the particles are indistinguishable, it is equally possible to have

$$\bar{\psi}\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t = t_0\right) = \psi_0\left(\boldsymbol{x}_2, t_0\right)\psi_0'\left(\boldsymbol{x}_1, t_0\right) , \tag{4.5}$$

as a wavefunction of the system. If ψ is a solution of Schrödinger's equation at time t_0, then, $\bar{\psi}$ should also be a solution, since by hypothesis

$$H\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right) = H\left(\boldsymbol{x}_2, \boldsymbol{x}_1\right) . \tag{4.6}$$

We have here an exchange degeneracy. In fact, ψ and $\bar{\psi}$ are different states. This can be explicitly seen by noticing that they are orthogonal to each other:

$$\int \mathrm{d}^3x_1\,\mathrm{d}^3x_2\,\psi^*\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t_0\right)\bar{\psi}\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t_0\right)$$
$$= \underbrace{\int \mathrm{d}^3x_1\,\psi_0^*\left(\boldsymbol{x}_1, t_0\right)\psi_0'\left(\boldsymbol{x}_1, t_0\right)}_{=0}\underbrace{\int \mathrm{d}^3x_2\,\psi_0'^*\left(\boldsymbol{x}_2, t_0\right)\psi_0\left(\boldsymbol{x}_2, t_0\right)}_{=0} = 0 , \tag{4.7}$$

where each integral vanishes since by hypothesis, each wavepacket had no overlap with the other.

Let us now consider the time evolution of the system, where we assume that the particles approach each other. We will have in general a wavefunction not in the form of a product, but still two possible wavefunctions to describe the system, namely ψ and $\bar{\psi}$. Even more, we can also consider linear combinations, since the Schrödinger equation being linear, if both ψ and $\bar{\psi}$ are solutions, any linear combination is also a solution. In particular, we can have a symmetric and an antisymmetric combination

$$\begin{aligned}
\psi^S &= \frac{1}{\sqrt{2}}\left(\psi + \bar{\psi}\right)\\
\psi^A &= \frac{1}{\sqrt{2}}\left(\psi - \bar{\psi}\right)
\end{aligned} \tag{4.8}$$

The linear combinations above are symmetric or antisymmetric upon a permutation of the particles. Also a linear combination of them should be solution of Schrödinger's equation if each one of them is. We therefore consider now

$$\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t\right) = \alpha\,\psi^A\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t\right) + \beta\,\psi^S\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t\right) , \tag{4.9}$$

with $\mid \alpha \mid^2 + \mid \beta \mid^2 = 1$. The probability of finding a particle (either 1 or 2) at $\boldsymbol{x}$ and the other at $\boldsymbol{x}'$ is

$$\begin{aligned}
P\left(\boldsymbol{x}, \boldsymbol{x}'\right) &= \mid \Psi\left(\boldsymbol{x}, \boldsymbol{x}'\right)\mid^2 + \mid \Psi\left(\boldsymbol{x}', \boldsymbol{x}\right)\mid^2\\
&= \mid \alpha \mid^2 \mid \psi^A\left(\boldsymbol{x}, \boldsymbol{x}'\right)\mid^2 + \mid \beta \mid^2 \mid \psi^S\left(\boldsymbol{x}, \boldsymbol{x}'\right)\mid^2\\
&\quad + \alpha^*\beta\,\psi^{A*}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\psi^S\left(\boldsymbol{x}, \boldsymbol{x}'\right) + \beta^*\alpha\,\psi^{S*}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\psi^A\left(\boldsymbol{x}, \boldsymbol{x}'\right)\\
&\quad + \mid \alpha \mid^2 \mid \psi^A\left(\boldsymbol{x}', \boldsymbol{x}\right)\mid^2 + \mid \beta \mid^2 \mid \psi^S\left(\boldsymbol{x}', \boldsymbol{x}\right)\mid^2\\
&\quad + \alpha^*\beta\,\psi^{A*}\left(\boldsymbol{x}', \boldsymbol{x}\right)\psi^S\left(\boldsymbol{x}', \boldsymbol{x}\right) + \beta^*\alpha\,\psi^{S*}\left(\boldsymbol{x}', \boldsymbol{x}\right)\psi^A\left(\boldsymbol{x}', \boldsymbol{x}\right)\\
&= 2\left[\mid \alpha \mid^2 \mid \psi^A\left(\boldsymbol{x}, \boldsymbol{x}'\right)\mid^2 + \mid \beta \mid^2 \mid \psi^S\left(\boldsymbol{x}, \boldsymbol{x}'\right)\mid^2\right] . \tag{4.10}
\end{aligned}$$

Since all linear combinations are physically equivalent, the probability P should be independent of α and β. This can be accomplished only if

$$\mid \psi^A \left(\boldsymbol{x}, \boldsymbol{x}' \right) \mid = \mid \psi^S \left(\boldsymbol{x}, \boldsymbol{x}' \right) \mid \ . \tag{4.11}$$

Let us now assume that the particles do not interact with each other. Then, the wavefunction of the total system can be written as a product of the one-particle wavefunctions even in the case that both particles are approaching each other. Recalling (4.4), we have

$$\mid \psi^{S,A} \left(\boldsymbol{x}, \boldsymbol{x}' \right) \mid = \frac{1}{\sqrt{2}} \mid \psi_0 \left(\boldsymbol{x} \right) \psi_0' \left(\boldsymbol{x}' \right) \pm \psi_0 \left(\boldsymbol{x}' \right) \psi_0' \left(\boldsymbol{x} \right) \mid \ . \tag{4.12}$$

For $\boldsymbol{x} = \boldsymbol{x}'$, we have

$$\mid \psi^S \left(\boldsymbol{x}, \boldsymbol{x}' \right) \mid = \sqrt{2} \mid \psi_0 \left(\boldsymbol{x} \right) \psi_0' \left(\boldsymbol{x} \right) \mid \neq 0 \ , \tag{4.13}$$

but $\mid \psi^A \left(\boldsymbol{x}, \boldsymbol{x}' \right) \mid = 0$. This is a contradiction, that will be solved by introducing a postulate that until now was not contradicted by experiments (but we should discuss this in more detail).

4.1.1 Permutation operators

Let us consider first only two particles. We take a complete set of one-particle states $\{\mid u_i >\}$, such that a basis of two-particle states can be obtained as a product

$$\mid u_i^{(1)} > \otimes \mid u_j^{(2)} > \equiv \mid u_i^{(1)}; u_j^{(2)} > \ . \tag{4.14}$$

We introduce a *permutation operator* that exchanges particles:

$$P \mid u_i^{(1)}; u_j^{(2)} > = \mid u_i^{(2)}; u_j^{(1)} > \ . \tag{4.15}$$

By applying twice such an operator, we recover the original state. Since this fact is independent of the states used, such an operator fulfills in general

$$P^2 = 1 \ . \tag{4.16}$$

Furthermore, we can show that P is hermitian, by considering any matrix element:

$$< u_i^{(1)}; u_j^{(2)} \mid P \mid u_{i'}^{(1)}; u_{j'}^{(2)} > = < u_i^{(1)}; u_j^{(2)} \mid u_{i'}^{(2)}; u_{j'}^{(1)} > = \delta_{ij'} \delta_{ji'} \ . \tag{4.17}$$

Since all matrix elements are real, $P^\dagger = P$. Moreover, since $P^2 = 1$, we have

$$PP = P^\dagger P = 1 \ , \tag{4.18}$$

that is, P is unitary.

Let us consider finally the eigenvalues of P. If $\mid \psi >$ is an eigenvector of P, since $P^2 = 1$, we have

$$P^2 \mid \psi > = \lambda^2 \mid \psi > \quad \Longrightarrow \quad \lambda = \pm 1 \ . \tag{4.19}$$

The eigenstates with eigenvalue $+1$ are symmetric, the ones with eigenvalue -1 are antisymmetric.

$$
\begin{aligned}
P \mid \psi_S > &= \mid \psi_S > \\
P \mid \psi_A > &= - \mid \psi_A > \ .
\end{aligned}
\tag{4.20}
$$

Let us examine next the case with $N > 2$ particles. Generalizing what we did with two particles, we construct a basis for the N-particle state as a product of one-particle states.

$$
\mid u_{i_1}^{(1)}, u_{i_2}^{(2)}, \ldots, u_{i_N}^{(N)} >= \mid u_{i_1}^{(1)} > \otimes \mid u_{i_2}^{(2)} > \otimes \cdots \otimes \mid u_{i_N}^{(N)} > \ .
\tag{4.21}
$$

In general, there are $N!$ possible permutations. We denote a general permutation by

$$
P_{\ell_1 \cdots \ell_N} \ , \quad \text{with} \quad \ell_j = 1, \ldots, N; \ j = 1, \ldots, N \ .
\tag{4.22}
$$

As an example let us consider the case $N = 3$. There are $3! = 6$ possible permutations: P_{123}, P_{231}, P_{312}, P_{213}, P_{321}, and P_{132}. The action of the permutation operator is then, e.g.

$$
P_{312} \mid u_{i_1}^{(1)}, u_{i_2}^{(2)}, u_{i_3}^{(3)} >= \mid u_{i_1}^{(3)}, u_{i_2}^{(1)}, u_{i_3}^{(2)} >= \mid u_{i_2}^{(1)}, u_{i_3}^{(2)}, u_{i_1}^{(3)} > \ .
\tag{4.23}
$$

Properties of permutation operators

The permutation operators build a group since

i) The product of two permutation operators is a permutation operator. This can be easily seen in our example with $N = 3$, where e.g. $P_{312} P_{213} = P_{132}$

$$
\begin{aligned}
P_{312} P_{213} \mid u_{i_1}^{(1)}, u_{i_2}^{(2)}, u_{i_3}^{(3)} > &= P_{312} \mid u_{i_1}^{(2)}, u_{i_2}^{(1)}, u_{i_3}^{(3)} > \\
&= P_{312} \mid u_{i_2}^{(1)}, u_{i_1}^{(2)}, u_{i_3}^{(3)} > \\
&= \mid u_{i_2}^{(3)}, u_{i_1}^{(1)}, u_{i_3}^{(2)} > \\
&= P_{132} \mid u_{i_1}^{(1)}, u_{i_2}^{(2)}, u_{i_3}^{(3)} > \ .
\end{aligned}
$$

ii) The identity is also a permutation operator. Again in our example, the identity is P_{123}.

iii) The inverse of a permutation is also a permutation. In our example we have

$$
\begin{aligned}
P_{123}^{-1} &= P_{123} \ , & P_{231}^{-1} &= P_{312} \\
P_{312}^{-1} &= P_{231} \ , & P_{213}^{-1} &= P_{213} \\
P_{321}^{-1} &= P_{321} \ , & P_{132}^{-1} &= P_{132} \ .
\end{aligned}
$$

In general, permutations do not commute. This can be also seen in our example: $P_{213}P_{312} = P_{321} \neq P_{132}$, as we obtained in i).

A permutation where only two particles are permuted is called a *transposition*. In our example they are P_{132}, P_{321}, and P_{213}. As we have already shown for the case $N = 2$, transpositions are hermitian and unitary. Furthermore, each permutation operator can be expressed as a product of transpositions. In our example $P_{312} = P_{132}P_{213}$. The *parity* of a permutation is given by the parity of the number of transpositions in which a permutation can be splitted. In our example P_{132} is odd but P_{312} is even. Since a permutation can be expressed as a product of transpositions, and transpositions are unitary, permutations are unitary (recall that the product of unitary operators is unitary). But since permutations do not commute in general, although transpositions are hermitian, a general permutation is not.

Symmetrization and antisymmetrization operators

Here we discuss possible eigenstates of permutation operators. Let us look for states that are eigenstates of all permutation operators in a system with N particles. We number with an index p all possible $N!$ permutations and let $\mid \psi >$ be such that

$$P_p \mid \psi >= c_p \mid \psi > \quad \forall \, p \, . \tag{4.24}$$

The easiest case is that of a transposition, where we have already seen (case $N = 2$), that $c_p^{(transp)} = \pm 1$. Since $\mid \psi >$ is assumed to be an eigenvector of all permutations, it should be an eigenvector of all transpositions. Furthermore, if the particles are indistinguishable, the eigenvalue of the transposition cannot depend on the particular transposition, and therefore, the eigenvalue should be the same for all transpositions, i.e. ± 1. Therefore, the eigenvalue for a permutation should be

$$c_p = (\pm 1)^{n_p} \, , \tag{4.25}$$

where n_p is the number of transpositions in which the p-th permutation can be splitted. It is even or odd depending on whether the permutation is even or odd. This means that there are only two possible cases

  a) Totally symmetric case

$$P_p \mid \psi_S >=\mid \psi_S > \quad \Longrightarrow \quad c_p = 1 \quad \forall \, p. \tag{4.26}$$

  b) Totally antisymmetric case

$$P_p \mid \psi_A >= \epsilon_p \mid \psi_A > \quad \text{with} \begin{cases} \epsilon_p &= +1 & P_p \text{ an even permutation} \\ \epsilon_p &= -1 & P_p \text{ an odd permutation} \end{cases} \tag{4.27}$$

The set of all totally symmetric states spans a subspace of the total Hilbert space which we call $\mathcal{H}_S$, and correspondingly $\mathcal{H}_A$ for the totally antisymmetric states. We can easily see that the states of these two subspaces are orthogonal to each other:

$$< \psi_S \mid \psi_A >=< \psi_S \mid P_p^\dagger \mid \psi_A >=< \psi_S \mid P_p^{-1} \mid \psi_A >= - < \psi_S \mid \psi_A > , \tag{4.28}$$

where we assumed that the parity of P_p^{-1} is odd.

Finally, let us construct projection operators on the subspaces $\mathcal{H}_S$ and $\mathcal{H}_A$, such that we can obtain elements of either subspace from any given state. We define the following operators

$$S \;=\; \frac{1}{N!} \sum_p P_p \qquad \text{symmetrization operator ,} \qquad (4.29)$$

$$A \;=\; \frac{1}{N!} \sum_p \epsilon_p P_p \qquad \text{antisymmetrization operator ,} \qquad (4.30)$$

where we sum over the $N!$ permutations. Since P_p is unitary, $P^\dagger = P^{-1}$ is also a permutation operator. This implies that $S^\dagger = S$, and $A^\dagger = A$, i.e. both operators are hermitian. Furthermore, we see that for any permutation operator P_{p_0}, the following holds:

$$
\begin{aligned}
P_{p_0} S \;=\;& \frac{1}{N!} \sum_p P_{p_0} P_p = \frac{1}{N!} \sum_{p'} P_{p'} = S \;, \\
P_{p_0} A \;=\;& \frac{1}{N!} \sum_p \epsilon_p P_{p_0} P_p = \frac{1}{N!} \sum_p \epsilon_{p_0}^2 \epsilon_p P_{p_0} P_p \\
\;=\;& \epsilon_{p_0} \frac{1}{N!} \sum_p \underbrace{\epsilon_{p_0} \epsilon_p}_{\tilde{\epsilon}_p} \underbrace{P_{p_0} P_p}_{\tilde{P}_p} = \epsilon_{p_0} A \;.
\end{aligned}
\qquad (4.31)
$$

With the results above, we can prove that

$$S^2 \;=\; S \frac{1}{N!} \sum_p P_p = \frac{1}{N!} \sum_p \underbrace{S P_p}_{=S} = S \qquad (4.32)$$

$$A^2 \;=\; A \frac{1}{N!} \sum_p \epsilon_p P_p = \frac{1}{N!} \sum_p \epsilon_p \underbrace{A P_p}_{=\epsilon_p A} = A \qquad (4.33)$$

$$SA \;=\; S \frac{1}{N!} \sum_p \epsilon_p P_p = \frac{1}{N!} \sum_p \epsilon_p S P_p = S \frac{1}{N!} \sum_p \epsilon_p = 0 \;. \qquad (4.34)$$

Equations (4.32) and (4.33) show that S and A are projection operators, whereas (4.34) shows that they project onto orthogonal subspaces.

4.1.2   The symmetrization postulate

We have seen in the case of two indistinguishable particles, that if we allow any superposition of symmetric and antisymmetric states, we arrive at a contradiction. On the other hand, in the general case of N indistinguishable particles, it is possible to project any state into the subspace of totally symmetric or antisymmetric states. However, this leaves open what happens with the rest of possible states.

In order to resolve this situation, we introduce a symmetrization postulate: "The physical states of a system with N indistinguishable particles are all either totally

symmetric or totally antisymmetric. The particles with symmetric states are called *bosons* and the particles with antisymmetric states are called *fermions*". This is an additional postulate to the ones that constitute the foundation of quantum mechanics. As a consequence of this postulate it is not any more possible to construct the Hilbert space of N particles as a product of the subspaces of each particle. The subspace for bosons is $\mathcal{H}_S$ and for fermions $\mathcal{H}_A$.

Although this seems at this point rather arbitrary, we should recall that in the frame of non-relativistic quantum mechanics, spin had also to be introduced by Pauli's postulate. It is relativistic quantum mechanics, specifically Dirac's equation, that tells us that there are particles with a new quantum number, namely spin. In fact, there is a so-called *spin-statistics theorem* that demonstrates that in a local relativistic quantum field-theory (in 4 space-time dimensions) particles with half-integer spin are fermions and particles with integer spin are bosons. Other spins are not allowed, since as was already shown (suppossedly) in non-relativistic quantum mechanics, the algebra of spins, i.e. the SU(2) algebra, admits eigenvalues of $\boldsymbol{S}^2$ with the form $s(s+1)$, where s is half-integer or integer. In fact, until now no violation of the postulate was observed. However, systems in lower dimensions may show departures from the rule. We discuss this point qualitatively in the following.

- <u>$d = 1$</u>. Let us think in a purely one-dimensional system, with quantum mechanical particles with a hard core. Since particles cannot pass each other, there cannot be exchange processes during the time evolution of the system. Therefore, up to some extent, the statistical properties do not play a role. In fact, in one dimension it is possible to map hard-core bosons into fermions with the help of a so-called *Jordan-Wigner transformation*. Actually, it is possible to construct even more general statistics. Furthermore, in one dimension it is possible to map the low energy properties of bosons (not only hard-core ones) into fermions and viceversa by a procedure called *bosonization*. Although all this lies beyond the scope ot these lectures, it is usefull to know that such possibilities exist.

- <u>$d = 2$</u>. In this case we have particles on a plane. Let us imagine two such particles. As we have discussed above, a permutation of two particles (transposition) performed twice brings the particles to the initial situation. However, if we imagine a rope attached to the particles, we can distinguish both states since there will be a difference in the number of windings of the rope around one of the particles, if the particles are not rotated during the whole process. This shows that in two dimensions an additional number of topological character can be used and the concept of *fractional statistics* arises. This has immediate consequences for experimentally relevant systems like those in *fractional quantum Hall effect*.

- <u>$d = 3$</u>. The topological case discussed above does not subsist in 3 dimensions, such that in this case, all particles are either bosons or fermions.

The symmetrization postulate resolves the problem of exchange degeneracy since only states belonging to $\mathcal{H}_S$ or $\mathcal{H}_A$ are allowed. In this case, an arbitrary permutation does not bring a state to another one, but it leaves it invariant:

i) Bosons: $S \mid \psi >=\mid \psi >$.

$$\Longrightarrow P \mid \psi >= PS \mid \psi >= S \mid \psi >=\mid \psi > \ . \tag{4.35}$$

ii) Fermions: $A \mid \psi >=\mid \psi >$.

$$\Longrightarrow P_p \mid \psi >= P_p A \mid \psi >= \epsilon_p A \mid \psi >= \epsilon_p \mid \psi > \ . \tag{4.36}$$

In this case the permutation generates only a state that is linearly dependent on the original one.

4.1.3   Occupation-number states for bosons

We start with N particles, where each particle can occupy one-particle states $\mid u_i >$, where in principle $i = 1, \ldots, \infty$. As we already discussed repeatedly, if the one-particle states $\{\mid u_i >\}$ form a basis, we can use as a basis for the N particles the tensor product $\mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots >$, where n_i is the number of particles in state $\mid u_i >$. Of course, it should hold that

$$\sum_{i=1}^{\infty} n_i = N \ . \tag{4.37}$$

As we have already seen, the discussion above holds for distinguishable particles. If we are working with indistinguishable particles, we should apply the projector S on the states (4.37), such that the physical states are then given by

$$S \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots >= \frac{1}{N!} \sum_p P_p \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots > \ . \tag{4.38}$$

In order to properly normalize the state above, let us discuss more in detail the action of the permutation operators on the states. Among the permutations entering (4.38), there are some of them that permute particles within some state $\mid u_i^{n_i} >$. Given n_i particles, there are $n_i!$ such permutations. These permutations do not change the state $\mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots >$. Writing out the state $\mid u_i^{n_i} >$ explicitely,

$$\mid u_i^{n_i} >=\mid u_i^{(1)}, u_i^{(2)}, \ldots, u_i^{(n_i)} > \ , \tag{4.39}$$

we can immediately see, e.g. using the rules for the action of a permutation operator as displayed in the example (4.23), that $\mid u_i^{n_i} >$ is not changed by such permutations that only permute the particles within that state. There are in total $\prod_{j=1}^{\infty} n_j!$ such permutations. Due to (4.37), there are many states with $n_j = 0$, but this is not a problem since $0! = 1$. All other permutations do change the vector

$\mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots >$. To see this, let us consider in detail the vectors $\mid u_1^{n_1} >$ and $\mid u_2^{n_2} >$. Each one can be explicitely written as

$$
\begin{aligned}
\mid u_1^{n_1} > &= \mid u_1^{(1)}, \ldots, u_1^{(\alpha)}, \ldots, u_1^{(n_1)} > , \\
\mid u_2^{n_2} > &= \mid u_2^{(n_1+1)}, \ldots, u_2^{(\beta)}, \ldots, u_2^{(n_1+n_2)} > .
\end{aligned}
\tag{4.40}
$$

Now imagine a transposition between the α-th particle in state 1, with $1 \le \alpha \le n_1$ and the β-th particle in state 2, with $n_1 + 1 \le \beta \le n_1 + n_2$. Since after the transposition, the α-th particle is in state 2 and the β-th particle in state 1, we have a vector different from the initial one. Moreover, they are orthogonal, since the states $\mid u_i >$ are basis vectors.

We can now calculate the norm of the vector (4.38).

$$
\begin{aligned}
< u_1^{n_1}, u_2^{n_2}, &\ldots, u_j^{n_j}, \ldots \mid S^\dagger S \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots > \\
&= < u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots \mid \underbrace{SS}_{=S} \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots > \\
&= \frac{1}{N!} \sum_p < u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots \mid P_p \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots > \\
&= \frac{\prod_{j=1}^{\infty} n_j!}{N!} .
\end{aligned}
\tag{4.41}
$$

This means that given a one-particle basis $\{\mid u_i >\}$, a normalized state for N bosons is given by

$$
\mid \psi_S >= \left(\frac{N!}{\prod_{j=1}^{\infty} n_j!} \right)^{\frac{1}{2}} S \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots > .
\tag{4.42}
$$

Next we consider the construction of a basis in $\mathcal{H}_S$. As before, we consider a basis for the N-particle system given by a product of the one-particle states. They give a basis of $\mathcal{H}$, the Hilbert space obtained as a tensorial product of the Hilbert spaces of each particle. The subspace of totally symmetric states upon permutation was already denoted as $\mathcal{H}_S$, with $\mathcal{H}_S \subset \mathcal{H}$. Then, any vector $\mid \psi_S > \in \mathcal{H}_S$ is also an element of $\mathcal{H}$, such that, it can be expanded in the basis of $\mathcal{H}$

$$
\mid \psi_S >= \sum_{i_1, \ldots, i_N} a_{i_1, \ldots, i_N} \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} > .
\tag{4.43}
$$

From what we have discussed in Sec. 4.1.1, we know that if $\mid \psi_S > \in \mathcal{H}_S$, then $S \mid \psi_S >= \mid \psi_S >$, such that

$$
\mid \psi_S >= S \mid \psi_S >= \sum_{i_1, \ldots, i_N} a_{i_1, \ldots, i_N} S \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} > .
\tag{4.44}
$$

Since $S \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} >$ are elements of $\mathcal{H}_S$, we can expect that they are close to be members of a basis of $\mathcal{H}_S$. In order to see whether this is the case, let us introduce a vector

$$
\mid n_1, \ldots, n_i, \ldots >= cS \mid u_1^{n_1}, \ldots, u_i^{n_i}, \ldots > ,
\tag{4.45}
$$

and discuss its properties.

i) <u>Scalar product.</u>

$$< n_1, \ldots, n_i, \ldots \mid n'_1, \ldots, n'_i, \ldots > \neq 0 \ , \tag{4.46}$$

only then, when $n_i = n'_i$ for $i = 1, 2, \ldots$ This can be seen by looking at the vector $\mid u_1^{n_1}, \ldots, u_i^{n_i}, \ldots >$. If two vectors have a different number of particles in a given state, it means that there are particles in different states in each vector, and hence, they are orthogonal.

ii) <u>Normalization.</u> As we have seen in (4.41), the normalization constant c is given by

$$c = \left(\frac{N!}{\prod_{j=1}^{\infty} n_j!} \right)^{\frac{1}{2}} \ . \tag{4.47}$$

iii) <u>Basis.</u> Equation (4.44) shows that any state in $\mathcal{H}_S$ can be expanded in states proportional to $\mid n_1, \ldots, n_i, \ldots >$. Furthermore, in *i)* and *ii)*, it was shown that they are orthonormalized. Therefore, they constitute a basis of $\mathcal{H}_S$.

Once we found a basis of $\mathcal{H}_S$, we still have to translate the coefficients of the expansion appearing in (4.44). In order to do so, we express the summation in (4.44) over all possible states for N particles as a summation over all possible occupation numbers with the constraint that the total number of particles is N and a summation over all the states that are compatible with a given configuration of occupation numbers.

$$\sum_{i_1, \ldots, i_N} = \sum_{\substack{n_1, \ldots, n_j, \ldots \\ \sum_i n_i = N}} \sum_{\substack{i_1, \ldots, i_N \\ \binom{i_1, \ldots, i_N}{n_1, \ldots, n_j, \ldots}}} \tag{4.48}$$

Using the reformulation of the sums above, we have

$$\mid \psi_S >= \sum_{\substack{n_1, \ldots, n_j, \ldots \\ \sum_i n_i = N}} \frac{1}{c} \sum_{\substack{i_1, \ldots, i_N \\ \binom{i_1, \ldots, i_N}{n_1, \ldots, n_j, \ldots}}} a_{i_1, \ldots, i_N} \mid n_1, \ldots, n_i, \ldots > \ . \tag{4.49}$$

We recall now that we are dealing with identical particles. This means, that given a configuration of the occupation numbers $n_1, \ldots, n_j, \ldots$, the coefficients $a_{i_1, \ldots, i_N}$ are the same, irrespective of the particular distribution of particles in the different states, i.e.

$$\sum_{\substack{i_1, \ldots, i_N \\ \binom{n_1, \ldots, n_j, \ldots}}} a_{i_1, \ldots, i_N} = a_{n_1, \ldots, n_j, \ldots} \sum_{\substack{i_1, \ldots, i_N \\ \binom{n_1, \ldots, n_j, \ldots}}}$$

$$= a_{n_1, \ldots, n_j, \ldots} \frac{N!}{n_1! \cdots n_j! \cdots} \ . \tag{4.50}$$

Taking into account the coefficient $1/c$ in (4.49), we can define coefficients

$$c_{n_1,\ldots,n_j,\ldots} = \sqrt{\frac{N!}{n_1! \cdots n_j! \cdots}} \, a_{n_1,\ldots,n_j,\ldots} \, , \qquad (4.51)$$

such that

$$| \, \psi_S > = \sum_{n_1,\ldots,n_j,\ldots} c_{n_1,\ldots,n_j,\ldots} \, | \, n_1,\ldots,n_j,\ldots > \, , \qquad (4.52)$$

where

$$\sum_{n_1,\ldots,n_j,\ldots} | \, c_{n_1,\ldots,n_j,\ldots} \, |^2 = 1 \, , \qquad (4.53)$$

with the condition (4.37).

4.1.4   Bose-Einstein statistics

Once we have a formal description of the space $\mathcal{H}_S$ with a general prescription that allows to go from a basis of one-particle states to a basis of N-particle states, fulfilling the requirements of the symmetrization postulate, we recall some concepts of statistical mechanics, that are fundamental for dealing with an N-particle system.

When we are working with a macroscopic number of particles, we have the idea that there is the notion of temperature and we would like to be able to calculate the physical properties of the system in a statistical manner starting from our knowledge of the energy levels of the system. In this case, we will have in general a statistical mixing of states (in contrast to a coherent superposition) and the statistical properties can be calculated using the density matrix ρ. In the case of a statistical mixture of states, we assign a probability p_n to a state $| \, \psi_n >$, such that the density matrix is given by

$$\rho = \sum_n p_n \, | \, \psi_n > < \psi_n \, | \, . \qquad (4.54)$$

From this definition we obtain the basic properties of the density matrix

   i) Normalization

$$\mathrm{Tr}\rho = 1 \, . \qquad (4.55)$$

   ii) Expectation value of an operator

$$< A > = \mathrm{Tr}\,(\rho A) \, . \qquad (4.56)$$

Canonical ensemble

Here we consider a system with $N \gg 1$ particles at a temperature T. The temperature of the system is given by putting the system in contact with a heat bath. We assume that the walls of the system allow for an exchange of energy but the number of particles in the system under consideration (we call it '1') is constant, i.e. there is no exchange of particles with the bath. We are then dealing with a canonical ensemble. In the following we discuss how to obtain the density matrix for this statistical ensemble.

We assume that the whole system (system 1 + bath) is isolated, such that,

$$E = E_1 + E_2 = \text{cte} , \tag{4.57}$$

where we denote with '2' the heat bath, and E is the total energy. We recall that the heat bath is allways assumed to be much larger than the system under consideration, such that $E_2 \gg E_1$, the energy being an extensive quantity. The probability of system 1 to have an energy E_1 should be proportional to the number of states in system 2 that are compatible with an energy E_2:

$$p\left(E_1\right) \sim \Gamma_2\left(E_2\right) . \tag{4.58}$$

A measure of the number of states for a given energy is given by the entropy, in fact

$$S_2\left(E_2\right) = k_B \ln \Gamma_2\left(E_2\right) , \tag{4.59}$$

where k_B is Boltzmann's constant. For S_2 we can write

$$S_2\left(E_2\right) = S_2\left(E - E_1\right) \simeq S_2(E) - E_1 \frac{\partial S}{\partial E} , \tag{4.60}$$

From the first law of thermodynamics

$$\mathrm{d}E = T\mathrm{d}S - P\mathrm{d}V , \tag{4.61}$$

we have at constant volume that

$$\frac{\partial S}{\partial E} = \frac{1}{T} , \tag{4.62}$$

such that from (4.59) and (4.60) we have that

$$\Gamma_2\left(E_2\right) \sim \exp\left[\frac{S_2(E)}{k_B}\right] \exp\left(-\frac{E_1}{k_B T}\right) , \tag{4.63}$$

and hence, inserting the result above into (4.58), we have

$$p\left(E_1\right) \sim \exp\left(-\frac{E_1}{k_B T}\right) . \tag{4.64}$$

This is the probability of having the system at the energy E_1, given the temperature T. Once the probability for a given energy is found, we have that the density matrix should be given by

$$\rho = \frac{\exp\left(-\beta H\right)}{\operatorname{Tr}\exp\left(-\beta H\right)} , \tag{4.65}$$

with $\beta = \left(k_B T\right)^{-1}$.

Grand canonical ensemble

In this case fluctuations in the number of particles is allowed, i.e. the system under consideration and the thermal bath can exchange also particles. The fluctuation of particles induces in general a fluctuation of the energy, that can be described by introducing the chemical potential, defined as follows

$$\mu = \left. \frac{\partial E}{\partial N} \right|_V . \tag{4.66}$$

Since N is actually a discrete quantity, we should consider $\Delta N = 1$, so that the chemical potential describes the change in energy when the number of particles is increased by one. In order to obtain the density matrix in this case we have to repeat the discussion for the canonical ensemble taking into account the change in the number of particles. The first law of thermodynamics is now

$$\mathrm{d}E = T\mathrm{d}S - P\mathrm{d}V + \mu\mathrm{d}N , \tag{4.67}$$

leding to

$$\mathrm{d}S = \frac{1}{T} \left(\mathrm{d}E - \mu\mathrm{d}N \right) \tag{4.68}$$

at constant volume. Taking into account that $E_1 \ll E_2$ and $N_1 \ll N_2$, with a total energy $E = E_1 + E_2$ and a total number of particles $N = N_1 + N_2$, the probability of having energy E_1 and number of particles N_1 in the system under consideration is

$$p\left(E_1, N_1\right) \sim \Gamma_2\left(E_2, N_2\right) \tag{4.69}$$

and the entropy is given by

$$
\begin{aligned}
S_2\left(E_2, N_2\right) &= S_2\left(E - E_1, N - N_1\right) \\
&\simeq S_2\left(E, N\right) - E_1\frac{\partial S}{\partial E} - N_1\frac{\partial S}{\partial N} \\
&= S_2\left(E, N\right) - \frac{E_1}{T} - \frac{\mu N_1}{T} .
\end{aligned} \tag{4.70}
$$

Then,

$$p\left(E_1, N_1\right) \sim \exp\left[-\frac{1}{k_B T}\left(E_1 - \mu N_1\right) \right] . \tag{4.71}$$

Accordingly, the density matrix is given by

$$\rho = \frac{\exp\left[-\beta\left(H - \mu\hat{N}\right) \right]}{\mathrm{Tr}\exp\left[-\beta\left(H - \mu\hat{N}\right) \right]} , \tag{4.72}$$

where $\hat{N}$ is the particle-number operator.

Bose-Einstein statistics

Once we have determined the density matrix in the canonical and the grand-canonical ensemble in general, we examine how it acts in the subspace $\mathcal{H}_S$. We consider here the so-called *ideal Bose-gas*, that is an ensemble of N bosons that do not interact with each other. In this case, the Hamiltonian can be written as the sum of N Hamiltonians.

$$H = H^{(1)} + H^{(2)} + \cdots + H^{(N)} . \tag{4.73}$$

Let us denote the energy levels by ε_i, $i = 1, \ldots, \infty$. Then, the partition function is given by

$$\begin{aligned} Z &= \operatorname{Tr} \exp\left[-\beta\left(H - \mu\hat{N}\right)\right] \\ &= \sum_{n_1,\ldots,n_\infty} < n_1 \cdots n_\infty \mid \exp\left[-\beta\left(H - \mu\hat{N}\right)\right] \mid n_1 \cdots n_\infty > . \end{aligned} \tag{4.74}$$

The particle number operator acts on the occupation-number states as follows

$$\hat{N} \mid n_1 \cdots n_\infty >= \sum_i n_i \mid n_1 \cdots n_\infty > , \tag{4.75}$$

whereas for the Hamiltonian we have

$$H \mid n_1 \cdots n_\infty >= \sum_i \varepsilon_i\, n_i \mid n_1 \cdots n_\infty > . \tag{4.76}$$

Inserting the results above into (4.74), we have

$$\begin{aligned} Z &= \sum_{n_1,\ldots,n_\infty} < n_1 \cdots n_\infty \mid \exp\left[\beta\left(\mu\sum_i n_i - \sum_i \varepsilon_i\, n_i\right)\right] \mid n_1 \cdots n_\infty > \\ &= \sum_{n_1} \exp\left[\beta\left(\mu\, n_1 - \varepsilon_1\, n_1\right)\right] \times \cdots \times \sum_{n_\infty} \exp\left[\beta\left(\mu\, n_\infty - \varepsilon_\infty\, n_\infty\right)\right] \\ &= \prod_i^\infty \underbrace{\sum_{n=0}^\infty \left\{\exp\left[\beta(\mu - \varepsilon_i)\right]\right\}^n}_{\text{geometric series}} = \prod_i^\infty \frac{1}{1 - \exp\left[\beta(\mu - \varepsilon_i)\right]} . \end{aligned} \tag{4.77}$$

From the knowledge of the partition function, we can calculate the expectation value of the number operator:

$$\begin{aligned} <\hat{N}> &= \frac{\operatorname{Tr}\hat{N}\rho}{\operatorname{Tr}\rho} = \frac{\operatorname{Tr}\hat{N}\exp\left[-\beta\left(H - \mu\hat{N}\right)\right]}{\operatorname{Tr}\exp\left[-\beta\left(H - \mu\hat{N}\right)\right]} \\ &= k_B T\, \frac{\partial}{\partial\mu} \ln \operatorname{Tr}\exp\left[-\beta\left(H - \mu\hat{N}\right)\right]\Big|_{T,V} \\ &= k_B T\, \frac{\partial}{\partial\mu} \ln\left\{\prod_i^\infty \frac{1}{1 - \exp\left[\beta(\mu - \varepsilon_i)\right]}\right\} \\ &= \sum_{i=1}^\infty \frac{1}{\exp\left[\beta(\varepsilon_i - \mu)\right] - 1} . \end{aligned} \tag{4.78}$$

Since the expectation value of $\hat{N}$ is the sum of the mean occupation numbers (we call them $\tilde{n}_i$) for each level i, we have the well known result

$$\tilde{n}_i = \frac{1}{\exp\left[\beta(\varepsilon_i - \mu)\right] - 1} \ . \tag{4.79}$$

From here, it is possible to show for free bosons that as $T \to 0$, the occupation number of the lowest state diverges in the thermodynamic limit, namely *Bose-Einstein condensation* results. Unfortunately this is beyond the scope of this lectures, so that it will not be discussed here. However, this phenomenon show, how quantum mechanical indistinguishable particles can lead to phenomena radically different from those possible in classical physics.

4.1.5 Fermions and the exclusion principle. Slater determinant.

We can essentially repeat here what we have done for bosons in Sec. 4.1.3, however we should pay attention to the fact that now we are dealing with particles in $\mathcal{H}_A$. Given a state vector $\mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots >$ as in the bosonic case, we have now to apply the antisymmetrization operator in order to project it down to $\mathcal{H}_A$.

$$A \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots >= \frac{1}{N!} \sum_p (-1)^p P_p \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots > \ . \tag{4.80}$$

We notice now that if $n_i \geq 2$ for some state i, such a state is symmetric under under a transposition of two particles in that state. This means that

$$\mid u_1^{n_1}, \ldots, u_i^{n_i}, \ldots >= \frac{1}{2}\left[1 + P_{\alpha_i \beta_i}\right] \mid u_1^{n_1}, \ldots, u_i^{n_i}, \ldots > \ . \tag{4.81}$$

However, we have already seen in Sec. 4.1.1 that

$$P_p A = A P_p = (-1)^p A \ . \tag{4.82}$$

The identity has even parity but a transposition has odd parity, such that

$$A\left[1 + P_{\alpha_i \beta_i}\right] = A - A = 0 \ . \tag{4.83}$$

Consequently whenever the operator A encounters a state with $n_i \geq 2$ for some state i, it will annihilate it. Such a fact corresponds to *Pauli's exclusion principle* that states that two fermions cannot occupy the same state. Hence, in the case of fermions, each one-particle state can be at most singly occupied, i.e. $n_i = 0$ or 1. For the norm of the state, we can repeat the calculation in (4.41), but now since $n_i = 0$ or 1, $n_i! = 1$, it leads to

$$\mid \psi_A >= \sqrt{N!} \, A \mid u_1^{n_1}, u_2^{n_2}, \ldots, u_j^{n_j}, \ldots > \ . \tag{4.84}$$

A practical way of obtaining a totally antisymmetric wavefunction starting from one-particle states is the so-called *Slater determinant*. Let us rewrite $\mid \psi_A >$ above in a way, where we see explicitely the one-particle states that the N fermions are occupying

$$
\begin{aligned}
\mid \psi_A > &= \sqrt{N!}\, A \mid u_1^{(1)}, u_2^{(2)}, \dots, u_N^{(N)} > \\
&= \sqrt{N!}\, \frac{1}{N!} \sum_p (-1)^p\, P_p \mid u_1^{(1)}, u_2^{(2)}, \dots, u_N^{(N)} > \\
&= \frac{1}{\sqrt{N!}}\, \varepsilon_{i_1 i_2 \cdots i_N} \mid u_1^{(i_1)}, u_2^{(i_2)}, \dots, u_N^{(i_N)} > \\
&= \frac{1}{\sqrt{N!}}
\begin{vmatrix}
\mid u_1^{(1)} > & \mid u_1^{(2)} > & \cdots & \mid u_1^{(N)} > \\
\mid u_2^{(1)} > & \mid u_2^{(2)} > & \cdots & \mid u_2^{(N)} > \\
\vdots & \vdots & \vdots & \vdots \\
\mid u_N^{(1)} > & \mid u_N^{(2)} > & \cdots & \mid u_N^{(N)} >
\end{vmatrix}
\end{aligned}
\tag{4.85}
$$

In the third line above, we introduced the Levi-Civita symbol in N dimensions, and a summation is understood for repeated indices. This symbol guarantees that we have the correct sign according to the parity of the permutation. However, such an expression corresponds to the determinant of a matrix $\mid u_i^{(j)} >$. The Slater determinant makes the exclusion principle explicit, since a determinant vanishes if two columns or two rows are equal.

The occupation number states can be introduced in the same way as done in Sec. 4.1.3 for bosons, taking into account now that $n_i = 0, 1$. Then, without repeating the steps we already performed in the case of bosons, we just remark that the occupation number states can be obtained as follows:

$$
\mid n_1, \dots, n_i, \dots >= cA \mid u_1^{n_1}, \dots, u_i^{n_i}, \dots > ,
\tag{4.86}
$$

with the properties listed below

i) <u>Scalar product</u>.

$$
< n_1, \dots, n_i, \dots \mid n_1', \dots, n_i', \dots > \neq 0 ,
\tag{4.87}
$$

only then, when $n_i = n_i'$ for $i = 1, 2, \dots$ with $n_i = 0, 1$.

ii) <u>Normalization</u>. As we have seen in (4.84), the normalization constant c is given by

$$
c = \sqrt{N!} .
\tag{4.88}
$$

iii) <u>Basis</u>. By the same reasons as in Sec. 4.1.3, $\mid n_1, \dots, n_i, \dots >$ constitute a basis of $\mathcal{H}_A$.

In the same way that led to an expansion of a totally symmetric state in (4.43), a totally antisymmetric state can be as well expressed as a linear superposition of elements of the basis in $\mathcal{H}$ since $\mathcal{H}_A \subset \mathcal{H}$.

$$
\begin{aligned}
\mid \psi_A > \; &= \; A \mid \psi_A >= \sum_{i_1,\ldots,i_N} a_{i_1,\ldots,i_N} A \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} > \\
&= \; \frac{1}{N!} \sum_{i_1,\ldots,i_N} a_{i_1,\ldots,i_N} \sum_p \epsilon_p P_p \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} > ,
\end{aligned}
\tag{4.89}
$$

where we recall that P_p permutes the particles. We show this explicitely in the following discussion introducing the notation

$$
P_p \longrightarrow P_p [(1), \ldots, (N)] .
\tag{4.90}
$$

Due to Pauli's exclusion principle, the sum over indices $i_1, \ldots, i_N$ can only contain terms, where all indices from i_1 to i_N are different. As a consequence of this, when we go from a sum over states to a sum over occupation numbers as done in (4.48) for bosons,

$$
\sum_{i_1,\ldots,i_N} = \sum_{\substack{n_1,\ldots,n_j,\ldots \\ \sum_i n_i = N}} \sum_{\substack{i_1,\ldots,i_N \\ \left(n_1,\ldots,n_j,\ldots \right)}} ,
\tag{4.91}
$$

the second summation above, performed for a given distribution of occupation numbers (only zero or one), amounts to a permutation of the indices i_i to i_N:

$$
\sum_{\substack{i_1,\ldots,i_N \\ \left(n_1,\ldots,n_j,\ldots \right)}} = \sum_{\substack{p \\ \left(n_1,\ldots,n_j,\ldots \right)}} P_p (i_1, \ldots, i_N) .
\tag{4.92}
$$

Then, for (4.89) we have

$$
\begin{aligned}
\mid \psi_A > \; = \; \frac{1}{N!} \sum_{\substack{n_1,\ldots,n_j,\ldots \\ \sum_i n_i = N}} \sum_{\substack{p' \\ \left(n_1,\ldots,n_j,\ldots \right)}} P_{p'} (i_1, \ldots, i_N) \, a_{i_1,\ldots,i_N} \\
\times \sum_p \epsilon_p \, P_p [(1), \ldots, (N)] \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} > .
\end{aligned}
\tag{4.93}
$$

Since the permutations constitute a group, we can write the following

$$
\begin{aligned}
P_p [(1), \ldots, (N)] \; &= \; P_{p'} [(1), \ldots, (N)] \, P_{p'}^{-1} [(1), \ldots, (N)] \\
&\quad \times P_p [(1), \ldots, (N)] \\
&= \; P_{p'} [(1), \ldots, (N)] \, P_{\bar{p}} [(1), \ldots, (N)] ,
\end{aligned}
\tag{4.94}
$$

and it also holds that

$$
\epsilon_p = \epsilon_{p'} \, \epsilon_{\bar{p}} .
\tag{4.95}
$$

Using the manipulations above, we can write

$$\sum_{p'} P_{p'}(i_1, \ldots, i_N)\, a_{i_1,\ldots,i_N} \sum_{p} \epsilon_p\, P_p\,[(1), \ldots, (N)] \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} >$$

$$= \sum_{p'} P_{p'}(i_1, \ldots, i_N)\, a_{i_1,\ldots,i_N}\, \epsilon_{p'}\, P_{p'}\,[(1), \ldots, (N)]$$

$$\times \sum_{\bar{p}} \epsilon_{\bar{p}}\, P_{\bar{p}}\,[(1), \ldots, (N)] \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} > \quad . \quad (4.96)$$

Here we should realize that if we perform a permutation of the states given by the indices $i_1, \ldots, i_N$, and the same permutation is performed on the particles, the vector $\mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} >$ does not change. Therefore, we can consider the summation over permutations p' and $\bar{p}$ above independently from each other, i.e.

$$(4.96) = \left[\sum_{p'} P_{p'}(i_1, \ldots, i_N)\, a_{i_1,\ldots,i_N}\, \epsilon_{p'} \right]$$

$$\times \left[\sum_{\bar{p}} \epsilon_{\bar{p}}\, P_{\bar{p}}\,[(1), \ldots, (N)] \mid u_{i_1}^{(1)}, \ldots u_{i_N}^{(N)} > \right] \quad . \quad (4.97)$$

The first term on the r.h.s. of the equation above is zero if the coefficients $a_{i_1,\ldots,i_N}$ are symmetric with respect to permutations. Since they cannot be symmetric, they should be antisymmetric in the case of transpositions. Since each permutation can be expressed as a product of transpositions, the coefficients $a_{i_1,\ldots,i_N}$ should have the parity of the permutation, i.e.

$$P_p(i_1, \ldots, i_N)\, a_{i_1,\ldots,i_N} = \epsilon_p\, a_{i_1,\ldots,i_N} \quad . \quad (4.98)$$

This means that

$$\sum_{p'} \epsilon_{p'}\, P_{p'}(i_1, \ldots, i_N)\, a_{i_1,\ldots,i_N} = N!\, a_{i_1,\ldots,i_N} \equiv \sqrt{N!}\, c_{n_1,\ldots,n_j,\ldots} \quad . \quad (4.99)$$

Using the result above together with (4.86), we finally have

$$\mid \psi_A > = \sum_{n_1,\ldots,n_j,\ldots} c_{n_1,\ldots,n_j,\ldots} \mid n_1, \ldots, n_j, \ldots > \quad , \quad (4.100)$$

where

$$\sum_{n_1,\ldots,n_j,\ldots} \mid c_{n_1,\ldots,n_j,\ldots} \mid^2 = 1 \quad . \quad (4.101)$$

4.1.6 Fermi-Dirac statistics

The arguments that lead to the density matrix (4.65) for the canonical and (4.72) for the grand canonical ensemble in Sec. 4.1.4 were of general character and therefore, the density matrices deduced there can be also used in the case of fermions.

Let us now consider again the partition function in the grand canonical ensemble. We do so for generality. In the case one wants to consider the canonical ensemble, one needs only to put $\mu = 0$, and fix the number of particles. As in Sec. 4.1.4, we look at a system of non-interacting particles, in this case, an *ideal Fermi gas*.

$$
\begin{aligned}
Z &= \text{Tr} \exp\left[-\beta\left(H - \mu\hat{N}\right)\right] \\
&= \sum_{n_1,\dots,n_\infty} < n_1 \cdots n_\infty \mid \exp\left[-\beta\left(H - \mu\hat{N}\right)\right] \mid n_1 \cdots n_\infty > \\
&= \sum_{n_1,\dots,n_\infty} < n_1 \cdots n_\infty \mid \exp\left[\beta\left(\mu\sum_i n_i - \sum_i \varepsilon_i n_i\right)\right] \mid n_1 \cdots n_\infty > \\
&= \prod_i^\infty \sum_{n=0}^1 \left\{\exp\left[\beta(\mu - \varepsilon_i)\right]\right\}^n = \prod_i^\infty \left\{1 + \exp\left[\beta(\mu - \varepsilon_i)\right]\right\} . \quad (4.102)
\end{aligned}
$$

Once we obtained the partition function, we calculate as in the case of bosons, the expectation value of the number operator.

$$
\begin{aligned}
< \hat{N} > &= k_B T \frac{\partial}{\partial\mu} \ln\left(\prod_i^\infty \left\{1 + \exp\left[\beta(\mu - \varepsilon_i)\right]\right\}\right) \\
&= k_B T \sum_i \frac{\partial}{\partial\mu} \ln\left(1 + \exp\left[\beta(\mu - \varepsilon_i)\right]\right) \\
&= \sum_i \frac{1}{\exp\left[-\beta(\mu - \varepsilon_i)\right] + 1} , \quad (4.103)
\end{aligned}
$$

such that the *Fermi-Dirac distribution* is obtained

$$
\tilde{n}_i = \frac{1}{\exp\left[\beta(\varepsilon_i - \mu)\right] + 1} . \quad (4.104)
$$

In the limit of $T \longrightarrow 0$ (i.e. $\beta \longrightarrow \infty$), it is easy to see that

$$
\tilde{n}_i = \begin{cases} 1 & \text{for } \varepsilon_i < \mu \\ 0 & \text{for } \varepsilon_i > \mu \end{cases} \quad (4.105)
$$

Therefore, $\mu(T = 0) = E_F$, where E_F, the Fermi-energy, was introduced already in Sec. 3.1.2.

4.1.7   The Schrödinger equation for N identical particles.

Once we have seen the structure of states for N quantum mechanical identical particles, we should consider now the Hamiltonian and the Schrödinger equation, in order to see, how the whole formalism works in the case of many particles.

Let us look at a Hamiltonian in a rather general in form, with a kinetic energy part and an interaction part containing pairwise interactions. This is not the most general Hamiltonian for a many particle system, but the one of interest for us, since

we are going to consider only the consequences of Coulomb interaction, as we said at the very beginning of these lectures.

$$H = \sum_{i=1}^{N} T_i + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V_{ij} \; . \tag{4.106}$$

The Schrödinger equation looks as follows

$$i\hbar \frac{\partial}{\partial t} \mid \psi_1, \ldots, \psi_N, t > = H \mid \psi_1, \ldots, \psi_N, t > \; . \tag{4.107}$$

In order to obtain a solution, we proceed as in Secs. 4.1.3 and 4.1.5. We start by taking one-particle states $\mid u_i >$, that build a complete set of one-particle states $\{\mid u_i >\}$. A basis in the Hilbert space of N particles is constructed using product states. Since these N-particle states consitute a basis, they are time independent. The solution of the Schrödinger equation can be expressed as a linear combination of such states.

$$\mid \psi_1, \ldots, \psi_N, t > = \sum_{\alpha_1, \ldots, \alpha_N} a\left(\alpha_1, \ldots, \alpha_N, t\right) \mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} > \; , \tag{4.108}$$

where the time dependence is in the coefficients of the expansion. The next step is to distinguish between bosons and fermions, that is to project the states to either $\mathcal{H}_S$ or $\mathcal{H}_A$. We consider first the bosonic case, then, as we have already seen, the same kind of steps have to be taken in the fermionic case but with the restriction imposed on the ocupation numbers due to Pauli's exclusion principle. Of course, also the appropriate changes of sign should be taken into account.

Bosons

In the case of bosons, we use the totally symmetric projector S:

$$\begin{aligned} S \mid \psi_1, \ldots, \psi_N, t > &= \sum_{\alpha_1, \ldots, \alpha_N} a\left(\alpha_1, \ldots, \alpha_N, t\right) S \mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} > \\ &= \sum_{n_1, \ldots, n_j, \ldots} c_{n_1, \ldots, n_j, \ldots}(t) \mid n_1, \ldots, n_j, \ldots > \; , \end{aligned} \tag{4.109}$$

where in going to the second line, we used (4.52), and according to (4.51),

$$c_{n_1, \ldots, n_j, \ldots}(t) = \sqrt{\frac{N!}{n_1! \cdots n_j! \cdots}} \, a\left(\alpha_1, \ldots, \alpha_N, t\right) \; , \tag{4.110}$$

We can now insert this state into Schrödinger's equation (4.107), and consider first the left hand side, i.e. the time derivative.

$$i\hbar \frac{\partial}{\partial t} S \mid \psi_1, \ldots, \psi_N, t > = i\hbar \sum_{n_1, \ldots, n_j, \ldots} \frac{\partial}{\partial t} c_{n_1, \ldots, n_j, \ldots}(t) \mid n_1, \ldots, n_j, \ldots > \tag{4.111}$$

Next we multiply from the left by $< u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid$,

$$i\hbar < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid \frac{\partial}{\partial t} S \mid \psi_1, \ldots, \psi_N, t >$$

$$= i\hbar \sum_{n_1, \ldots, n_j, \ldots} \frac{\partial}{\partial t} c_{n_1, \ldots, n_j, \ldots}(t) < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid n_1, \ldots, n_j, \ldots > . \quad (4.112)$$

Due to the orthogonality of the one-particle states, only those states will remain, where the same number of particles per state are present in $\mid n_1, \ldots, n_j, \ldots >$ as in $< u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid$, that is only one term survives in the summation. The overlap gives, according to (4.45),

$$< u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid n_1, \ldots, n_j, \ldots >$$

$$= \sqrt{\frac{N!}{\prod_{j=1}^{\infty} n_j!}} \frac{1}{N!} \underbrace{\sum_p < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid P_p \mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >}_{= \prod_{j=1}^{\infty} n_j!}$$

$$= \sqrt{\frac{\prod_{j=1}^{\infty} n_j!}{N!}} , \quad (4.113)$$

where $\prod_{j=1}^{\infty} n_j!$ is given by the particular configuration in $\mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >$. Finally, we have

$$i\hbar < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid \frac{\partial}{\partial t} S \mid \psi_1, \ldots, \psi_N, t >= \sqrt{\frac{\prod_{j=1}^{\infty} n_j!}{N!}} i\hbar \frac{\partial}{\partial t} c_{n_1, \ldots, n_j, \ldots}(t) . \quad (4.114)$$

Next we consider the kinetic part.

$$\sum_{i=1}^{N} T_i \, S \mid \psi_1, \ldots, \psi_N, t >$$

$$= \sum_{i=1}^{N} T_i \sum_{n_1, \ldots, n_j, \ldots} c_{n_1, \ldots, n_j, \ldots}(t) \mid n_1, \ldots, n_j, \ldots > . \quad (4.115)$$

Again we multiply from the left by $< u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid$,

$$< u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid \sum_{i=1}^{N} T_i \, S \mid \psi_1, \ldots, \psi_N, t >$$

$$= \sum_{n_1, \ldots, n_j, \ldots} c_{n_1, \ldots, n_j, \ldots}(t) < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid \sum_{i=1}^{N} T_i \mid n_1, \ldots, n_j, \ldots > . (4.116)$$

In order to calculate the matrix elements for the kinetic energy operator, we use again (4.45)

$$< u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid \sum_{i=1}^{N} T_i \mid n_1, \ldots, n_j, \ldots >$$

$$= \sqrt{\frac{N!}{\prod_{j=1}^{\infty} n_j!}} \frac{1}{N!} \sum_{i,p} < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid T_i P_p \mid u_{\beta_1}^{(1)}, \ldots, u_{\beta_N}^{(N)} >, \quad (4.117)$$

where we have chosen labels β that are in general different from α, but they should be compatible with the specific configuration $n_1, \ldots, n_j, \ldots$. Since T_i is a one-particle operator that acts on particle i, it leaves unaffected all other particles. This means, that all the levels β_j, where particle i is not present, should have the same number of particles as the levels α_j, $j \neq i$. As a consequence of this,

i) the number of particles in levels different from α_i and β_i, in the sum over $n_1, \ldots, n_j, \ldots$ in (4.116) is restricted to those given by the state $\mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >$;

ii) the sum over permutations in (4.117) gives a factor

$$\prod_{\beta_\ell \neq \beta_i, \alpha_i} n_{\beta_\ell}! \times (n_{\alpha_i} - 1)! \, (n_{\beta_i} - 1)! \, , \tag{4.118}$$

where we took also into account that there are $(n_{\alpha_i} - 1)$ particles in level α_i and $(n_{\beta_i} - 1)$ particles in level β_i that remain unaffected by the operator T_i.

On the other hand, we have in general matrix elements of the form

$$< u_{\alpha_i}^{(i)} \mid T_i \mid u_{P(\beta_i)}^{(i)} > \, , \tag{4.119}$$

where $P(\beta_i)$ denotes the state to which particle i went after the permutation P. Since the particles are indistinguishable, the same matrix element appears for all possible particles in level β_i. This gives an additional factor n_{β_i} and the sum over permutations is reduced to a sum over levels β_i that are reached by the permutations. Although there are in general much more levels than those that can be reached by performing the permutations, since the factor n_{β_i} is present, we can extend the sum to all possible levels. Let us summarize the discussion above by rewriting (4.116) with the corresponding modifications.

$$(4.116) \quad = \quad \sum_{n_1, \ldots, n_j, \ldots} \sqrt{\frac{N!}{\prod_{j=1}^{\infty} n_j!}} \frac{1}{N!} c_{n_1, \ldots, n_j, \ldots}(t)$$
$$\times \sum_i \sum_{\beta_i} \prod_{\beta_\ell \neq \beta_i, \alpha_i} n_{\beta_\ell}! \, (n_{\alpha_i} - 1)! n_{\beta_i}! \, < u_{\alpha_i}^{(i)} \mid T_i \mid u_{\beta_i}^{(i)} > \tag{4.120}$$

where we still have to discuss which values take the occupation numbers $n_1, \ldots, n_j, \ldots$. Since the operator T_i connects a state $\mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >$ where particle i is in state $\mid u_{\alpha_i}^{(i)} >$ with a state $\mid u_{\beta_1}^{(1)}, \ldots, u_{\beta_N}^{(N)} >$, where particle i is in state $\mid u_{\beta}^{(i)} >$, then, the state $\mid u_{\beta_1}^{(1)}, \ldots, u_{\beta_N}^{(N)} >$ should have $n_\beta + 1$ particles in level β if state $\mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >$ has n_β particles in that level, and similarly $n_{\alpha_i} - 1$ particles in level α_i. Furthermore, since the particles are indistinguishable, we can go from a sum over particles i over to a sum over levels α as follows

$$\sum_i < u_{\alpha_i}^{(i)} \mid T_i \mid u_{\beta_i}^{(i)} > \rightarrow \sum_\alpha < \alpha \mid T \mid \beta > n_\alpha \, , \tag{4.121}$$

where we took into account the number of particles n_α in each level α. Before going to the final result, we should take care to consider two different cases. Until

now we assumed that in general states $\mid \alpha >$ and $\mid \beta >$ are different. It could happen however, that the operator T can also have non-vanishing matrix elements for $\mid \alpha >= \mid \beta >$. In this case, the state $\mid u_{\beta_1}^{(1)}, \ldots, u_{\beta_N}^{(N)} >$ will have the same number of particles in state $\mid \alpha >$ as the state $\mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >$. Taking this into account, we have

$$
(4.120) \quad = \quad \sum_\alpha \sqrt{\frac{n_1! \cdots n_\alpha! \cdots}{N!}} \, c_{n_1,\ldots,n_\alpha,\ldots}(t) < \alpha \mid T \mid \alpha > n_\alpha
$$
$$
+ \sum_{\alpha \neq \beta} \sqrt{\frac{n_1! \cdots (n_\alpha - 1)! \cdots (n_\beta + 1)! \cdots}{N!}} \, c_{n_1,\ldots,n_\alpha-1,\ldots,n_\beta+1,\ldots}(t)
$$
$$
\times < \alpha \mid T \mid \beta > n_\alpha \, . \quad (4.122)
$$

Before going to the interaction term, let us consider Schrödinger's equation only with the kinetic energy part, in order to have a first look at its form. We have on the one hand (4.114), where the occupation numbers are the same as in $\mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >$, whereas (4.122) has occupations numbers in general differing by one in levels α and β. This leads to

$$
i\hbar \frac{\partial}{\partial t} c_{n_1,\ldots,n_\alpha,\ldots}(t) \quad = \quad \sum_\alpha < \alpha \mid T \mid \alpha > n_\alpha \, c_{n_1,\ldots,n_\alpha,\ldots}(t)
$$
$$
+ \sum_{\alpha \neq \beta} < \alpha \mid T \mid \beta > \sqrt{n_\alpha (n_\beta + 1)}
$$
$$
\times c_{n_1,\ldots,n_\alpha-1,\ldots,n_\beta+1,\ldots}(t) \, . \quad (4.123)
$$

Already without taking into account the interaction, we have a set of coupled differential equations, with a huge number of equations, in principle infinite. We see therefore, that to work with a many particle system in first quantization appears as an extemely hard task.

Let us consider finally the interaction term. Here we have,

$$
\frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N V_{ij} \, S \mid \psi_1, \ldots, \psi_N, t >
$$
$$
= \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N V_{ij} \sum_{n_1,\ldots,n_j,\ldots} c_{n_1,\ldots,n_j,\ldots}(t) \mid n_1, \ldots, n_j, \ldots > \, . \quad (4.124)
$$

Again we multiply from the left by $< u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid$,

$$
\frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid V_{ij} \, S \mid \psi_1, \ldots, \psi_N, t >
$$
$$
= \frac{1}{2} \sum_{n_1,\ldots,n_j,\ldots} c_{n_1,\ldots,n_j,\ldots}(t) \sum_{\substack{i,j=1 \\ i \neq j}}^N < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid V_{ij} \mid n_1, \ldots, n_j, \ldots >
$$

$$= \frac{1}{2} \sum_{n_1,\ldots,n_j,\ldots} c_{n_1,\ldots,n_j,\ldots}(t)$$

$$\times \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \sqrt{\frac{N!}{\prod_{j=1}^{\infty} n_j!}} \frac{1}{N!} \sum_p < u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} \mid V_{ij} P_p \mid u_{\beta_1}^{(1)}, \ldots, u_{\beta_N}^{(N)} > \ . \ (4.125)$$

The same arguments can be repeated here as for the kinetic energy, with the only difference, that instead of having one state that is affected, we have to consider two. The matrix elements that have to be considered are of the form

$$< u_{\alpha_i}^{(i)} u_{\alpha_j}^{(j)} \mid V_{ij} \mid u_{\beta_i}^{(i)} u_{\beta_j}^{(j)} > , \tag{4.126}$$

This means, that in general the state $\mid u_{\beta_1}^{(1)}, \ldots, u_{\beta_N}^{(N)} >$ will have $n_{\alpha_i} - 1$, $n_{\alpha_j} - 1$, $n_{\beta_i} + 1$, and $n_{\beta_j} + 1$ particles if the state $\mid u_{\alpha_1}^{(1)}, \ldots, u_{\alpha_N}^{(N)} >$ has n_{α_i}, n_{α_j}, n_{β_i}, and n_{β_j} particles in the corresponding states. As in the case of a one-particle operator, we go from a sum over particles over to a sum over states. However, we have to take into account that $i \neq j$, and therefore, distinguish whether the the two particles are sitting in different states or on the same state

i) Particles on different states. Since we have two different states, $i \neq j$.

$$\sum_{\substack{i,j=1 \\ i \neq j}} < u_{\alpha_i}^{(i)} u_{\alpha_j}^{(j)} \mid \ \longrightarrow \ \sum_{\alpha \neq \alpha'} n_\alpha n_{\alpha'} < \alpha \alpha' \mid \ . \tag{4.127}$$

ii) Particles on the same state. Since $i \neq j$, one particle can be identified with one of the n_α particles in that state, but for the other one there are only $n_\alpha - 1$ possibilities.

$$\sum_{\substack{i,j=1 \\ i \neq j}} < u_{\alpha_i}^{(i)} u_{\alpha_j}^{(j)} \mid \ \longrightarrow \ \sum_\alpha n_\alpha (n_\alpha - 1) < \alpha \alpha \mid \ . \tag{4.128}$$

Taking into account the discussion above, we have

$$(4.125) \ \longrightarrow \ \frac{1}{2} \sqrt{\frac{\prod_{j=1}^{\infty} n_j!}{N!}} \sum_{\substack{\alpha, \alpha' \\ \beta, \beta'}} n_\alpha (n_{\alpha'} - \delta_{\alpha \alpha'}) < \alpha \alpha' \mid V \mid \beta \beta' >$$

$$\times c_{n_1,\ldots,n_\alpha - 1,\ldots,n_\beta + 1,\ldots,n_{\alpha'} - 1,\ldots,n_{\beta'} + 1,\ldots} \ . \tag{4.129}$$

As in the kinetic energy part, we have also to treat separately cases where $\alpha = \beta$, etc.. There are in total 15 different possibilities. They correspond to all different (1), two indices equal and all the other different (6), indices equal in pairs (3), three indices equal (4), and all equal (1). Let us consider just two of them in order to see, the kind of fafctors that arise.

i) $\alpha \neq \alpha', \alpha \neq \beta, \alpha \neq \beta', \alpha' \neq \beta, \alpha' \neq \beta', \beta \neq \beta'$.
In this case we have a factor $n_\alpha n_{\alpha'}$ from (4.127), and from the normalization factors

$$\sqrt{(n_\alpha - 1)! \, (n_{\alpha'} - 1)! \, (n_\beta + 1)! \left(n'_\beta + 1\right)!} \,, \tag{4.130}$$

such that after cancelling the normalization on both sides of Schrödinger equation, such a term contains a factor

$$\sqrt{n_\alpha n_{\alpha'} \left(n_\beta + 1\right) \left(n'_\beta + 1\right)} \,. \tag{4.131}$$

ii) $\alpha = \alpha', \alpha \neq \beta, \alpha \neq \beta', \beta \neq \beta'$.
In this case we have a factor $n_\alpha \left(n_\alpha - 1\right)$ from (4.127), and from the normalization factors

$$\sqrt{(n_\alpha - 2)! \, (n_\beta + 1)! \left(n'_\beta + 1\right)!} \,, \tag{4.132}$$

such that after cancelling the normalization on both sides of Schrödinger equation, such a term contains a factor

$$\sqrt{n_\alpha \left(n_\alpha - 1\right) \left(n_\beta + 1\right) \left(n'_\beta + 1\right)} \,. \tag{4.133}$$

Putting all results together, the Schrödinger equation has the following form

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} c_{n_1,\ldots,n_\alpha,\ldots}(t) \;=\; & \sum_\alpha <\alpha \mid T \mid \alpha> n_\alpha \, c_{n_1,\ldots,n_\alpha,\ldots}(t) \\
& + \sum_{\alpha \neq \beta} <\alpha \mid T \mid \beta> \sqrt{n_\alpha \left(n_\beta + 1\right)} \\
& \qquad\qquad\qquad \times c_{n_1,\ldots,n_\alpha - 1,\ldots,n_\beta + 1,\ldots}(t) \\
& + \frac{1}{2} \sum_{\alpha \neq \alpha' \neq \beta \neq \beta'} <\alpha\alpha' \mid V \mid \beta\beta'> \\
& \qquad \times \sqrt{n_\alpha n_{\alpha'} \left(n_\beta + 1\right) \left(n'_\beta + 1\right)} \\
& \qquad \times c_{n_1,\ldots,n_\alpha - 1,\ldots,n_\beta + 1,\ldots,n_{\alpha'} - 1,\ldots,n_{\beta'} + 1,\ldots}(t) \\
& + \frac{1}{2} \sum_{\alpha = \alpha' \neq \beta \neq \beta'} <\alpha\alpha \mid V \mid \beta\beta'> \\
& \qquad \times \sqrt{n_\alpha \left(n_\alpha - 1\right) \left(n_\beta + 1\right) \left(n'_\beta + 1\right)} \\
& \qquad \times c_{n_1,\ldots,n_\alpha - 2,\ldots,n_\beta + 1,\ldots,n_{\beta'} + 1,\ldots}(t) \\
& + \quad 13 \text{ other terms} \,.
\end{aligned} \tag{4.134}
$$

This shows that to solve a many-body problem in first quantization is rather hopeless, since just to write them down becomes rather demanding.

Fermions

A general fermionic state can be expanded in terms of occupation-number states as shown in (4.89),

$$
\begin{aligned}
A \mid \psi_1, \ldots, \psi_N, t > \; &= \sum_{\alpha_1, \ldots, \alpha_N} a\left(\alpha_1, \ldots, \alpha_N, t\right) A \mid u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} > \\
&= \sum_{n_1, \ldots, n_j, \ldots} c_{n_1, \ldots, n_j, \ldots}(t) \mid n_1, \ldots, n_j, \ldots > ,
\end{aligned}
\tag{4.135}
$$

where the relation between $a\left(\alpha_1, \ldots, \alpha_N, t\right)$ and $c_{n_1, \ldots, n_j, \ldots}(t)$ is given by (4.99). As in the bosonic case, we multiply the Schrödinger equation from the left by $< u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} \mid$, and taking into account that Pauli's exclusion principle only allows $n_i = 0, 1$, we have for the time derivative

$$
i\hbar < u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} \mid \frac{\partial}{\partial t} A \mid \psi_1, \ldots, \psi_N, t > = \sqrt{\frac{1}{N!}} \, i\hbar \frac{\partial}{\partial t} c_{n_1, \ldots, n_j, \ldots}(t) .
\tag{4.136}
$$

For the treatment of the kinetic energy and the interaction term, we should now take into account the fact that in the case of fermions, there are phase factors associated with the permutations. In order to follow these phase factors, we will assume a particular ordering of the levels for $< u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} \mid$, namely

$$
\alpha_1 < \alpha_2 < \cdots < \alpha_N .
\tag{4.137}
$$

With the assumption above, we have in analogy to the bosonic case (4.116)

$$
\begin{aligned}
&< u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} \mid \sum_{i=1}^{N} T_i \, A \mid \psi_1, \ldots, \psi_N, t > \\
&= \sum_{n_1, \ldots, n_j, \ldots} c_{n_1, \ldots, n_j, \ldots}(t) < u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} \mid \sum_{i=1}^{N} T_i \mid n_1, \ldots, n_j, \ldots > .
\end{aligned}
\tag{4.138}
$$

However, the matrix elements have now the following form

$$
\begin{aligned}
&< u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} \mid \sum_{i=1}^{N} T_i \mid n_1, \ldots, n_j, \ldots > \\
&= \frac{1}{\sqrt{N!}} \sum_{i,p} (-1)^p < u^{(1)}_{\alpha_1}, \ldots, u^{(N)}_{\alpha_N} \mid T_i P_p \mid u^{(1)}_{\beta_1}, \ldots, u^{(N)}_{\beta_N} > .
\end{aligned}
\tag{4.139}
$$

We use now the fact that the states are ordered as discussed above in order to determine the phase factor in eq. (4.139), recalling that the kinetic operator is a one-particle operator that connects the state α_i with the state β_i. There are two cases to be considered

i) $\beta_i < \alpha_i$.

In this case, the number of transpositions is given by the number of occupied states between β_i and α_i, such that

$$
(-1)^p = (-1)^{n_{\beta_i+1} + n_{\beta_i+2} + \cdots + n_{\alpha_i-1}} .
\tag{4.140}
$$

ii) $\beta_i > \alpha_i$.

Here we need to count the number of occupied states between α_i and β_i.

$$(-1)^p = (-1)^{n_{\alpha_i+1} + n_{\alpha_i+2} + \cdots + n_{\beta_i-1}} \ . \tag{4.141}$$

The rest of the calculation for the kinetic energy term goes along the lines discussed for bosons, such that using (4.139) with the phase factors discussed above, we finally have similarly to the bosonic case

$$(4.138) = \sqrt{\frac{1}{N!}} \sum_{\alpha,\beta} (-1)^{n_{\alpha+1} + n_{\alpha+2} + \cdots + n_{\beta-1}}$$

$$\times < \alpha \mid T \mid \beta > c_{n_1,\ldots,n_\alpha-1,\ldots,n_\beta+1,\ldots}(t) \ , \tag{4.142}$$

where the phase factors are to be understood as counting the number of occupied states between α and β.

We do not deal here directly with the interaction terms, since from the discussion of the kinetic energy term, we see that a similar structure as in the bosonic case is obtained with the addition of phase factors. This means, that also a complicated set of differential equations is obtained here and the formulation in first quantization is of doubtfull use.

4.2 Second quantization

Second quantization was originally introduced in order to deal with relativistic quantum mechanics, realizing that a consistent way of formulating a relativistic field theory had to go beyond first quantization. In our case, we stay in the realms of non-relativistic quantum mechanics, but second quantization will allow us to describe a many-body system in a transparent way, on the basis of the occupation-number states that we discussed in the previous section. We start with bosons and then discuss fermions.

4.2.1 Bosons in second quantization

Occupation-number states appear already in the discussion of the harmonic oscillator in an elementary course in quantum mechanics. In fact, we have already seen them in our chapter of phonons. Let us recall the discussion in the case of a harmonic oscillator. There we have operators b, $b^\dagger$ that fulfill the following commutation relation:

$$\left[b, b^\dagger \right] = 1 \ . \tag{4.143}$$

Furthermore, we can define an occupation-number operator $\hat{n} = b^\dagger b$, with eigenstates $\mid n >$, such that

$$\hat{n} \mid n >= n \mid n > , \qquad n \geq 0 \ . \tag{4.144}$$

As a consequence of the commutation relation above, it is easy to show that

$$\begin{aligned}
\hat{n}\, b \mid n > & = & (n-1)\, b \mid n > , \\
\hat{n}\, b^{\dagger} \mid n > & = & (n+1)\, b^{\dagger} \mid n > ,
\end{aligned} \qquad (4.145)$$

i.e. $b \mid n >$ and $b^{\dagger} \mid n >$ are eigenstates of the occupation-number operator with a quantum less or more. Therefore, they are called annihilation and creation operators. With the assumption that $\mid n >$ is normalized, we have already seen that

$$\begin{aligned}
b \mid n > & = & \sqrt{n} \mid n-1 > , \\
b^{\dagger} \mid n > & = & \sqrt{n+1} \mid n+1 > .
\end{aligned} \qquad (4.146)$$

We generalize in the following the properties discussed above to, in principle, an infinite number of modes $i = 1, \ldots, \infty$, in such a way that the occupation-number states $\mid n_1, \ldots, n_i, \ldots >$ we had in the previous sections, are eigenstates of occupation-number operators $\hat{n}_i = b_i^{\dagger} b_i$, where the commutation relations are generalized as follows:

$$\begin{aligned}
\left[b_i, b_j^{\dagger} \right] & = & \delta_{ij} , \\
\left[b_i, b_j \right] & = & \left[b_i^{\dagger}, b_j^{\dagger} \right] = 0 .
\end{aligned} \qquad (4.147)$$

The action of the occupation-number operators on the states is a simple generalization, where the occupation number states is seen as a tensorial product of eigenstates of infinitely many harmonic oscillators:

$$\hat{n}_i \mid n_1, \ldots, n_i, \ldots > = n_i \mid n_1, \ldots, n_i, \ldots > . \qquad (4.148)$$

Then, using again the commutation relations (4.147), we obtain the action of annihilation and creation operators on the occupation-number states

$$\begin{aligned}
b_i \mid n_1, \ldots, n_i, \ldots > & = & \sqrt{n_i} \mid n_1, \ldots, n_i - 1, \ldots > , \\
b_i^{\dagger} \mid n_1, \ldots, n_i, \ldots > & = & \sqrt{n_i + 1} \mid n_1, \ldots, n_i + 1, \ldots > .
\end{aligned} \qquad (4.149)$$

The space containing all the occupation-number states is called the *Fock-space*. It is a vector space as the Hilbert space but it contains all possible numbers of particles. Acting with an annihilation or creation operator on one state of the Fock-space brings us from one state to another one in the same Fock-space.

Let us reconsider the Schrödinger equation we discussed in Sec. 4.1.7 and translate it from first to second quantization. We had there a general state

$$\mid \psi(t) > = \sum_{n_1, \ldots, n_i, \ldots} c_{n_1, \ldots, n_i, \ldots}(t) \mid n_1, \ldots, n_i, \ldots > . \qquad (4.150)$$

Recalling the form we finally obtained for the Schrödinger equation, let us examine the different contributions on the right hand side of (4.134), where we consider only the terms that were written down explicitely. Actually, in (4.134) we arrived at a set of coupled differential equations, only in terms of the coefficients $c_{n_1, \ldots, n_i, \ldots}(t)$ of the linear combination above. But since the states $\mid n_1, \ldots, n_i, \ldots >$ constitute a basis in $\mathcal{H}_S$, we can reconstruct the evolution of the state $\mid \psi(t) >$ by multiplying in (4.134) both sides by $\mid n_1, \ldots, n_i, \ldots >$ and summing over all indices $n_1, \ldots, n_i, \ldots$.

1. Time derivative.

$$i\hbar \frac{\partial}{\partial t} c_{n_1,\ldots,n_\alpha,\ldots}(t) \quad \rightarrow \quad i\hbar \frac{\partial}{\partial t} \sum_{n_1,\ldots,n_i,\ldots} c_{n_1,\ldots,n_i,\ldots}(t) \mid n_1, \ldots, n_i, \ldots >$$

$$= \quad i\hbar \frac{\partial}{\partial t} \mid \psi(t) > . \tag{4.151}$$

2. Kinetic terms.

   i) Diagonal part.

$$\sum_i < i \mid T \mid i > n_i \, c_{n_1,\ldots,n_i,\ldots}(t)$$

$$\rightarrow \quad \sum_{n_1,\ldots,n_i,\ldots} \sum_i < i \mid T \mid i > n_i \, c_{n_1,\ldots,n_i,\ldots}(t)$$

$$\times \mid n_1, \ldots, n_i, \ldots > . \tag{4.152}$$

   Since

$$n_i \mid n_1, \ldots, n_i, \ldots >= b_i^\dagger b_i \mid n_1, \ldots, n_i, \ldots > , \tag{4.153}$$

   we have

$$(4.152) \quad = \quad \sum_{n_1,\ldots,n_i,\ldots} \sum_i < i \mid T \mid i > b_i^\dagger b_i \, c_{n_1,\ldots,n_i,\ldots}(t) \mid n_1, \ldots, n_i, \ldots >$$

$$= \quad \sum_i b_i^\dagger < i \mid T \mid i > b_i \mid \psi(t) > . \tag{4.154}$$

   ii) Off-diagonal part

$$\sum_{i \neq j} < i \mid T \mid j > \sqrt{n_i(n_j+1)} \, c_{n_1,\ldots,n_i-1,\ldots,n_j+1,\ldots}(t)$$

$$\rightarrow \quad \sum_{n_1,\ldots,n_i,\ldots} \sum_{i \neq j} < i \mid T \mid j > \sqrt{n_i(n_j+1)}$$

$$\times c_{n_1,\ldots,n_i-1,\ldots,n_j+1,\ldots}(t) \mid n_1, \ldots, n_i, \ldots > . \tag{4.155}$$

   since we are summing over all possible values of the n_i's, we can rename them as follows

$$n_i - 1 = n_i' , \quad n_j + 1 = n_j' , \quad n_k = n_k' , \quad \text{for} \quad k \neq i, \ k \neq j . \tag{4.156}$$

   Notice that the condition $\sum_i n_i = N$ is also fulfilled by the new variables. With the changes above, we have

$$(4.155) \quad = \quad \sum_{n_1',\ldots,n_i',\ldots} \sum_{i \neq j} < i \mid T \mid j > \sqrt{(n_i'+1)\,n_j'} \, c_{n_1',\ldots,n_i',\ldots,n_j',\ldots}(t)$$

$$\times \mid n_1', \ldots, n_i'+1, \ldots, n_j'-1, \ldots > . \tag{4.157}$$

The original occupation numbers fulfilled the condition $n_i \geq 0$. We can also restrict the new variables to the same range of values since if $n_i = 0$, then $n'_i = -1$ but $\sqrt{(n'_i + 1)\, n'_j} = 0$. We can also admit $n'_j = 0$ in spite of the fact that this implies $n_j = -1$, since $\sqrt{(n'_i + 1)\, n'_j} = 0$ also. Finally, we need only to realize that

$$\sqrt{(n'_i + 1)\, n'_j} \mid n'_1, \ldots, n'_i + 1, \ldots, n'_j - 1, \ldots >$$
$$= b_i^\dagger b_j \mid n'_1, \ldots, n'_i, \ldots >, \quad (4.158)$$

such that

$$(4.157) \quad = \quad \sum_{i \neq j} b_i^\dagger < i \mid T \mid j > b_j \mid \psi(t) > \ . \quad\quad (4.159)$$

Putting together the results (4.154) and (4.159), we have a rather simple expression for the kinetic energy operator:

$$\sum_{i=1}^{N} T_i \rightarrow \sum_{i,j} b_i^\dagger < i \mid T \mid j > b_j \ , \quad\quad (4.160)$$

where it is not anymore necessary to distinguish the different cases.

3. Interaction terms.
Here we have to distinguish the 15 cases we mentioned before. However, after having seen that second quantization leads to expressions, where different cases are all incorporated without an explicit division of cases, we just examine the two terms we already discussed and see, whether the same happens as in in the case of the kinetic energy.

   i) Matrix elements with all four different states.

$$\frac{1}{2} \sum_{i \neq j \neq k \neq \ell} < ij \mid V \mid k\ell > \sqrt{n_i n_j \left(n_k + 1 \right) \left(n_\ell + 1 \right)}$$
$$\times c_{n_1, \ldots, n_i - 1, \ldots, n_k + 1, \ldots, n_j - 1, \ldots, n_\ell + 1, \ldots}(t)$$
$$\rightarrow \frac{1}{2} \sum_{n_1, \ldots, n_i, \ldots} \sum_{i \neq j \neq k \neq \ell} < ij \mid V \mid k\ell >$$
$$\times \sqrt{n_i n_j \left(n_k + 1 \right) \left(n_\ell + 1 \right)}$$
$$\times c_{n_1, \ldots, n_i - 1, \ldots, n_k + 1, \ldots, n_j - 1, \ldots, n_\ell + 1, \ldots}(t)$$
$$\times \mid n_1, \ldots, n_i, \ldots > \ . \quad\quad (4.161)$$

As before, we rename the variables:

$$n_i - 1 \ = \ n'_i \,, \quad n_j - 1 = n'_j \,, \quad n_k + 1 = n'_k \,, \quad n_\ell + 1 = n'_\ell$$
$$n_m \ = \ n'_m \,, \quad \text{for} \quad m \neq i, j, k, \ell \ . \quad\quad (4.162)$$

Repeating the steps we made in $2.ii$), we arrive at

$$(4.161) = \frac{1}{2} \sum_{i \neq j \neq k \neq \ell} b_i^\dagger b_j^\dagger < ij \mid V \mid k\ell > b_k b_\ell . \qquad (4.163)$$

ii) Matrix elements with two states equal.

$$\frac{1}{2} \sum_{i=j \neq k \neq \ell} < ii \mid V \mid k\ell > \sqrt{n_i \big(n_i - 1\big)\big(n_k + 1\big)(n_\ell + 1)}$$

$$\times c_{n_1, \ldots, n_i - 2, \ldots, n_k + 1, \ldots, n_\ell + 1, \ldots}(t)$$

$$\rightarrow \frac{1}{2} \sum_{n_1, \ldots, n_i, \ldots} \sum_{i=j \neq k \neq \ell} < ii \mid V \mid k\ell >$$

$$\times \sqrt{n_i \big(n_i - 1\big)\big(n_k + 1\big)(n_\ell + 1)}$$

$$\times c_{n_1, \ldots, n_i - 2, \ldots, n_k + 1, \ldots, n_\ell + 1, \ldots}(t)$$

$$\times \mid n_1, \ldots, n_i, \ldots > . \qquad (4.164)$$

Here we rename the variables as follows:

$$n_i - 2 = n_i' , \quad n_k + 1 = n_k' , \quad n_\ell + 1 = n_\ell'$$
$$n_m = n_m' , \quad \text{for} \quad m \neq i, k, \ell . \qquad (4.165)$$

Then, we have

$$(4.164) = \frac{1}{2} \sum_{i \neq k \neq \ell} b_i^\dagger b_i^\dagger < ii \mid V \mid k\ell > b_k b_\ell . \qquad (4.166)$$

We see that it is again not necessary to taken into account the different cases explicitly, since the algebra of creation and annihilation operators does this automatically. Finally, we have for the interaction term

$$\frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V_{ij} = \frac{1}{2} \sum_{i,j,k,\ell} b_i^\dagger b_j^\dagger < ij \mid V \mid k\ell > b_k b_\ell . \qquad (4.167)$$

After having discussed the different terms, we can summarize the Schrödinger equation in second quantization:

$$i\hbar \frac{\partial}{\partial t} \mid \psi(t) >= H \mid \psi(t) > , \qquad (4.168)$$

where the Hamiltonian in second quantization is

$$H = \sum_{i,j} b_i^\dagger < i \mid T \mid j > b_j + \frac{1}{2} \sum_{i,j,k,\ell} b_i^\dagger b_j^\dagger < ij \mid V \mid k\ell > b_k b_\ell . \qquad (4.169)$$

The statistics of the particles is now contained in the commutation relation of the creation and annihilation operators. To see this explicitely, let us consider the

vacuum, i.e. the state that is annihilated by any annihilation operator. This is the generalization of the ground state of the harmonic oscillator $\mid 0 >$:

$$b \mid 0 >= 0 \qquad \longrightarrow \qquad b_i \mid 0 >= 0 \ . \tag{4.170}$$

A particle in state i is obtained by acting with a creation operator on the vacuum:

$$b_i^\dagger \mid 0 >= \mid i > \ . \tag{4.171}$$

Due to the commutation relation obeyed by bosons, we have

$$b_i^\dagger b_j^\dagger = b_j^\dagger b_i^\dagger \quad \Rightarrow \quad b_i^\dagger b_j^\dagger \mid 0 >= b_j^\dagger b_i^\dagger \mid 0 > \quad \Rightarrow \quad \mid ij >= \mid ji > \ , \tag{4.172}$$

such that a transposition does not lead to a different state.

4.2.2   Fermions in second quantization

In the case of fermions, we can also define creation and annihilation operators $f_i^\dagger$, f_i, such that an occupation-number operator is given by $\hat{n}_i = f_i^\dagger f_i$, with the property

$$\hat{n}_i \mid n_1, \ldots, n_i, \ldots > \ = \ n_i \mid n_1, \ldots, n_i, \ldots > \ . \tag{4.173}$$

We have seen in the case of bosons, that the commutation relations guarantee that the properties that result from the symmtrization postulate are respected. We can try here to look for commutation relations that also lead to states that respect the symmetrization postulate for fully antisymmetric states. A main property in this respect is that fermions should be antisymmetric with respect to transpositions. Let us ask as in the case of bosons that a vacuum exists, such that

$$f_i \mid 0 >= 0 \ . \tag{4.174}$$

On this vacuum we can create a particle

$$f_i^\dagger \mid 0 >= \mid i > \ . \tag{4.175}$$

We can as well create two particles and ask the corresponding states to be antisymmetric with respect to a transposition.

$$\begin{aligned}
f_i^\dagger f_j^\dagger \mid 0 > \ &= \ \mid ij > \\
\hookrightarrow f_j^\dagger f_i^\dagger \mid 0 > \ &= \ \mid ji >= - \mid ij >= -f_i^\dagger f_j^\dagger \mid 0 > \\
\Longrightarrow f_i^\dagger f_j^\dagger + f_j^\dagger f_i^\dagger \ &\equiv \ \left\{ f_i^\dagger, f_j^\dagger \right\} = 0 \ .
\end{aligned} \tag{4.176}$$

Therefore, fermion creation and annihilation operators anticommute. This property, that results from the symmetry properties under transpositions, also leads to Pauli's exclusion principle. In order to see this, we just need to take $i = j$. In this case we have

$$f_i^\dagger f_i^\dagger + f_i^\dagger f_i^\dagger = 2 f_i^\dagger f_i^\dagger = 0 \ , \tag{4.177}$$

showing that two fermions cannot be created in the same state. Taking the hermitian conjugate of (4.176), we arrive at

$$
\begin{aligned}
\left\{ f_i^\dagger, f_j^\dagger \right\}^\dagger &= \left(f_i^\dagger f_j^\dagger + f_j^\dagger f_i^\dagger \right)^\dagger \\
&= f_j f_i + f_i f_j = \{ f_i, f_j \} = 0 \; .
\end{aligned}
\tag{4.178}
$$

Next we have to discuss the commutation relations between creation and annihilation operators for fermions. Since the occupation number operator counts the number of particles in a given state, we have

$$
\begin{aligned}
\hat{n}_i \mid 0 > &= f_i^\dagger f_i \mid 0 >= 0 \; , \\
\hat{n}_i \mid i > &= f_i^\dagger f_i \mid i >= \mid i > \; .
\end{aligned}
\tag{4.179}
$$

On the other hand, from (4.175), we have

$$
\begin{aligned}
f_i \mid i > &= f_i f_i^\dagger \mid 0 >= \mid 0 > \; , \\
f_i f_i^\dagger \mid i > &= f_i f_i^\dagger f_i^\dagger \mid 0 >= 0 \; .
\end{aligned}
\tag{4.180}
$$

Then,

$$
\begin{aligned}
\left(f_i f_i^\dagger + f_i^\dagger f_i \right) \mid 0 > &= \mid 0 > \; , \\
\left(f_i f_i^\dagger + f_i^\dagger f_i \right) \mid i > &= \mid i > \; ,
\end{aligned}
\tag{4.181}
$$

such that

$$
f_i f_j^\dagger + f_j^\dagger f_i = \left\{ f_i, f_j^\dagger \right\} = \delta_{ij} \; .
\tag{4.182}
$$

We arrived then, at the anticommutation relations fulfilled by fermion creation and annihilation operators:

$$
\left\{ f_i, f_j^\dagger \right\} = \delta_{ij} \; , \quad \left\{ f_i^\dagger, f_j^\dagger \right\} = \left\{ f_i, f_j \right\} = 0 \; .
\tag{4.183}
$$

With the anticommutation relations obtained above, we can go back to the Schrödinger equation for fermions, where, as in the case of bosons, we start with a general state

$$
\mid \psi(t) >= \sum_{n_1, \ldots, n_i, \ldots} c_{n_1, \ldots, n_i, \ldots}(t) \mid n_1, \ldots, n_i, \ldots > \; ,
\tag{4.184}
$$

the difference with bosonic states being that $n_i = 0, 1$. We restrict the discussion to the kinetic term in order to see how the transformation is done. Recalling (4.142) we have to see whether the creation and annihilation operators introduced here are able to take into account the phase factors that appeared there. Let us then express the occupation number states in terms of the creation operators:

$$
\mid n_1, \ldots, n_i, \ldots > = \left(f_1^\dagger \right)^{n_1} \cdots \left(f_i^\dagger \right)^{n_i} \cdots \mid 0 > \; ,
\tag{4.185}
$$

with the constraint that $\sum_i n_i = N$. As we already discussed in Sec. 4.1.7, in the case of fermions it is important to keep track of the ordering of states. This is done above by applying the creation operators in a definite order. Let us now look at the action of an annihilation operator on such a state

$$
\begin{aligned}
f_j \mid n_1, \ldots, n_i, \ldots > \; &= \; f_j \left(f_1^\dagger\right)^{n_1} \cdots \left(f_i^\dagger\right)^{n_i} \cdots \mid 0 > \\
&= \; (-1)^{n_1+n_2+\cdots+n_{j-1}} \\
&\quad \times \left(f_1^\dagger\right)^{n_1} \cdots \left(f_{j-1}^\dagger\right)^{n_{j-1}} f_j \left(f_j^\dagger\right)^{n_j} \cdots \mid 0 > \; . \quad (4.186)
\end{aligned}
$$

Here we have to distinguish two cases

   i) $n_j = 0$. In this case the result is zero since $f_j \mid 0 >= 0$.

   ii) $n_j = 1$. In this case we would have

$$
f_j f_j^\dagger = 1 - f_j^\dagger f_j \; , \quad\quad\quad (4.187)
$$

   where the second term cancels because again the annihilation operator acts on the vacuum.

Going back to (4.186) we have

$$
\begin{aligned}
(4.186) \; &= \; (-1)^{n_1+n_2+\cdots+n_{j-1}} \left(f_1^\dagger\right)^{n_1} \cdots \left(f_{j-1}^\dagger\right)^{n_{j-1}} \left(f_{j+1}^\dagger\right)^{n_{j+1}} \cdots \mid 0 > \\
&= \; (-1)^{n_1+n_2+\cdots+n_{j-1}} \mid n_1, \ldots, n_{j-1}, n_j - 1, n_{j+1}, \ldots > \; . \quad (4.188)
\end{aligned}
$$

The same happens when considering the action of a creation operator, where in this case, zero results if $n_j = 1$. The result is

$$
\begin{aligned}
f_i^\dagger \mid n_1, \ldots, n_i, \ldots > \; &= \; (-1)^{n_1+n_2+\cdots+n_{i-1}} \\
&\quad \times \mid n_1, \ldots, n_{i-1}, n_i + 1, n_{i+1}, \ldots > \; . \quad (4.189)
\end{aligned}
$$

Putting together (4.188) and (4.189) we have

$$
\begin{aligned}
f_i^\dagger f_j \mid n_1, \ldots, n_i, \ldots, n_j, \ldots > \; &= \; (-1)^{n_{i+1}+n_{i+2}+\cdots+n_{j-1}} \\
&\quad \times \mid n_1, \ldots, n_i + 1, \ldots, n_j - 1, \ldots > (4.190)
\end{aligned}
$$

With this result, we can rewrite the kinetic term (4.142):

$$
\begin{aligned}
&\sum_{n_1,\ldots,n_i,\ldots} \sum_{i,j} < i \mid T \mid j > (-1)^{n_{i+1}+n_{i+2}+\cdots+n_{j-1}} \\
&\quad \times c_{n_1,\ldots,n_i+1,\ldots,n_j-1,\ldots}(t) \mid n_1, \ldots, n_i + 1, \ldots, n_j - 1, \ldots > \\
&= \sum_{i,j} f_i^\dagger < i \mid T \mid j > f_j \underbrace{\sum_{n_1,\ldots,n_i,\ldots} c_{n_1,\ldots,n_i,\ldots,n_j,\ldots}(t) \mid n_1, \ldots, n_i, \ldots >}_{|\psi(t)>} (4.191)
\end{aligned}
$$

where we performed a change of variables in the summation over $n_1, \ldots,$ with $n_i + 1 \rightarrow n_i$ and $n_j - 1 \rightarrow n_j$, as we did in the bosonic case.

The interaction can be transformed in a similar way. The final result for the Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t} \mid \psi(t) > = H \mid \psi(t) > , \tag{4.192}$$

where the Hamiltonian in second quantization is

$$H = \sum_{i,j} f_i^\dagger < i \mid T \mid j > f_j + \frac{1}{2} \sum_{i,j,k,\ell} f_i^\dagger f_j^\dagger < ij \mid V \mid k\ell > f_\ell f_k . \tag{4.193}$$

We see that the Hamiltonian the same form has for bosons as well as for fermions. The information about the statistical properties of the particles considered resides solely in the commutation or anticommutation relations of the creation and annihilation operators.

4.2.3   Field operators

The creation and annihilation operators $b_i^\dagger$, b_i for bosons and $f_i^\dagger$, f_i for fermions create and annihilate a particle in a state $\mid i >$, that was taken from a certain one-particle basis. In the following we discuss changes of basis and since the same steps are valid both for bosons and for fermions, let us use as a notation operators $c_i^\dagger$, c_i for particles, without specifying their statistics.

We introduce now a linear combination of operators as follows,

$$\begin{aligned}
\hat{\psi}(\boldsymbol{x}) &\equiv \sum_i \psi_i(\boldsymbol{x})\, c_i , \\
\hat{\psi}^\dagger(\boldsymbol{x}) &\equiv \sum_i \psi_i^*(\boldsymbol{x})\, c_i^\dagger ,
\end{aligned} \tag{4.194}$$

where the coefficients of the expansion $\psi_i(\boldsymbol{x})$ are one-particle wavefunctions for the quantum numbers i and the summation goes over a complete set of states associated with the quantum number i. These are called *field operators*.

With the definitions above we can rewrite the kinetic energy term:

$$\begin{aligned}
\sum_{i,j} & c_i^\dagger < i \mid T \mid j > c_j \\
&= \int \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{x}' \sum_{i,j} c_i^\dagger < i \mid \boldsymbol{x} >< \boldsymbol{x} \mid T \mid \boldsymbol{x}' >< \boldsymbol{x}' \mid j > c_j \\
&= \int \mathrm{d}\boldsymbol{x}\, \hat{\psi}^\dagger(\boldsymbol{x}) \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 \right) \hat{\psi}(\boldsymbol{x}) ,
\end{aligned} \tag{4.195}$$

where in going from the second to the third line we used that

$$< \boldsymbol{x} \mid T \mid \boldsymbol{x}' > = \delta(\boldsymbol{x} - \boldsymbol{x}') \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_{\boldsymbol{x}}^2 \right) . \tag{4.196}$$

We see that using the field operators, the kinetic energy term has exactly the same form as the expectation value in first quantization but instead of the wavefunctions we have operators that act on states of the Fock space. Hence the name second quantization. We can depict this situation as follows

$$H_{classic} \xrightarrow{q,p \to \hat{q},\hat{p}} H_{1st\ quantization} \xrightarrow{\psi \to \hat{\psi}} H_{2nd\ quantization} \ . \tag{4.197}$$

For the interaction term we have

$$\sum_{i,j,k,\ell} c_i^\dagger c_j^\dagger < ij \mid V \mid k\ell > c_\ell c_k$$

$$= \int d\boldsymbol{x}\, d\boldsymbol{x}'\, d\boldsymbol{x}''\, d\boldsymbol{x}''' \sum_{i,j,k,\ell} c_i^\dagger c_j^\dagger < i \mid \boldsymbol{x} > < j \mid \boldsymbol{x}' >$$

$$\times < \boldsymbol{x}\boldsymbol{x}' \mid V \mid \boldsymbol{x}''\boldsymbol{x}''' > < \boldsymbol{x}'' \mid k > < \boldsymbol{x}''' \mid \ell > c_\ell c_k \ . \tag{4.198}$$

Since V is a two-particle interaction potential, it can only depend on two coordinates. This means

$$< \boldsymbol{x}\boldsymbol{x}' \mid V \mid \boldsymbol{x}''\boldsymbol{x}''' > \ = \ < \boldsymbol{x}\boldsymbol{x}' \mid V \mid \boldsymbol{x}\boldsymbol{x}' > \delta\left(\boldsymbol{x}''' - \boldsymbol{x}'\right) \delta\left(\boldsymbol{x}'' - \boldsymbol{x}\right) \ . \tag{4.199}$$

With this choice we have

$$(4.198) \ = \ \int d\boldsymbol{x}\, d\boldsymbol{x}'\, \hat{\psi}^\dagger(\boldsymbol{x})\, \hat{\psi}^\dagger(\boldsymbol{x}')\, V(\boldsymbol{x}, \boldsymbol{x}')\, \hat{\psi}(\boldsymbol{x}')\, \hat{\psi}(\boldsymbol{x}) \ . \tag{4.200}$$

There are of course other possible choices to group four coordinates into two. However the choice above is the one that guarantees that H is hermitian. Putting together the results for the kinetic energy (4.195) and interaction (4.200) terms, we have the Hamiltonian in terms of field operators:

$$
\begin{aligned}
H \ = \ & \int d\boldsymbol{x}\, \hat{\psi}^\dagger(\boldsymbol{x}) \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\right) \hat{\psi}(\boldsymbol{x}) \\
& + \frac{1}{2} \int d\boldsymbol{x}\, d\boldsymbol{x}'\, \hat{\psi}^\dagger(\boldsymbol{x})\, \hat{\psi}^\dagger(\boldsymbol{x}')\, V(\boldsymbol{x}, \boldsymbol{x}')\, \hat{\psi}(\boldsymbol{x}')\, \hat{\psi}(\boldsymbol{x}) \ .
\end{aligned}
\tag{4.201}
$$

The commutation and anticommutation relations for field operators can be easily deduced from the respective relations for creation and annihilation operators:

$$
\begin{aligned}
\left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^\dagger(\boldsymbol{x}')\right]_\mp \ &= \ \sum_{i,j} \psi_i(\boldsymbol{x})\, \psi_j^*(\boldsymbol{x}') \underbrace{\left[c_i, c_j^\dagger\right]_\mp}_{=\delta_{ij}} \\
&= \ \sum_i \psi_i(\boldsymbol{x})\, \psi_i^*(\boldsymbol{x}') = \delta\left(\boldsymbol{x} - \boldsymbol{x}'\right) \ ,
\end{aligned}
\tag{4.202}
$$

where the upper (lower) sign in the square brackets corresponds to bosons (fermions), and to obtain the final result we used that $\{\psi_i(\boldsymbol{x})\}$ build a complete set of wavefunctions.

What we did above with the Hamiltonian can be done for any operator in first quantization, giving a form in second quantization. For example, for any one-particle operator,

$$J = \sum_{i=1}^{N} J_i \tag{4.203}$$

we have in second quantization, following the same steps we performed for the kinetic energy term,

$$
\begin{aligned}
\hat{J} &= \sum_{i,j} < i \mid J \mid j > c_i^\dagger c_j \\
&= \int \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{x}' \sum_i \psi_i^*(\boldsymbol{x})\, c_i^\dagger < \boldsymbol{x} \mid J \mid \boldsymbol{x}' > \sum_j \psi_j(\boldsymbol{x}')\, c_j \\
&= \int \mathrm{d}\boldsymbol{x}\, \hat{\psi}^\dagger(\boldsymbol{x})\, J(\boldsymbol{x})\, \hat{\psi}(\boldsymbol{x}) \;,
\end{aligned}
\tag{4.204}
$$

where we used, as we did for the kinetic energy term that

$$< \boldsymbol{x} \mid J \mid \boldsymbol{x}' > = J(\boldsymbol{x})\, \delta(\boldsymbol{x} - \boldsymbol{x}') \;. \tag{4.205}$$

A particularly important one-particle operator is the *density operator*. In first quantization it is

$$n(\boldsymbol{x}) = \sum_{i=1}^{N} \delta(\boldsymbol{x} - \boldsymbol{x}_i) \;. \tag{4.206}$$

Using the prescription above, we have

$$\hat{n}(\boldsymbol{x}) = \int \mathrm{d}\tilde{\boldsymbol{x}}\, \mathrm{d}\tilde{\boldsymbol{x}}' \sum_i \psi_i^*(\tilde{\boldsymbol{x}})\, c_i^\dagger < \tilde{\boldsymbol{x}} \mid \delta(\tilde{\boldsymbol{x}} - \boldsymbol{x}) \mid \tilde{\boldsymbol{x}}' > \sum_j \psi_j(\tilde{\boldsymbol{x}}')\, c_j, \tag{4.207}$$

where for the matrix element we know that

$$< \tilde{\boldsymbol{x}} \mid \delta(\tilde{\boldsymbol{x}} - \boldsymbol{x}) \mid \tilde{\boldsymbol{x}}' > = \delta(\tilde{\boldsymbol{x}} - \boldsymbol{x})\, \delta(\tilde{\boldsymbol{x}} - \tilde{\boldsymbol{x}}') \;, \tag{4.208}$$

such that

$$\hat{n}(\boldsymbol{x}) = \hat{\psi}^\dagger(\boldsymbol{x})\, \hat{\psi}(\boldsymbol{x}) \;. \tag{4.209}$$

Given the density operator with the field operators, we can obtain the *particle number operator*

$$\hat{N} = \int \mathrm{d}\tilde{\boldsymbol{x}}\, \hat{n}(\boldsymbol{x}) = \int \mathrm{d}\tilde{\boldsymbol{x}}\, \hat{\psi}^\dagger(\boldsymbol{x})\, \hat{\psi}(\boldsymbol{x}) \;. \tag{4.210}$$

It can be easily shown, that $\hat{N}$ commutes with the Hamiltonian (4.201).

4.3 Non-interacting electrons. The Fermi gas

As a first application of second quantization, we consider the simplest model for electrons in a metal, namely non-interacting, free electrons, i.e. not even in the presence of a periodic potential, as is normaly the case in solids. We have already seen in Chapter 3 the consequences of such a potential and also introduced some concepts like Fermi energy, Fermi surface, and density of states. We will calculate them now for the simplest possible situation. Although this seems to be an oversimplification, it is rather surprising that such results obtained by Sommerfeld around 1926, could explain the behavior of specific heat and also Pauli paramagnetism for simple metals at low temperatures. As we have seen in Sec. 3.2, if the periodic potential is weak enough, the electronic band-structure can be well described over most of the Brillouin by essentially free electrons, and therefore, this could be in these cases a good approximation. Only those points where degeneracies appear will present departures, since there a band gap opens. The Coulomb interaction, however, cannot be considered as weak since it diverges when two electrons come close together. It is one of Landau's merits to have clarified the situation by introducing the idea of a Fermi liquid. Although we are not going to look at it in detail, we will try at least to give a general idea, why most fermionic systems (simple metals, ^{3}He, nuclear matter) can be regarded as composed of weakly interacting fermions, namely quasi-particles with the same quantum numbers as the original constituents but with renormalized masses.

4.3.1 Hamiltonian, Fermi momentum and Fermi energy

We consider non-interacting electrons in a homogeneous three-dimensional box with sides of length L, with periodic boundary conditions, as introduced in Sec. 1.2.2. Then, only the following wavevectors are allowed

$$k_i = \frac{2\pi n_i}{L} , \quad i = x, y, z , \quad n_i \text{ integer} . \tag{4.211}$$

The Hamiltonian has the following form in first quantization

$$H = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} . \tag{4.212}$$

As we have seen in Sec. 4.2, in second quantization, the Hamiltonian takes the form

$$H = \sum_{\alpha,\beta} f_\alpha^\dagger < \alpha \mid \frac{\boldsymbol{p}_i^2}{2m} \mid \beta > f_\beta , \tag{4.213}$$

where the indices α and β denote quantum numbers of a one-particle basis. In our case, the quantum number is the wavevector $\boldsymbol{k}$ and it also contains the spin of the electrons, such that

$$\mid \alpha > \longrightarrow \mid \boldsymbol{k}, \sigma > , \tag{4.214}$$

where $\boldsymbol{k}$ takes the values given in (4.211) and $\sigma = \pm 1/2$ gives the possible projections of the spin along a certain quantization axis. Then, the matrix elements to be calculated are

$$
\begin{aligned}
< \alpha \mid \frac{\boldsymbol{p}_i^2}{2m} \mid \beta > \quad \rightarrow \quad & < \boldsymbol{k}_1, \sigma_1 \mid -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} \mid \boldsymbol{k}_2, \sigma_2 > \\
= \quad & \frac{1}{2mL^3} \int \mathrm{d}\boldsymbol{x} \, \exp\left(-i\boldsymbol{k}_1 \cdot \boldsymbol{x}\right) \left(-\hbar^2 \boldsymbol{\nabla}^2\right) \exp\left(i\boldsymbol{k}_2 \cdot \boldsymbol{x}\right) \\
& \qquad\qquad\qquad\qquad\qquad \times < \sigma_1 \mid \sigma_2 > \\
= \quad & \frac{\hbar^2 \boldsymbol{k}_2^2}{2mV} \delta_{\sigma_1,\sigma_2} \int \mathrm{d}\boldsymbol{x} \, \exp\left[i\left(\boldsymbol{k}_2 - \boldsymbol{k}_1\right) \cdot \boldsymbol{x}\right] \\
= \quad & \frac{\hbar^2 \boldsymbol{k}_2^2}{2m} \delta_{\sigma_1,\sigma_2} \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \, ,
\end{aligned}
\tag{4.215}
$$

leading to the Hamiltonian in second quantization

$$
H = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \, f_{\boldsymbol{k},\sigma}^\dagger f_{\boldsymbol{k},\sigma} \, ,
\tag{4.216}
$$

with

$$
\epsilon_{\boldsymbol{k}} = \frac{\hbar^2 \boldsymbol{k}^2}{2m} \, .
\tag{4.217}
$$

Given N electrons, the ground state energy is obtained by filling up the lowest levels with them. As a consequence of Pauli's exclusion principle, we can have up to two electrons per level, since for the same momentum we have two possibilities for the spin. In this case one speaks of a degenerate electron gas.
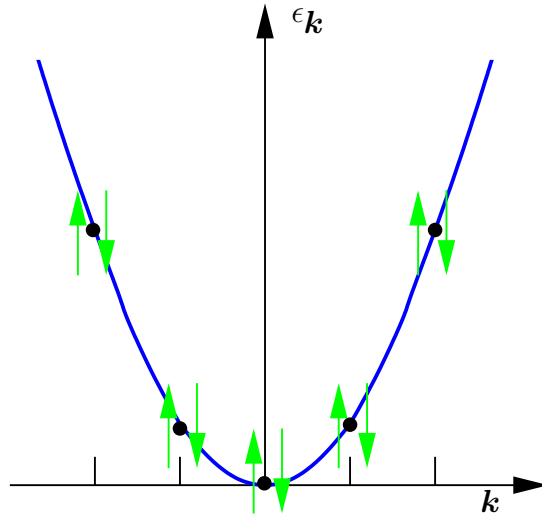

Figure 4.1: Dispersion relation for free electrons.

As seen in Fig. 4.1, given N electrons, there is a maximal wavevector that corresponds to the last occupied states. It is the Fermi wavevector and its energy is

the Fermi energy. In order to determine the Fermi wavevector, we can calculate the expectation value of the particle number operator.

$$
\begin{aligned}
N &= <G \mid \hat{N} \mid G> \\
&= \sum_{\boldsymbol{k},\sigma} <G \mid f^{\dagger}_{\boldsymbol{k},\sigma} f_{\boldsymbol{k},\sigma} \mid G> = \sum_{\boldsymbol{k},\sigma} \theta\left(k_F - \mid \boldsymbol{k} \mid\right) ,
\end{aligned} \tag{4.218}
$$

where $\theta(x)$ is the Heavyside function defined as

$$
\theta(x) = \begin{cases} 1 & x \geq 0 , \\ 0 & x < 0 . \end{cases} \tag{4.219}
$$

This leads to

$$
\begin{aligned}
(4.218) &= g\left(\frac{L}{2\pi}\right)^3 \int \mathrm{d}^3 k \, \theta\left(k_F - \mid \boldsymbol{k} \mid\right) \\
&= \frac{gV}{2\pi^2} \int_0^{k_F} k^2 \, \mathrm{d}k = \frac{gV}{6\pi^2} k_F^3 ,
\end{aligned} \tag{4.220}
$$

where g is the degree of degeneracy (in this case $g = 2$). From the result above we can obtain the Fermi-wavevector

$$
k_F = \left(\frac{6\pi^2}{g} \frac{N}{V}\right)^{\frac{1}{3}} , \tag{4.221}
$$

that is, k_F is proportional to the cubic root of the density of particles. Actually, $(V/N)^{1/3}$ defines a length, the average separation of particles, such that k_F can be thought as the inverse of the average separation of electrons.

Once we obtained the Fermi wavevector, it is straightforward to calculate the Fermi energy:

$$
E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{6\pi^2}{g} \frac{N}{V}\right)^{\frac{2}{3}} . \tag{4.222}
$$

4.3.2 Ground-state properties of the Fermi gas

Here we will concentrate on the ground-state energy and the density of states.

Ground-state energy

It is given by the expectation value of H:

$$
\begin{aligned}
E_G &= <G \mid H \mid G> \\
&= \frac{\hbar^2}{2m} \sum_{\boldsymbol{k},\sigma} \boldsymbol{k}^2 <G \mid f^{\dagger}_{\boldsymbol{k},\sigma} f_{\boldsymbol{k},\sigma} \mid G> \\
&= g\frac{\hbar^2}{2m}\left(\frac{L}{2\pi}\right)^3 \int \mathrm{d}^3 k \, \boldsymbol{k}^2 \, \theta\left(k_F - \mid \boldsymbol{k} \mid\right)
\end{aligned}
$$

$$= \frac{\hbar^2}{m}\frac{V}{2\pi^2}\int_0^{k_F}k^4\,\mathrm{d}k = \frac{\hbar^2}{2m}\frac{V}{\pi^2}\frac{k_F^5}{5}$$

$$= \underbrace{\frac{\hbar^2 k_F^2}{2m}}_{=E_F}\frac{1}{5}\underbrace{\frac{Vk_F^3}{\pi^2}}_{=3N} = \frac{3}{5}NE_F \ , \tag{4.223}$$

such that the ground-state energy per particle is

$$\frac{E_G}{N} = \frac{3}{5}E_F \ . \tag{4.224}$$

This last result shows that the Fermi energy is the only energy scale in the system.

Density of states

In the particular case of the Fermi gas, it is very easy to calculate the density of states, since in this case we know that the surfaces of constant energy are given by the surface of spheres with radius k. Then, we can use the same reasoning as in Sec. 3.1.3 based on Fig. 3.6, where

$$N(E)\mathrm{d}E \ = \ \frac{g}{(2\pi)^3}\frac{4\pi}{3}\left\{\left[\frac{2m}{\hbar^2}\left(E+\mathrm{d}E\right)\right]^{\frac{3}{2}} - \left(\frac{2m}{\hbar^2}E\right)^{\frac{3}{2}}\right\}$$

$$\simeq \ \frac{g}{(2\pi)^3}\frac{4\pi}{3}\left(\frac{2mE}{\hbar^2}\right)^{\frac{3}{2}}\left[\left(1+\frac{\mathrm{d}E}{E}\right)^{\frac{3}{2}} - 1\right]$$

$$\hookrightarrow N(E) \ = \ \frac{g}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}E^{\frac{1}{2}} \ . \tag{4.225}$$

This is a result that is valid for simple metals.

4.3.3   Low temperature properties of the Fermi gas

We have already seen in Sec. 4.1.6 some elementary properties of fermions at finite temperatures, where we obtained the Fermi-Dirac distribution. In the following we consider several thermodynamic quantities at low temperatures.

We focus first on the so-called thermodynamic potential, that is defined as follows:

$$\Omega\left(T,V,\mu\right) = -k_B T \ln Z_G \ , \tag{4.226}$$

where we denote with Z_G the partition function in the grand canonical ensemble, with

$$Z_G = \mathrm{Tr}\exp\left[-\beta\left(H - \mu\hat{N}\right)\right] \ . \tag{4.227}$$

The thermodynamic potential is related with entropy as follows

$$\Omega\left(T,V,\mu\right) = E - TS - \mu N \ . \tag{4.228}$$

Since the independent variables of the thermodynamic potential are T, V, and μ, the entropy can be obtained as

$$S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu} . \tag{4.229}$$

From the entropy, finally, we can obtain the specific heat. Another quantity that we may need in the calculation of the specific heat is the chemical potential. Since it is one of the independent variables in Ω, we can obtain it from the relation

$$N = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} . \tag{4.230}$$

We therefore need as a first step to calculate the thermodynamic potential. For this we just need to recall our previous calculation for the Fermi gas (4.102), and insert the corresponding quantum numbers, such that

$$\Omega = -k_B T \sum_{\boldsymbol{k},\sigma} \ln\left\{1 + \exp\left[\beta\left(\mu - \epsilon_{\boldsymbol{k}}\right)\right]\right\} . \tag{4.231}$$

A procedure that is very often usefull is to go from a summation over wavevectors over to an integral over energy with the help of the density of states. This is especially easy in the case of the Fermi gas. Let us first consider a summation over states.

$$\sum_{\boldsymbol{k},\sigma} = \frac{V}{(2\pi)^3}\, g \int \mathrm{d}^3 k = \frac{V}{(2\pi)^3}\, g\, 4\pi \int k^2\, \mathrm{d}k , \tag{4.232}$$

where for the last equality we assumed that the quantity to be summed over depends only on the dispersion, and use explicitely, that the Fermi gas has an isotropic energy dispersion. On the other hand, we have the relation (3.19), such that

$$N(E)\, \mathrm{d}E = \frac{g}{(2\pi)^3}\, 4\pi k^2\, \mathrm{d}k . \tag{4.233}$$

In this way, for some function $f\left(\epsilon_{\boldsymbol{k}}\right)$, we can go over to an integral over energies:

$$\sum_{\boldsymbol{k},\sigma} f\left(\epsilon_{\boldsymbol{k}}\right) = V \int N(E)\, f(E)\, \mathrm{d}E . \tag{4.234}$$

For the summation (4.231) we are interested in, this means

$$\begin{aligned}
\Omega &= -k_B T V \frac{g}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \int_0^\infty E^{\frac{1}{2}} \ln\left\{1 + \exp\left[\beta\left(\mu - E\right)\right]\right\}\, \mathrm{d}E \\
&= -\frac{gV}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \frac{2}{3} \int_0^\infty \mathrm{d}E\, \frac{E^{\frac{3}{2}}}{\exp\left[\beta(E - \mu)\right] + 1} .
\end{aligned} \tag{4.235}$$

Next we calculate the integral in the limit of low temperatures.

$$I = \int_0^\infty dE \frac{E^{\frac{3}{2}}}{1 + \exp\left[-\beta(\mu - E)\right]} \tag{4.236}$$

First we introduce a change of variables

$$x \equiv \frac{E - \mu}{k_B T} \tag{4.237}$$

and define

$$\alpha \equiv \frac{\mu}{k_B T} . \tag{4.238}$$

With the changes above, we have

$$I = (k_B T)^{\frac{5}{2}} I(\alpha) , \tag{4.239}$$

with

$$\begin{aligned}
I(\alpha) &\equiv \int_{-\alpha}^\infty dx \frac{(x + \alpha)^{\frac{3}{2}}}{e^x + 1} \\
&= \int_{-\alpha}^0 dx \frac{(x + \alpha)^{\frac{3}{2}}}{e^x + 1} + \int_0^\infty dx \frac{(x + \alpha)^{\frac{3}{2}}}{e^x + 1} \\
&= \int_0^\alpha dx \frac{(\alpha - x)^{\frac{3}{2}}}{e^{-x} + 1} + \int_0^\infty dx \frac{(x + \alpha)^{\frac{3}{2}}}{e^x + 1} \\
&= \int_0^\alpha dx \, (\alpha - x)^{\frac{3}{2}} \\
&\quad + \int_0^\infty dx \frac{(x + \alpha)^{\frac{3}{2}} - (\alpha - x)^{\frac{3}{2}}}{e^x + 1} + \int_\alpha^\infty dx \frac{(\alpha - x)^{\frac{3}{2}}}{e^x + 1} .
\end{aligned} \tag{4.240}$$

The three integrals can be computed in the low temperature limit, where, since $\mu \longrightarrow E_F$, with E_F finite, $\alpha \longrightarrow \infty$. In this limit we have for the last integral,

$$\int_\alpha^\infty dx \frac{(\alpha - x)^{\frac{3}{2}}}{e^x + 1} \sim e^{-\alpha} \longrightarrow 0 . \tag{4.241}$$

Furthermore, we have

$$(x + \alpha)^{\frac{3}{2}} - (\alpha - x)^{\frac{3}{2}} \stackrel{\alpha \to \infty}{\longrightarrow} 3x\alpha^{\frac{1}{2}} + \mathcal{O}\left(\alpha^{-\frac{1}{2}}\right) , \tag{4.242}$$

such that the corresponding integral gives

$$3\alpha^{\frac{1}{2}} \int_0^\infty dx \frac{x}{e^x + 1} = 3\alpha^{\frac{1}{2}} \frac{1}{2} \Gamma(2) \zeta(2) , \tag{4.243}$$

where $\Gamma(n) = (n-1)!$, for n a positive integer, is the Gamma function (i.e. $\Gamma(2) = 1$), and

$$\zeta(z) = \sum_{p=1}^\infty p^{-z} , \quad \text{Re } z > 1 , \tag{4.244}$$

is the Riemann zeta function. It turns out that (see tables) that $\zeta(2) = \pi^2/6$. For the first integral we have

$$\int_0^\alpha \mathrm{d}x\, (\alpha - x)^{\frac{3}{2}} = -\frac{2}{5}(\alpha - x)^{\frac{5}{2}}\Big|_0^\alpha = \frac{2}{5}\alpha^{\frac{5}{2}} \ . \tag{4.245}$$

Putting all the results together we have finally

$$I \;=\; (k_B T)^{\frac{5}{2}} \left[\frac{2}{5}\left(\frac{\mu}{k_B T}\right)^{\frac{5}{2}} + \frac{\pi^2}{4}\left(\frac{\mu}{k_B T}\right)^{\frac{1}{2}} + \cdots\right] \ , \tag{4.246}$$

leading to

$$\Omega \;=\; -\frac{gV}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{2}{3}\left[\frac{2}{5}\mu^{\frac{5}{2}} + \frac{\pi^2}{4}\mu^{\frac{1}{2}}(k_B T)^2 + \cdots\right] \ . \tag{4.247}$$

Once we obtained the thermodynamic potential, we can proceed to calculate different thermodynamic quantities.

Chemical potential

As already anticipated in eq. (4.230), given the number of particles N, we should in principle be able to calculate the temperature dependence of the chemical potential, at least in the limit of low temperatures. Using (4.230), we have

$$N \;=\; -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V}$$
$$=\; \frac{gV}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{2}{3}\left[\mu^{\frac{3}{2}} + \frac{\pi^2}{8}\mu^{-\frac{1}{2}}(k_B T)^2 + \cdots\right] \ . \tag{4.248}$$

From eq. (4.222), and the result above, we have

$$\frac{N}{V} \;=\; \left(E_F\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{g}{6\pi^2}$$
$$=\; \frac{g}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{2}{3}\left[\mu^{\frac{3}{2}} + \frac{\pi^2}{8}\mu^{-\frac{1}{2}}(k_B T)^2 + \cdots\right] \ , \tag{4.249}$$

leading to

$$\mu = E_F\left[1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\mu}\right)^2 + \cdots\right]^{-\frac{2}{3}} \ . \tag{4.250}$$

Up to $\mathcal{O}(T^2)$,

$$\mu = E_F\left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{E_F}\right)^2 + \cdots\right] \ . \tag{4.251}$$

Since in general $E_F \sim 1 - 10\ \mathrm{eV} \sim 10^4 - 10^5 K$, it is a good approximation for most relevant temperatures in condensed matter physics to set $\mu \simeq E_F$.

Specific heat

The specific heat is defined as

$$c_V = \left(\frac{\partial E}{\partial T}\right)_{V,N} , \tag{4.252}$$

where the internal energy $E = E(S, V, N)$. This quantity can be extracted from the thermodynamic potential, since as we have already seen in (4.228), $E = \Omega + TS + \mu N$. From this, and taking into account that $\Omega = \Omega(T, V, \mu)$, we have

$$c_V = T\left(\frac{\partial S}{\partial T}\right)_{V,N} . \tag{4.253}$$

On the other hand, knowing the thermodynamic potential, we can obtain the entropy as in (4.229)

$$
\begin{aligned}
S &= -\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu} \\
&= \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{2}{3}\left[\frac{\pi^2}{2}k_B^2 T\mu^{\frac{1}{2}} + \ldots\right]
\end{aligned}
\tag{4.254}
$$

From (4.248), we have in lowest order,

$$N = \frac{gV}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{2}{3}\mu^{\frac{3}{2}} \tag{4.255}$$

such that we can now express S as a function of T, V, and N, as we need it in order to calculate the specific heat according to (4.253):

$$
\begin{aligned}
S(T, V, N) &\simeq Nk_B\frac{\pi^2}{2}\frac{k_B T}{E_F} , \\
\hookrightarrow c_V &= Nk_B\frac{\pi^2}{2}\frac{k_B T}{E_F} .
\end{aligned}
\tag{4.256}
$$

We can express also the specific heat in another way by recalling the form of the density of states (4.225) and noticing that

$$N(E_F) = \frac{g}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} E_F^{\frac{1}{2}} , \tag{4.257}$$

such that

$$c_V = V\frac{\pi^2 k_B}{3}N(E_F)k_B T . \tag{4.258}$$

Both forms of the specific heat show that the specific heat of a Fermi gas increases linearly with temperature for $k_B T \ll E_F$. This is in clear contrast to the behavior

of a classical system of free particles, where the equipartition theorem states that each degree of freedom carries an energy $k_B T/2$, and hence, predicts a total internal energy

$$E^{(classical)} = \frac{1}{2} N k_B T \ , \tag{4.259}$$

such that

$$c_V^{(classical)} \ = \ \left(\frac{\partial E}{\partial T} \right)_V = \text{cte} \ . \tag{4.260}$$

The difference between the classical and the quantum mechanical prediction is a direct consequence of Pauli's exclussion principle. The fraction of the total number of degrees of freedom that can contribute to the specific heat for a given temperature is of the order of $k_B T$, such that

$$\Delta E(T) = N \frac{k_B T}{E_F} \, k_B T \ , \tag{4.261}$$

leading to the linear temperature dependence of the specific heat. Equation (4.258) also shows that the specific heat is a measure of the density of states at the Fermi energy. Certainly this is so in a metal, but for an insulator where at low temperatures the Fermi energy is generally in the band gap, this linear contribution vanishes, since the density of states should also vanish at the Fermi energy.

4.4   Green's functions for many-body systems.

The solution of the Schrödinger equation for an interacting system should be the next step, after having discussed non-interacting electrons. In this section we consider formal solutions of the Schrödinger equation in the form of a Green's function, one of the central objects in quantum field theory. Although no direct calculations will be performed before discussing perturbation theory in the next section, a great deal of physical information can be extracted from the Green's function on general grounds.

4.4.1   Evolution operator in different pictures

A central role in the development of quantum field theory is played by the evolution operator, that, as we shall see, can be formulated in different ways. Here one speaks of the Schrödinger picture, where states are in general time dependent but the Hamiltonian and in general operators are not. There is also the Heisenberg picture, where the states is time independent but the operators are time dependent, and finally, the interaction picture, where the time evolution of the operators and states is determined by the part of the Hamiltonian around which the perturbation theory is developed, in general, the non-interacting system.

Schrödinger picture

This is the usual formulation used in elementary quantum mechanics, where the states are in general time dependent but operators are not. The operators are obtained applying the usual rules of quantization, i.e. elevating to operators with appropriate commutation rules the dynamical variables of a classical system. Of course, in the following discussion we assume that they are expressed in second quantization as discussed in Sec. 4.2. Then, the Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t} \mid \Psi_S(t) >= H \mid \Psi_S(t) > . \tag{4.262}$$

The solution of this equation in the case of a time independent Hamiltonian can be written formally, given the initial state at time t_0, as

$$\mid \Psi_S(t) >= \exp\left[-\frac{i}{\hbar} H (t - t_0)\right] \mid \Psi_S(t_0) > . \tag{4.263}$$

Therefore, the evolution operator is in this case

$$U_S(t, t_0) = \exp\left[-\frac{i}{\hbar} H (t - t_0)\right] . \tag{4.264}$$

Since the evolution operator is unitary, it preserves the norm of the wavefunction.

Interaction picture

Let us assume that the Hamiltonian is given by a part H_0 that can be solved exactly and an interaction term H_I.

$$H = H_0 + H_I . \tag{4.265}$$

Let us define a state vector from the one in the Schrödinger picture as follows

$$\mid \Psi_I(t) >= \exp\left[\frac{i}{\hbar} H_0 t\right] \mid \Psi_S(t) > , \tag{4.266}$$

and consider its time evolution

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} \mid \Psi_I(t) > \ = \ & -H_0 \exp\left[\frac{i}{\hbar} H_0 t\right] \mid \Psi_S(t) > \\
& + \exp\left[\frac{i}{\hbar} H_0 t\right] i\hbar \frac{\partial}{\partial t} \mid \Psi_S(t) > \\
= \ & \left\{ - H_0 \right. \\
& \left. + \exp\left[\frac{i}{\hbar} H_0 t\right] H \exp\left[-\frac{i}{\hbar} H_0 t\right] \right\} \mid \Psi_I(t) > \\
= \ & H_I(t) \mid \Psi_I(t) > ,
\end{aligned}
\tag{4.267}
$$

where we defined

$$H_I(t) \equiv \exp\left[\frac{i}{\hbar}H_0\,t\right] H_I \exp\left[-\frac{i}{\hbar}H_0\,t\right] . \tag{4.268}$$

Since in general H_0 and H_I do not commute, we have to respect the order in which they appear. The definition we introduced for $H_I(t)$ can be extended to other operators. To see this, we consider an arbitrary matrix element of some operator

$$
\begin{aligned}
< \Psi_S(t) \mid \hat{\mathcal{O}}_S \mid \Psi_S(t) > &= < \Psi_I(t) \mid \underbrace{e^{iH_0\,t/\hbar}\hat{\mathcal{O}}_S\,e^{-iH_0\,t/\hbar}}_{\equiv \hat{\mathcal{O}}_I(t)} \mid \Psi_I(t) > \\
&= < \Psi_I(t) \mid \hat{\mathcal{O}}_I(t) \mid \Psi_I(t) > .
\end{aligned}
\tag{4.269}
$$

We see then, that in the interaction picture both states and operators depend on time. The time evolution of the operators can be easily obtained,

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{\mathcal{O}}_I(t) &= e^{iH_0\,t/\hbar}\left(\hat{\mathcal{O}}_S H_0 - H_0\hat{\mathcal{O}}_S\right) e^{-iH_0\,t/\hbar} \\
&= \left[\hat{\mathcal{O}}_I(t), H_0\right] ,
\end{aligned}
\tag{4.270}
$$

that is, it is simply determined by the non-interacting part.

Next we consider an evolution operator for the state in the interaction picture. It should be unitary and able to give the state at time t, knowing the state at time t_0:

$$\mid \Psi_I(t) >= U(t, t_0) \mid \Psi_I(t_0) > . \tag{4.271}$$

Apart from the condition of being unitary, U should also fulfill

$$U(t_0, t_0) = 1 . \tag{4.272}$$

From (4.267) and (4.271), we have

$$i\hbar\frac{\partial}{\partial t}U(t, t_0) = H_I(t)\,U(t, t_0) . \tag{4.273}$$

Integrating this equation from time t_0 to time t, we have

$$U(t, t_0) - U(t_0, t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\,H_I(t')\,U(t', t_0) , \tag{4.274}$$

or, given the initial condition,

$$U(t, t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,H_I(t')\,U(t', t_0) . \tag{4.275}$$

This is an integral equation, and an iterative solution can be at least formally proposed.

$$
\begin{aligned}
U(t, t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,H_I(t') \\
&\quad + \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,H_I(t')\,H_I(t'') + \cdots
\end{aligned}
\tag{4.276}
$$

Since, as we remarked earlier, in general H_0 and H_I do not commute, the time ordering of the operators should be respected. We can, nevertheless, try to bring the expressions above to a more symmetric appearance. For this, let us consider the term with two integrals above.

$$
\begin{aligned}
\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \, H_I(t') \, H_I(t'') &= \int_{t_0}^t dt'' \int_{t''}^t dt' \, H_I(t') \, H_I(t'') \\
&= \int_{t_0}^t dt' \int_{t'}^t dt'' \, H_I(t'') \, H_I(t') \,, \qquad (4.277)
\end{aligned}
$$

where the first equality is due to the fact that the integration regions are equal as shown in Fig. 4.2. The last equality is obtained by a simple change of variables.
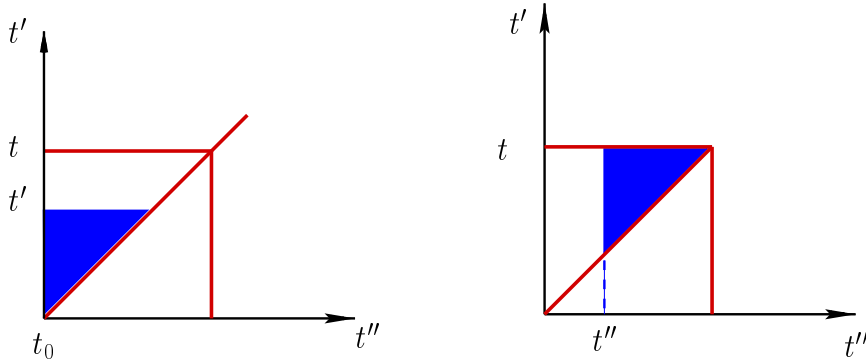

Figure 4.2: Regions of integration for the first two integrals in eq. (4.277).

Using (4.277), we can write for the contribution in second order for the evolution operator

$$
\begin{aligned}
\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \, H_I(t') \, H_I(t'') &= \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^t dt'' \Big[H_I(t') \, H_I(t'') \, \theta(t' - t'') \\
&\qquad\qquad + H_I(t'') \, H_I(t') \, \theta(t'' - t') \Big] \\
&= \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^t dt'' \, T\left[H_I(t') \, H_I(t'') \right] \,, \qquad (4.278)
\end{aligned}
$$

where we introduced a time ordered product of operators, denoted by T standing in front of the operators affected by it, with the operator at later time to the left of the operator at earlier time. This can be generalized to all orders, by properly taking into account the number of possible time orderings at each order, which is given by the permutations of n time variables at order n, i.e. we have to devide by $n!$.

$$
\begin{aligned}
U(t, t_0) &= \sum_{n=0}^\infty \frac{1}{n!} \left(-\frac{i}{\hbar} \right)^n \int_{t_0}^t dt_1 \cdots \int_{t_0}^t dt_n \, T\left[H_I(t_1) \cdots H_I(t_n) \right] \\
&= T \exp\left[-\frac{i}{\hbar} \int_{t_0}^t dt' \, H_I(t') \right] \,. \qquad (4.279)
\end{aligned}
$$

Heisenberg picture

In this case we define a state vector as follows

$$| \Psi_H(t) > \equiv \exp\left[\frac{i}{\hbar}H\,t\right] | \Psi_S(t) > , \tag{4.280}$$

Using the Schrödinger equation for $| \Psi_S(t) >$, one can immediately see that

$$i\hbar\frac{\partial}{\partial t} | \Psi_H(t) > = 0 , \tag{4.281}$$

i.e. the state in the Heisenberg picture is time independent. As in the interaction picture, by considering an arbitrary matrix element, we can obtain the operators in the Heisenberg picture.

$$< \Psi_S(t) | \hat{\mathcal{O}}_S | \Psi_S(t) > = < \Psi_H(t) | \mathrm{e}^{iH\,t/\hbar}\hat{\mathcal{O}}_S\,\mathrm{e}^{-iH\,t/\hbar} | \Psi_H(t) > , \tag{4.282}$$

such that operators in the Heisenberg picture are related to operators in the Schrödinger picture as follows

$$\hat{\mathcal{O}}_H(t) = \mathrm{e}^{iH\,t/\hbar}\hat{\mathcal{O}}_S\,\mathrm{e}^{-iH\,t/\hbar} . \tag{4.283}$$

Therefore, in the Heisenberg picture, the state is time independent, whereas the whole time dependence is contained in the operators, as opposed to the Schrödinger picture. The evolution of the system is given by

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{\mathcal{O}}_H(t) &= \mathrm{e}^{iH\,t/\hbar}\left(\hat{\mathcal{O}}_S H - H\hat{\mathcal{O}}_S\right)\mathrm{e}^{-iH\,t/\hbar} \\ &= \left[\hat{\mathcal{O}}_H(t), H\right] . \end{aligned} \tag{4.284}$$

This equation tells us immediately, which operators correspond to a constant of motion.

From the definitions of the state vectors in all three pictures, it is readily seen that

$$| \Psi_H >=| \Psi_S(t=0) >=| \Psi_I(t=0) > . \tag{4.285}$$

Since the eigenstates of the Hamiltonian correspond to stationary solutions of the Schrödinger equation, the relation above shows that the states in the Heisenberg representation are the exact eigenstates of the system.

4.4.2   The one-particle Green's function

Let us first define the Green's function and then proceed to discuss the motivation to introduce it. We will consider in these lectures only the $T = 0$ case, since it is somewhat simpler than the general case of finite temperatures and will serve as a

first step to get an insight in theoretical techniques for a many-body system. The one-particle Green's function is defined as

$$iG_{\alpha\beta}\left(\boldsymbol{x}, t; \boldsymbol{x}', t'\right) \equiv \frac{< \Psi_0 \mid T \left[\hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right) \hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}', t'\right)\right] \mid \Psi_0 >}{< \Psi_0 \mid \Psi_0 >} , \quad (4.286)$$

where $\mid \Psi_0 >$ is the ground-state of the interacting system, and $\hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right)$ is a field operator in the Heisenberg picture

$$\hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right) = \mathrm{e}^{iHt/\hbar} \hat{\psi}_{S\alpha}\left(\boldsymbol{x}\right) \mathrm{e}^{-iHt/\hbar} , \quad (4.287)$$

with α a set of quantum numbers characterizing the particle, like spin in the case of electrons. In the following we are going to concentrate on electrons for definitness, such that α can only take the values $\pm 1/2$ corresponding to the possible spin projections. Furthermore, the field operators are anticommuting ones.

The name 'one-particle' comes from the fact that the object defined in (4.286) can be seen as giving the evolution in the exact ground-state of a particle with spin β that is created at $\boldsymbol{x}'$ at time t' and annihilated at $\boldsymbol{x}$ at time t with spin α. Therefore, it is also called the one-particle propagator. The time ordered product is as follows

$$T \left[\hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right) \hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}', t'\right)\right] = \begin{cases} \hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right) \hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}', t'\right) & t > t' \\ -\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}', t'\right) \hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right) & t' > t \end{cases} \quad (4.288)$$

The minus sign corresponds to the fact that the field operators anticommute, such that a permutation in their order has to carry the corresponding phase factor.

Equation of motion for the Green's function

Since we are interested in the behavior of interacting electrons in condensed matter physics, let us concentrate on a specific Hamiltonian, namely the one corresponding to a two-particle interaction as given in (4.201). Taking into account spins, it becomes

$$\begin{aligned} H = &\int \mathrm{d}\boldsymbol{x}\, \hat{\psi}_{\alpha}^{\dagger}\left(\boldsymbol{x}\right) \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U\left(\boldsymbol{x}\right)\right] \hat{\psi}_{\alpha}\left(\boldsymbol{x}\right) \\ &+\frac{1}{2} \int \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{x}'\, \hat{\psi}_{\alpha}^{\dagger}\left(\boldsymbol{x}\right) \hat{\psi}_{\beta}^{\dagger}\left(\boldsymbol{x}'\right) V\left(\mid \boldsymbol{x} - \boldsymbol{x}' \mid\right) \hat{\psi}_{\beta}\left(\boldsymbol{x}'\right) \hat{\psi}_{\alpha}\left(\boldsymbol{x}\right) , \quad (4.289) \end{aligned}$$

where again we use the convention that a summation takes place for repeated indices, and included a potential acting on the electrons as in the case of electrons in a lattice. The field operators in (4.286) obey an equation of motion as in (4.284):

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right) = \left[\hat{\psi}_{H\alpha}\left(\boldsymbol{x}, t\right), H\right] , \quad (4.290)$$

and similarly for the creation operator. With this, we can obtain an equation of motion for the Green's function.

$$i\hbar\frac{\partial}{\partial t}G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = (-i)\,i\hbar\frac{\partial}{\partial t}\Bigg[\theta\left(t-t'\right)<\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)>$$

$$-\theta\left(t'-t\right)<\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)>\Bigg]\,, \qquad (4.291)$$

where we introduced the notation

$$<\hat{\mathcal{O}}> = \frac{<\Psi_0\mid\hat{\mathcal{O}}\mid\Psi_0>}{<\Psi_0\mid\Psi_0>}\,. \qquad (4.292)$$

On performing the time derivative, we have

$$(4.291) = \hbar\Bigg[\delta\left(t-t'\right)<\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)+\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)>$$

$$+\theta\left(t-t'\right)<\frac{\partial}{\partial t}\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)>$$

$$-\theta\left(t'-t\right)<\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)\frac{\partial}{\partial t}\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)>\Bigg]\,. \qquad (4.293)$$

Since at equal times

$$\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t\right)+\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t\right)\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)$$

$$= \mathrm{e}^{iHt/\hbar}\left\{\hat{\psi}_{S\alpha}\left(\boldsymbol{x}\right),\hat{\psi}_{S\beta}^{\dagger}\left(\boldsymbol{x}'\right)\right\}\mathrm{e}^{-iHt/\hbar} = \delta\left(\boldsymbol{x}-\boldsymbol{x}'\right)\delta_{\alpha\beta}\,, \quad (4.294)$$

and using (4.290) in (4.293), we have for the Green's function

$$i\frac{\partial}{\partial t}G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = \delta\left(\boldsymbol{x}-\boldsymbol{x}'\right)\delta\left(t-t'\right)\delta_{\alpha\beta}$$

$$+<T\left\{-\frac{i}{\hbar}\left[\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right),H\right]\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)\right\}>\,. (4.295)$$

The commutator can be easily transformed in a commutator for field operators in the Schrödinger picture:

$$\left[\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right),H\right] = \mathrm{e}^{iHt/\hbar}\left[\hat{\psi}_{S\alpha}\left(\boldsymbol{x}\right),H\right]\mathrm{e}^{-iHt/\hbar}\,. \qquad (4.296)$$

For the last commutator, we have

$$\left[\hat{\psi}_{\alpha}\left(\boldsymbol{x}\right),H\right] = \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+U\left(\boldsymbol{x}\right)\right]\hat{\psi}_{\alpha}\left(\boldsymbol{x}\right)$$

$$+\int\mathrm{d}\boldsymbol{x}'\,\hat{\psi}_{\beta}^{\dagger}\left(\boldsymbol{x}'\right)V\left(\mid\boldsymbol{x}-\boldsymbol{x}'\mid\right)\hat{\psi}_{\beta}\left(\boldsymbol{x}'\right)\hat{\psi}_{\alpha}\left(\boldsymbol{x}\right)\,, \quad (4.297)$$

and going back to the Heisenberg picture, we have

$$
\left[\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right),H\right] = \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U\left(\boldsymbol{x}\right)\right]\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)
$$
$$
+ \int \mathrm{d}\boldsymbol{x}'\,\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t\right)V\left(\mid\boldsymbol{x}-\boldsymbol{x}'\mid\right)
$$
$$
\times\hat{\psi}_{H\beta}\left(\boldsymbol{x}',t\right)\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\ . \quad (4.298)
$$

For the last term, we can make a simple change that will be usefull later, namely we introduce

$$
V\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) \equiv V\left(\mid\boldsymbol{x}-\boldsymbol{x}'\mid\right)\delta\left(t-t'\right)\ , \quad (4.299)
$$

such that finally, inserting the results obtained above into (4.295), the equation of motion for the Green's function is as follows

$$
\mathbf{1} = \left\{i\frac{\partial}{\partial t} - \frac{1}{\hbar}\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U\left(\boldsymbol{x}\right)\right]\right\}G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right)
$$
$$
+\frac{i}{\hbar}\int\mathrm{d}\boldsymbol{x}''\,\mathrm{d}t''\,V\left(\boldsymbol{x},t;\boldsymbol{x}'',t''\right)
$$
$$
\times < T\left[\hat{\psi}_{H\gamma}^{\dagger}\left(\boldsymbol{x}'',t''\right)\hat{\psi}_{H\gamma}\left(\boldsymbol{x}'',t''\right)\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)\right] >, (4.300)
$$

where we introduced the notation

$$
\mathbf{1} = \delta\left(\boldsymbol{x}-\boldsymbol{x}'\right)\delta\left(t-t'\right)\delta_{\alpha\beta}\ . \quad (4.301)
$$

This is an integro-differential equation for the Green's function, that in general has no explicit solution. In the non-interacting case, the equation above reduces to

$$
\left\{i\frac{\partial}{\partial t} - \frac{1}{\hbar}\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U\left(\boldsymbol{x}\right)\right]\right\}G_{\alpha\beta}^{(0)}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = \mathbf{1}\ , \quad (4.302)
$$

i.e. $G_{\alpha\beta}^{(0)}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right)$ is the resolvent of a differential equation, and hence, the name Green's function, as in e.g. electrodynamics. Formally, the solution is

$$
G_{\alpha\beta}^{(0)}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = \left\{i\frac{\partial}{\partial t} - \frac{1}{\hbar}\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U\left(\boldsymbol{x}\right)\right]\right\}^{-1}\ , \quad (4.303)
$$

where we can view the linear differential equation above as a matrix equation with an infinite number of continuous and discrete indices. Given the potential $U\left(\boldsymbol{x}\right)$, it is in many cases (as in the case of a periodic potential), possible to obtain an explicit solution for the propagator.

We can in the same spirit express the whole eq. (4.300) in such a way that a formal solution can be obtained as in the non-interacting case. For that purpose, a new quantity is introduced.

$$
\frac{i}{\hbar}\int\mathrm{d}\boldsymbol{x}''\,\mathrm{d}t''\,V\left(\boldsymbol{x},t;\boldsymbol{x}'',t''\right)
$$
$$
\times < T\left[\hat{\psi}_{H\gamma}^{\dagger}\left(\boldsymbol{x}'',t''\right)\hat{\psi}_{H\gamma}\left(\boldsymbol{x}'',t''\right)\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\hat{\psi}_{H\beta}^{\dagger}\left(\boldsymbol{x}',t'\right)\right] >
$$
$$
\equiv -\int\mathrm{d}\boldsymbol{x}''\,\mathrm{d}t''\,\Sigma_{\alpha\gamma}^{*}\left(\boldsymbol{x},t;\boldsymbol{x}'',t''\right)G_{\gamma\beta}\left(\boldsymbol{x}'',t'';\boldsymbol{x}',t'\right)\ . \quad (4.304)
$$

Going back to (4.300), we can write

$$\left[G^{(0)\,-1} - \Sigma^*\right] G \;=\; \mathbf{1}\,, \tag{4.305}$$

where we use the matrix notation mentioned above. Again a formal solution is

$$G \;=\; \left[G^{(0)\,-1} - \Sigma^*\right]^{-1}\,, \tag{4.306}$$

or

$$G \;=\; G^{(0)} + G^{(0)}\,\Sigma^*\,G\,. \tag{4.307}$$

The last equation is an integral equation for the one-particle Green's function, that is called Dyson equation. The kernel of the integral equation is the so-called one-particle irreducible part of the self-energy. We will discuss the Dyson equation when we arrive at the development of a perturbation theory and diagrams. The physical meaning of the self-energy should become clear in the next section.

4.4.3   Physical interpretation of the one-particle Green's function and the self-energy

Without still considering the full structure of the formalism that gives the frame for the Green's function theory, we discuss a number of features on a general level that allow us to understand the physical meaning of the different quantities introduced before and make connection to their experimental relevance.

The Lehmann representation

We consider again the exact Green's function given by eq. (4.286). We assume in the following that the ground-state is normalized such that $< \Psi_0 \mid \Psi_0 >= 1$ and, hence,

$$iG_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) \;=\; < \Psi_0 \mid T\left[\hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right)\,\hat{\psi}^\dagger_{H\beta}\left(\boldsymbol{x}',t'\right)\right] \mid \Psi_0 > \,. \tag{4.308}$$

We assume further, that we have the complete set of eigenstates $\{\mid \Psi_n >\}$ of the Hamiltonian and insert them between the creation and annihilation operators.

$$
\begin{aligned}
iG_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) \;=\; \sum_n \Big[& \theta\left(t-t'\right) < \Psi_0 \mid \hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right) \mid \Psi_n > \\
& \times < \Psi_n \mid \hat{\psi}^\dagger_{H\beta}\left(\boldsymbol{x}',t'\right) \mid \Psi_0 > \\
& -\theta\left(t'-t\right) < \Psi_0 \mid \hat{\psi}^\dagger_{H\beta}\left(\boldsymbol{x}',t'\right) \mid \Psi_n > \\
& \times < \Psi_n \mid \hat{\psi}_{H\alpha}\left(\boldsymbol{x},t\right) \mid \Psi_0 > \Big]. \tag{4.309}
\end{aligned}
$$

Since the creation and annihilation operators are in the Heisenberg picture, as given by (4.283), and the set of states considered here are eigenstates of H, we have

$$
\begin{aligned}
iG_{\alpha\beta}\left(\boldsymbol{x}, t; \boldsymbol{x}', t'\right) = & \sum_{n} \left[\theta\left(t-t'\right) \exp\left[-\frac{i}{\hbar}\left(E_n - E_0\right)\left(t-t'\right)\right] \right. \\
& \times <\Psi_0 \mid \hat{\psi}_\alpha\left(\boldsymbol{x}\right) \mid \Psi_n ><\Psi_n \mid \hat{\psi}_\beta^\dagger\left(\boldsymbol{x}'\right) \mid \Psi_0> \\
& -\theta\left(t'-t\right) \exp\left[\frac{i}{\hbar}\left(E_n - E_0\right)\left(t-t'\right)\right] \\
& \times <\Psi_0 \mid \hat{\psi}_\beta^\dagger\left(\boldsymbol{x}'\right) \mid \Psi_n ><\Psi_n \mid \hat{\psi}_\alpha\left(\boldsymbol{x}\right) \mid \Psi_0>, (4.310)
\end{aligned}
$$

where E_n is the eigenvalue of H for $\mid \Psi_n >$, and E_0 is the ground-state energy. Since we assumed a time independent Hamiltonian, G depends only on the difference $t-t'$.

Next we consider the θ functions that appear as a consequence of time ordering. It will be usefull for the discussion right after, to give an integral representation of this function that looks as follows

$$
\theta\left(t-t'\right) = \lim_{\eta\to 0^+} -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{e^{-i\omega(t-t')}}{\omega + i\eta} \ . \tag{4.311}
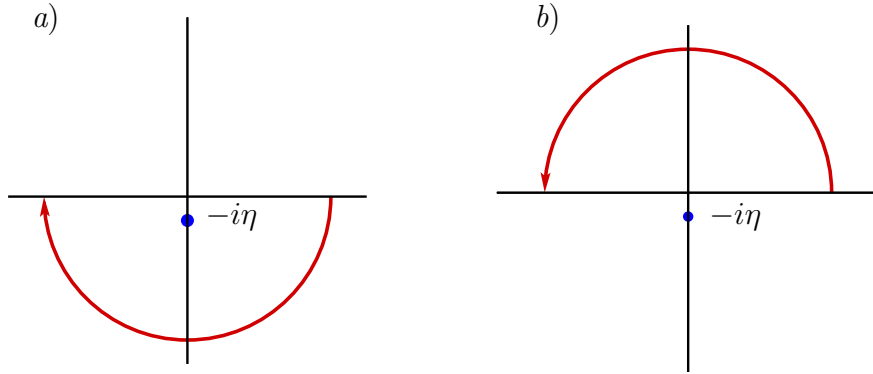$$

Figure 4.3: *a*) Contour integral for $t > t'$.*b*) Contour integral for $t < t'$.

As shown by Fig. 4.3, after an analytic continuation in the complex ω-plane and applying the theorem of residues, the desired result is obtained. After having introduced the integral representation of the θ function, we can perform a Fourier transformation of the Green's function. Let us consider explicitly the first term in (4.310), where we use the notation $\tau \equiv t - t'$.

$$
\begin{aligned}
\int d\tau\, e^{i\omega\tau} G_{\alpha\beta}\left(\boldsymbol{x}, \boldsymbol{x}'; \tau\right) \ \to\ & (-i) \int d\tau\, e^{i\omega\tau}\, \theta(\tau)\, e^{-i(E_n - E_0)\tau/\hbar} \\
= & -(-i) \int \frac{d\omega'}{2\pi i} \frac{1}{\omega' + i\eta} \\
& \times \int d\tau\, e^{i\omega\tau}\, e^{-i\omega'\tau}\, e^{-i(E_n - E_0)\tau/\hbar} \\
= & \frac{1}{\omega - \frac{1}{\hbar}\left(E_n - E_0\right) + i\eta} \ . \tag{4.312}
\end{aligned}
$$

Let us give a close look to the energy difference that appeared in the denominator above. This energy denominator belong to a term with matrix elements

$$(E_n - E_0) \quad \leftrightarrow \quad < \Psi_0 \mid \hat{\psi}_\alpha(\boldsymbol{x}) \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}') \mid \Psi_0 > \ . \qquad (4.313)$$

Since $\mid \Psi_0 >$ is the ground-state for N particles, the state $\mid \Psi_n >$ should correspond to an excited state with $N + 1$ particles. This means that E_n corresponds to the energy of an excited state of the system with $N + 1$ particles, and we denote it explicitely as $E_n \to E_n(N + 1)$. Then, the energy denominator in (4.312) can be written as follows.

$$\begin{aligned} E_n - E_0 &= E_n(N+1) - E_0(N) \\ &= E_n(N+1) - E_0(N+1) + E_0(N+1) - E_0(N) \\ &= \epsilon_n(N+1) + \mu \ , \end{aligned} \qquad (4.314)$$

where

$$\epsilon_n(N+1) = E_n(N+1) - E_0(N+1) \qquad (4.315)$$

is the excitation energy of the system with $N + 1$ particles, and

$$\mu = E_0(N+1) - E_0(N) \ , \qquad (4.316)$$

is the chemical potential, and since we are working at $T = 0$, it is the Fermi energy. A similar calculation leads to the corresponding results for the second term in (4.310). The final result is

$$\begin{aligned} G_{\alpha\beta}(\boldsymbol{x}, \boldsymbol{x}'; \omega) &= \hbar \sum_n \left[\frac{< \Psi_0 \mid \hat{\psi}_\alpha(\boldsymbol{x}) \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}') \mid \Psi_0 >}{\hbar\omega - \mu - \epsilon_n(N+1) + i\eta} \right. \\ &\quad \left. + \frac{< \Psi_0 \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}') \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\alpha(\boldsymbol{x}) \mid \Psi_0 >}{\hbar\omega - \mu + \epsilon_n(N-1) - i\eta} \right] . (4.317) \end{aligned}$$

The expression above shows, that the poles of the one-particle Green's function give the exact one-particle excitations of the interacting system. The first term correspond to the excitations of a particle added to the system, and hence, are particle excitations, that have energies above the chemical potential since $\epsilon_n > 0$. The second term corresponds to one particle less in the system, and hence they are hole excitations, with energies below the chemical potential. Figure 4.4 shows location of the singularities of the Green's function in the Lehmann representation.

We can easily calculate the Green's function in the case of the Fermi gas, since there, all the excited states are known, and we can express the field operators in terms of creation and annihilation operators in momentum space.

$$\hat{\psi}_\alpha(\boldsymbol{x}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} f_{\boldsymbol{k}\alpha} \exp\left(i\boldsymbol{k} \cdot \boldsymbol{x}\right) \qquad (4.318)$$

$$\hat{\psi}_\beta^\dagger(\boldsymbol{x}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} f_{\boldsymbol{k}\beta}^\dagger \exp\left(-i\boldsymbol{k} \cdot \boldsymbol{x}\right) \qquad (4.319)$$
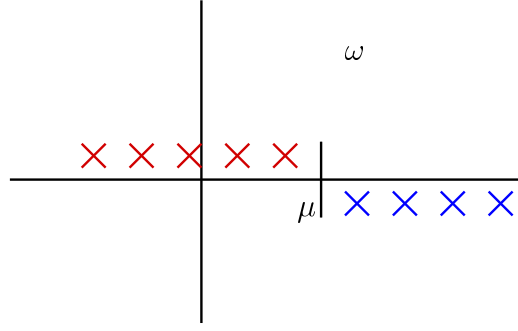
Figure 4.4: Schematic location of the poles of $G(\omega)$ in the complex ω plane. The red crosses correspond to hole excitations below the chemical potential, whereas the blue crosses correspond to particle excitations.

Then, for the matrix elements in (4.317), we have

$$< \Psi_0 \mid \hat{\psi}_\alpha(\boldsymbol{x}) \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}') \mid \Psi_0 >$$
$$= \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} \exp(i\boldsymbol{k} \cdot \boldsymbol{x}) \exp(-i\boldsymbol{k}' \cdot \boldsymbol{x}')$$
$$\times < \Psi_0 \mid f_{\boldsymbol{k}\alpha} \mid \Psi_n >< \Psi_n \mid f_{\boldsymbol{k}'\beta}^\dagger \mid \Psi_0 > , \quad (4.320)$$

and with eigenstates $\mid \Psi_n >= \mid \boldsymbol{k}\alpha >$,

$$(4.320) = \frac{1}{V} \sum_{\boldsymbol{k}} \exp[i\boldsymbol{k} \cdot (\boldsymbol{x} - \boldsymbol{x}')]$$
$$\times < \Psi_0 \mid f_{\boldsymbol{k}\alpha} \mid \boldsymbol{k} >< \boldsymbol{k} \mid f_{\boldsymbol{k}\alpha}^\dagger \mid \Psi_0 > \delta_{\alpha\beta} . \quad (4.321)$$

Inserting this expression into (4.317) would lead to a propagator that depends only on the difference $\boldsymbol{x} - \boldsymbol{x}'$, as it should, since the Fermi gas corresponds to a homogeneous system. This means that we can Fourier transform the corresponding expression, obtaining the following result.

$$G_{\alpha\beta}(\boldsymbol{k},\omega) = \delta_{\alpha\beta}\,\hbar \left[\frac{|< \Psi_0 \mid f_{\boldsymbol{k}\alpha} \mid \boldsymbol{k} >|^2}{\hbar\omega - \epsilon_{\boldsymbol{k}} + i\eta} + \frac{|< \Psi_0 \mid f_{\boldsymbol{k}\alpha}^\dagger \mid \boldsymbol{k} >|^2}{\hbar\omega - \epsilon_{\boldsymbol{k}} - i\eta} \right]. \quad (4.322)$$

Here we see explicitly that the poles of the one-particle Green's function correspond to the one-particle excitation energies for particles and holes, where the energies of particle states are above the chemical potential whereas the states for holes have energies below the chemical potential, since $\epsilon_{\boldsymbol{k}} > 0$, as anticipated in the general discussion above. Notice that after inserting the actual values for $\epsilon_n(N \pm 1)$, the chemical potetial is cancelled, since $\epsilon_n(N \pm 1) = E_n(N \pm 1) - E_0(N \pm 1)$ gives the difference in energy for a particle (hole) created above (below) the Fermi energy, with respect to the Fermi energy.

We can also obtain the matrix elements, since, as we have already seen, the ground state of the Fermi gas corresponds to all states occupied up to E_F, i.e. up to $\mid \boldsymbol{k} \mid = k_F$. Therefore, in this specially simple case,

$$
\begin{aligned}
\mid < \Psi_0 \mid f_{\boldsymbol{k}\alpha} \mid \boldsymbol{k} > \mid^2 &= \theta\left(k - k_F\right) , \\
\mid < \Psi_0 \mid f_{\boldsymbol{k}\alpha}^\dagger \mid \boldsymbol{k} > \mid^2 &= \theta\left(k_F - k\right) .
\end{aligned}
\tag{4.323}
$$

Once we have seen how the propagator of free electrons looks like, let us, before we go into the discussion of further many-body formalism, consider the case of a solid, i.e. electrons in the presence of a periodic potential, as we have at least partly discussed in Chapter 3. As we have shown in Sec. 4.2.3, field operators are related to a one-particle basis with appropriate quantum numbers. As we have seen in Chapter 3, the quantum numbers for a one-particle basis in a periodic potential are wavevectors in the first Brillouin zone, as a consequence of Bloch's theorem, and eventually an index for the bands. Furthermore, without external fields, the Hamiltonian of a solid in the very general form given in (4.289) conserves spin, and, hence, the states can be also labeled by the spin projection. Therefore, quite generally, we have very similarly as for the Fermi gas,

$$
\begin{aligned}
\hat{\psi}_\alpha\left(\boldsymbol{x}\right) &= \sum_{n,\boldsymbol{k}} f_{n\boldsymbol{k}\alpha}\, u_{n\boldsymbol{k}} \exp\left(i\boldsymbol{k}\cdot\boldsymbol{x}\right) , \\
\hat{\psi}_\beta^\dagger\left(\boldsymbol{x}\right) &= \sum_{n,\boldsymbol{k}} f_{n\boldsymbol{k}\beta}^\dagger\, u_{n\boldsymbol{k}}^* \exp\left(-i\boldsymbol{k}\cdot\boldsymbol{x}\right) ,
\end{aligned}
\tag{4.324}
$$

with the difference, that the summation over $\boldsymbol{k}$ is now restricted to the first Brillouin zone.

As in the case of the Fermi gas, we focus now on the matrix elements in (4.317),

$$
\begin{aligned}
< \Psi_0 &\mid \hat{\psi}_\alpha\left(\boldsymbol{x}\right) \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\beta^\dagger\left(\boldsymbol{x}'\right) \mid \Psi_0 > \\
&= \sum_{\substack{n,n' \\ \boldsymbol{k},\boldsymbol{k}'}} u_{n\boldsymbol{k}}\left(\boldsymbol{x}\right) u_{n'\boldsymbol{k}'}^*\left(\boldsymbol{x}'\right) \exp\left(i\boldsymbol{k}\cdot\boldsymbol{x}\right) \exp\left(-i\boldsymbol{k}'\cdot\boldsymbol{x}'\right) \\
&\qquad\qquad \times < \Psi_0 \mid f_{n\boldsymbol{k}\alpha} \mid \Psi_n >< \Psi_n \mid f_{n'\boldsymbol{k}'\beta}^\dagger \mid \Psi_0 > ,
\end{aligned}
\tag{4.325}
$$

From the matrix element $< \Psi_0 \mid f_{n\boldsymbol{k}\alpha} \mid \Psi_n >$, we see that $\mid \Psi_n >$ should be a state that differs from the ground-state by one particle in the one-particle state with quantum numbers n, $\boldsymbol{k}$, α. We name it accordingly

$$
\mid \Psi_n > \rightarrow \mid n\boldsymbol{k}\alpha > ,
\tag{4.326}
$$

and consequently, $\beta = \alpha$, $\boldsymbol{k}' = \boldsymbol{k}$, $n' = n$, and

$$
\epsilon_n(N+1) \rightarrow \epsilon_{n\boldsymbol{k}} .
\tag{4.327}
$$

Inserting those modifications in the matrix elements (4.325), and the matrix elements together with the one-particle excitations in (4.317), we have finally for the

Green's function of a periodic system,

$$
\begin{aligned}
G_{\alpha\beta}\left(\boldsymbol{x},\boldsymbol{x}';\omega\right) &= \hbar\delta_{\alpha\beta}\sum_{n\boldsymbol{k}}u_{n\boldsymbol{k}}\left(\boldsymbol{x}\right)u_{n'\boldsymbol{k}'}^{*}\left(\boldsymbol{x}'\right)\exp\left[i\boldsymbol{k}\cdot\left(\boldsymbol{x}-\boldsymbol{x}'\right)\right] \\
&\times\left[\frac{<\Psi_{0}\mid f_{n\boldsymbol{k}\alpha}\mid n\boldsymbol{k}\alpha><n\boldsymbol{k}\alpha\mid f_{n\boldsymbol{k}\alpha}^{\dagger}\mid\Psi_{0}>}{\hbar\omega-\epsilon_{n\boldsymbol{k}}+i\eta}\right. \\
&\left.+\frac{<\Psi_{0}\mid f_{n\boldsymbol{k}\alpha}^{\dagger}\mid n\boldsymbol{k}\alpha><n\boldsymbol{k}\alpha\mid f_{n\boldsymbol{k}\alpha}\mid\Psi_{0}>}{\hbar\omega-\epsilon_{n\boldsymbol{k}}-i\eta}\right]\;.\,(4.328)
\end{aligned}
$$

In order to obtain the form of the Green's function in reciprocal space, we recall the fact that the functions $u_{n\boldsymbol{k}}\left(\boldsymbol{x}\right)$ are periodic with the periodicity of the lattice, and hence, as shown in (3.22), they can be expanded in a Fourier summation over reciprocal lattice vectors, such that

$$
\begin{aligned}
G_{\alpha\beta}\left(\boldsymbol{x},\boldsymbol{x}';\omega\right) &\sim \frac{1}{\Omega}\sum_{\boldsymbol{k},\boldsymbol{G},\boldsymbol{G}'}{}^{v}\boldsymbol{G}\,{}^{v}\boldsymbol{G}'^{*} \\
&\times\exp\left[i\left(\boldsymbol{k}+\boldsymbol{G}\right)\cdot\boldsymbol{x}\right]\exp\left[-i\left(\boldsymbol{k}+\boldsymbol{G}'\right)\cdot\boldsymbol{x}'\right]\cdots(4.329)
\end{aligned}
$$

where Ω is the volume of the unit cell. This shows that in general, the Fourier-transform of a *non-local function* on a lattice will be of the form

$$
G(\boldsymbol{x},\boldsymbol{x}')\rightarrow G\left(\boldsymbol{k}+\boldsymbol{G},\boldsymbol{k}+\boldsymbol{G}'\right)\;. \tag{4.330}
$$

This can be seen quite generally, since if $G(\boldsymbol{x},\boldsymbol{x}')$ describes a periodic system, the following should be fulfilled

$$
G(\boldsymbol{x},\boldsymbol{x}')=G(\boldsymbol{x}+\boldsymbol{R},\boldsymbol{x}'+\boldsymbol{R})\;. \tag{4.331}
$$

Then, a double Fourier transformation leads to

$$
\begin{aligned}
G\left(\boldsymbol{k},\boldsymbol{k}'\right) &= \frac{1}{V}\int\mathrm{d}^{3}x\,\mathrm{d}^{3}x'\,\exp\left(-i\boldsymbol{k}\cdot\boldsymbol{x}\right)\exp\left(i\boldsymbol{k}'\cdot\boldsymbol{x}'\right)G(\boldsymbol{x},\boldsymbol{x}') \\
&= \exp\left[i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\cdot\boldsymbol{R}\right] \\
&\times\frac{1}{V}\int\mathrm{d}^{3}x\,\mathrm{d}^{3}x'\,\exp\left(-i\boldsymbol{k}\cdot\boldsymbol{x}\right)\exp\left(i\boldsymbol{k}'\cdot\boldsymbol{x}'\right)G(\boldsymbol{x},\boldsymbol{x}')\;,\;\;(4.332)
\end{aligned}
$$

i.e. $\boldsymbol{k}-\boldsymbol{k}'=\boldsymbol{G}$. Therefore, a non-local function in a periodic system will be in general a function of $\boldsymbol{k}\in$ first Brillouin zone, $\boldsymbol{G}$, and $\boldsymbol{G}'$.

In the case of models on a lattice, as frequently used by theoreticians, the degrees of freedom are only defined on the lattice sites. This means, that a natural choice is to go over to Wannier functions. As shown in (3.63), Bloch functions are the lattice Fourier-transform of Wannier functions, such that

$$
u_{n\boldsymbol{k}}\left(\boldsymbol{x}\right) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}}\varphi_{n}\left(\boldsymbol{x}-\boldsymbol{R}\right)\exp\left[i\left(\boldsymbol{R}-\boldsymbol{x}\right)\cdot\boldsymbol{k}\right]\;. \tag{4.333}
$$

A possible choice of a Wannier function is

$$\varphi_n (\boldsymbol{x} - \boldsymbol{R}) = \delta (\boldsymbol{x} - \boldsymbol{R}) \exp\left[-i (\boldsymbol{R} - \boldsymbol{x}) \cdot \boldsymbol{k}\right] , \tag{4.334}$$

such that the phase factor is cancelled out. Inserting the resulting $u_{n\boldsymbol{k}} (\boldsymbol{x})$ into (4.328), we can consider again the double Fourier transform (4.332), and obtain,

$$
\begin{aligned}
G (\boldsymbol{k}, \boldsymbol{k}') &= \frac{1}{NV} \sum_{\boldsymbol{R}, \boldsymbol{R}'} \int \mathrm{d}^3 x \, \mathrm{d}^3 x' \, \delta (\boldsymbol{x} - \boldsymbol{R}) \, \delta (\boldsymbol{x} - \boldsymbol{R}') \\
&\quad \times \sum_{n, \tilde{\boldsymbol{k}}} \exp\left[-i \left(\boldsymbol{k} - \tilde{\boldsymbol{k}}\right) \cdot \boldsymbol{x}\right] \exp\left[i \left(\boldsymbol{k}' - \tilde{\boldsymbol{k}}\right) \cdot \boldsymbol{x}'\right] \times \cdots \\
&= \frac{1}{NV} \sum_{n, \tilde{\boldsymbol{k}}} \sum_{\boldsymbol{R}, \boldsymbol{R}'} \exp\left[-i \left(\boldsymbol{k} - \tilde{\boldsymbol{k}}\right) \cdot \boldsymbol{R}\right] \exp\left[i \left(\boldsymbol{k}' - \tilde{\boldsymbol{k}}\right) \cdot \boldsymbol{R}'\right] \\
&\qquad\qquad\qquad \times \cdots \\
&= \frac{N}{V} \delta_{\boldsymbol{k}, \boldsymbol{k}'} \sum_n \cdots \tag{4.335}
\end{aligned}
$$

Therefore, in the case of a model on a lattice, where the degrees of freedom are only defined on the lattice sites, we have for the one-particle Green's function,

$$
G_{\alpha\beta} (\boldsymbol{k}, \omega) = \frac{\hbar}{\Omega} \delta_{\alpha\beta} \sum_n \left[\frac{|< \Psi_0 \mid f_{n\boldsymbol{k}\alpha} \mid n\boldsymbol{k}\alpha >|^2}{\hbar\omega - \epsilon_{n\boldsymbol{k}} + i\eta} \right.
$$
$$
\left. + \frac{|< \Psi_0 \mid f^\dagger_{n\boldsymbol{k}\alpha} \mid n\boldsymbol{k}\alpha >|^2}{\hbar\omega - \epsilon_{n\boldsymbol{k}} - i\eta} \right] . \tag{4.336}
$$

In particular, in the case of a non-interacting system, with only one band, say a tight binding model with only nearest neighbor hopping on a hypercubic lattice in d dimensions, where the dispersion relation is given by

$$\epsilon_{\boldsymbol{k}} = -2t \sum_{i=1}^d \cos (\boldsymbol{k} \cdot \boldsymbol{a}_i) , \tag{4.337}$$

the Green's function is

$$G_{\alpha\beta} (\boldsymbol{k}, \omega) = \frac{\hbar}{\Omega} \delta_{\alpha\beta} \left[\frac{\theta (k - k_F)}{\hbar\omega - \epsilon_{n\boldsymbol{k}} + i\eta} + \frac{\theta (k_F - k)}{\hbar\omega - \epsilon_{n\boldsymbol{k}} - i\eta} \right] . \tag{4.338}$$

Spectral functions

For the following discussion we concentrate on the case of a lattice model (4.336), in order to keep the notation simple, and not to be restricted to a homogeneous system.

Let us introduce two *spectral functions* $A^+ (\boldsymbol{k}, \omega)$ and $A^- (\boldsymbol{k}, \omega)$ that give the probability of a particle $(+)$ or a hole $(-)$ with momentum $\boldsymbol{k}$ and energy ω to be in

an exact eigenstate of the system with $N + 1$ or $N - 1$ particles respectively. They are defined as

$$A^+ (\boldsymbol{k}, \omega) \equiv \frac{1}{\Omega} \sum_n |< \Psi_0 \mid f_{n\boldsymbol{k}\alpha} \mid n\boldsymbol{k}\alpha >|^2 \ \delta \left(\hbar\omega - \epsilon_{n\boldsymbol{k}} \right) \ ,$$

$$A^- (\boldsymbol{k}, \omega) \equiv \frac{1}{\Omega} \sum_n |< \Psi_0 \mid f^\dagger_{n\boldsymbol{k}\alpha} \mid n\boldsymbol{k}\alpha >|^2 \ \delta \left(\hbar\omega - \epsilon_{n\boldsymbol{k}} \right) \ , \qquad (4.339)$$

From the definitions above it is clear that these functions are real and positive definite. These expressions are very similar to those of the density of states we discussed in Chapter 3, with the difference that in that chapter, we were dealing with non-interacting particles, and hence, all the possible eigenstates of the system were one-particle states. In this case, the matrix elements specify that we are considering only those states related with one particle more or less in the system, and therefore, we are looking at the density of states of one-particle states resolved in momentum. These quantities are in fact accessible experimentally with *angular resolved photoemission or inverse photoemission spectroscopy*, in short ARPES for photoemission. For inverse photoemission progress has still to be reached in order to have accurate results. The density of states for one-particle excitations is obtained by integrating over momentum.

$$N(\omega) = \frac{1}{N} \sum_{\boldsymbol{k}} \left[A^+ (\boldsymbol{k}, \omega) + A^- (\boldsymbol{k}, \omega) \right] \ , \qquad (4.340)$$

where this quantity measures the density of states of both states above and below the Fermi energy.

By comparing (4.339) with (4.317), we see that the spectral functions and the one-particle Green's function are related as follows

$$G (\boldsymbol{k}, \omega) = \int_{-\infty}^{\infty} \mathrm{d}\omega' \left[\frac{A^+ (\boldsymbol{k}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega' + i\eta} + \frac{A^- (\boldsymbol{k}, \omega')}{\omega - \frac{\mu}{\hbar} + \omega' - i\eta} \right] \qquad (4.341)$$

Since we have an integral that passes through a singularity, we have to use the concept of a principal value of an integral, that is summarized symbolically for real ω as follows

$$\frac{1}{\omega \pm i\eta} = \mathcal{P} \frac{1}{\omega} \mp i\pi \ \delta(\omega) \ . \qquad (4.342)$$

Here $\mathcal{P}$ means that the real part of the integral is to be calculated as a principal value, e.g.

$$G (\boldsymbol{k}, \omega) = \mathcal{P} \int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{A^+ (\boldsymbol{k}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega'} - i\pi A^+ \left(\boldsymbol{k}, \omega - \frac{\mu}{\hbar} \right) \qquad (4.343)$$

for $\hbar\omega > \mu = E_F$. Since the integral in now real, we can summarize the result above as

$$A^+ \left(\boldsymbol{k}, \omega - \frac{\mu}{\hbar} \right) = -\frac{1}{\pi} \mathrm{Im} G (\boldsymbol{k}, \omega) \quad \text{for } \omega > \frac{\mu}{\hbar} \ ,$$

$$A^- \left(\boldsymbol{k}, \frac{\mu}{\hbar} - \omega \right) = \frac{1}{\pi} \mathrm{Im} G (\boldsymbol{k}, \omega) \quad \text{for } \omega < \frac{\mu}{\hbar} \ . \qquad (4.344)$$

That is, the one particle Green's function gives the spectral function for particles and holes measured from the chemical potential (or Fermi energy). Since the density of states is given by the sum over momentum of the spectral functions, it is given by the local Green's function

$$
\begin{aligned}
N\left(\omega - \frac{\mu}{\hbar}\right) &= -\frac{1}{\pi}\operatorname{Im}G\left(\boldsymbol{R},\boldsymbol{R}\,;\omega\right) \quad \text{for } \omega > \frac{\mu}{\hbar}\,, \\
N\left(\frac{\mu}{\hbar} - \omega\right) &= \frac{1}{\pi}\operatorname{Im}G\left(\boldsymbol{R},\boldsymbol{R}\,;\omega\right) \quad \text{for } \omega < \frac{\mu}{\hbar}\,,
\end{aligned}
\tag{4.345}
$$

where again, we made explicit, that the energies are measured from the Fermi energy. We therefore see, that the one-particle Green's function is directly related to experimentally accessible quantities like the spectral function (angular resolved photoemission and inverse phototemission), and the density of states (integrated photoemission).

Quasiparticles

Once we have seen that the Green' function allows to access the one-particle states, we discuss here, which are the signals and characteristics of those states.

We consider first non-interacting fermions with some dispersion relation $\epsilon_{\boldsymbol{k}}$.
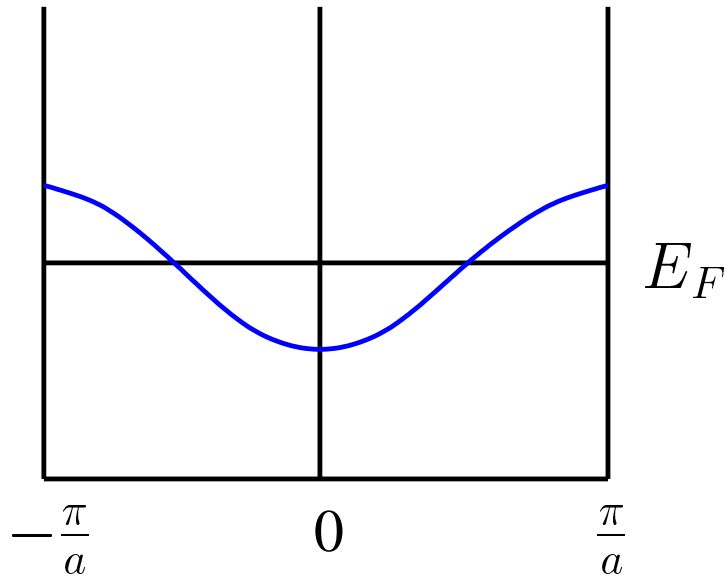
Figure 4.5: Dispersion relation for free electrons in one dimension.

Figure 4.5 displays an example in one dimension for a tight-binding model with nearest neighbor hopping t and a dispersion $\epsilon_k = -2t\cos ka$. The Green's function for a non interacting case was already calculated in (4.338), with the result

$$
G\left(\boldsymbol{k},\omega\right) = \frac{\hbar}{\Omega}\left[\frac{\theta\left(k - k_F\right)}{\hbar\omega - \epsilon_{\boldsymbol{k}} + i\eta} + \frac{\theta\left(k_F - k\right)}{\hbar\omega - \epsilon_{\boldsymbol{k}} - i\eta}\right]\,,
\tag{4.346}
$$

and according to (4.344), we have

$$
\begin{aligned}
A^+\left(\boldsymbol{k}, \hbar\omega - E_F\right) &= \frac{\hbar}{\Omega}\delta\left(\hbar\omega - \epsilon_{\boldsymbol{k}}\right) \quad \text{for } k > k_F \ , \\
A^-\left(\boldsymbol{k}, E_F - \hbar\omega\right) &= \frac{\hbar}{\Omega}\delta\left(\hbar\omega - \epsilon_{\boldsymbol{k}}\right) \quad \text{for } k < k_F \ .
\end{aligned}
\tag{4.347}
$$
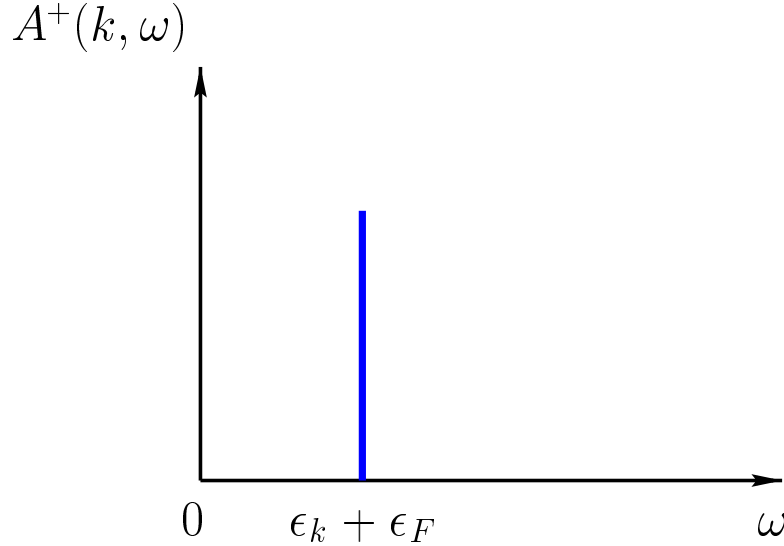
Figure 4.6: Spectral weight for free fermions.

Each state has a weight that is unity apart from the normalization factor. Since we are dealing with a non-interacting system, all the weight is on the one-particle state. This corresponds to a particle (or a hole) in that state.

Let us now consider an interacting system. As we saw in (4.306), a formal solution is obtained in the form

$$
G = \left[G^{(0)\,-1} - \Sigma^*\right]^{-1} \ ,
\tag{4.348}
$$

where in general the propagators and the self-energy have to be considered as non-local functions depending in general on two point in space and time or in momenta and energies. However, as we have discussed in the case of the Green's function, being on a lattice renders these quantities diagonal in momentum, such that we can write (without paying attention to the normalization factors)

$$
G\left(\boldsymbol{k}, \omega\right) = \frac{1}{\hbar\omega - \epsilon_{\boldsymbol{k}}^0 - \Sigma^*\left(\boldsymbol{k}, \omega\right)} \ ,
\tag{4.349}
$$

where $\epsilon_{\boldsymbol{k}}^0$ correspond to the dispersion obtained for the non-interacting fermions, i.e. the dispersion contained in $G^{(0)}$. In general, $\Sigma^*\left(\boldsymbol{k}, \omega\right)$ is a complicated complex function but let us assume that at least a part of $\Sigma^*\left(\boldsymbol{k}, \omega\right)$ is well behaved, meaning

that it is a function with a finite range in momentum and energy, and it can be isolated such that the energy dispersion is modified as

$$\epsilon_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}}^0 + \mathrm{Re}\tilde{\Sigma}\left(\boldsymbol{k},\omega\right) \ . \tag{4.350}$$

and also an imaginary part can be separated, such that

$$G\left(\boldsymbol{k},\omega\right) \ = \ \frac{z\left(\boldsymbol{k}\right)}{\hbar\omega - \epsilon_{\boldsymbol{k}} + i\Gamma} + G_{inc} \ , \tag{4.351}$$

where Γ gives a *lifetime* to the particle with dispersion $\epsilon_{\boldsymbol{k}}$. G_{inc} contains the rest, where no poles are present, and is called the incoherent part since it does not describe a particle that propagates coherently. In contrast to it, we call the first term G_c, the coherent part, since it corresponds to a coherently propagating particle at least for times $t < 1/\Gamma$. This can be seen by taking the Fourier transform of $G_c\left(\boldsymbol{k},\omega\right)$ in order to see its evolution in time. Here we take $t > 0$ and $\Gamma > 0$.

$$\begin{aligned} G_c\left(\boldsymbol{k},t\right) \ &= \ \int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{e}^{-i\omega t} \frac{z\left(\boldsymbol{k}\right)}{\omega - \epsilon_{\boldsymbol{k}} + i\Gamma} \\ &\sim \ z\left(\boldsymbol{k}\right) \exp\left\{-i\left[\epsilon_{\boldsymbol{k}} - i\Gamma\right]t\right\} \ , \end{aligned} \tag{4.352}$$

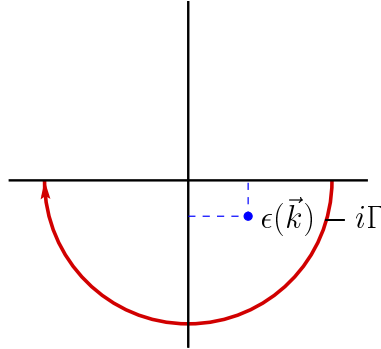The contour integral can be performed in the lower half-plane for $t > 0$. Since

Figure 4.7: Contour used to evaluate $G_c(t)$ for $t > 0$.

Γ was assumed to be positive, we see that the Green's function describes a plane wave that decays with the lifetime $1/\Gamma$. Furthermore, the residue of the pole $z\left(\boldsymbol{k}\right)$ gives the weight of the particle. Since in this case, the particle has not an infinite lifetime like in the non-interacting case, one speaks of a quasiparticle. Accordingly, $z\left(\boldsymbol{k}\right)$ is called the quasiparticle weight. In the case that it vanishes, there are no quasiparticles, i.e. an electron with momentum $\boldsymbol{k}$ and spin α has not finite overlap with the excitations of the system.

We can consider now the contribution of G_c to the spectral function. We can rewrite it as follows

$$G_c \ = \ \frac{z\left(\boldsymbol{k}\right)\left(\hbar\omega - \epsilon_{\boldsymbol{k}} - i\Gamma\right)}{\left(\hbar\omega - \epsilon_{\boldsymbol{k}}\right)^2 + \Gamma^2} \ , \tag{4.353}$$

such that

$$
\begin{aligned}
A^+\left(\boldsymbol{k}, \hbar\omega - E_F\right) &= -\frac{1}{\pi}\,\mathrm{Im}G\left(\boldsymbol{k}, \omega\right) \\
&\to \frac{z\left(\boldsymbol{k}\right)\Gamma}{\left(\hbar\omega - \epsilon_{\boldsymbol{k}}\right)^2 + \Gamma^2}\ .
\end{aligned}
\tag{4.354}
$$

The coherent part of the one-particle propagator leads to a Lorentzian peaked at $\epsilon_{\boldsymbol{k}}$, with a width that is given by the inverse of the lifetime and proportional to the quasiparticle weight. A similar result is obtained for the hole, taking into account that there, $\Gamma < 0$.
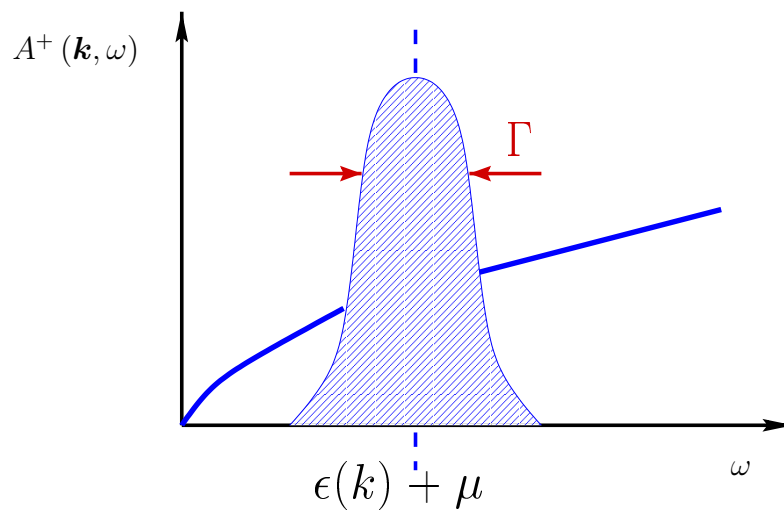
Figure 4.8: . Sketch of the spectral function for a quasiparticle with finite lifetime.

Figure 4.8 gives a sketch of the contribution from the coherent part of the propagator to the spectral function. The background is due to the incoherent part of the propagator. If the quasiparticle weight vanishes, then the background is the only remaining par of the spectral function.

Momentum distribution function

The momentum distribution function plays an important role for fermionic systems since it determines whether a Fermi surface is present or not, at least in translational invariant systems, where momentum is a good quantum number. It is defined as follows

$$
n_\sigma\left(\boldsymbol{k}\right) = \ < \Psi_0 \mid f^\dagger_{\boldsymbol{k},\sigma} f_{\boldsymbol{k},\sigma} \mid \Psi_0 >\ ,
\tag{4.355}
$$

where we use a definition that distinguishes the spin projection. As we have already discussed in Sec. 4.3, in the ground-state of a non-interacting system all electrons

are sitting in the lowest levels, up to the Fermi momentum, such that in this case,

$$
n_\sigma(\boldsymbol{k}) \;=\; \begin{cases} 1 & \text{for } k < k_F \\ 0 & \text{for } k > k_F \end{cases} \tag{4.356}
$$

where we assume that the number of electrons with for each spin projection is equal.

In the interacting case, we have to look for the relation of this quantity with the Green's function. Since for the evaluation of the Green's function, the time ordering of operators matters, we can obtain (4.355), where the creation operator is at the left of the destruction operator by the follwing limiting procedure

$$
n_\sigma(\boldsymbol{k}) \;=\; -iG\left(\boldsymbol{k}; t, t^+\right) \;, \tag{4.357}
$$

where t^+ is an infinitesimal later that t, such that the operators appear in the desired order. The minus sign compensates the sign due to the application of the time ordering operator. We can now insert the Green's function on the Lehman representation and Fourier transform it from frequency back to time.

$$
\begin{aligned}
(4.357) &= \frac{-i}{2\pi} \int d\omega\, G(\boldsymbol{k}, \omega)\, e^{-i\omega\left(t - t^+\right)} \\
&= \frac{1}{2\pi i} \int_C d\omega\, G(\boldsymbol{k}, \omega) \\
&= \frac{1}{2\pi i} \int_C d\omega\, \left[G_c(\boldsymbol{k}, \omega) + G_{inc}(\boldsymbol{k}, \omega)\right] \;.
\end{aligned} \tag{4.358}
$$

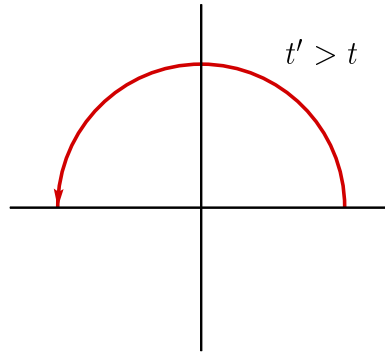Figure 4.9 show the contour of integration C in (4.358) that is appropriate for

Figure 4.9: Contour of integration C for $t' > t$.

$t - t^+ < 0$. In the last equality we explicitly wrote the coherent and incoherent parts of the Green's function, since they give different contributions to the integral. The coherent part has a pole that is on the upper half of the complex plane for energies below E_F, and hence for $k < k_F$, since in that case $\Gamma < 0$. Therefore, given the contour C, G_c gives a contribution to $n(\boldsymbol{k})$ that is the residue of the pole, namely $z(\boldsymbol{k})$. On the other hand, for energies above E_F, the poles of G_c lie

in the lower half-plane since $\Gamma > 0$. Therefore, there is no contribution from the coherent part to $n(\boldsymbol{k})$. On the other hand, the incoherent part has no poles and gives a continuous contribution to the integral. The result of the discussion above is summarized in Fig. 4.10, where the blue line shows $n(\boldsymbol{k})$ for the non-interacting case, and the red line the result for the interacting case. In the non-interacting
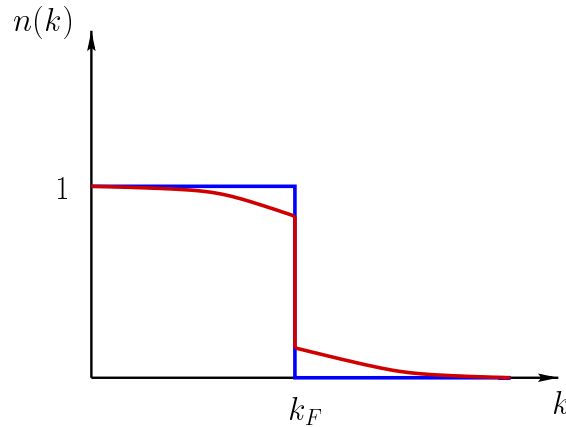

Figure 4.10: $n(\boldsymbol{k})$ for non-interacting fermions (blue line) and for interacting ones (red line).

case, the Green's function has only a coherent part and the residue of the poles is $z(\boldsymbol{k}) = 1$. This gives a jump at the Fermi momentum k_F as shown by the blue line. For the interacting case, however, $z(\boldsymbol{k}) < 1$ and there is moreover an additional continuous contribution from G_{inc}. Nevertheless, as long as $z(\boldsymbol{k}) \neq 0$, there is a jump at the Fermi momentum and, hence a sharp Fermi surface. Only in the case that $z(\boldsymbol{k}) = 0$, the jump disappears, signaling that there are no quasiparticles. Therefore, the existence of a Fermi surface is directly related to the existence of quasiparticles. In this case, one speaks of a *Fermi liquid*.

There is a well known case and well defined at least from the theoretical side, where $z(k) = 0$ and close to k_F,

$$n(k) \;=\; \frac{1}{2} - \operatorname{sign}(k - k_F)\; |\,k - k_F\,|^{\alpha}\,, \tag{4.359}$$

where the exponent $\alpha > 0$. This case corresponds to a universality class called Luttinger liquid, that encompasses interacting one-dimensional fermionic systems. Although Luttinger liquids are beyond the scope of these lectures, let us mention that in this case it can be proved that $z(k) = 0$, and therefore, one-particle excitations are not connected to quasiparticles. Instead, in the case of electrons in one-dimension, it can be shown at least in generic models, that they decay in two kind of excitations. One group is called *holons*, and they carry charge $+e$ but no spin and the others are called *spinons* with spin $S = 1/2$ but zero charge. This phenomenon is known as *charge-spin separation*.

At present, materials that present deviations from Fermi liquids are at the center of research in solid state, one of the most prominent candidates being high temperature superconductors. To which extent charge-spin separation plays a role in these systems is a matter of active debate.

Lifetime close to the Fermi surface

In the discussion above we have shown that if there is a coherent part of the Green's function, then, there are quasiparticles and their existence implies a Fermi surface. We should still discuss, how the lifetime of the quasiparticles behaves when we approach the Fermi surface, since if it would tend to zero or remain finite at the Fermi surface, such a concept would be of doubtfull value.

In the following we will assume that $z(k) \neq 0$, such that a Fermi surface exists. For simplicity, we can think of a homogeneous and isotropic system such that the Fermi surface is a sphere. Let us focus on a quasiparticle with energy close to the Fermi surface, i.e.

$$\epsilon = E_F + \delta \ , \quad \text{with } \frac{\delta}{E_F} \ll 1 \ , \tag{4.360}$$

In general, the quasiparticle will be scattered by particles in the Fermi sea, i.e. with $\epsilon' < E_F$. We denote the final states with a subscript '1'. The scattering rate
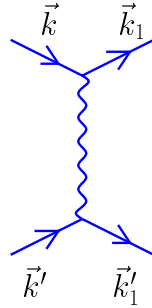

Figure 4.11: Schematic representation of a scattering event.

should be proportional to the number of available initial and final states, given by the momenta depicted in Fig. 4.11, such that

$$\Gamma_{\boldsymbol{k}} \propto \int \mathrm{d}\boldsymbol{k}' \int \mathrm{d}\boldsymbol{k}_1 \int \mathrm{d}\boldsymbol{k}_1' \, \delta \left[\boldsymbol{k} + \boldsymbol{k}' - (\boldsymbol{k}_1 + \boldsymbol{k}_1') \right] \ , \tag{4.361}$$

where we took into account explicitly momentum conservation. Since all the states below the Fermi energy are occupied, both particles should be in general scattered to states above the Fermi energy. During the scattering process also energy conservation should be respected, i.e.

$$\epsilon + \epsilon' = \epsilon_1 + \epsilon_1' \ . \tag{4.362}$$

Taking

$$
\begin{aligned}
\epsilon &= E_F + \delta & \epsilon_1 &= E_F + \delta_1 \,, \\
\epsilon' &= E_F + \delta' & \epsilon_1' &= E_F + \delta_1' \,,
\end{aligned}
\tag{4.363}
$$

we have $\delta' = \delta_1 + \delta_1' - \delta$. Since $\delta/E_F \ll 1$, and $\delta' < 0$, it follows that $\delta_1, \delta_1', \mid \delta' \mid \ll E_F$. We can now go back to (4.361) and change the integrations over momenta into integrations over energy intoducing density of states

$$
\begin{aligned}
\Gamma_{\boldsymbol{k}} &\propto \int_{-\infty}^{E_F} \mathrm{d}\epsilon' \, N(\epsilon') \int_{E_F}^{\infty} \mathrm{d}\epsilon_1 \, N(\epsilon_1) \int_{E_F}^{\infty} \mathrm{d}\epsilon_1' \, N(\epsilon_1') \, \delta\left[\epsilon + \epsilon' - (\epsilon_1 + \epsilon_1')\right] \\
&\leq \int_{E_F}^{E_F+\delta} \mathrm{d}\epsilon_1 \, N(\epsilon_1) \int_{E_F}^{E_F+\delta} \mathrm{d}\epsilon_1' \, N(\epsilon_1') \, N(\epsilon_1 + \epsilon_1' - \epsilon) \\
&\sim N(E_F)^3 \, \delta^2 \,.
\end{aligned}
\tag{4.364}
$$

We therefore see that $\Gamma \sim (\epsilon - E_F)^2$, as we get closer to the Fermi energy, showing that as long as a Fermi surface exists, quasiparticles become better and better defined as we approach the Fermi surface and they have infinite lifetime on it, since we know on the other hand, that Γ has to change sign on crossing the Fermi surface. The phase space arguments used above do not depend on the specific form of the interaction, but only on Fermi statistics and are, therefore, quite general. They were shown to be valid in all orders of perturbation theory by Luttinger (J.M. Luttinger, *Phys. Rev.* **121** (1961), 942). They were also rederived in the frame of renormalization group theory by Shankar (R. Shankar, *Rev. Mod. Phys.* **66**, 129 (1994)). The arguments above fail, when divergencies appear in some form, such that except for the free system, the Fermi surface is destroyed, as in the one-dimensional case.

4.4.4   Perturbation theory and Feynman diagrams

After having discussed general features of the Green's function, we give in this subsection the basic arguments needed in order to perform a perturbation expansion and to discuss Feynman diagrams for a fermionic system. The exposition is far from complete, the main aim being to give a basis to understand diagrams. A thorough discussion may be found e.g. in *Quantum Theory of Many-Particle Systems* by A. Fetter and J.D. Walecka.

Adiabatic "switching on" and the Gell-Mann and Low theorem

The results discussed here will give a link between the Green's function as defined in (4.286) and perturbation theory through the evolution operator (4.279) defined in the interaction picture.

We already discussed the adiabatic theorem in Chapter 2 and have seen, how the eigenstates of a Hamiltonian at a time t_0 are connected to the eigenstates of the Hamitltonian at a later time, if the Hamiltonian is time dependent but this

time dependence is sufficiently slow. In the present case, the interest is to connect the states of the exactly soluble Hamiltonian H_0, where in principle everything is known, and the ones of the full Hamiltonian $H = H_0 + H_I$. For this purpose, we introduce the following time-dependent Hamiltonian

$$H = H_0 + e^{-\epsilon|t|} H_I \; , \tag{4.365}$$

where $\epsilon > 0$ and very small. For $|t| \to \infty$, the Hamiltonian (4.365) reduces to H_0, whereas at $t = 0$, it becomes the interacting problem we are interested in. Therefore it is said that in the limit $\epsilon \to 0$, the interaction is switched on adiabatically.

   Given the Hamiltonian (4.365), we can go to the interaction picture and replace in the results obtained in Sec. 4.4.1

$$H_I \longrightarrow e^{-\epsilon|t|} H_I \; . \tag{4.366}$$

This leads to an evolution operator like (4.279), with the corresponding changes

$$U_\epsilon(t, t_0) \;\; = \;\; \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} \right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n$$
$$\times e^{-\epsilon(|t_1| + \cdots + |t_n|)} \, T \left[H_I(t_1) \cdots H_I(t_n) \right] \; . \tag{4.367}$$

As $t_0 \to -\infty$, the effect of the interaction vanishes and one approaches H_0, with

$$H_0 \mid \Phi_0 > = E^{(0)} \mid \Phi_0 > \; . \tag{4.368}$$

Therefore, as $t_0 \to -\infty$, $\mid \Psi_I(t_0) > \to \mid \Phi_0 >$. Recalling the relation among state vectors in the different pictures (4.285), we have in particular for the states vectors in the Heisenberg and interaction pictures,

$$\mid \Psi_H > = \mid \Psi_I(0) > = U_\epsilon(0, -\infty) \mid \Phi_0 > \; , \tag{4.369}$$

such that the evolution operator in the interaction picture gives us the link between the eigenstates of the non-interacting system and the eigenstates of the full interacting one, since as we already mentioned, the states vectors in the Heisenberg picture correspond to the eigenvectors of the interacting system.

   It only remains to see what happens in the limit $\epsilon \to 0$. This is shown by the Gell-Mann and Low theorem that states the following. *If the following quantity exists to all orders in perturbation theory,*

$$\lim_{\epsilon \to 0} \frac{U_\epsilon(0, -\infty) \mid \Phi_0 >}{< \Phi_0 \mid U_\epsilon(0, -\infty) \mid \Phi_0 >} \equiv \frac{\mid \Psi_0 >}{< \Phi_0 \mid \Psi_0 >} \; , \tag{4.370}$$

then, it is an eigenstate of H

$$H \frac{\mid \Psi_0 >}{< \Phi_0 \mid \Psi_0 >} = E \frac{\mid \Psi_0 >}{< \Phi_0 \mid \Psi_0 >} \; . \tag{4.371}$$

The theorem demonstrates that starting with an eigenstates of H_0, in the limit $\epsilon \to 0$, an eigenstate of the full Hamiltonian develops from $| \Phi_0 >$. In order to avoid an exceedingly formal presentation, we defer the reader to Sec. 3.6 of the book by Fetter and Walecka for a demonstration of this theorem. Since the adiabatic switching on was defined in such a way that also for $t \to \infty$, we reach the non-interacting system, the proof applies equally well to

$$\frac{U_\epsilon(0, \infty) \mid \Phi_0 >}{< \Phi_0 \mid U_\epsilon(0, \infty) \mid \Phi_0 >} \, , \tag{4.372}$$

where

$$U_\epsilon(0, \infty) = U_\epsilon^\dagger(\infty, 0) \, . \tag{4.373}$$

One-particle Green's function as power series in the interaction

Once we could connect the eigenstates of the non-interacting system with the ones of the full interacting one, by appropriately passing through the interaction picture, we still have to somehow relate operators in the Heisenberg picture, as they appear in the definition of the Green's function, to the evolution operators that belong to the interaction picture. For this, it is usefull to relate an operator in the Heisenberg picture to an operator in the interaction picture. We recall the relations between operators in the Heisenberg picture and those in the Schroedinger picture (4.283) and between operators in the interaction picture and the Schrödinger picture

$$\begin{aligned} \hat{\mathcal{O}}_H(t) &= e^{iHt/\hbar} \, \hat{\mathcal{O}}_S \, e^{-iHt/\hbar} \\ &= e^{iHt/\hbar} \, e^{-iH_0 t/\hbar} \, \hat{\mathcal{O}}_I(t) \, e^{iH_0 t/\hbar} \, e^{-iHt/\hbar} \, . \end{aligned} \tag{4.374}$$

In order to identify the product of exponentials, we need to recall the definition of a state in the interaction picture (4.266), and the evolution operator there (4.271). From (4.266) we have

$$\begin{aligned} | \Psi_I(t) > &= \exp\left[\frac{i}{\hbar} H_0 t\right] | \Psi_S(t) > \\ &= \exp\left[\frac{i}{\hbar} H_0 t\right] \exp\left[-\frac{i}{\hbar} H(t - t_0)\right] | \Psi_S(t_0) > \\ &= \exp\left[\frac{i}{\hbar} H_0 t\right] \exp\left[-\frac{i}{\hbar} H(t - t_0)\right] \exp\left[-\frac{i}{\hbar} H_0 t_0\right] | \Psi_I(t_0) > \end{aligned} \tag{4.375}$$

But, due to (4.271),

$$U(t, t_0) = \exp\left[\frac{i}{\hbar} H_0 t\right] \exp\left[-\frac{i}{\hbar} H(t - t_0)\right] \exp\left[-\frac{i}{\hbar} H_0 t_0\right] \, . \tag{4.376}$$

We have here another way to express the evolution operator in the interaction picture. This form is usefull in connection with (4.374), since it shows that

$$\hat{\mathcal{O}}_H(t) = U(0, t) \, \hat{\mathcal{O}}_I(t) \, U(t, 0) \, . \tag{4.377}$$

In the case of two operators, the case that is of interest to calculate the Green's function, we would have

$$
\begin{aligned}
\hat{\mathcal{O}}_H(t)\,\hat{\mathcal{O}}_H(t') &= U(0,t)\,\hat{\mathcal{O}}_I(t)\,U(t,0)\,U(0,t')\,\hat{\mathcal{O}}_I(t')\,U(t',0) \\
&= U(0,t)\,\hat{\mathcal{O}}_I(t)\,U(t,t')\,\hat{\mathcal{O}}_I(t')\,U(t',0)\;,
\end{aligned}
\tag{4.378}
$$

where in going from the first to the second line we used the fact that

$$
U(t,t') = U(t,t_1)\,U(t_1,t')\;,
\tag{4.379}
$$

for any t, t_1, and t', since for any pair of states fulfilling (4.271), we can perform the evolution in one step, i.e.

$$
\begin{aligned}
\mid \Psi_I(t) > &= U(t,t_1)\mid \Psi_I(t_1) > \\
&= U(t,t_1)\,U(t_1,t')\mid \Psi_I(t') >\;.
\end{aligned}
\tag{4.380}
$$

We have now the elements to formulate a perturbative form for the Green's function. There we need recalling eq. (4.286) on the one hand, the ground-state of the interacting system. According to the Gell-Mann and Low theorem we have for the normalization of the Green' function

$$
\begin{aligned}
\frac{<\Psi_0\mid\Psi_0>}{\mid<\Phi_0\mid\Psi_0>\mid^2} &= \frac{<\Phi_0\mid U_\epsilon(\infty,0)\,U_\epsilon(0,-\infty)\mid\Phi_0>}{\mid<\Phi_0\mid\Psi_0>\mid^2} \\
&= \frac{<\Phi_0\mid \hat{S}\mid\Phi_0>}{\mid<\Phi_0\mid\Psi_0>\mid^2}\;,
\end{aligned}
\tag{4.381}
$$

where we defined

$$
\hat{S} = U_\epsilon(\infty,0)\,U_\epsilon(0,-\infty) = U_\epsilon(\infty,-\infty)\;.
\tag{4.382}
$$

Since from the Gell-Mann and Low theorem we only know that the ratio exists in the limit $\epsilon \to 0$, we keep the denominator in calculating the norm of the ground-state.

We need on the other hand, the expectation value in the ground-state of the field operators. Again we keep the denominator coming from (4.370).

$$
\begin{aligned}
&\frac{<\Psi_0\mid \hat{\psi}_{H\alpha}(\boldsymbol{x},t)\,\hat{\psi}^\dagger_{H\beta}(\boldsymbol{x}',t')\mid\Psi_0>}{\mid<\Phi_0\mid\Psi_0>\mid^2} \\
&= \frac{1}{\mid<\Phi_0\mid\Psi_0>\mid^2}<\Phi_0\mid U_\epsilon(\infty,0)\,U(0,t)\,\hat{\psi}_{I\alpha}(\boldsymbol{x},t)\,U(t,t') \\
&\qquad\qquad\times\hat{\psi}^\dagger_{I\beta}(\boldsymbol{x}',t')\,U(t',0)\,U_\epsilon(0,-\infty)\mid\Phi_0> \\
&= \frac{<\Phi_0\mid U_\epsilon(\infty,t)\,\hat{\psi}_{I\alpha}(\boldsymbol{x},t)\,U(t,t')\,\hat{\psi}^\dagger_{I\beta}(\boldsymbol{x}',t')\,U_\epsilon(t',-\infty)\mid\Phi_0>}{\mid<\Phi_0\mid\Psi_0>\mid^2}
\end{aligned}
\tag{4.383}
$$

Then, the Green's function defined in (4.286) can be expressed as

$$
iG_{\alpha\beta}(x,x') = \frac{<\Phi_0\mid U_\epsilon(\infty,t)\,\hat{\psi}_{I\alpha}(x)\,U(t,t')\,\hat{\psi}^\dagger_{I\beta}(x')\,U_\epsilon(t',-\infty)\mid\Phi_0>}{<\Phi_0\mid\hat{S}\mid\Phi_0>},
\tag{4.384}
$$

where the denominator coming from (4.370) is cancelled out. We also introduced the short writing $(\boldsymbol{x}, t) \longrightarrow x$.

In order to explicitly show that (4.384) corresponds to a perturbative expansion, we recall the form of the evolution operator (4.279), where a series expansion in H_I appears. Each of the three evolution operators above gives rise to such a series expansion with a time ordering operator. Since the definition of the Green's function itself also contains a time ordering operator, we can use the time ordered product for all the terms, such that the proper ordering is kept. Without writing the whole expression explicitly, let us concentrate on the main elements we have to reconsider in order to find a compact expression. As shown in eq. (4.279), from each evolution operator we have an infinite summation, such that in the numerator of (4.384) we should have

$$U_\epsilon\left(\infty, t\right) \hat{\psi}_{I\alpha}\left(x\right) U(t, t') \hat{\psi}_{I\beta}^\dagger\left(x'\right) U_\epsilon\left(t', -\infty\right)$$

$$\rightarrow \sum_\ell \frac{1}{\ell!}\left(-\frac{i}{\hbar}\right)^\ell \sum_m \frac{1}{m!}\left(-\frac{i}{\hbar}\right)^m \sum_p \frac{1}{p!}\left(-\frac{i}{\hbar}\right)^p \times \cdots, \quad (4.385)$$

where $\cdots$ correspond to the various integrals and time ordered products of H_I's and field operators. Now we notice that an infinite summation with all possible $r!$ ordering of times (denoted by $\cdots$), can be split in the following way

$$\begin{aligned}
\sum_r \frac{1}{r!}\left(-\frac{i}{\hbar}\right)^r \times \cdots &= \sum_m \sum_p \sum_r \frac{1}{r!} \delta_{r, m+p} \binom{r}{m}\left(-\frac{i}{\hbar}\right)^r \times \cdots \\
&= \sum_m \left(-\frac{i}{\hbar}\right)^m \sum_p \left(-\frac{i}{\hbar}\right)^p \\
&\quad \times \frac{1}{(m+p)!} \binom{m+p}{m} \times \cdots \\
&= \sum_m \frac{1}{m!}\left(-\frac{i}{\hbar}\right)^m \sum_p \frac{1}{p!}\left(-\frac{i}{\hbar}\right)^p \times \cdots \quad (4.386)
\end{aligned}$$

That is, all three summations in (4.385) can be reduced to one single summation by applying repeatedly the reasoning above. Since we had time ordered products, we can view the whole product as time ordered and extend the integral to the outermost limits, i.e. from $-\infty$ to ∞. Finally, returning to (4.384), we have for the one-particle Green's function,

$$\begin{aligned}
iG_{\alpha\beta}\left(x, x'\right) &= \sum_n \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{\infty} \mathrm{d}t_1 \cdots \mathrm{d}t_n \\
&\quad \times \frac{<\Phi_0 \mid T\left[H_I\left(t_1\right) \cdots H_I\left(t_n\right) \hat{\psi}_{I\alpha}\left(x\right) \hat{\psi}_{I\beta}^\dagger\left(x'\right)\right] \mid \Phi_0>}{<\Phi_0 \mid \hat{S} \mid \Phi_0>} \quad (4.387)
\end{aligned}$$

Thus, we arrive at an expression appropriate for perturbation theory, where the one-particle Green's function is explicitly written as an expansion in powers of the perturbation H_I.

Once an explicit expansion in powers of the interaction was achieved, it remains to perform the evaluations of the different terms entering (4.387). For this, we need Wick's theorem, that will allow us to reduce the time ordered products into c-numbers, and hence, expressions that can be readily evaluated.

Wick's theorem

Although this is the central theorem for the posterior diagrammatic expansion for the one-particle Green's function and all other imaginable physical quantities, its explicit demonstration will not be presented here to avoid an overloading on the formal side. The demonstration can be found in Sec. 3.8 of the above mentioned book by Fetter and Walecka. Nevertheless, we will discuss here the necessary elements to be able to understand the demonstration and also to reach a general understanding of the elements entering in the construction of diagrams.

As a first step, we will realize that a large number of terms in (4.387) are actually zero. For this, let us consider what happens when we act with a destruction field operator on a certain eigenstate of H_0. In general it will destroy a particle at some point x, where this particle can have some weight on states above the Fermi energy and some below it. As we discussed in the previous section, the states above the Fermi energy, are particle states (i.e. states that can be occupied ba a particle added to the system), and hence, acting with $\hat{\psi}$ on these states corresponds to the destruction of a particle. On the other hand, the states below the Fermi energy correspond to hole states. That is, destroying a particle below the Fermi energy corresponds to the creation of a hole. We can therefore, formally distinguish these two different kind of actions of a destruction operator by splitting $\hat{\psi}$ as follows

$$\hat{\psi}(x) = \hat{\psi}^{(+)}(x) + \hat{\psi}^{(-)\dagger}(x) \ , \tag{4.388}$$

where the superscritp $(+)$ corresponds to particle states and $(-)$ to hole states. In particular for the non-interacting ground-state $\mid \Phi_0 >$ entering (4.387) we have

$$\hat{\psi}^{(+)} \mid \Phi_0 >= 0 \ , \tag{4.389}$$

such that $\mid \Phi_0 >$ is the vacuum for $\hat{\psi}^{(+)}$. For the Fermi gas, we can give explicitly the form of $\hat{\psi}^{(+)}$ and $\hat{\psi}^{(-)\dagger}$:

$$
\begin{aligned}
\hat{\psi}_\alpha(x) &= \sum_{k>k_F} \frac{1}{\sqrt{V}} \exp\left[i\left(\boldsymbol{k}\cdot\boldsymbol{x} - \frac{\epsilon_{\boldsymbol{k}}}{\hbar}t\right)\right] a_{\alpha\boldsymbol{k}} \\
&+ \sum_{k<k_F} \frac{1}{\sqrt{V}} \exp\left[i\left(\boldsymbol{k}\cdot\boldsymbol{x} - \frac{\epsilon_{\boldsymbol{k}}}{\hbar}t\right)\right] b^{\dagger}_{\alpha\boldsymbol{k}} \\
&\equiv \hat{\psi}^{(+)}(x) + \hat{\psi}^{(-)\dagger}(x) \ . \tag{4.390}
\end{aligned}
$$

In the same way, if we consider a creation field operator, it can create a particle on a particle state or one on a hole state, i.e. destroy a hole. Just taking the hermitian conjugate of (4.388), we have

$$\hat{\psi}^{\dagger}(x) = \hat{\psi}^{(+)\dagger}(x) + \hat{\psi}^{(-)}(x) \ , \tag{4.391}$$

and again

$$\hat{\psi}^{(-)} \mid \Phi_0 >= 0 \ , \tag{4.392}$$

since in the ground-state there are no holes present.

The fact that $\hat{\psi}^{(\pm)}$ annihilate the non-interacting ground-state, leads us to try to shift allway such operators to the right until they encounter $\mid \Phi_0 >$ giving thus zero. A product of operators in second quantization, where all the creation operators are on the left and destruction operators on the right, is called a *normal ordered product*, and denoted by N (not to be confused with the number of particles). As in the case of the time ordering, it takes into account the statistics of the particles considered, such that

$$N \left(\hat{A}\hat{B} \right) = -N \left(\hat{B}\hat{A} \right) \tag{4.393}$$

for $\hat{A}$ and $\hat{B}$ creation or annihilation operators for fermions. In the case of the creation and annihilation operators introduced above, we have

$$N \left[\hat{\psi}^{(+)}(x) \, \hat{\psi}^{(-)\dagger}(x') \right] = -\hat{\psi}^{(-)\dagger}(x') \, \hat{\psi}^{(+)}(x) \ . \tag{4.394}$$

We need now to see how to go from a time ordered product as it appears in e.g. (4.387) to normal ordered products. Since the expectation value in the ground-state of normal ordered products vanishes, the rest is what needs to be evaluated. The difference between a time ordered product of two operators and the normal product is called *contraction*

$$\hat{A}^\bullet \hat{B}^\bullet \equiv T \left(\hat{A}\hat{B} \right) - N \left(\hat{A}\hat{B} \right) \tag{4.395}$$

In order to see the meaning of a contraction, let us apply the definition above to the Green's function of a non-interacting system $G^{(0)} \left(x, x' \right)$, where since the interaction part is absent, the operators in the interaction picture and the Heisenberg picture are identical, and hence, all the discussion above can be applied.

$$\begin{aligned} iG^{(0)} \left(x, x' \right) &= \ < \Phi_0 \mid T \left[\psi(x) \, \psi^\dagger(x') \right] \mid \Phi_0 > \\ &= \ < \Phi_0 \mid \psi(x)^\bullet \, \psi^\dagger(x')^\bullet \mid \Phi_0 > \\ &\quad + < \Phi_0 \mid N \left[\psi(x) \, \psi^\dagger(x') \right] \mid \Phi_0 > \ . \end{aligned} \tag{4.396}$$

Since the expectation value in the ground-state of the normal ordered product is zero, it turns out that each contraction of two field operators leads to a non-interacting Green's function. This happens whenever we have a creation and an annihilation operator. It remains to see what happens when we have two creation or annihilation operators. We look at a pair of annihilation operators since from there, we can also obtain the result for a couple of creation operators.

$$\begin{aligned} < \Phi_0 \mid \psi(x)^\bullet \, \psi(x')^\bullet \mid \Phi_0 > &= \ < \Phi_0 \mid T \left[\psi(x) \, \psi(x') \right] \mid \Phi_0 > \\ &\quad - < \Phi_0 \mid N \left[\psi(x) \, \psi(x') \right] \mid \Phi_0 > \ . \end{aligned} \tag{4.397}$$

Again the normal ordered product vanishes, but now the time ordered product also vanishes, since the number of particles in $\psi(x)\,\psi(x') \mid \Phi_0 >$ is different from the number of particles in $< \Phi_0 \mid$, and hence, these states are orthogonal. Therefore, in this case the contraction is zero and similarly when two creation operators are present.

After having seen what happens with the time ordered product of two operators, we need to have the result for an arbitrary number of operators, as they occur in (4.387). For this, we have Wick's theorem:

$$
\begin{aligned}
T\left(\hat{A}_1 \cdots \hat{A}_n\right) \;=\;\; & N\left(\hat{A}_1 \cdots \hat{A}_n\right) \\
& +N \,(\text{sum over all possible contractions}) \ . \quad (4.398)
\end{aligned}
$$

From what we said above, when we take the expectation value in the ground-state, we need only to consider contractions between a creation and an annihilation operator. Furthermore, from all normal ordered products only those containing only contractions will survive. This is the basis for a diagramatic expansion.

Feynman diagrams

In order to see how diagrams can be used to describe the different terms in perturbation theory, we go back to the expansion of the Green's function in powers of H_I, eq. (4.387). Let us consider first the numerator up to $\mathcal{O}\left(H_I\right)$,

$$
iG_{\alpha\beta} \rightarrow iG_{\alpha\beta}^{(0)} + i\tilde{G}_{\alpha\beta}^{(1)} \ , \qquad (4.399)
$$

with

$$
i\tilde{G}_{\alpha\beta}^{(1)} = -\frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t_1 \; < \Phi_0 \mid T\left[H_I\left(t_1\right)\,\hat{\psi}_\alpha\left(x\right)\,\hat{\psi}_\beta^\dagger\left(x'\right)\right] \mid \Phi_0 > \ , \qquad (4.400)
$$

where we introduced the tilde in order to remember that we are considering only the numerator in (4.387). Recalling the form of H_I in eq. (4.289), and using a notation similar to (4.299),

$$
V_{\mu\nu\nu'\mu'}\left(\boldsymbol{x}, t; \boldsymbol{x}', t'\right) \;\equiv\; V\left(\mid \boldsymbol{x} - \boldsymbol{x}' \mid\right)\,\delta\left(t - t'\right)\delta_{\mu\mu'}\delta_{\nu\nu'} \ , \qquad (4.401)
$$

we have

$$
\begin{aligned}
i\tilde{G}_{\alpha\beta}^{(1)} \;=\;\; & -\frac{i}{\hbar}\frac{1}{2}\sum_{\substack{\mu\mu' \\ \nu\nu'}} \int_{-\infty}^{\infty} \mathrm{d}^4x_1\,\mathrm{d}^4x_1'\, V_{\mu\nu\nu'\mu'}\left(x_1, x_1'\right) \\
& \times < \Phi_0 \mid T\Big[\hat{\psi}_\mu^\dagger\left(x_1\right)\,\hat{\psi}_\nu^\dagger\left(x_1'\right)\,\hat{\psi}_{\nu'}\left(x_1'\right)\,\hat{\psi}_{\mu'}\left(x_1\right) \\
& \hspace{5cm} \times\hat{\psi}_\alpha\left(x\right)\,\hat{\psi}_\beta^\dagger\left(x'\right)\Big] \mid \Phi_0 > \ . \quad (4.402)
\end{aligned}
$$

Since we have to contract creation and annihilation operators in pairs, we have here six possible different ways of contracting all six operators. For each contraction we

have a non-interacting Green's function, such that

$$
\begin{aligned}
(4.402) \quad = \quad & -\frac{i}{\hbar}\frac{1}{2}\sum_{\substack{\mu\mu'\\ \nu\nu'}}\int_{-\infty}^{\infty}\mathrm{d}^4x_1\,\mathrm{d}^4x_1'\,V_{\mu\nu\nu'\mu'}\left(x_1,x_1'\right)\\
& \times\Bigg\{iG_{\alpha\beta}^{(0)}\left(x,x'\right)\left[iG_{\mu'\mu}^{(0)}\left(x_1,x_1\right)\,iG_{\nu'\nu}^{(0)}\left(x_1',x_1'\right)\right.\\
& \hspace{6cm}\left.-iG_{\mu'\nu}^{(0)}\left(x_1,x_1'\right)\,iG_{\nu'\mu'}^{(0)}\left(x_1',x_1\right)\right]\\
& +iG_{\alpha\mu}^{(0)}\left(x,x_1\right)\left[iG_{\mu'\nu}^{(0)}\left(x_1,x_1'\right)\,iG_{\nu'\beta}^{(0)}\left(x_1',x'\right)\right.\\
& \hspace{6cm}\left.-iG_{\mu'\beta}^{(0)}\left(x_1,x'\right)\,iG_{\nu'\nu}^{(0)}\left(x_1',x_1'\right)\right]\\
& +iG_{\alpha\nu}^{(0)}\left(x,x_1'\right)\left[iG_{\nu'\mu}^{(0)}\left(x_1',x_1\right)\,iG_{\mu'\beta}^{(0)}\left(x_1,x'\right)\right.\\
& \hspace{6cm}\left.-iG_{\nu'\beta}^{(0)}\left(x_1',x'\right)\,iG_{\mu'\mu}^{(0)}\left(x_1,x_1\right)\right]\Bigg\}\,.(4.403)
\end{aligned}
$$

At this stage we see that expressions in perturbation theory become rather lengthy, so that a short description of the different contributions would be usefull. This is achieved by Feynman diagrams.

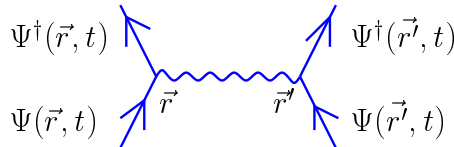Let us start by introducing a graph for the interaction. The wavy line represents

Figure 4.12: Graph representing the interaction vertex.

the Coulomb interaction between two points. As can be seen from (4.289), there are two field operators at one point and two on the other. Destruction operators are represented by the lines ending at the interaction vertex, whereas creation operators are depicted by lines starting there. On performing a contraction, creation and annihilation operators build up a non-interacting Green's function. The different
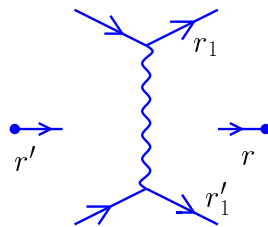

Figure 4.13: Lines to be joined in first order.

contractions are obtained by joining starting and ending lines. Figure (4.13) shows

these lines prior to the contraction. The contractions written in (4.403) can be obtained by performing all possible connection of the lines starting at r' in Fig. 4.13 and joining them with the lines ending at r_1, r'_i or r. In doing so, there are two kinds of diagrams as depicted in Fig. 4.14.   There is a set of diagrams with all
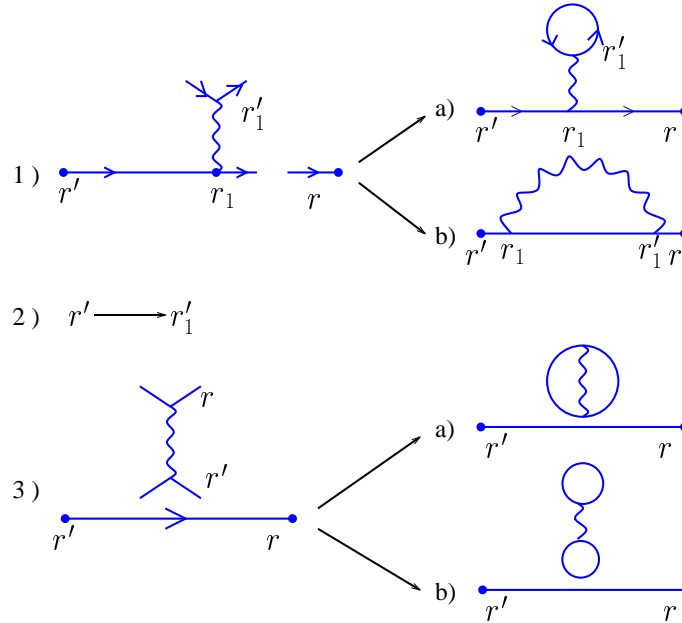

Figure 4.14: Diagrams obtained in first order. For further explanation see the text.

parts connected, like those corresponding to 1). In 2) the same diagrams as in 1) are obtained but with r_1 and r'_1 exchanged. The other set depicted under 3) has disconnected parts. Furthermore, there are pairs of diagrams where an exchange occurs in the contraction with r, whereas the point r' has the same contraction. One speaks in this case of exchange diagrams. This will be discussed in more detail when we arrive at the treatment of the so-called Hartree-Fock approximation. From the way in which diagrams are built up, it is natural to have a sense of time, given by the arrows in each line. We have as a convention that time increases to the right, such that particles propagate from left to right, whereas holes do so from right to left. In the diagrams depicted in Fig. 4.14 there are lines starting and ending at the same point. They correspond to contributions of the form $G^{(0)}_{\mu'\mu}(x_1, x_1)$ in (4.403). In order to have a definite order of the corresponding times, we have to recall that they stem from the interaction term, where the creation operators were standing at the left of the annihilation ones. Therefore, they should be understood in the same way as in (4.357), corresponding to electronic densities. Figure 4.15 shows that after evaluating all the contributions up to $\mathcal{O}(H_I)$, a common factor can be extracted, as can be directly verified from (4.403). The common factor can be indeed identified with the denominator of (4.387). There we have no external points, such that all

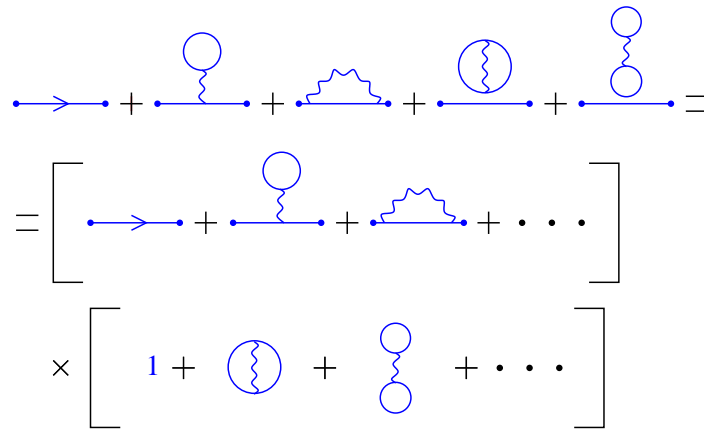the diagrams arising from that term should be closed ones. Up to first order in H_I,

Figure 4.15: A common factor can be extracted from the first order diagrams.

it gives

$$
\begin{aligned}
< \Phi_0 \mid \hat{S} \mid \Phi_0 > \\
=&< \Phi_0 \mid U_\epsilon \left(\infty, -\infty\right) \mid \Phi_0 > \\
=&< \Phi_0 \mid \Phi_0 > - \frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t_1 \; < \Phi_0 \mid T\, H_I\left(t_1\right) \mid \Phi_0 > \\
=& 1 - \frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}^4 x_1 \, \mathrm{d}^4 x_1' \, V_{\mu\nu\nu'\mu'}\left(x_1, x_1'\right) \\
& \times < \Phi_0 \mid T\left[\hat{\psi}_\mu^\dagger\left(x_1\right) \hat{\psi}_\nu^\dagger\left(x_1'\right) \hat{\psi}_{\nu'}\left(x_1'\right) \hat{\psi}_{\mu'}\left(x_1\right)\right] \mid \Phi_0 > \; . \quad (4.404)
\end{aligned}
$$

Figure 4.16 shows the diagrams corresponding to the first order contribution of the
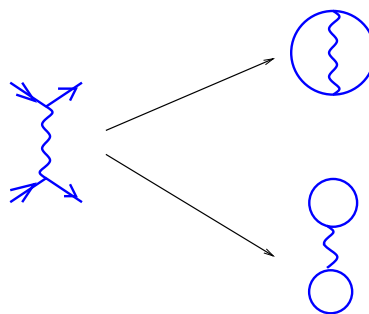

Figure 4.16: Diagrams for the denominator of the Green's function in first order.

denominator of (4.387). This means that at least to this order, the denominator cancels the disconnected diagrams in the numerator of (4.387), leaving only connected diagrams. In fact, it can be proved (see Fetter-Walecka Sec. 3.8) that disconnected diagrams are cancelled to all orders, such that, the Green's functions is given by

the sum of all connected diagrams. Here one speaks of the *linked cluster* theorem or expansion.

$$
\begin{aligned}
iG_{\alpha\beta}\,&(x,x') \\
&= \sum_n \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{\infty} \mathrm{d}t_1 \cdots \mathrm{d}t_n \\
&\quad \times < \Phi_0 \mid T\left[H_I\,(t_1)\cdots H_I\,(t_n)\ \hat{\psi}_{I\alpha}\,(x)\ \hat{\psi}_{I\beta}^{\dagger}\,(x')\right] \mid \Phi_0 >_{connected} . \quad (4.405)
\end{aligned}
$$

We can finally give the rules for Feynman diagrams. We give them first in direct space and then in momentum space. For direct space we have for the n-th order contribution to the one-particle Green's function:

a) Draw all topologically distinct connected diagrams with n interaction lines V and $2n + 1$ Green's functions $G^{(0)}$.

b) Label each vertex with a point in space-time x_i.

c) Each solid line represents a Green's function $G^{(0)}\,(x,x')$ running from x' to x.

d) Each wavy line corresponds to the interaction (4.401).

e) Integrate all internal variables over space and time. Sum over all internal spin indices.

f) Each diagram carries a factor $(-1)^L$, where L is the number of closed fermion loops in the diagram.

g) Each diagram contributes to $G(x,x')$ with a factor $-i(-i/\hbar)^n(i)^{2n+1} = (i/\hbar)^n$.

For the Feynman diagrams in momentum space we restrict ourselves to homogeneous systems or models on a lattice, such that the Green's function is diagonal in momentum and frequency. Furthermore, we assume the interaction to be such that it is also diagonal in momentum, and being instantaneous, such that its Fourier-transform has no frequency dependence. Then, the rules in this case are as follows.

a) Draw all topologically distinct connected diagrams with n interaction lines V and $2n + 1$ Green's functions $G^{(0)}$.

b) Assign a direction to each interaction line; associate directed momentum and frequency to each line and conserve energy and momentum at each vertex.

c) Each solid line represents a Green's function $G_{\alpha\beta}^{(0)}\,(\boldsymbol{k},\omega)$.

d) Each wavy line corresponds to the Fourier trnsform of the interaction (4.401).

e) Integrate over the n internal momenta and frequencies. Sum over all internal spin indices.

f) Each diagram carries a factor $(-1)^L$, where L is the number of closed fermion loops in the diagram. From the Fourier transformations there is an additional factor $(2\pi)^{-4n}$.

g) Each diagram contributes to $G(\boldsymbol{k}, \omega)$ with a factor $-i(-i/\hbar)^n(i)^{2n+1} = (i/\hbar)^n$.

4.5 The Hartree-Fock approximation

After having discussed in general the treatment of a many-body fermionic system, we deal here with one of the most popular approximations for a such systems, the Hartree-Fock approximation. This approximation is the first one that is generally used for nuclear, atomic and solid-state systems. As we will see, it is not perturbative in the sense that the Green's function will contain all powers in the interaction, but only a selected class of diagrams enters. This approximation gives a first sight of interacting systems, giving in the case of atoms, metals and semiconductors a qualitative first picture but with quantitative failures. Although not accurate, this approximation fulfills a variational principle, and hence is to some extent controlled.

4.5.1 Self-energy in the Hartree-Fock approximation

As we have seen in the previous section, up to first order in the interaction, the one-particle Green's function is given by the diagrams depicted in Fig. 4.17. We
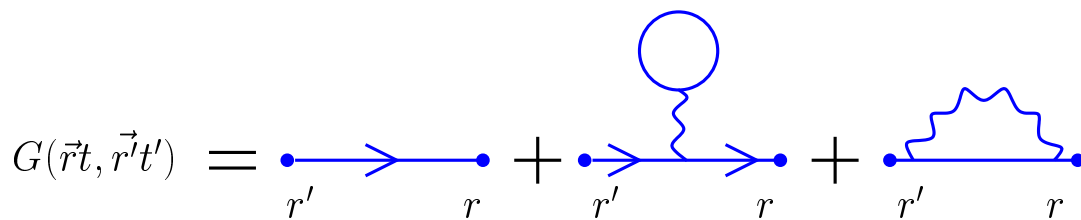

$$G(\vec{r}t, \vec{r'}t') =$$

Figure 4.17: One-particle Green's function up to first order in the interaction.

can view the propagator in Fig. 4.17 as the lowest order contribution for the one-particle Green's function with a self-energy that corresponds to the two diagrams shown there, i.e.

$$G = G^{(0)} + G^{(0)}\Sigma^*G^{(0)} + \cdots \tag{4.406}$$

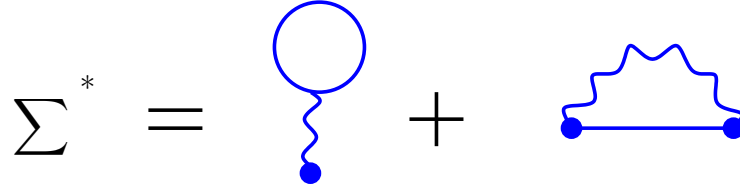In this case, the self-energy is given by Fig. 4.18.

Figure 4.18: Self-energy in first order of the interaction.

Using Dyson's eq. (4.307), which we repeat here for clarity,

$$G = G^{(0)} + G^{(0)} \Sigma^* G \,, \tag{4.407}$$

we can now generate a Green's function with the interaction in all orders but with just a restricted set of diagrams. The diagramatic representation of Dyson's equation is given in Fig. 4.19, where the double line represents the full one-particle Green's function and the fact that it appears on both sides of the equation corresponds to the fact that we are dealing with a self-consistent equation. The shaded circle represents the one-particle irreducible self-energy. We will discuss this denomination later. For the moment it just contains the diagrams shown in Fig. 4.18.   The explicit solution
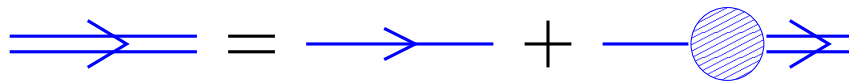

Figure 4.19: Diagramatic representation of Dyson's equation.

of Dyson's equation with the self-energy depicted in Fig. 4.18 is shown in Fig. 4.20 At this point, it is instructive to calculate the actual expression for the self-energy. Since we have already calculated all the contributions in first order, we need just to recall the result (4.403), where we have to consider only those contributions related with connected diagrams. The result for the first order contribution to the Green's function is

$$\begin{aligned}
G^{(1)}_{\alpha\beta}(x, x') = \;& \frac{i}{\hbar} \sum_{\substack{\mu\mu' \\ \nu\nu'}} \int_{-\infty}^{\infty} \mathrm{d}^4 x_1 \, \mathrm{d}^4 x_1' \, V_{\mu\nu\nu'\mu'}(x_1, x_1') \\
& \times G^{(0)}_{\alpha\mu}(x, x_1) \Big[G^{(0)}_{\mu'\nu}(x_1, x_1') \, G^{(0)}_{\nu'\beta}(x_1', x') \\
& \hspace{4cm} - G^{(0)}_{\mu'\beta}(x_1, x') \, G^{(0)}_{\nu'\nu}(x_1', x_1') \Big].
\end{aligned} \tag{4.408}$$

We recall the fact that the zero-th order Green's function is diagonal in spin, such
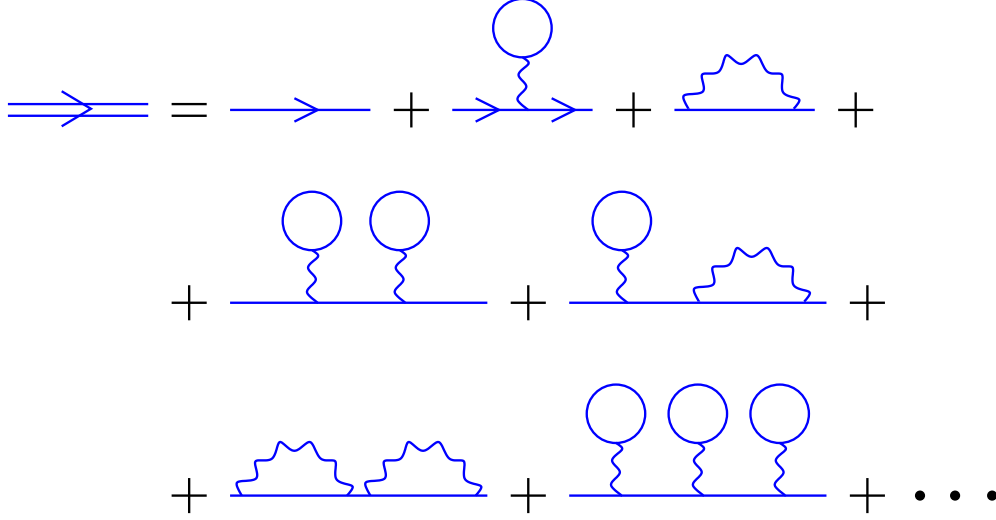

Figure 4.20: Expansion of the Green's function with the irreducible self-energy given by Fig. 4.18.

that it is convenient to introduce the following notation:

$$G^{(0)}_{\alpha\beta} \equiv \delta_{\alpha\beta} \, \bar{G}^{(0)} \, , \qquad (4.409)$$

where $\bar{G}^{(0)}$ contains the rest. Furthermore, recalling (4.401), the spin dependence of the interaction has the form $V_{\mu\nu\nu'\mu'} \sim \delta_{\mu\mu'}\delta_{\nu\nu'}$, whereas the time dependence is $\sim \delta(t - t')$. Putting all these facts together, we obtain

$$\begin{aligned}
\Sigma^{*(1)}_{\alpha\beta}(x, x') &= -\frac{1}{\hbar} \, \delta_{\alpha\beta} \, \delta(t - t') \\
&\times \Bigg[\delta(\boldsymbol{x} - \boldsymbol{x}') \, (2S + 1) \int \mathrm{d}^3 x_1 \, i\bar{G}^{(0)}\left(x_1, x_1^+\right) \, V(|\, \boldsymbol{x} - \boldsymbol{x}_1 \,|) \\
&\quad - V(|\, \boldsymbol{x} - \boldsymbol{x}' \,|) \, i\bar{G}^{(0)}\left(\boldsymbol{x}, t; \boldsymbol{x}', t^+\right) \Bigg] \, , \qquad (4.410)
\end{aligned}$$

where S is the spin of the fermions, i.e $S = 1/2$ in the case of electrons. In order to grasp the physical meaning of these terms, let us concentrate on the first one. From the definition of the Green's function (4.286), we have

$$\begin{aligned}
iG_{\alpha\beta}\left(x, x^+\right) &= -\frac{< \Psi_0 \mid \hat{\psi}^\dagger_{H\beta}(x) \, \hat{\psi}_{H\alpha}(x) \mid \Psi_0 >}{< \Psi_0 \mid \Psi_0 >} \\
&= -\delta_{\alpha\beta} < n_\alpha(x) > \, , \qquad (4.411)
\end{aligned}$$

in the case of a system with spin rotational invariance. This means that

$$i\bar{G}^{(0)}\left(x_1, x_1^+\right) = -n^{(0)}(x_1) \, , \qquad (4.412)$$

the density per spin of the non-interacting system. That is, this term of the self-energy gives the Coulomb interaction of the particle we consider with the density of all other particles, since we integrate in space over the whole system. But this cannot be correct, since if the particle we consider interacts with the other particles, they themselve should interact with each other. In order to correct for this, we should consider the density of the interacting system. This is easily done, if we replace $G^{(0)}$ by the full G in (4.410). Although at this point we still do not clearly see the role of the second term in (4.410), we include it and discuss it at the end. This leads to

$$
\begin{aligned}
\Sigma_{HF}^{*}\left(x, x^{\prime}\right) \;=\; & -\frac{1}{\hbar} \delta\left(t-t^{\prime}\right) \\
& \times\left[\delta\left(\boldsymbol{x}-\boldsymbol{x}^{\prime}\right)(2 S+1) \int \mathrm{d}^{3} x_{1}\, iG\left(x_{1}, x_{1}^{+}\right) V\left(\mid \boldsymbol{x}-\boldsymbol{x}_{1}\mid\right)\right. \\
& \left.-V\left(\mid \boldsymbol{x}-\boldsymbol{x}^{\prime}\mid\right) iG\left(\boldsymbol{x}, t ; \boldsymbol{x}^{\prime}, t^{+}\right)\right],
\end{aligned}
\tag{4.413}
$$

The result is depicted in Fig. 4.21. Before we discuss the physical meaning of these diagrams, let us first remark a clear difference between the diagrams appearing in Fig. 4.20 and in Fig. 4.21. Whereas in the diagrams of Fig. 4.20, we could devide diagrams by cutting one propagator, this is not possible in the diagrams of Fig. 4.21. The diagrams in Fig. 4.20 are therefore called one-particle reducible diagrams, whereas those of Fig. 4.21 are one-particle irreducible, and hence the name one-particle irreducible self-energy. We can now try to understand the physical meaning
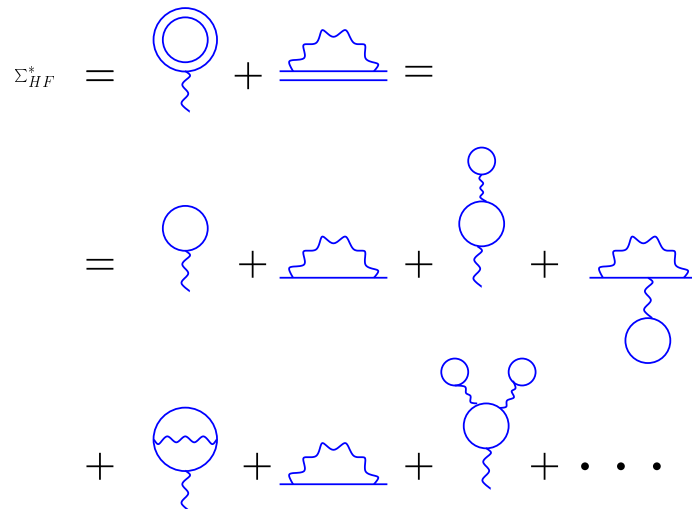

Figure 4.21: Hartree-Fock irreducible part of the self-energy .

of the terms entering 4.413. As a first step we notice that Σ^{*} is proportional to $\delta\left(t-t^{\prime}\right)$, and hence, will be frequency independent. It will be therefore, convenient

to perform a Fourier transformation in time. For this, we have

$$G\left(\boldsymbol{x}, t; \boldsymbol{x}', t'\right) = \frac{1}{2\pi} \int \mathrm{d}\omega \, \mathrm{e}^{-i\omega(t-t')} \, G\left(\boldsymbol{x}, \boldsymbol{x}', \omega\right) , \qquad (4.414)$$

such that

$$G\left(\boldsymbol{x}, t; \boldsymbol{x}', t^{+}\right) = \lim_{\delta \to 0^{+}} \frac{1}{2\pi} \int \mathrm{d}\omega \, \mathrm{e}^{i\omega\delta} \, G\left(\boldsymbol{x}, \boldsymbol{x}', \omega\right) . \qquad (4.415)$$

Then, we can write after Fourier transforming in time,

$$
\begin{aligned}
\hbar\Sigma^{*}\left(\boldsymbol{x}, \boldsymbol{x}'\right) = & -i\left(2S+1\right) \delta\left(\boldsymbol{x} - \boldsymbol{x}'\right) \\
& \times \int \mathrm{d}^3 x_1 \, V\left(\mid \boldsymbol{x} - \boldsymbol{x}_1 \mid\right) \frac{1}{2\pi} \int \mathrm{d}\omega \, \mathrm{e}^{i\omega\delta} \, G\left(\boldsymbol{x}_1, \boldsymbol{x}_1, \omega\right) \\
& + iV\left(\mid \boldsymbol{x} - \boldsymbol{x}' \mid\right) \frac{1}{2\pi} \int \mathrm{d}\omega \, \mathrm{e}^{i\omega\delta} \, G\left(\boldsymbol{x}, \boldsymbol{x}', \omega\right) , \qquad (4.416)
\end{aligned}
$$

where it is understood that we take the limit $\delta \to 0^{+}$. To proceed further, let us consider the Lehmann representation of the fully interacting Green's function (4.317)

$$
\begin{aligned}
G\left(\boldsymbol{x}, \boldsymbol{x}', \omega\right) = & \hbar \sum_{n} \left[\frac{< \Psi_0 \mid \hat{\psi}\left(\boldsymbol{x}\right) \mid \Psi_n >< \Psi_n \mid \hat{\psi}^{\dagger}\left(\boldsymbol{x}'\right) \mid \Psi_0 >}{\hbar\omega - \mu - \epsilon_n(N+1) + i\eta} \right. \\
& \left. + \frac{< \Psi_0 \mid \hat{\psi}^{\dagger}\left(\boldsymbol{x}'\right) \mid \Psi_n >< \Psi_n \mid \hat{\psi}\left(\boldsymbol{x}\right) \mid \Psi_0 >}{\hbar\omega - \mu + \epsilon_n(N-1) - i\eta} \right]. \quad (4.417)
\end{aligned}
$$

Since Σ^{*} is frequency independent, we will look for a solution that has the same form as the non-interacting Green's function, but with the corresponding changes due to interaction. Since we are at $T = 0$, $\mu = E_F$. Furthermore, we set

$$
\begin{aligned}
\epsilon_n(N+1) &= \tilde{\epsilon}_n - E_F , \\
\epsilon_n(N-1) &= E_F - \tilde{\epsilon}_n , \qquad (4.418)
\end{aligned}
$$

and

$$G\left(\boldsymbol{x}, \boldsymbol{x}', \omega\right) = \hbar \sum_{n} \psi_n\left(\boldsymbol{x}\right) \psi_n^{*}\left(\boldsymbol{x}'\right) \left[\frac{\theta\left(\tilde{\epsilon}_n - E_F\right)}{\hbar\omega - \tilde{\epsilon}_n + i\eta} + \frac{\theta\left(E_F - \tilde{\epsilon}_n\right)}{\hbar\omega - \tilde{\epsilon}_n - i\eta} \right] . (4.419)$$

Here we introduced a complete set of orthonormal wavefunctions $\{\psi_n\left(\boldsymbol{x}\right)\}$, which we should determine in order to solve the problem. With such a form for the Green's function, we can now evaluate Σ^{*}. For this we need only to perform the ω-integration in (4.416). The integrals we have to perform have the form

$$\int \mathrm{d}\omega \, \mathrm{e}^{i\omega\delta} \, G\left(\boldsymbol{x}, \boldsymbol{x}', \omega\right) , \qquad (4.420)$$

where since $\delta > 0$, the contour of integration has to close on the upper half plane, i.e. Im $\omega > 0$, such that only poles on the upper half-plane give a contribution, that is, according to (4.419), the terms proportional to $\theta\left(E_F - \tilde{\epsilon}_n\right)$. Therefore, we have

$$
\begin{aligned}
\hbar\Sigma^*\left(\boldsymbol{x}, \boldsymbol{x}'\right) \ =\ & (2S+1)\,\delta\left(\boldsymbol{x} - \boldsymbol{x}'\right)\int \mathrm{d}^3x_1\, V\left(\mid \boldsymbol{x} - \boldsymbol{x}_1 \mid\right) \\
& \times \sum_n \mid \psi_n\left(\boldsymbol{x}_1\right) \mid^2\ \theta\left(E_F - \tilde{\epsilon}_n\right) \\
& -V\left(\mid \boldsymbol{x} - \boldsymbol{x}' \mid\right) \sum_n \psi_n\left(\boldsymbol{x}\right) \psi_n^*\left(\boldsymbol{x}'\right) \theta\left(E_F - \tilde{\epsilon}_n\right)\ . \quad (4.421)
\end{aligned}
$$

The one-particle wavefunctions were chosen in a similar way as in the non-interacting system. They are the one-particle wavefunctions to be determined from the equation of motion of the Green's function. In particular, as we already mentioned,

$$
\begin{aligned}
(2S+1)\,G\left(\boldsymbol{x}, t; \boldsymbol{x}, t^+\right) \ =\ & \lim_{\delta \to 0^+} (2S+1)\,\frac{1}{2\pi}\int \mathrm{d}\omega\, \mathrm{e}^{i\omega\delta}\, G\left(\boldsymbol{x}, \boldsymbol{x}, \omega\right) \\
=\ & (2S+1)\sum_n \mid \psi_n\left(\boldsymbol{x}_1\right) \mid^2\ \theta\left(E_F - \tilde{\epsilon}_n\right) \\
=\ & n(\boldsymbol{x})\ . \quad (4.422)
\end{aligned}
$$

We therefore have a self-energy that reflects the fact that the particle in question is interacting with a density of interacting particles.

In order to find the solution for the wavefunctions introduced, we can go to the explicit form of Dyson's equation, i.e. to the equation of motion for the Green's function, as already deduced in (4.305).

$$
G^{(0)\,-1}\, G - \Sigma^*\, G\ =\ \mathbf{1}\ . \quad (4.423)
$$

Let us recall the general form of $G^{(0)}$, as given by (4.303), where we take into account the possibility of an external static potential. Then,

$$
G^{(0)\,-1}\left(\boldsymbol{x}, \boldsymbol{x}'; \omega\right) \ =\ \omega - \frac{1}{\hbar}\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U\left(\boldsymbol{x}\right)\right]\ . \quad (4.424)
$$

Inserting the form chosen for the Green's function (4.419), and the result above for $G^{(0)\,-1}$ into (4.423), we have

$$
\begin{aligned}
\delta\left(\boldsymbol{x} - \boldsymbol{x}'\right) \ =\ & \left[\hbar\omega + \frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - U\left(\boldsymbol{x}\right)\right] \\
& \times \sum_n \psi_n\left(\boldsymbol{x}\right)\psi_n^*\left(\boldsymbol{x}'\right)\left[\frac{\theta\left(\tilde{\epsilon}_n - E_F\right)}{\hbar\omega - \tilde{\epsilon}_n + i\eta} + \frac{\theta\left(E_F - \tilde{\epsilon}_n\right)}{\hbar\omega - \tilde{\epsilon}_n - i\eta}\right] \\
& -\int \mathrm{d}^3x_1\, \hbar\Sigma^*\left(\boldsymbol{x}, \boldsymbol{x}_1\right) \\
& \times \sum_n \psi_n\left(\boldsymbol{x}_1\right)\psi_n^*\left(\boldsymbol{x}'\right)\left[\frac{\theta\left(\tilde{\epsilon}_n - E_F\right)}{\hbar\omega - \tilde{\epsilon}_n + i\eta} + \frac{\theta\left(E_F - \tilde{\epsilon}_n\right)}{\hbar\omega - \tilde{\epsilon}_n - i\eta}\right]\ . (4.425)
\end{aligned}
$$

Finally, we use the fact that the wavefunctions $\psi_n(\boldsymbol{x})$ are assumed to be orthonormal and multiply both sides of the equation by $\psi_j(\boldsymbol{x}')$ and integrate over $\boldsymbol{x}'$. Then, we are left with a set of Schrödinger-like equations for the eigenfunctions $\psi_j(\boldsymbol{x})$ and eigenvalues $\tilde{\epsilon}_j$.

$$
\begin{aligned}
&\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U(\boldsymbol{x}) \right]\psi_j(\boldsymbol{x}) \\
&+ (2S+1)\sum_n \int \mathrm{d}^3 x_1\, V(|\,\boldsymbol{x}-\boldsymbol{x}_1\,|)\,|\,\psi_n(\boldsymbol{x}_1)\,|^2\ \psi_j(\boldsymbol{x})\,\theta(E_F-\tilde{\epsilon}_n) \\
&- \sum_n \int \mathrm{d}^3 x_1\, V(|\,\boldsymbol{x}-\boldsymbol{x}_1\,|)\,\psi_n(\boldsymbol{x})\,\psi_n^*(\boldsymbol{x}_1)\,\psi_j(\boldsymbol{x}_1)\,\theta(E_F-\tilde{\epsilon}_n) \\
&= \tilde{\epsilon}_j\,\psi_j(\boldsymbol{x})\ .
\end{aligned}
\tag{4.426}
$$

These are the Hartree-Fock equations as they were originally obtained. Since there is a non-local part (the last term), the solution of these equations is in general not straightforward. Furthermore, the fact that they have to be solved self-consistently, since the solution determines the potentials, corresponds to the fact that the Coulomb interaction is taken into account in all orders. However, not all possible scattering processes are included, only those shown by Fig. 4.21. The effect of Coulomb interaction (or any other two-particle interaction due to a potential of the form $V(|\,\boldsymbol{x}-\boldsymbol{x}_1\,|)$), is given by two distinct parts. The first one corresponds as we already mentioned, to an interaction with the density and is given by a local potential, in the case of Coulomb interaction corresponding to an electrostatic potential. The second part is characterized by a non-local potential, and is called the exchange term, since it differs from the first one by an exchange $\psi_n(\boldsymbol{x}_1) \leftrightarrow \psi_j(\boldsymbol{x})$.