LECTURE NOTES
OF
INTRODUCTION TO MANY BODY THEORY
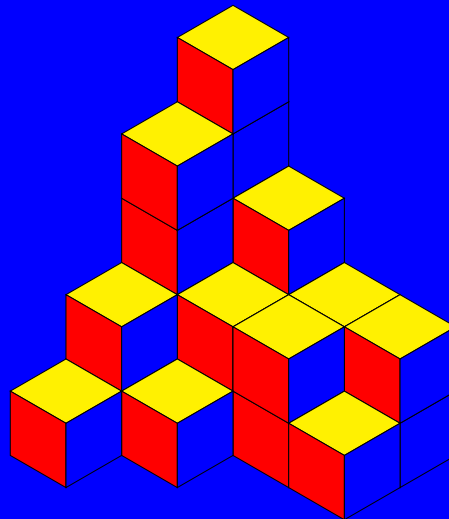
Collection of the lectures notes of professor Silvestrelli.

EDITED BY

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ACADEMIC YEAR 2019-2020

Abstract

In this document I have tried to reorder the notes of the "Introduction to Many-Body Theory" course held by Professor Pier Luigi Silvestrelli at the Department of Physics of the University of Padua during the second semester of the 2019-20 academic year of the master's degree. There may be formatting errors, wrong marks, missing exponents etc. If you find errors, let me know (alice.pagano@studenti.unipd.it) and I will correct them, so that this document can be a good study support.

Padova, Friday 8$^{\text{th}}$ May, 2020   Alice Pagano

Contents

Introduction

Useful informations

Reference textbook:

- Fetter A.L., Walecka J.D., "Quantum Theory of Many-Particle Systems" (1971,2003)

- H. Bruns, K. Flensberg, "Many-Body Quantum theory in Condensed Matter Physics" (2002)

There are two options for the exam:

- Homeworks (detailed calculations, send the solution to the professor by a PDF file in 10 days) + "simplified" oral exam (quantitative concepts, no long calculations).

- Standard oral exam.

Outline of the course

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Chapter 1

Second quantization

1.1 Introduction

The classical picture of the world, that essentially could be described by the Netwon's laws, is that the world is made by *many* ($N \gg 1$) *interacting* particles that move in space and in time. In the past years, this scenario has changed. Firstly, some scientists (as Faraday, Maxwell...) have introduced the concept of field, then space and time, that were two distinct concepts, were unified by Einstein. After that, the concept of quantum mechanics was developed (by Schrödinger, Bohr, Dirac, Einstein, Planck, Jordan) and in this scenario all the property of a system are fully described by a time dependent Schrödinger equation as

$$i\hbar \frac{\mathrm{d}\psi(\dots)}{\mathrm{d}t} = H\psi(\dots)$$

A further step was trying to unify the concept of field with the one of quantum mechanics: we arrive at the definition of a **quantum field theory** (Dirac, Feymann, Dyson...). In this formalism, the classical particles are described in term of quanta of a given field. We emphasize that in this course, we will use the formalism of quantum field theory, even if our approach will be a *non-relativistic* one.

1.2 Quantum many-body problem

Let us describe the the property of a quantum many-body system. In principle, the solution of a quantum many-body problem is very easy. Let us consider a N-body quantum wave function that is a function of the coordinates of all the particles of the system, the solution of the problem is given by the N-body Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\psi(x_1, \dots, x_N, t) = H\psi(x_1, \dots, x_N, t)$$

If we are able to solve the equation, we will have all the properties of our system, but in practice it is not possible in an exact way, even using the most powerful computers. In order to deal with such a problem, we can:

- use approximations;

- use alternative approaches as:

  - adopting some concepts by quantum field theory (non-relativistic approach) as the formalism of the second quantization;

  - or, adopting the formalism of quantum statistical mechanics (we have a lot of particles, so it is important the collective behaviour of the particles);

− or, even by using the concept of the Green's function.

To summarize, we can quote Paul Dirac:

> The fundamental law necessary for the mathemtical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficultly lies only in the fact that application of these laws leads to equations that are too complex to be solved.

Hence, in principle we know what we have to do, but we are unable to do it in practice.

1.2.1   Green's function

Typically if we know the Green's function, we are able to compute:

- the expectation value of single-particle operators (as the kinetic term);

- the ground state energy of the system;

- describe the excitations (elementary excitation spectrum);

- finally, we are able to have results to use in a linear response theory, that is important for connections with the experiments. Indeed, the way we are able to investigate systems is by exciting them: we send a beam (an excitation, as electromagnetic radiation) to the system, then the system is excited (it is no longer in a ground state) and it has, if the temperature is not too high, a response. In particular, we want a linear response (i.e. linear with respect to this perturbation): this happens if the perturbation is small enough and it is not a general situation.

In general, we will assume that the temperature is $T = 0$, but eventually we will see what happens when the system as a finite temperature $T > 0$.

Unfortunately, we cannot exactly determine the interacting N-body Green's function. One is forced to use approximations and, in particular, one of the most useful approach is the **perturbative** one: typically we start from a non interacting system and we extend the study to an interacting system by tuning on the perturbation. In general, we not only need many term in the expansion, but even an *infinite* number of terms, because usually the interaction is a Coulomb one that is a strong interaction. To deal with such perturbative approach we will introduce very useful tecniques as the Feymann diagrams, that are very useful tools to emphasize the most important concepts of the derivation of the expansion.

Typically, our reference system is the *degenerate electron gas*, or "**Jellium**", that is a system made by interacting electrons (fermions) on top of uniform positive background which is introduced using all terms neutral (???). This system could be useful also to describe plasma or metal and most of our work will be on such a model system. Since it is a system made by fermions (electrons), it is better that we image the system at a zero temperature, but in the course we will briefly see what change when we increase the temperature.

1.3   Second quantization formalism

The first subject of the course is the topic of second quantization, which is an alternative way to study quantum system using quantum field theory (chapter 1 Fetter). This topic is important because we define a new approach which of course is the same of the approaches to solve Schrödinger equation, but it gives great simplification to deal with many body quantum interacting bodies. In particular, it introduces the

concept of 'creation' and 'annichilation' of particles by using suitable operators and it allows to keep track of the proper symmetry of wave function in a very efficient and confortable way. Even if we do not use relativistic approach, the concept of creation and annichilation of particles is very useful to manage with the difficult problem of interacting particles.

Remark. By convention the original form of quantum mechanics is denoted *first quantization*, while quantum field theory (that, as said, is the formalism we adopt to study many body interactin particles) is formulated in the language of *second quantization*.

Let us consider a N-body problem, we have to solve the time dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x_1,\ldots,x_N,t) = H\psi(x_1,\ldots,x_N,t) + \text{boundary conditions for } \psi \qquad (1.1)$$

where ψ is the N-body wave function and it is suitable to specific boundary conditions that depend in the system we are studying. In particular, the typical form of the Hamiltonian is the following:

$$H = \sum_{k=1}^{N} T(x_k) + \frac{1}{2}\sum_{\substack{k,l=1 \\ (k\neq l)}}^{N} V(x_k,x_l) \qquad (1.2)$$

where the green term incorporates the kinetic term and the single particle 1-body potential, while the yellow term corresponds to the potential term characterizing the interaction of the particles. In front of this factor there is the term $1/2$ to avoid to count twice every interaction between a pair of particles and of course we have also to omit the self interaction (a particle is not allowed to interact with itself and we have to neglect that term). Moreover, the coordinates x_k has to be considered as 'general' coordinates, i.e. all the coordinates that are necessary to characterize a single particle. For instance, if we consider a fermion with spin, the generalized coordinates could be the space coordinates of the particle (a vector with 3 component), but we should also incorporate the spin variable for fermions. Similar considerations are applied to all the other particles.

We have also satisfy the following properties:

- the Hamiltonian that characterize the system should be *symmetric* under exchange of particles, because we are considering indistinguishable particles;

- we should consider *normalized* wave functions, i.e.

$$\|\psi\|^2 = \int dx_1 \ldots dx_N \, |\psi(x_1,\ldots,x_N)|^2 = 1 \qquad (1.3)$$

The first step is to expand the N-body wave function ψ using a complete basis set of time-independent single particle wave functions (with periodic boundary conditions): $\{\psi_{E_k}(x_k)\}$. We do this expansion because if we omit the interaction potential term in the Hamiltonian, we obtain a 1-body problem (non interacting problem), which solution is a product of a sequence of single particle wave functions and depending on the system, we should consider proper boundary condition. After we have solved this problem, we try to turn on the interaction.

Example 1

For instance let us consider an homogeneous system inside a cubic box characterized by the length of the side of the box L of volume $V = L^3$. The complete

basis set for such a system is completely made by plane-waves. In general, we consider the thermodynamic limit for which we have $N \to \infty, V \to \infty$ with the constraint $n = N/V$ finite.

Another example is a crystal lattice whose most useful basis set can be represented by Block-functions.

The index E_k denotes a *complete set of single particles quantum numbers* and it is again a general expression that depends on the specific system we are considering.

Example 2

For example, if we have spinless bosons in a box the complete set of quantum numbers is $\{\vec{p}\}$.

Instead, for a homogeneous system of fermsions we have to add also the spin variable $\{\vec{p}, s_z\}$.

Now, let us expand the N-body function as a function of the complete basis set:

$$\psi(x_1, \ldots, x_N, t) = \sum_{E_1, \ldots, E_N} c(E_1, \ldots, E_N, t) \varphi_{E_1}(x_1) \ldots \varphi_{E_N}(x_N) \qquad (1.4)$$

where the first particle in the quantum state is denoted by E_1. Note that the single particle wave functions are time independent, while the coefficients c are time dependent due to the presence of the interactions. We have to force that the basis set is orthonormal:

$$\langle \varphi_{E_i} | \varphi_{E_j} \rangle = \delta_{ij} \qquad (1.5)$$

The completeness relations are:

$$\sum_i |\varphi_{E_i}\rangle \langle \varphi_{E_i}| = \mathbb{1} \qquad (1.6a)$$

$$\sum_i \varphi_{E_i}^\dagger(x) \varphi_{E_i}(x') = \sigma(x - x') \qquad (1.6b)$$

It is trivial to show that the orthonormality condition on the single particle basis set leads to a similar orthonormality condition on the expansion coefficients:

$$\sum_{E_1, \ldots, E_N} |c(E_1, \ldots, E_N, t)|^2 = 1 \qquad (1.7)$$

This means that the square modulus is nothing else than the probability and that the coefficients can be interpeted as *probability amplitude.*

Moreover, we suppose that the particles are indistinguishable: it means that if we take the square modulus of the particles wave function and we interchange the pair of particles we should obtain the same quantity:

$$|\psi(x_1, \ldots, x_i, \ldots, x_j, \ldots, t)|^2 = |\psi(x_1, \ldots, x_j, \ldots, x_i, \ldots, t)|^2$$

so ψ incorporates the particle statistics. The N-body wave function could be *symmetric* or *antisymmetric* in the upon the exchange of two particles.

$$\psi(x_1, \ldots, x_i, \ldots, x_j, \ldots, t) = \pm\psi(x_1, \ldots, x_j, \ldots, x_i, \ldots, t) \qquad (1.8)$$

Again, since we are considering the expansion of ψ, we obtain the same condition for the expansion coefficients:

$$c(E_1, \ldots, E_i, \ldots, E_j, \ldots, t) = \pm c(E_1, \ldots, E_j, \ldots, E_i, \ldots, t) \qquad (1.9)$$

where the $+$ sign refers to the kind of particles called **boson**, while the $-$ sign refers to **fermion**.

We assume that the $\{E_k\}$ sum over an infinite set of *ordered* quantum numbers $\varepsilon_1, \varepsilon_2, \ldots$ with values increasing. For example, if we consider the energy, we suppose that the quantum numbers go to increasing single particles energies (essentially they are the eigenvalues of the single particle of the system).

In this description, we have included both bosons and fermions, but now, for a while, we will consider only bosons. Indeed, since in the case of boson we have a plus sign the situation, it is simpler to introduce the new formalism of second quantization.

1.3.1 Case: bosons particles

Let us consider the case of only bosons particles. Another important concept to introduce, in order to write the Schrödinger equation in second quantization, is the one of **occupation number**. Let us start with an example.

Occupation number

Example 3

How many times is ε_i present in the particular set $\{E_1, \ldots, E_N\}$ (where $i = 1, \ldots, N$ is a single particle index)? Let us consider a system with only three particles ($N = 3$) and let us suppose that our coefficients can be written as:

$$c(E_1, E_2, E_3, t) = c(\varepsilon_5, \varepsilon_3, \varepsilon_2, t)$$

This means that

- $E_1 = \varepsilon_5$, hence the 1st particle is in the ε_5 state;

- $E_2 = \varepsilon_3$, hence the 2nd particle is in the ε_3 state;

- $E_3 = \varepsilon_2$, hence the 3rd particle is in the ε_2 state.

Then, by expliciting the syemmtry of c we can order (for example by assuming creasing values of ε_i numbers) and re-group (in case of multiple occupation) the eigenvalues:

- eiganvalue 1: empty;

- eigenvalue 2: occupied (1);

- eigenvalue 3: occupied (1);

- eigenvalue 4: empty;

- eigenvalue 5: occupied (1);

- eigenvalue $i \geq 6$: empty. Let us note that the index i now refers to the eigenvalue index that is different from the particle index.

Now, it is convenient to introduce new coefficients which emphasize the occupation numbers:

$\bar{c}$ coefficients

$$\bar{c}(n_1, n_2, \ldots, n_\infty, t)$$

where n_1 refers to the occupation number of the 1st level. For instance, in the above example we can write the new coefficients as $\bar{c}(0, 1, 1, 0, 1, 0, \ldots, 0, t)$. The occupation number concept is a crucial point. In fact, given that we cannot distinguish particles, what is important is how many particles occupied a given state rather than which state a given particle occupies.

Remark. This is the first step to introduce a quantum field theory approach, where the particles are to be interpreted as quanta of a specific field.

Using the normalization condition, we arrive to the result:

$$\sum_{E_1,\ldots,E_N} |c(E_1,\ldots,E_N,t)|^2 = 1 = \sum_{\substack{n_1,n_2,\ldots,n_\infty \\ \left(\sum_{i=1}^\infty n_i = N\right)}} \sum_{\substack{E_1,\ldots,E_N \\ (n_1,n_2,\ldots,n_\infty)}} |c(E_1,\ldots,E_N,t)|^2$$
(1.10)

where the green sum is a sum over occupation number set consistent with the total particle number N costraint, while the yellow sum is the sum over quantum number set consistent with the particular occupation number set fixed.

Then, by exploiting the symmetry of c we obtain new $\bar{c}$ coefficients:

$$\sum_{\substack{n_1,n_2,\ldots,n_\infty \\ \left(\sum_{i=1}^\infty n_i = N\right)}} |\bar{c}(n_1,n_2,\ldots,n_\infty,t)|^2 \sum_{\substack{E_1,\ldots,E_N \\ (n_1,n_2,\ldots,n_\infty)}} 1 = 1 \qquad (1.11)$$

where the red term is equivalent to the problem of locating N identical objects in an infinite number of boxes, so that we have n_1 objects in the first box, n_2 objects in the second box and so on. By considering all the possibilities, this can be done in a number of ways that is equal to

$$\frac{N}{n_1! n_2! \ldots n_\infty!}$$

Example 4

For instance, let us consider only $N = 3$ particles. We want to check all the possible ways to put $n_1 = 2$ particles in the first box, $n_2 = 1$ in the second one and no particle in all the other boxes. Computing the factorial of the occupation numberm we obtain:

$$\frac{N}{n_1! n_2! \ldots n_\infty!} = \frac{3!}{2!1!\ldots 1!} = 3$$

(remember that $0! = 1 = 1!$). It corresponds to the different particles that can occupy the second state which has occupation equal to one.

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f coefficients

It is convenient to define a new (normalized) coefficient:

$$f(n_1,n_2,\ldots,n_\infty,t) \equiv \left(\frac{N!}{n_1! n_2! \ldots n_\infty!}\right)^{1/2} \bar{c}(n_1,n_2,\ldots,n_\infty,t) \qquad (1.12)$$

that is related to the coefficient $\bar{c}$ up to a multiplicative factor. It has the propoerty of being normalized:

$$\sum_{\substack{n_1,n_2,\ldots,n_\infty \\ \left(\sum_{i=1}^N n_i = N\right)}} |f(n_1,n_2,\ldots,n_\infty,t)|^2 = 1$$

Hence, the f coefficients correspond to the probability of having n_1 particles in the ε_1 state, n_2 in ε_2 and so on.

Let us rewrite the original N-body wave function as a function of single particle wave function with the f coefficients as weights:

Expansion of the N-body wave function

$$\psi(x_1, \ldots, x_N, t) = \sum_{E_1, \ldots, E_N} c(E_1, \ldots, E_N, t)\varphi_{E_1}(x_1) \ldots \varphi_{E_N}(x_N)$$

$$= \sum_{\substack{n_1, n_2, \ldots, n_\infty \\ (\sum_{i=1}^N n_i = N)}} \bar{c}(n_1, n_2, \ldots, n_\infty, t) \sum_{\substack{E_1, \ldots, E_N \\ (n_1, n_2, \ldots, n_\infty)}} \varphi_{E_1}(x_1) \ldots \varphi_{E_N}(x_N)$$

$$\overset{(a)}{=} \sum_{\substack{n_1, n_2, \ldots, n_\infty \\ (\sum_{i=1}^N n_i = N)}} f(n_1, n_2, \ldots, n_\infty, t)\Phi_{n_1 n_2 \ldots n_\infty}(x_1, x_2, \ldots, x_N)$$

$$\equiv \sqrt{\frac{\prod_i n_i!}{N!}} \sum_{\substack{E_1, \ldots, E_N \\ (n_1, n_2, \ldots, n_\infty)}} \varphi_{E_1}(x_1) \ldots \varphi_{E_N}(x_N)$$

where in (a) we have simplified the formula by defining a new set of many body N-particle wave functio Φ which is in any case independent on time. Hence, we are been able to express the original time dependent N-body wave function into a set of *completely symmetric* (under the exchange of 2 particles) function Φ, which also obey the **orthonormality condition**:

$$\int dx_1 \ldots dx_N \, \Phi^\dagger_{n'_1 n'_2 \ldots n'_\infty}(x_1, \ldots, x_N)\Phi_{n_1 n_2 \ldots n_\infty}(x_1, \ldots, x_N) = \delta_{n'_1, n_1} \ldots \delta_{n'_\infty n_\infty}$$

To summarize, the original N-body wave function ψ can be expanded in a *complete* and *orthonormal* basis set made of *completely symmetrized* functions defined in terms of *occupation numbers*: $\{\Phi_{n_1 \ldots n_\infty}(x_1, \ldots, x_N)\}$.

Example 5

In the previous example of the 3 spinless bosons, we had: $n_1 = 2, n_2 = 1$ and $n_i = 0$ for $i > 2$ (all the other states are empty). In this case, the function Φ is defined as:

$$\Phi_{210\ldots0}(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}\Big[\varphi_1(x_1)\varphi_1(x_2)\varphi_2(x_3) + \varphi_1(x_1)\varphi_2(x_2)\varphi_1(x_3)$$
$$+ \varphi_2(x_1)\varphi_1(x_2)\varphi_1(x_3)\Big]$$

where we have a normalization factor and the sum of the three possibilities corresponding to the three possible ways of distribution the three particles satisfying the constraint of the occupation number above choosen.

Now, let us make a step further. We remember that implicitily we are working in coordinate representation space, $\varphi = \langle x|\varphi \rangle$; hence, we can write the N-body wave function formally as

$$\Phi_{n_1 n_2 \ldots n_\infty}(x_1, \ldots, x_N) = \langle x_1 \ldots x_N | n_1 \ldots n_\infty \rangle$$

where $\{|n_1 n_2 \ldots n_\infty \rangle\}$ is the set of **abstract state vectors** (independent on time) in the Hilbert space, with $n_i \geq 0 \, \forall i$. In this way, these vectors are no more linked to a specific space representation: we have the only essential information concerning the list of occupation numbers, with the constraint that the occupation number must be positive.

Abstract representation

Clearly, due to the property of the original wave function it is easy to check that this basis set has the correct property:

- It must be **orthogonal**: $\langle n'_1 n'_2 \ldots n'_\infty | n_1 n_2 \ldots n_\infty \rangle = \delta_{n'_1 n_1} \delta_{n'_2 n_2} \ldots \delta_{n'_\infty n_\infty}$.

- It must be **complete**: $\sum_{n_1 n_2 \ldots n_\infty} |n_1 n_2 \ldots n_\infty \rangle\langle n_1 n_2 \ldots n_\infty | = \mathbb{1}$.

In order to manipulate the abstract state vectors, we introduce suitable (bosonic), time-independent operators: $b_k, b_k^\dagger$ so that they satisfy the following *commutaion rules*[1]:

$$\begin{cases} [b_k, b_{k'}] = [b_k^\dagger, b_{k'}^\dagger] = 0 \\ [b_k, b_{k'}] = \delta_{k,k'} \end{cases} \tag{1.13}$$

which are the same commutaion rules for the "creation" and "destruction" operator of the quantum harmonic oscillator. For the harmonic oscillator, the combination of these operators gives the so called **number operator** $\hat{n}_k$:

$$b_k^\dagger b_k \left| n_k \right\rangle \equiv \hat{n}_k \left| n_k \right\rangle = n_k \left| n_k \right\rangle \tag{1.14}$$

By applying it into a state characterized by an occupation number $\left| n_k \right\rangle$ it gives the corresponding state multiplyed by the occupation number itself.

Let us focus on a given state k:

$$\hat{n} = b^\dagger b$$

is **hermitian**. In particular, it means that

$$\hat{n} = b^\dagger b = \left(b^\dagger b \right)^\dagger = \hat{n}^\dagger$$

This relation implies that the eigenvalues are real which is consistent with our assumption and that $\hat{n}$ is also **positive definite**:

$$n = \left\langle n \right| b^\dagger b \left| n \right\rangle = \sum_m \left\langle n \right| b^\dagger \left| m \right\rangle \left\langle m \right| b \left| n \right\rangle = \sum_m \left| \left\langle m \right| b \left| n \right\rangle \right|^2 \geq 0$$

where we have inserted the completness relation and then we wrote the square modulus. We have shown that the eigenvalues are non negative. Eventually, as said, the interpretation of the $\hat{n}$ is number particle operator.

Since we have $[b, b^\dagger] = bb^\dagger - b^\dagger b = 1$ (for a given state $k = k'$), we obtain two important relations:

$$[b^\dagger b, b] = b^\dagger bb - bb^\dagger b = -b \tag{1.15a}$$

$$[b^\dagger b, b^\dagger] = b^\dagger bb^\dagger - b^\dagger b^\dagger b = b^\dagger \tag{1.15b}$$

By applying this operator to the state $\left| n \right\rangle$ and using the above relations, we obtain:

$$b^\dagger b(b \left| n \right\rangle) = b \left(b^\dagger b \right) \left| n \right\rangle - b \left| n \right\rangle = b \left(b^\dagger b - 1 \right) \left| n \right\rangle$$
$$= b(\hat{n} - 1) \left| n \right\rangle = (n-1)b \left| n \right\rangle$$

It means that if the state $\left| n \right\rangle$ is an eigenstate of the operator $\hat{n} = b^\dagger b$ with eigenvalue n, $b \left| n \right\rangle$ is eigenstate of $\hat{n}$ with eigenvalue $(n-1)$:

$$b \left| n \right\rangle \rightarrow \left| n - 1 \right\rangle$$

so we refers to b as the *destruction operator*: it reduces the occupation number of a given state by a factor 1, one particle. Similarly, $b^\dagger \left| n \right\rangle$ is eigenstate of $\hat{n}$ with eigenvalue $(n+1)$:

$$b^\dagger \left| n \right\rangle \rightarrow \left| n + 1 \right\rangle$$

and we refers to $b^\dagger$ as the *creation operator*.

More precisely, by taking the normalization condition into account, we obtain:

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[1]The commutator is defined as $[a, b] \equiv ab - ba$.

- For the **destruction operator** b: $(\langle n| b)^{\dagger}(b\,|n\rangle) = \langle n|\, b^{\dagger}b\,|n\rangle = n = n\,\langle n-1|n-1\rangle$. Hence,

$$b\,|n\rangle = \sqrt{n}\,|n-1\rangle \qquad\qquad (1.16)$$

- For the **creation operator** $b^{\dagger}$: $\left(\langle n|\, b^{\dagger}\right)^{\dagger}\left(b^{\dagger}\,|n\rangle\right) = \langle n|\, bb^{\dagger}\,|n\rangle = \langle n|n\rangle + \langle n|\, b^{\dagger}b\,|n\rangle = 1 + n = (1+n)\,\langle n+1|n+1\rangle$. Finally:

$$b^{\dagger}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad\qquad (1.17)$$

Remark. Applying b many times eventually give "0" (*empty state*) and the $|n\rangle$ state can be obtained by applying the creation operator $b^{\dagger}$ "n" times to it.

Until now, for simplicity, we have made some considerations focusing on just a given state, so now we want to see what happens if we generalize this definition to all the states of our system. In fact, this procedure can be generalized to many levels[2] and the generic state can be obtained by repeated applications of $b_{k}^{\dagger}$ operators to the "vacuum" (empty) state $|0\rangle$. To be more precise: *Generic state*

$$|n_1 n_2 \dots n_\infty\rangle = \frac{\left(b_1^{\dagger}\right)^{n_1}}{\sqrt{(n_1+1)!}}\frac{\left(b_2^{\dagger}\right)^{n_2}}{\sqrt{(n_2+1)!}}\cdots\frac{\left(b_\infty^{\dagger}\right)^{n_\infty}}{\sqrt{(n_\infty+1)!}}\,|0\rangle$$

where of course we have to include the normalization factors.

Let us come back to the original Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x_1,\dots,x_N,t) = H\psi(x_1,\dots,x_N,t) = (T+V)\psi(x_1,\dots,x_N,t)$$

where, in the Hamiltonian, we have a single-particle and one-body term (T), and a two-particle and interacting potential energy term (V). In particular, the explicit expression of the kinetic energy term is

$$T = \sum_{k=1}^{N} T_k = \sum_{k=1}^{N}\left(-\frac{\hbar^2\boldsymbol{\nabla}_k^2}{2m}\right)$$

and by definition only acts on one particle. For instance, by fixing k as quantum number, it can only act on the corresponding single particle wave function $\varphi_{E_k}(x_k)$.

Now we expand the N-body wave function considering a superposition of single particle wave functions, where the weights are the time dependent c coefficients. In particular, we use the E' notations because it is convenient for the subsequent demsotration. The expansion is:

$$\psi(x_1,\dots,x_N,t) = \sum_{E_1',\dots,E_N'} c(E_1',\dots E_N',t)\varphi_{E_1'}(x_1)\dots\varphi_{E_N'}(x_N)$$

Considering that the wave functions are orthonormal:

$$\int \mathrm{d}x_i\,\varphi_{E_i}^{\dagger}(x_i)\varphi_{E_i'}(x_i) = \delta_{E_i'E_i}$$

lets multiply the right hand of the Schrödinger equation by product of the wave functions $\varphi_{E_i}^{\dagger}(x_i)$ and then integrate over all the coordinates of the particles. The result is: *Focus on the kinetic term*

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[2]Recall that the occupations numbers operators relative to different states commute: $[\hat{n}_k, \hat{n}_{k'}] = 0$ if $\vec{k} \neq \vec{k}'$.

$$\int \mathrm{d}x_1 \ldots \mathrm{d}x_N \, \varphi_{E_1}^\dagger(x_1) \ldots \varphi_{E_N}^\dagger(x_N) \sum_{k=1}^N T_k \sum_{E_1',\ldots,E_N'} c(E_1',\ldots E_N',t) \varphi_{E_1'}(x_1) \ldots \varphi_{E_N'}(x_N) =$$

$$= \sum_{k=1}^N \sum_{E_k'} c(E_1,\ldots,\boxed{E_k'},\ldots,E_N,t) \int \mathrm{d}x_k \, \varphi_{E_k}^\dagger(x_k) T_k \varphi_{E_k'}(x_k)$$

where for a given k, E_k' can be different from E_k. What happens is that since the kinetic term only acts to the corresponding single particle wave function, if k has a given value, essentially the sum is eliminated due to the presence of the delta terms, for all the terms. It means that only the E_i' reduces to the i state on the left with an exception for the term relative to the k state, because in this case the coefficients can be different. In other words, in the sum $\sum_{E_i'} c(E_i')$ the only term that survies is the sum over E_k'.

This procedure can be applied also to the potential energy term and for the left hand of the Schrödinger equation. For the latter, the procedure is trivial, while for the potential energy the computing is more complicated (see [1] for details), because we have to consider pairs of particles, so we will implicitly assumed to do this. The Schrödinger equation transform as:

$$i\hbar \frac{\partial}{\partial t} c(E_1,\ldots,E_N,t) = \sum_{k=1}^N \sum_{E_k} c(E_1,\ldots,E_k',\ldots,E_N,t) \langle \varphi_{E_k}| T |\varphi_{E_k}\rangle + (\ldots V \ldots)$$

(1.18)

Basically, by considering this equation and focusing on the kinetic energy contribution, we note that only the difference between the coefficients c in both sides is that in the right term we have the E_k' term instead of E_k on the left.

By focusing on the kinetic term and introducing the occupation number coefficients:

$$\sum_{k=1}^N \sum_{E_k'} c(E_1,\ldots,E_k',\ldots,E_N,t) \langle \varphi_{E_k}| T \left|\varphi_{E_k'}\right\rangle =$$

$$= \sum_{k=1}^N \sum_{E_k'} \bar{c}(n_1,n_2,\ldots,(n_{E_k}-1),\ldots,(n_{E_k}+1),\ldots,t) \langle \varphi_{E_k}| T \left|\varphi_{E_k'}\right\rangle$$

Now we can replace the sum over k (sum of total number of particles, $k = 1,\ldots,N$) with the sum over *states* that forms an infinite set of levels (the sum is infinite). We can do this because every time we observe that E_k assume the same value in the summation over k (for ex. E), it gives the same contribution to the sum (since the particles are indistinguishable); if it occurs n_E times:

$$\sum_{k=1}^N \to \sum_E n_E$$

To make the notation more symmetric we replace E_k' with w. Eventually, we obtain

$$\sum_E \sum_w n_E \bar{c}(n_1,\ldots,(n_E-1),\ldots,(n_w+1),\ldots,n_\infty,t) \langle E| T |w\rangle \qquad (1.19)$$

Example 6

The last procedure is not completely easy to understand at first glance and to better understand why it works it is better to make an exercise. Let us consider for instance the simple case of $N = 3$ particles. The occupation numbers in this quantum states are $n_1 = 2, n_2 = 1$. If we try to repeat the procedure followed for the general case for a very simple case, by considering all the possibilities of the sum, we should easily understand that we can replace the sum by multiplying it for the occupation number of the state n_E.

Now, we remember that the $\bar{c}$ cofficients are also defined by f cofficients. The relation is:

$$\bar{c}(n_1, \ldots, n_\infty, t) = \sqrt{\frac{\prod_i n_i!}{N!}} f(n_1, \ldots, n_\infty, t)$$

To make the notation even more symmetric (using the same notation of [1]), in the double sum we replace the E and w state with i and j. If we consider the result in Eq. (1.19) and if we consider the relation between $\bar{c}$ and f, we arrive easily at the new form of the Schrödinger equation as a function of the f coefficients:

$$i\hbar \frac{\partial}{\partial t} f(n_1, \ldots, n_\infty, t) \sqrt{\frac{\prod_i n_i!}{N!}} = \sum_{i,j=1}^{\infty} n_i f(n_1, \ldots, (n_i - 1), \ldots, (n_j + 1), \ldots, n_\infty, t) \cdot$$

$$\cdot \sqrt{\frac{\prod_l {}^{"} n_l!}{N!} (n_j + 1)!(n_i + 1)!} \langle i | T | j \rangle + (\ldots V \ldots)$$

(1.20)

where, as said, for the potential energy term contribution we have assumed to have done the same procedure however we have not done it explicitly. In particular, the $\prod {}^{"}$ means the productory with $l \neq i$ and $l \neq j$. In fact, we have:

$$\prod_i n_i! = \prod_l {}^{"} n_l! n_i! n_j!$$

$$(n_j + 1)! = (n_j + 1) n_j!$$

$$(n_i - 1)! = \frac{n_i!}{n_i}$$

and we can rewrite very easily the constant factor in this way:

$$n_i \sqrt{\prod_l {}^{"} n_l!(n_j + 1)!(n_i - 1)!} = \sqrt{n_i}\sqrt{(n_j + 1)}\sqrt{\prod_i n_i!}$$

The Schrödinger becomes:

$$i\hbar \frac{\partial}{\partial t} f(n_1, \ldots, n_\infty, t) = \sum_{i,j}^{\infty} \sqrt{n_i}\sqrt{n_j + 1}$$

$$\cdot f(n_1, \ldots, (n_i - 1), \ldots, (n_j + 1), \ldots, n_\infty, t) \langle i | T | i \rangle + (\ldots V \ldots)$$

We can also consider

$$|\psi(t)\rangle = \sum_{n_1 \ldots n_\infty} f(n_1, \ldots, n_\infty, t) |n_1, \ldots, n_\infty\rangle$$

and write

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \sum_{n_1, \ldots, n_\infty} \langle i | T | j \rangle f(n_1, \ldots, (n_i - 1), \ldots, (n_j + 1), \ldots, n_\infty, t) \cdot$$

$$\cdot \sqrt{n_i}\sqrt{n_j + 1} |n_1, \ldots, n_\infty\rangle + (\ldots V \ldots)$$

Now, let us change the occupation numbers by introducing a new set:

$$\begin{cases} n_i' \equiv n_i - 1 \\ n_j' \equiv n_j + 1 \\ n_k' \equiv n_k \qquad (k \neq i, j) \end{cases}$$

with the constraint

$$\sum_l n_l' = \sum_l n_l = N$$

Remark. It is possible to sum the new occupation numbers over exactly the same values of the original ones, because $\sqrt{n_i}\sqrt{n_j + 1} = 0$ for $n_j' = 0$ and $n_i' = -1$. In fact,

- $n_j' = 0$ would correspond to $n_j = -1$ that is absent in the original sum, because occupation numbers can be not negative. Hence, $\sqrt{n_j + 1} = 0$.

- $n_i' = -1$ is absent in the new sum, but $n_i = 0$ implies $\sqrt{n_i} = 0$.

By considering now the n' occupation number we arrive to this expression:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \sum_{\substack{n_1' \ldots n_\infty' \\ (\sum_i n_i' = N)}} \sum_{i,j} \langle i| T |j\rangle f(n_1', \ldots, n_i', \ldots, n_j', \ldots, n_\infty', t) \cdot$$
$$\cdot \sqrt{(n_i' + 1)} \sqrt{n_j'} |\ldots (n_i' + 1) \ldots (n_j' + 1) \ldots\rangle + (\ldots V \ldots) \tag{1.22}$$

If we now recall the definition of the (bosonic) creation and destruction operators (with the proper normalization):

$$b_k |n_k\rangle = \sqrt{n_k} |n_k - 1\rangle$$
$$b_k^\dagger |n_k\rangle = \sqrt{n_k + 1} |n_k + 1\rangle$$

clearly we see that we can write:

$$\sqrt{(n_i' + 1)} \sqrt{n_j'} |\ldots (n_i' + 1) \ldots (n_j' - 1) \ldots\rangle = b_i^\dagger b_j |\ldots n_i' \ldots n_j' \ldots\rangle$$

Eventually, we rewrite the Schrödinger equation in a very compact way:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \sum_{i,j} \langle i| T |j\rangle b_i^\dagger b_j |\psi(t)\rangle + (\ldots V \ldots) \tag{1.24}$$

In conclusion, we have explicitly seen how we can transform the Schrödinger equation, by expressing the kinetic term in terms of the creation and destruction operators. We can say that the kinetic part of H is expressed in the **second quantization form**! We can repeat exactly the same procedure for the potential term but it is much complicated and longer. However, the strategy is very similar so we do not do it explicitly (for the final result look at [1]).

To be more precise, in the previous derivation we have implicitly assumed that in all the cases the i and j coefficients where different. In order to be complete, we have also to take into account the $i = j$ case; the result is the number operator $\hat{n}_i = b_i^\dagger b_i$. Again, this is done explicitly for the kinetic energy term, but for the potential energy contribution the computation results more complicated.

Now, summurazing the contribution corresponding to the kinetic energy term and potential energy term we can rewrite the equation in the second quantization formalism

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \tag{1.25}$$

where $\hat{H}$ is an operator in the abstract occupation-number space, expressed in terms of $b_i^\dagger$ and b_i:

$$\hat{H} = \sum_{ij} b_i^\dagger \langle i| T |j\rangle b_j + \frac{1}{2} \sum_{\substack{ij \\ kl}} b_i^\dagger b_j^\dagger \langle ij| V |kl\rangle b_l b_k \qquad (1.26)$$

Remark. In the second quantization formalism the matrix elements $\langle i| T |j\rangle$ and $\langle ij| V |kl\rangle$ are simply complex numbers, while the quantum statistics is now incorporated into the $b_i^\dagger, b_i$ operators (with their commutation properties).

Equation (1.25) and (1.26) toghether restate the Schrödinger euqation in second quantization, and all of the statistics and operator properties are contined into creation and destruction operators. The physical problem is clearly unchanged by the new formulation. In particular the coefficients f specify the connection between first and second quantization.

For every solution [1] to the original time-dependent many particle Schrödingereuqation there exists a set of expansion coefficients f. Given this set of expansion coefficients f, it is possible to construct a solution to the problem in second quantization, as shown above. Conversely, if the problem is solved in second quantization, we can determine a set of expansion coefficients f, which then yield a solution to the original time-dependent many particle Schrödinger equation.
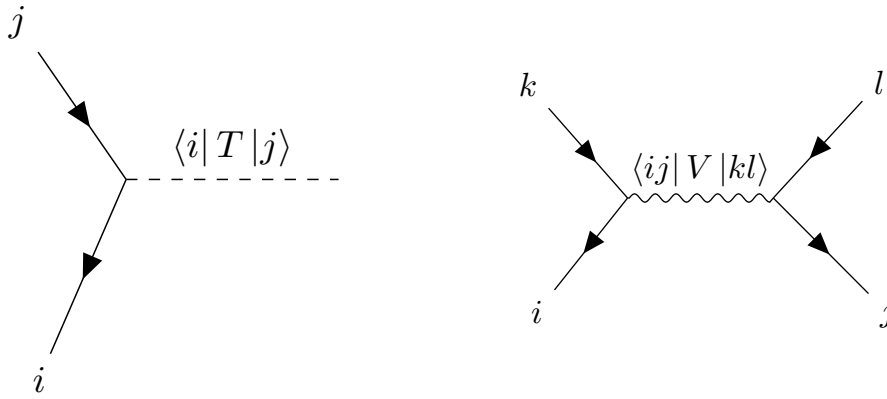
Figure 1.1: It is interesting to see a graphical representation of one and two-particle operators in the second quantization formalism. The incoming/outcoming arrows represent initial/final states. On the left, the dashed line represents the transition amplitude for one-particle process, while on the right, the sinusoidal lines represents the transition amplitude for two-particle process (for instance the Coulomb interaction). As we will see in the future, this representation is strictly connected to Feymann diagrams.

1.3.2 Case: fermions particles

Let us now repeat the same procedure for fermions particles and in particular let us decompose the N-body wave function as:

$$\psi(x_1, \ldots, x_N, t) = \sum_{E_1, \ldots, E_N} c(E_1, \ldots, E_N, t) \varphi_{E_1}(x_1) \ldots \varphi_{E_N}(x_N)$$

The difference is that now the time dependent c coefficients are antisymmetric in order to respect the symmetry of the system:

$$c(\ldots, E_1, \ldots, E_j, \ldots, t) = -c(\ldots, E_j, \ldots, E_i, \ldots, t)$$

Hence we should have $E_i \neq E_j$, otherwise we would obtain $c = 0$. As a conseuqnce, we cannot have two particle in the same quantum state (**Pauli exclusion principle**) and the occupation number n_i for each state can assume only the value 0 or 1. As done for the boson case, we can arrange the quantum numbers in the coefficient c in an increasing sequence as $c(\ldots, E_i^0 < E_j^0 < E_k^0, \ldots, t)$ and introduce $\bar{c}$ coefficients:

$$\bar{c}(n_1, n_2, \ldots, n_\infty, t)$$

Actually, the procedure is the same as for bosons: we want to expand the N-body wave function. The difference is that for fermions the occupation number can be only 0 or 1, hence the ψ can be written as:

$$\psi(x_1, \ldots, x_N, t) = \sum_{n_1, \ldots, n_\infty = 0}^{1} f(n_1, \ldots, n_\infty, t) \Phi_{n_1, \ldots, n_\infty}(x_1, \ldots, x_N)$$

where now the Φ N-body time independent wave function should incorporate the symmetry of the system,

$$\Phi_{n_1, \ldots, n_\infty}(x_1, \ldots, x_N) = \sqrt{\frac{\prod_i n_i!}{N!}} \det \begin{bmatrix} \varphi_{E_1^0}(x_1) & \cdots & \varphi_{E_1^0}(x_N) \\ & \vdots & \\ \varphi_{E_N^0}(x_1) & \cdots & \varphi_{E_N^0}(x_N) \end{bmatrix} \tag{1.27}$$

where we are considering the normalized determinant (**Slater determinant**). The first line in the matrix corresponds to the occupation of the first state by all the possible particle of the system and similarly for the other rows.

The $\{\Phi(\ldots)\}$ forms a complete set of orthonormal, antisymmetric, time-independent many-particle wave functions. Hence, by going from the coordinate space representation ($\Phi_{n_1 \ldots n_\infty}(x_1, \ldots, x_N) = \langle x_1 \ldots x_N | n_1 \ldots n_\infty \rangle$) to the *abstract* occupation number space we obtain:

$$|\psi(t)\rangle = \sum_{n_1, \ldots, n_\infty} f(n_1, \ldots, n_\infty, t) |n_1, \ldots, n_\infty\rangle$$

where there is the well known connection between the f coefficients and $\bar{c}$ coefficients:

$$f(n_1, \ldots, n_\infty, t) = \sqrt{\frac{N!}{\prod_i n_i!}} \bar{c}(n_1, \ldots, n_\infty, t)$$

As for bosons, at this stage we should define suitable operators working in this abstract occupation-number space in such a way they incorporate the correct fermionic statistic[3]:

$$\begin{cases} \{a_i, a_j\} = \{a_i\dagger, a_j\dagger\} = 0 & \Rightarrow \begin{matrix} a_i a_j = -a_j a_i \\ a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger \end{matrix} \\ \{a_i, a_j^\dagger\} = \delta_{ij} \end{cases} \tag{1.28}$$

Let us check that these rules give the correct statistics (in particular, the occupation number cannot be larger than 1):

- Two particle cannot occupy the same state:

$$a_i^2 = \frac{1}{2}\{a_i, a_i\} = a_i^{\dagger 2} = \frac{1}{2} = \{a_i^\dagger, a_j^\dagger\} = 0 \Rightarrow a_i^\dagger a_i^\dagger |0\rangle = 0$$

---

[3]The **anticommutator** $\{\ldots\}$ is defined as $\{A, B\} \equiv AB + BA$

- The occupation number operator is defined as $\hat{n}_i = a_i^\dagger a_i$ and has the correct properties (for fermions), in fact:

$$\hat{n}_i^2 = a_i^\dagger a_i a_i^\dagger a_i = a_i^\dagger (1 - a_i^\dagger a_i) a_i = a_i^\dagger a_i - \underbrace{a_i^{\dagger 2}}_{=0} \underbrace{a_i^2}_{=0} = a_i^\dagger a_i = \hat{n}_i$$

Hence, $\hat{n}_i$ is a **projector** which has the property that eigenvalues can be 0 or 1.

Moreover, remember that for bosons we have introduced also this additional relationship in Eq. (1.15). The same relations also hold for fermions

Commutation properties

$$[a_i^\dagger a_i, a_j^\dagger] = a_j^\dagger \delta_{ij} \tag{1.29a}$$

$$[a_i^\dagger a_i, a_j] = -a_j \delta_{ij} \tag{1.29b}$$

Proof of (1.29a). Let us demonstrate explicitely only the first relation:

$$[a_i^\dagger a_i, a_j^\dagger] = a_i^\dagger a_i a_j^\dagger - a_j^\dagger a_i^\dagger a_i$$

$$= a_i^\dagger a_i a_j^\dagger \left(+a_j^\dagger a_i^\dagger a_i - a_i^\dagger a_j^\dagger a_i \right) - a_j^\dagger a_i^\dagger a_i$$

$$= a_i^\dagger \underbrace{\{a_i, a_j^\dagger\}}_{=\delta_{ij}} - \underbrace{\{a_i^\dagger, a_j^\dagger\}}_{=0} a_i = a_j^\dagger \delta_{ij}$$

∎

Now, if we consider the commutator between the occupation number operators:

$$[\hat{n}_i, \underbrace{\hat{n}_j}_{a_j^\dagger a_j}] = \hat{n}_i a_j^\dagger a_j - a_j^\dagger a_j \hat{n}_i$$

$$= \hat{n}_i a_j^\dagger a_j \left(-a_j^\dagger \hat{n}_i a_j + a_j^\dagger \hat{n}_i a_j \right) - a_j^\dagger a_j \hat{n}_i \tag{1.30}$$

$$= [\hat{n}_i, a_j^\dagger] a_j + a_j^\dagger [\hat{n}_i, a_j]) = [a_i^\dagger a_i, a_j^\dagger] a_j + a_j^\dagger [a_i^\dagger a_i, a_j]$$

$$= a_j^\dagger \delta_{ij} a_j + a_j^\dagger (-a_j \delta_{ij}) = 0$$

we can see that $\hat{n}_i$ and $\hat{n}_j$ commute: it allows the simultaneous diagonalization of the set $\{\hat{n}_i\}$, inline with the definition of the occupation number state vectors.

Giving these rules we can now write the generlalize abstract vector in this way:

Generic state

$$|n_1 n_2 \ldots n_\infty\rangle = \left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} \ldots \left(a_\infty^\dagger\right)^{n_\infty} |0\rangle \tag{1.31}$$

recalling that $\left(a_i^\dagger\right)^{n_i} = 0 \, \forall n_i > 1$ because of the exclusion principle. In particular:

$$a^\dagger |0\rangle = |1\rangle \quad a^\dagger |1\rangle = 0$$
$$a |0\rangle = 0 \qquad a |1\rangle = |0\rangle$$

Due to the anticommutator rules $(a_j^\dagger a_k^\dagger = -a_k^\dagger a_j^\dagger)$ it is essential to keep track of signs, for instance consider the action of $a_j^\dagger$ into the state:

Phase factor S_j

$$a_j^\dagger |n_1, n_2, \ldots, n_\infty\rangle = a_j^\dagger \left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} \ldots \left(a_\infty^\dagger\right)^{n_\infty} |0\rangle$$

$$\overset{\text{if} j \neq 1}{=} \left(a_1^\dagger\right)^{n_1} a_j^\dagger (-1)^{n_1} \left(a_2^\dagger\right)^{n_2} \ldots |0\rangle$$

$$\overset{\text{if} j \neq 2}{=} \left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} a_j^\dagger (-1)^{n_1} (-1)^{n_2} \ldots |0\rangle$$

$$= \ldots \ldots$$

At the end one gets to $\left(a_j^\dagger\right)^{n_j}$:

$$a_j^\dagger \left|n_1, n_2, \ldots, n_\infty\right\rangle = \underbrace{(-1)^{n_1+n_2+\cdots+n_{j-1}}}_{\equiv \text{phase factor} S_j} \left|n_1, \ldots (n_j+1) \ldots n_\infty\right\rangle$$

that is a state where we have and additional particle if the j state was empty $(n_j = 0)$, otherwise, if the state was already occupied $(n_j = 1)$, we get 0. The difference with the boson case is that now we have to take into account the **phase factor** S_j. Similarly if we apply the destruction operator:

$$a_j \left|n_1, n_2, \ldots, n_\infty\right\rangle = S_j \left|n_1, \ldots (n_j+1) \ldots n_\infty\right\rangle$$

Moreover, by combining the action of the two operators we have no phase factor:

$$a_j^\dagger a_j \left|\ldots n_j \ldots\right\rangle = n_j \left|\ldots n_j \ldots\right\rangle$$

Hence, we have seen efinition and properties for creation and destruction operators for fermions; now we can repeat the same derivation as for bosons starting from the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \left|\psi(t)\right\rangle = \hat{H} \left|\psi(t)\right\rangle$$

We introduce the c coefficients and we write the corresponding equation for them, by focusing on the kinetic term:

$$i\hbar \frac{\partial}{\partial t} c(E_1, \ldots, E_N, t) = \sum_{k=1}^{N} \sum_{E_k'} c(E_1, \ldots, E_k', \ldots, E_N, t) \left\langle E_k\right| T \left|E_k'\right\rangle \qquad (1.33)$$

the procedure is similar, but with the crucial difference that by reordering the quantum numbers on both sides of the equation one must carefully keep track of phase factors, since we are dealing with fermions.

At the end of the derivation [1]:

$$(-1)^{S_j - S_i} \left|\ldots (n_i'+1) \ldots (n_j'-1) \ldots\right\rangle = a_i^\dagger a_j \left|n_1' \ldots n_\infty'\right\rangle$$

We obtain an expression for H in SQ which is formally equal (the quantum statistic difference is incorporated in the properties of the $a_i, a_i^\dagger$ operators!) to that for bosons:

$$\hat{H} = \sum_{ij} a_i^\dagger \left\langle i\right| T \left|j\right\rangle a_j + \frac{1}{2} \sum_{\substack{ij \\ kl}} a_i^\dagger a_j^\dagger \left\langle ij\right| V \left|kl\right\rangle \; a_l a_k \qquad (1.34)$$

where the ordering of the final two operators in green is crucial (for bosons was irrelevant because the operators commute) to get that $\hat{H}$ is *hermitian* and correct (if the order is inverted a minues sign appears in the potential energy term!).

Remark. The formal expression for the kinetic energy term:

$$\hat{T} \equiv \sum_{ij} a_i^\dagger \left\langle i\right| T \left|j\right\rangle a_j$$

can be generalized for any single-particle operator; for example to the total moment can be expressed as

$$\hat{\vec{p}} = \sum_{ij} a_i^\dagger \left\langle i\right| \vec{p} \left|j\right\rangle a_j$$

1.4 Field operators

Now, we make a step further considering but we still consider the second quantization formalism. Let us define **field operators** formed by the linear combination of creation and destruction operators: they create and destroy particles in a *selected* point $\vec{\mathbf{x}}$:

$$\begin{cases} \hat{\psi}_\alpha(\vec{\mathbf{x}}) \equiv \sum_{\vec{\mathbf{k}}} \varphi_{\vec{\mathbf{k}},\alpha}(\vec{\mathbf{x}}) a_{\vec{\mathbf{k}},\alpha} \\ \hat{\psi}^\dagger_\alpha(\vec{\mathbf{x}}) \equiv \sum_{\vec{\mathbf{k}}} \varphi^\dagger_{\vec{\mathbf{k}},\alpha}(\vec{\mathbf{x}}) a^\dagger_{\vec{\mathbf{k}},\alpha} \end{cases} \tag{1.35}$$

Creation and destruction field operators

where in the specific case of fermions we have the wave vector index $\vec{\mathbf{k}}$ and the spin index α. We can see that by considering a linear combination of the creation and destruction operators with coefficients $\varphi_{\vec{\mathbf{k}},\alpha}$, that are single-particle wave functions, we obtain new operators which depend on the spatial space coordinates. Moreover, the $\sum_k$ in the creation field operator can be interpreted as the sum of all possible ways to add a particle at position $\vec{\mathbf{x}}$ through any of the basis states $\varphi_{\vec{\mathbf{k}},\alpha}$.

Crearly, for a *homogeneous* system of electrons we can consider the single-particle wave function made by normalized plane wave

$$\varphi_{\vec{\mathbf{k}},\alpha}(\vec{\mathbf{x}}) = \frac{e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}}{\sqrt{V}} \eta_\alpha$$

where V is the volume and η_α the spin function which can be $(1\ 0)^T$ or $(0\ 1)^T$.

For example, we want to write the kinetic term in second quantization using these new fields:

Kinetic term with field operators

$$\sum_{ij} a_i^\dagger \langle i| T |j\rangle a_j \underset{\substack{i\to\vec{\mathbf{k}},\alpha \\ j\to\vec{\mathbf{k}},\beta}}{\longrightarrow} \sum_{\substack{\vec{\mathbf{k}}\alpha \\ \vec{\mathbf{k}}\beta}} a^\dagger_{\vec{\mathbf{k}}\alpha} \left(\int \mathrm{d}^3 x\, \varphi^\dagger_{\vec{\mathbf{k}}\alpha}(\vec{\mathbf{x}}) \left(-\frac{\hbar^2 \boldsymbol{\nabla}_x^2}{2m} \right) \varphi_{\vec{\mathbf{k}}\beta}(\vec{\mathbf{x}}) \right) a_{\vec{\mathbf{k}},\beta} \sigma_{\alpha\beta}$$

$$= \sum_{\alpha\beta} \delta_{\alpha\beta} \int \mathrm{d}^3 x \underbrace{\left(\sum_{\vec{\mathbf{k}}\alpha} \varphi^\dagger_{\vec{\mathbf{k}}\alpha}(\vec{\mathbf{x}}) a^\dagger_{\vec{\mathbf{k}}\alpha} \right)}_{\hat{\psi}^\dagger_\alpha(\vec{\mathbf{x}})} \left(-\frac{\hbar^2 \boldsymbol{\nabla}_x^2}{2m} \right) \underbrace{\left(\sum_{\vec{\mathbf{k}}\beta} \varphi^\dagger_{\vec{\mathbf{k}}\beta}(\vec{\mathbf{x}}) a^\dagger_{\vec{\mathbf{k}}\beta} \right)}_{\hat{\psi}_\beta(\vec{\mathbf{x}})}$$

$$= \int \mathrm{d}^3 x \sum_{\alpha\beta} \hat{\psi}^\dagger_\alpha(\vec{\mathbf{x}}) \underbrace{\left(-\frac{\hbar^2 \boldsymbol{\nabla}_x^2}{2m} \right)}_{T(\vec{\mathbf{x}})} \hat{\psi}_\beta(\vec{\mathbf{x}}) \delta_{\alpha\beta}$$

where in the first step we have explicitly expressed the matrix element, where the kinetic energy term is diagonal on the spin index. Then we have grouped these terms and we have seen that the combinations obtained correspond to the field creation and destruction operators. Finally we have written the expression in function of these fields.

It is easy to demonstrate that these new field operators, since are nothing else of linear combination of the previous defined creation and destruction operators, satisfy the same commutation or anticommutation relations. For instance for fermions

$$\{\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{\psi}^\dagger_\beta(\vec{\mathbf{x}}')\} = \sum_{\vec{\mathbf{k}}\vec{\mathbf{k}}'} \psi_{\vec{\mathbf{k}},\alpha}(\vec{\mathbf{x}}) \psi^\dagger_{\vec{\mathbf{k}}',\beta}(\vec{\mathbf{x}}') \underbrace{\{a_{\vec{\mathbf{k}},\alpha}, a^\dagger_{\vec{\mathbf{k}}',\beta}\}}_{\delta_{\vec{\mathbf{k}},\vec{\mathbf{k}}'}\delta_{\alpha\beta}} = \sum_{\vec{\mathbf{k}}} \psi_{\vec{\mathbf{k}},\alpha}(\vec{\mathbf{x}}) \psi^\dagger_{\vec{\mathbf{k}},\beta} \delta_{\alpha\beta}$$

$$= \sum_{\vec{\mathbf{k}}} \langle \vec{\mathbf{x}}| \left| \psi_{\vec{\mathbf{k}},\alpha} \right\rangle \underbrace{\left\langle \psi_{\vec{\mathbf{k}},\beta} \right| |\vec{\mathbf{x}}'\rangle}_{\text{completness}} \delta_{\alpha\beta} = \delta(\vec{\mathbf{x}} - \vec{\mathbf{x}}') \delta_{\alpha\beta}$$

Bosons	Fermions	Field Operators
Commutation rules		
$[b_k, b_{k'}^\dagger] = \delta_{k,k'}$	$\{a_r, a_s^\dagger\} = \delta_{r,s}$	$[\hat{\psi}_\alpha(x), \hat{\psi}_\beta^\dagger(x')]_\pm = \delta_{\alpha\beta}\delta(x - x')$
$[b_k, b_{k'}] = 0$	$\{a_r, a_s\} = 0$	$[\hat{\psi}_\alpha(x), \hat{\psi}_\beta(x')]_\pm = 0$
$[b_k^\dagger, b_{k'}^\dagger] = 0$	$\{a_r^\dagger, a_s^\dagger\} = 0$	$[\hat{\psi}_\alpha^\dagger(x), \hat{\psi}_\beta^\dagger(x')]_\pm = 0$
Important relations		
$[b^\dagger b, b] = -b\delta_{kk'}$	$[a_r^\dagger a_r, a_s^\dagger] = a_s^\dagger \delta_{rs}$	
$[b^\dagger b, b^\dagger] = b^\dagger \delta_{kk'}$	$[a_r^\dagger a_r, a_s] = -a_s \delta_{rs}$	

Table 1.1: Commutation rules for creation and distruction operators, where the upper $+$ sign refers to bosons, while the lower $-$ sign to fermions (respectively commutator or anticommutator).

Also the interaction potential energy term can be expressed in terms of the field operators, so that we can rewrite in SQ the Hamiltonian with the field operators:

$$\hat{H} = \sum_\alpha \int \mathrm{d}^3x\, \hat{\psi}_\alpha^\dagger(\vec{\mathbf{x}}) T(\vec{\mathbf{x}}) \hat{\psi}_\alpha(\vec{\mathbf{x}}) + \frac{1}{2} \sum_{\alpha\beta} \int \mathrm{d}^3x \int \mathrm{d}^3x'\, \hat{\psi}_\alpha^\dagger(\vec{\mathbf{x}}) \hat{\psi}_\beta^\dagger(\vec{\mathbf{x}}') V(\vec{\mathbf{x}}, \vec{\mathbf{x}}')\, \hat{\psi}_\beta(\vec{\mathbf{x}}') \hat{\psi}_\alpha(\vec{\mathbf{x}})$$

$$(1.36)$$

where the order of the two final field operators, in green, should be at it is here due to the requirement that the hamiltonian is hermitian and that the fermionic statistic is correct. The quantities $\hat{\psi}$ and $\hat{\psi}^\dagger$ are not wave functions, however, but field operators; thus in second quantization the fields are the operators and the potential and kinetic energy are just complex coefficients.

To summarize:

- in first quantization:

$$\int \mathrm{d}^3x\, \underbrace{\psi^\dagger(\vec{\mathbf{x}}) V(\vec{\mathbf{x}}) \psi(\vec{\mathbf{x}})}_{\langle \psi | V | \psi \rangle}$$

  where the ψ are wave functions.

- in second quantization:

$$\int \mathrm{d}^3x\, \hat{\psi}^\dagger(\vec{\mathbf{x}}) V(x) \hat{\psi}(\vec{\mathbf{x}})$$

  where the $\hat{\psi}$ are field operators and $V(x)$ in the middle is just a complex coefficient.

Hence, the expressions for the potential term are very similar in both first and second quantization, but there is an important difference: in the second quantization the wave function are replaced with the fields. Namely, the wave functions are "transformed" into (field) operators.

It is easy to extend the derivation to any other operator; for instance for a general, one-body operator.

Example 7: Quantum angular momentum

For example in first quantization we have this term (quantum angular momentum, but could be any one body operator):

$$J = \sum_{i=1}^{N} J(\vec{\mathbf{x}}_i)$$

where the i is a particle index. In second quantization, we can write this expression in terms of the coefficients:

$$\hat{J} = \sum_{ij} \langle i| \, J \, |j\rangle \, c_i^\dagger c_j = \int \mathrm{d}^3x \, \hat{\psi}(\vec{\mathbf{x}}) J(x) \hat{\psi}(\vec{\mathbf{x}})$$

where now ij represents state index. We pointed out that in first quantization we have a sum over particles, while here we have sum over states: we used the same letters but the meaning is completely different!

Example 8: Number density operator

A useful quantity is the **number density operator**, which in first quantization can be written as

$$n(\vec{\mathbf{x}}) = \sum_{i=1}^{N} \delta(\vec{\mathbf{x}} - \vec{\mathbf{x}}_i)$$

Now, it is an easy exercise to demonstrate that in second quantization the expression is like

$$\hat{n}(\vec{\mathbf{x}}) = \sum_{ij} \phi_{E_i}^\dagger(\vec{\mathbf{x}}) \phi_{E_i} \vec{\mathbf{x}} c_i^\dagger c_j = \int \mathrm{d}^3x \, \hat{\psi}^\dagger(\vec{\mathbf{x}}') \delta(\vec{\mathbf{x}} - \vec{\mathbf{x}}') \hat{\psi}(\vec{\mathbf{x}}') = \hat{\psi}^\dagger(\vec{\mathbf{x}}) \hat{\psi}(\vec{\mathbf{x}}')$$

The expression $\hat{n}(\vec{\mathbf{x}}) = \hat{\psi}^\dagger(\vec{\mathbf{x}}) \hat{\psi}(\vec{\mathbf{x}}')$ in second quantization is formally similar to the familiar expresssion of quantum mechanics (in first quantization):

$$n(\vec{\mathbf{x}}) = \psi^*(\vec{\mathbf{x}}) \psi(\vec{\mathbf{x}}) = |\psi(\vec{\mathbf{x}})|^2$$

that the probability density is given by the product of complex conjiugate wave function for the wave function itself, which corresponds to the square modulus of the wave function. However, the meaning is different because in the first we have fields, while in the second we have wave functions.

Example 9: Total-number operator

Similarly, the **total-number operator** in second quantization is:

$$\hat{N} = \int \mathrm{d}^3x \, n(\vec{\mathbf{x}}) = \sum_i c_i^\dagger c_i = \sum_i \hat{n}_i = \int \mathrm{d}^3x \, \hat{\psi}^\dagger(\vec{\mathbf{x}}) \hat{\psi}(\vec{\mathbf{x}})$$

this can be easily obtained just considering that the single-particle wave functions (in the field definition oeprators) are orthonormal.

It is easy to show that the commutator between the total-number operator and the Hamiltonian is zero:

$$[\hat{N}, \hat{H}] = 0 \tag{1.37}$$

hence $\hat{N}$ can be diagonalized simultaneously with $\hat{H}$ (N =constant).
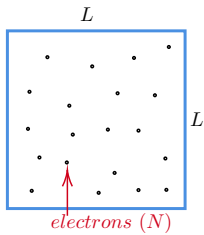
In conclusion, the second quantization formalism is just an alternative way to reformulate the original Schr*ö*dinger equation. Now the idea is trying to apply it to our N-body problem.

1.5   Application: Jellium model

Now we try to apply the second quantization formalism to an interesting physical model: "**degenerate electron gas**" or **Jellium model**. In particular, *"degenerate matter" means we are considering matter with high density, so high that the dominant contribution to its pressure rised from the Pauli exclusion principle*: we cannot force two electrons to occupy the same quantum state.

Many systems in the universe obey this property. For instance:

- electron gas in ordinary metals (Drude-Sommerfiled theory of metals);

- plasma;

- white dwarf stars. Ordinary stars cannot collapse due to the gravitational forcee bacause of the standard idrostatic pressure. In the interior of these particular dwarf stars, we have we have both α particles (He nuclei) and free electrons at high density, and the stability of the star is supported by the degeneracy pressure due to the Pauli exlusion principle. Hence, they not collapse because we cannot compress too much the electrons system if it is at high density.

- Neutron stars: the principle is as the one for dwarf stars, but in this case the degenerate particles are not electrons but neutrons.
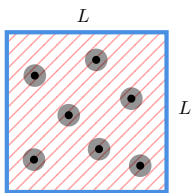
We assume that the Jellium model is included in a cubic box of side L, that is large. More specifically, we will assume that $L \to \infty$, in a way to focus only on bulk properties and to not deal with surfaces. In this box wa have essentially:

1. An interacting electron gas: N interacting electrons.

2. An uniformly distributed *positive* background, to ensure that the total system is neutral.

Let us consider the more common case of metals. A metal is constituted by free atoms merged into a solid. In particular, our system is constituted by nuclei, core electrons and ions (nuclei+core electrons) with mass M and charge $+Ze$. In a metal, while the core electrons remain rather closer to their nuclei, the so called "valence electrons" become very free and they are spread over all the system. Each valence electron has mass m and charge $-e$.

In a real metal the electron lattice potential is as in Fig. 1.4a. We have a characteristic behaviour due to the fact that electrons must move subject to the periodic potential made by positive ions. Now, in the Jellium model we make the drastic approximation to replace the periodic potential with a uniform positive background and so also the potential becomes smeared out. Hence, while in a real metal the positive charge is localized (for instance in the ionic coarse and crystal lattice), in the Jellium model the charge is uniform.

Moreover, we know that if the temperature is finite, also the ions vibrate and even at zero temperature there is the zero point energy. However, we completely neglect the ionic dinamical motion so this means that for instance we have no phonons and no lattice vibrations because only the electrons are the real dynamical variables. We also assume that we are in the thermodynamic limit, so the number of particle of electrons is very large and also the volume of the system (a cubic box) is very large, in such a way that the particle density is constant and finite.

Let us resume the drastic approximations involved in this model:

- in real metals (or in a plasma) the positive charge is not uniform, but localized in the ionic cores ("crystal lattice"). In Jellium, the positive charge is uniform

Figure 1.2: Cubic box of side L with N electrons and uniform positive background.

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Friday 20th March, 2020.
Compiled: Friday 8th May, 2020.

Figure 1.3: Cubic metal of volume L: nuclei are represented in black, core lectrons in grey and valence electron with the red pattern.

Drastical assumptions

(a) Real (metal) lattice periodic potential.

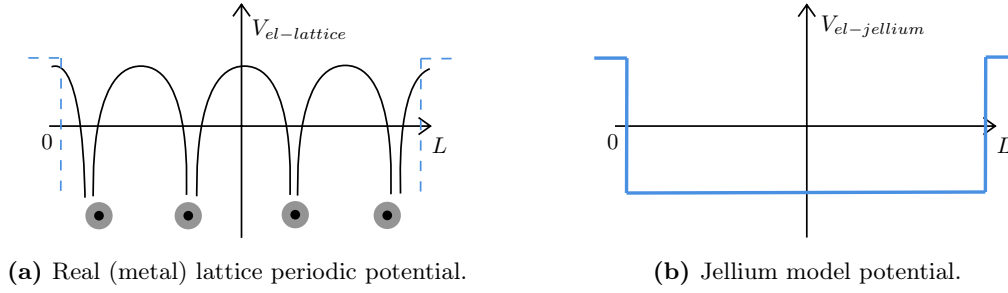(b) Jellium model potential.

Figure 1.4

distributed. The assumption of a uniform background is drastic and for this reason the present model can provide only a qualitative account of real metals.

- No dynamical motion of the positive charges (no phonons, namely lattice vibrations...), indeed the positive ions are much heavier than the electrons and it is permissible to neglect the ionic motion entirely. The dynamic motion is only the one of electrons.

- We assume thermodynamic limit: $N \to \infty$, namely $V = L^3 \to \infty$ (cubic box of side L) and with the particle density $n = N/V$ constant.

Let us write formally the total Hamiltonian of this system:

$$\hat{H} = \hat{H}_b + \hat{H}_{el-b} + \hat{H}_{el} \tag{1.38}$$

where H_b describes the positive background energy, the $\hat{H}_{el-b}$ the interaction between the electrons and positive background and the term relative to electrons $\hat{H}_{el} = \hat{T} + \hat{V}$ which has a kinetic term and a potential term which describes the electrons-electrons interaction. The last one is the most diffigult part of our N-body problem.

For simplicity since we are working with the coulomb interaction, we assume the GS unit system, namely:

$$\frac{1}{4\pi\varepsilon_0} \to 1$$

and we define also the **charge density** $\rho(\vec{\mathbf{x}})$ as a function of the **number density** $n(\vec{\mathbf{x}})$:   *Charge density*

$$\rho(\vec{\mathbf{x}}) = en(\vec{\mathbf{x}}) \tag{1.39}$$

Now, let us find the explicit expression for all the terms of the Hamiltonian in second quantization formalism.

Positive background Hamiltonian: $\hat{\mathbf{H}}_{\mathbf{b}}$

Let us start in trying to find the explicit expression for the positive background hamiltonian. It is easy to see that in principle $\hat{H}_b$ should be an operator, but actually is a purely c-number since the only dynamical variables are the electrons. Indeed, the interaction energy due to the positive background is just given by the usual electrostatic formula, where we have considered the Coulomb interaction:

$$\hat{H}_b = H_b = \frac{1}{2} \int_V \int_V \mathrm{d}^3x \, \mathrm{d}^3x' \, \frac{\rho_b(\vec{\mathbf{x}})\rho_b(\vec{\mathbf{x}'})}{|\vec{\mathbf{x}} - \vec{\mathbf{x}'}|}$$

Hence, by using the definition of ρ:

$$H_b = \frac{e^2}{2} \int_V \int_V \mathrm{d}^3x \, \mathrm{d}^3x' \, \frac{n_b(\vec{\mathbf{x}})n_b(\vec{\mathbf{x}'})}{|\vec{\mathbf{x}} - \vec{\mathbf{x}'}|}$$

$$\underset{\substack{n_b(\vec{\mathbf{x}})=n=\frac{N}{V} \\ \vec{\mathbf{y}}\equiv\vec{\mathbf{x}}-\vec{\mathbf{x}'}}}{=} \frac{e^2n^2}{2} \int_V \mathrm{d}^3x \int_V \mathrm{d}^3y \, \frac{1}{y} = 4\pi V \frac{e^2n^2}{2} \int_0^\infty \mathrm{d}y \, y \to \infty$$

where in the second step we have changed the variable in $\vec{y}$ (since is an infinite system is not a problem). We can immediately see that the integral diverge. It is a mathematical divergence, which reflects the fact that the Coulomb interaction is a long range interaction: it means that in our system every portion of the positive uniform background interact with every other portion of the same background and if we take into account all these contribution we get a divergence. Remind that, for the moment, we are just taking into account the first contribution of the Hamiltonian: the idea is that since the whole system is neutral, divergencies should disappear if we consider all the components.

In order to make the expression mathematically well defined at every step of the derivation we adopt a trick, we introduce an **artificial exponential convergence factor**:

Exponential convergence factor

$$\frac{e^2}{x} \to \frac{e^2}{x}e^{-\mu x}$$

where the constant $\mu > 0$. The idea is that at the end of the derivation since we want to recover the real Coulomb interaction, we have to take this term $\mu \to 0$ in such a way $e^{-\mu x} \to 1$. However, before to take the limit we should take the thermodynamic limit. The order of these steps is important:

1. Take the thermodynamic limit $L \to \infty, V \to \infty$.

2. Take the limit $\mu \to 0$.

It means that at every step we assume the effective range of the modified Coulomb interaction (the inverse of mu is a length!) is lower than the total size of the system:

$$\frac{1}{\mu} \ll L$$

Namely, it is no longer true that every positive portion interact with all the other positive portions. We can shift the origin of the integration freely, apart from surface corrections which are neglected, because we are interested in only bulk properties. Hence:

$$
\begin{aligned}
H_b &= 4\pi V \frac{e^2 n^2}{2} \int_0^\infty \mathrm{d}y\, y e^{-\mu y} = 4\pi V \frac{e^2 n^2}{2} \left[-\frac{y e^{-\mu y}}{\mu} \Big|_0^\infty + \frac{1}{\mu} \int_0^\infty \mathrm{d}y\, e^{-\mu y} \right] \\
&= 4\pi V \frac{e^2 n^2}{2} \left[-\frac{1}{\mu^2} e^{-\mu y} \right]_0^\infty = 4\pi V \frac{e^2 n^2}{2} \frac{1}{\mu^2} \underset{n=\frac{N}{V}}{=} \frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2} > 0
\end{aligned}
\tag{1.40}
$$

the integral is easily evaluated solved by parts. The final result is positive and consistent with what we expected: it should describe the repulsion between positive charges and in the limit $\mu \to 0$ we recover the divergence found before (every element of charge interacts with every other one).

Interaction term between electrons and background: $\hat{H}_{el-b}$

Let us analyze the interaction term between the particles and the background. Clearly, also in this case, we should have in principle a 1-body operator (electrons interact with an external field), but as we will see also we get a c-number. First, we write the electrostatic interaction between the electronic charge distribution and uniform positive one. Then, we introduce the exponential factor, we use the definition of electron density n_{el}:

$$n_{el}(\vec{x}') = \sum_{i=1}^N \delta(\vec{x}' - \vec{r}_i) \tag{1.41}$$

and we remember that he positive charge distribution is a constant $n_b(\vec{\mathbf{x}}) = n = N/V$. Making these substitution we obtain:

$$\hat{H}_{el-b} = H_{el-b} = -e^2 \int_V \int_V \mathrm{d}^3x \, \mathrm{d}^3x' \, \frac{n_{el}(\vec{\mathbf{x}}')n_b(\vec{\mathbf{x}})}{|\vec{\mathbf{x}} - \vec{\mathbf{x}}'|} e^{-\mu|\vec{\mathbf{x}} - \vec{\mathbf{x}}'|}$$

$$= -e^2 \sum_{i=1}^{N} \frac{N}{V} \int_V \mathrm{d}^3x \, \frac{e^{-\mu|\vec{\mathbf{x}} - \vec{\mathbf{r}}_i|}}{|\vec{\mathbf{x}} - \vec{\mathbf{r}}_i|} \overset{\vec{\mathbf{y}} \equiv \vec{\mathbf{x}} - \vec{\mathbf{r}}_i}{=\!=\!=} -\frac{e^2 N}{V} N \left(\int_V \mathrm{d}^3y \, \frac{e^{-\mu y}}{y} \right)$$

$$= -\frac{e^2 N^2}{V} 4\pi \underbrace{\left(\int_0^\infty \mathrm{d}y \, y e^{-\mu y} \right)}_{=1/\mu^2} = -e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2} < 0$$

The final expression is negative and this result is consistent because it describes attraction between negative electronic charge and positive charge. In particular, we note that there is a partial cancellation with the previous H_b contribution a part from an half factor. Of course, we hope that this cancellation will be perfect when we will consider the remaining term $\hat{H}_{el}$.

Electrons term: $\hat{H}_{el}$

It is the most interesting part but also the most difficult one because of the presence of the electron-electron potential term. This electron Hamiltonian written in second quantization formalism has the following expression:

$$\hat{H}_{el} = \hat{T} + \hat{V} = \sum_{ij} a_i^\dagger \langle i| T |j \rangle a_j + \frac{1}{2} \sum_{\substack{ij \\ kl}} a_i^\dagger a_j^\dagger \langle ij| V |kl \rangle a_l a_k$$

where we have creation and destruction particles and in the middle we have matrix element corresponding to the kinetic and potential energy contribution.

In order to evaluate these matrix element we should explicitly consider single-particle wave function. Since our system is uniform and infinite, all physical properties must be invariant under spatial translation, thus the natural choice is to take as single-particle wave function plane waves with *periodic boundary conditions*:

$$k_i = \frac{2\pi n_i}{L} \quad n_i = 0, \pm 1, \dots$$

To be more precise, in our specific case, the index $i = x, y, z$ is equivalent to pair of index $(\vec{\mathbf{k}}, \lambda)$. Eventually, the single-particle state can be denoted by:

$$\varphi_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}}) = \frac{e^{i\vec{\mathbf{k}} \cdot \vec{\mathbf{x}}}}{\sqrt{V}} \eta_\lambda$$

where $\vec{\mathbf{k}}$ is the wave vector, λ the spin index and the wave function is a normalized plane wave multiplied by spin wave function $\eta_\lambda = \left| \vec{\mathbf{k}}\lambda \right\rangle$.

Let us evaluate the two terms of the Hamiltonian:

- In order to evaluate the **kinetic energy term**, let us define the momentum operator, for which we have:

$$\hat{\vec{\mathbf{p}}} = -i\hbar \vec{\nabla} \quad \to \hat{p}^2 \left| \vec{\mathbf{k}}\lambda \right\rangle = \hbar^2 k^2 \left| \vec{\mathbf{k}}\lambda \right\rangle$$

namely, the spin state is an eigenstate of the momentum operator. Let us rewrite the kineti term:

$$\hat{T} \overset{(a)}{=} \sum_{\substack{\vec{\mathbf{k}}\lambda \\ \vec{\mathbf{k}}'\lambda'}} a^{\dagger}_{\vec{\mathbf{k}}\lambda} \left\langle \vec{\mathbf{k}}\lambda \right| \frac{p^2}{2m} \left| \vec{\mathbf{k}}'\lambda' \right\rangle a_{\vec{\mathbf{k}}'\lambda'} = \sum_{\substack{\vec{\mathbf{k}}\lambda \\ \vec{\mathbf{k}}'\lambda'}} \frac{\hbar^2 k^2}{2m} \delta_{\vec{\mathbf{k}}\vec{\mathbf{k}}'} \delta_{\lambda\lambda'} a^{\dagger}_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}'\lambda'}$$

$$\overset{(b)}{=} \sum_{\vec{\mathbf{k}}\lambda} \frac{\hbar^2 k^2}{2m} a^{\dagger}_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda} = \sum_{\vec{\mathbf{k}}\lambda} \frac{\hbar^2 k^2}{2m} \hat{n}_{\vec{\mathbf{k}}\lambda}$$

where in (a) we have considered that $\left| \vec{\mathbf{k}}\lambda \right\rangle$ is an eigenstate of $p^2/2m$ and the delta are due to orthonormality property of this basis set made by plane waves. In (b) we have exploit these delta functions. In the last step we have used the definition of the number operator. This expression has the meaning that to get the kinetic energy term we count the number of particles with wave-vector $\vec{\mathbf{k}}$ and spin λ. Each contribution is then multiplied by the term $\frac{\hbar^2 k^2}{2m}$.

- The procedure is more difficult for the **potential energy term**. First of all we should evaluate the matrix elements. Considering our specific case we have:

$$\langle ij| V |kl\rangle \rightarrow \left\langle \vec{\mathbf{k}}'\lambda', \vec{\mathbf{p}}'\mu' \right| V \left| \vec{\mathbf{k}}\lambda, \vec{\mathbf{p}}\mu \right\rangle =$$

$$= \int_V \mathrm{d}^3x \int_V \mathrm{d}^3x' \, \varphi^{\dagger}_{\vec{\mathbf{k}}'\lambda'}(\vec{\mathbf{x}}) \varphi^{\dagger}_{\vec{\mathbf{p}}'\mu'}(\vec{\mathbf{x}}') \overbrace{V(\vec{\mathbf{x}} - \vec{\mathbf{x}}')}^{\frac{e^2 e^{-\mu|\vec{\mathbf{x}} - \vec{\mathbf{x}}'|}}{|\vec{\mathbf{x}} - \vec{\mathbf{x}}'|}} \varphi_{\vec{\mathbf{k}}\lambda}(\vec{\mathbf{x}}) \varphi_{\vec{\mathbf{p}}\mu}(\vec{\mathbf{x}}')$$

$$= \frac{e^2}{V^2} \delta_{\lambda\lambda'} \delta_{\mu\mu'} \int_V \mathrm{d}^3x \int_V \mathrm{d}^3x' \, e^{i\vec{\mathbf{x}}\cdot(\vec{\mathbf{k}} - \vec{\mathbf{k}}')} e^{i\vec{\mathbf{x}}'\cdot(\vec{\mathbf{p}} - \vec{\mathbf{p}}')} \frac{e^{-\mu|\vec{\mathbf{x}} - \vec{\mathbf{x}}'|}}{|\vec{\mathbf{x}} - \vec{\mathbf{x}}'|}$$

where we have written explicitly in terms of the states and we have adopted the strategy to multiply by the expontential convergence term. Then we make the following substitution:

$$\vec{\mathbf{y}} \equiv \vec{\mathbf{x}} - \vec{\mathbf{x}}' \quad \rightarrow \vec{\mathbf{x}} = \vec{\mathbf{y}} + \vec{\mathbf{x}}'$$

obtaining:

$$\left\langle \vec{\mathbf{k}}'\lambda', \vec{\mathbf{p}}'\mu' \right| V \left| \vec{\mathbf{k}}\lambda, \vec{\mathbf{p}}\mu \right\rangle = \frac{e^2}{V^2} \delta_{\lambda\lambda'} \delta_{\mu\mu'} \int_V \mathrm{d}^3y \left(\int_V \mathrm{d}^3x' \, e^{i\vec{\mathbf{x}}'\cdot(\vec{\mathbf{k}} + \vec{\mathbf{p}} - \vec{\mathbf{k}}' - \vec{\mathbf{p}}')} \right) e^{i\vec{\mathbf{y}}\cdot(\vec{\mathbf{k}} - \vec{\mathbf{k}}')} \frac{e^{-\mu y}}{y}$$

Then we use an important relation, that will be exploit many times in the course:

$$\int_V \mathrm{d}^3x \, e^{i(\vec{\mathbf{k}}_2 - \vec{\mathbf{k}}_1)\cdot\vec{\mathbf{x}}} = V \delta_{\vec{\mathbf{k}}_1 \vec{\mathbf{k}}_2} \tag{1.42}$$

where the idea is that if we integrate over all the volume such term, we get that this contribution is different from zero only if $\vec{\mathbf{k}}_1$ is equal to $\vec{\mathbf{k}}_2$. In fact, by considering that the exponential is given by sum of sine and cosine (oscillating term), if the index are different, for every positive term there is a compensative negative term and overall the sum is zero. We obtain:

$$\left\langle \vec{\mathbf{k}}'\lambda', \vec{\mathbf{p}}'\mu' \right| V \left| \vec{\mathbf{k}}\lambda, \vec{\mathbf{p}}\mu \right\rangle = \frac{e^2}{V} \int_V \mathrm{d}^3y \, e^{i\vec{\mathbf{y}}\cdot(\vec{\mathbf{k}} - \vec{\mathbf{k}}')} \frac{e^{-\mu y}}{y} \delta_{\vec{\mathbf{k}} - \vec{\mathbf{k}}', \vec{\mathbf{p}}' - \vec{\mathbf{p}}} \delta_{\lambda,\lambda'} \delta_{\mu,\mu'}$$

Now, let us introduce another variable $\vec{\mathbf{q}} \equiv \vec{\mathbf{k}}' - \vec{\mathbf{k}}$, and we focus only on the first part of the last expression. We can estimate this integral by using polar, spherical coordinates: we must integrate over the solid angle

$$\mathrm{d}\Omega = \sin(\theta) \, \mathrm{d}\theta \, \mathrm{d}\varphi = - \mathrm{d}\cos(\theta) \, \mathrm{d}\varphi$$

where $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$. In particular the direction of $\vec{\mathbf{q}}$ represents the polar axis. The result is:

$$\int_V \mathrm{d}^3 y \, e^{-i\vec{\mathbf{y}}\cdot\vec{\mathbf{q}}} \frac{e^{-\mu y}}{y} = \int_0^\infty \mathrm{d}y \int \underbrace{\mathrm{d}\Omega}_{=-\mathrm{d}\cos(\theta)\mathrm{d}\varphi} y^2 \frac{e^{-\mu y}}{y} e^{-iqy\cos(\theta)}$$

$$\stackrel{t\equiv\cos(\theta)}{=} 2\pi \int_0^\infty \mathrm{d}y \, y e^{-\mu y} \underbrace{\left[\int_{-1}^1 \mathrm{d}t \, e^{-iqyt}\right]}_{\frac{e^{-iqyt}}{-iqy}\Big|_{-1}^1 = \frac{2\sin(qy)}{qy}}$$

$$= \frac{4\pi}{q} \underbrace{\left[\int_0^\infty \mathrm{d}y \, e^{-\mu y} \sin(qy)\right]}_{I}$$

where we can calculate the I integral by parts:

$$I = -\frac{e^{-\mu y}}{\mu} \cancel{\sin(qy)}\Big|_0^\infty + \frac{q}{\mu} \int_0^\infty \mathrm{d}y \, e^{-\mu y} \cos(qy)$$

$$= -\frac{q}{\mu^2} e^{-\mu y} \cos(qy)\Big|_0^\infty - \frac{q^2}{\mu^2} \underbrace{\left(\int_0^\infty \mathrm{d}y \, e^{-\mu y} \sin(qy)\right)}_{I}$$

and

$$I = \frac{q}{\mu^2} - \frac{q^2}{\mu^2} I \quad \Rightarrow I = \frac{q}{\cancel{\mu^2}} \frac{\cancel{\mu^2}}{q^2 + \mu^2} = \frac{q}{q^2 + \mu^2}$$

Eventually, we have:

$$\left\langle \vec{\mathbf{k}}'\lambda', \vec{\mathbf{p}}'\mu' \middle| V \middle| \vec{\mathbf{k}}\lambda, \vec{\mathbf{p}}\mu \right\rangle = \frac{4\pi e^2}{q^2 + \mu^2} \frac{1}{V} \delta_{\vec{\mathbf{k}}-\vec{\mathbf{k}}',\vec{\mathbf{p}}'-\vec{\mathbf{p}}} \delta_{\lambda\lambda'} \delta_{\mu\mu'}$$

This was just the matrix element but in order to obtain the complete second quantization expression for the potential energy term we should include also the creation and destruction operators and the half factor:

$$\hat{V} = \frac{e^2}{2V} \sum_{\substack{\vec{\mathbf{k}}'\lambda', \vec{\mathbf{p}}'\mu' \\ \vec{\mathbf{k}}\lambda, \vec{\mathbf{p}}\mu}} \delta_{\vec{\mathbf{k}}-\vec{\mathbf{k}}',\vec{\mathbf{p}}'-\vec{\mathbf{p}}} \delta_{\lambda\lambda'} \delta_{\mu\mu'} \frac{4\pi}{q^2 + \mu^2} a^\dagger_{\vec{\mathbf{k}}'\lambda'} a^\dagger_{\vec{\mathbf{p}}'\mu'} a_{\vec{\mathbf{p}}\mu} a_{\vec{\mathbf{k}}\lambda}$$

Remember that $\vec{\mathbf{q}} = -\vec{\mathbf{k}} + \vec{\mathbf{k}}' = \vec{\mathbf{p}} - \vec{\mathbf{p}}'$ (the second relation is because we can exploit the delta term $\delta_{\vec{\mathbf{k}}-\vec{\mathbf{k}}',\vec{\mathbf{p}}'-\vec{\mathbf{p}}}$), hence:

$$\vec{\mathbf{p}}' = \vec{\mathbf{p}} - \vec{\mathbf{q}}, \quad \vec{\mathbf{k}}' = \vec{\mathbf{k}} + \vec{\mathbf{q}}$$

Finally, the potential energy term in second quantization:

$$\hat{V} = \frac{e^2}{2V} \sum_{\substack{\vec{\mathbf{k}}\vec{\mathbf{p}}\vec{\mathbf{q}} \\ \lambda\mu}} \frac{4\pi}{q^2 + \mu^2} a^\dagger_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda} a^\dagger_{\vec{\mathbf{p}}-\vec{\mathbf{q}},\mu} a_{\vec{\mathbf{p}}\mu} a_{\vec{\mathbf{k}}\lambda}$$

where we have the sum over three wave vectors $\vec{\mathbf{k}}, \vec{\mathbf{p}}, \vec{\mathbf{q}}$ and two spin indexes λ, μ.

We can easily give a graphical representation of this process. On the bottom of Fig.1.5 we can see the effect of the two destruction operators $a_{\vec{\mathbf{p}}\mu} a_{\vec{\mathbf{k}}\lambda}$: we destroy the two particles $\vec{\mathbf{k}}_\lambda$ and $\vec{\mathbf{p}}_\mu$. Then, since we have two creation operators, as
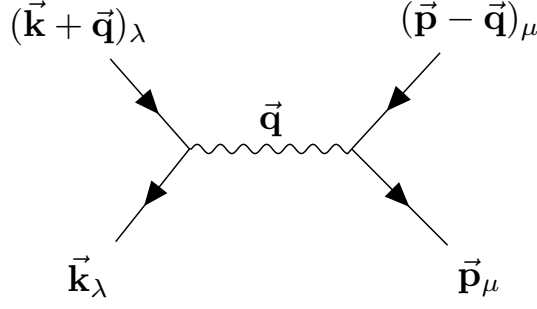
Figure 1.5: Graphical representation of the potential energy term in second quantization.

a consequence of the Coulomb interaction $\vec{q}$, we create two particles: $\left(\vec{k} + \vec{q}\right)$ with spin λ and $(\vec{p} - \vec{q})$ with spin μ. In particular, it is interesting to note that the particle with wave vector $\vec{k}$ is changed by the term $+\vec{q}$, while the other one ,$\vec{p}$, is changed by $\vec{q}$ in such a way that the total momentum of the system is conserved, namely by $-\vec{q}$. Hence, if one particle gains a momentum, the momentum is removed by the other in a way to be conserved, consistently with the assumption of considering a uniform system.

In summary, we have derived the second quantization form of the interaction potential term as a function of creation and destruction operators.

Now, in order to proceed, it is convenient to split the sum $\sum_{\vec{k},\vec{p},\vec{q}}$ into two parts: a part corresponding to $\vec{q} = 0$ and the rest containing terms with $\vec{q} \neq 0$.

Firstly, let us consider the $\vec{q} = 0$ term:

$$\hat{V}(\vec{q} = 0) = \frac{e^2}{2V} \frac{4\pi}{\mu^2} \sum_{\substack{\vec{k}\vec{p} \\ \lambda\mu}} a^{\dagger}_{\vec{k}\lambda} \; \boxed{a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu} a_{\vec{k}\lambda}}$$

By recalling the commutation rules:

$$[\hat{n}_{\vec{p}\mu}, a_{\vec{k}\lambda}] = [a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu}, a_{\vec{k}\lambda}] = \boxed{a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu} a_{\vec{k}\lambda}} - a_{\vec{k}\lambda} a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu} = -\delta_{\vec{k}\vec{p}} \delta_{\mu\lambda} a_{\vec{k}\lambda}$$

where the green term is corresponding to the green term in the $\hat{V}(\vec{q} = 0)$ contribution; hence, we can rewrite:

$$a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu} a_{\vec{k}\lambda} = a_{\vec{k}\lambda} a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu} - \delta_{\vec{k}\vec{p}} \delta_{\mu\lambda} a_{\vec{k}\lambda} = a_{\vec{k}\lambda} \left(a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu} - \delta_{\vec{k}\vec{p}} \delta_{\mu\lambda} \right)$$

Eventually, we can rewrite:

$$\hat{V}(\vec{q} = 0) = \frac{e^2}{2V} \frac{4\pi}{\mu^2} \sum_{\substack{\vec{k}\vec{p} \\ \lambda\mu}} \underbrace{a^{\dagger}_{\vec{k}\lambda} a_{\vec{k}\lambda}}_{\hat{n}_{\vec{k}\lambda}} \left(\underbrace{a^{\dagger}_{\vec{p}\mu} a_{\vec{p}\mu}}_{\hat{n}_{\vec{p}\mu}} - \delta_{\vec{k}\vec{p}} \delta_{\mu\lambda} \right)$$

$$\stackrel{(a)}{=} \frac{e^2}{2V} \frac{4\pi}{\mu^2} \underbrace{\left(\sum_{\vec{k}\lambda} \hat{n}_{\vec{k}\lambda} \right)}_{\hat{N}} \underbrace{\left(\sum_{\vec{p}\mu} \hat{n}_{\vec{p}\mu} \right)}_{\hat{N}} - \frac{e^2}{2V} \frac{4\pi}{\mu^2} \underbrace{\left(\sum_{\vec{k}\lambda} \hat{n}_{\vec{k}\lambda} \right)}_{\hat{N}}$$

$$\stackrel{(b)}{=} \frac{e^2}{2V} \frac{4\pi}{\mu^2} \left(\hat{N}^2 - \hat{N} \right) \stackrel{(c)}{=} \frac{e^2}{2V} \frac{4\pi}{\mu^2} \left(N^2 - N \right)$$

where in (a) we have separated the two sum over $\vec{k}$ and $\vec{p}$ and in (b) we have noted that by definition the sum of the number operator over all the wave vectors and spins gives the operator $\hat{N}$. Actually, in (c) we treated it as a c-number ($\hat{N} \rightarrow N$) because we are working with a constant number of particles and, in particular, this operator commutes with the total hamiltonian: $[\hat{H}, \hat{N}] = 0$.

We should also consider the thermodynamic limit: first of all we let $V \rightarrow \infty$ and the we take the limit $\mu \rightarrow 0$. Let us remind that the correct order is important, indeed the energy is an extensive quantity and if we consider the energy per particle we obtain:

$$\frac{e^2}{2V}\frac{4\pi}{\mu^2}(N^2 - N)\frac{1}{N} = \frac{e^2}{2}\frac{4\pi}{\mu^2}\left(\frac{N}{V}\right) - \frac{e^2}{2}\frac{4\pi}{\mu^2}\frac{1}{V}$$

where the second term vanishes in the thermodynamic limit, while we take μ finite in a way such that the above equation is describes a well defined quantity.

In practice, our $\vec{q} = 0$ contribution reduces to:

$$\hat{V}(\vec{q} = 0) \simeq \frac{e^2}{2}\frac{4\pi}{\mu^2}\frac{N^2}{V} > 0$$

that is a repulsion term between electrons (to be more precise, since $\vec{q} = 0$ it is a repulsion between *uniform* portion of electrons).

If we now sum this term to the others two terms H_b and H_{el-b}, we get that the results is equal to zero:

$$H_b + H_{el-b} + \hat{V}(\vec{q} = 0) = 0$$

In other words, $\hat{V}(\vec{q} = 0)$ completely cancels the remaining divergences that we had before. This is what we expected, since the system is neutral and that if we come back to the original expression of $\hat{V}$ (without the splitting of the sum), what remains is just the expression were we restrict to the sum over $\vec{q}$ different from zero:

Cancel divergences

$$\hat{V} = \frac{e^2}{2V}\sum_{\substack{\vec{k}\vec{p}\vec{q}\\\lambda\mu}}' \frac{4\pi}{q^2 + \mu^2}a^\dagger_{\vec{k}+\vec{q},\lambda}a^\dagger_{\vec{p}-\vec{q},\mu}a_{\vec{p}\mu}a_{\vec{k}\lambda}$$

where we have written the sum as $\sum'$ just to remember that we must take into account only the $\vec{q} \neq 0$ contribution. Of course, now there are no longer convergence problems and we can safely take the limit $\mu \rightarrow 0$, in such a way to recover the genuine Coulomb interaction and we obtain:

$$\hat{V} = \frac{e^2}{2V}\sum_{\substack{\vec{k}\vec{p}\vec{q}\\\lambda\mu}}' \frac{4\pi}{q^2}a^\dagger_{\vec{k}+\vec{q},\lambda}a^\dagger_{\vec{p}-\vec{q},\mu}a_{\vec{p}\mu}a_{\vec{k}\lambda}$$

Hence, the $\vec{q} \neq 0$ terms describe the electron-electron interactions that survive after the divergences cancellation.

Total Hamiltonian

Finally, the complete Hamiltonian of the degenerate electron gas is the following:

Hamiltonian of the system in second quantization

$$\hat{H} = \sum_{\vec{k}\lambda}\frac{\hbar^2 k^2}{2m}a^\dagger_{\vec{k}\lambda}a_{\vec{k}\lambda} + \frac{e^2}{2V}\sum_{\substack{\vec{k}\vec{p}\vec{q}\\\lambda\mu}}' \frac{4\pi}{q^2}a^\dagger_{\vec{k}+\vec{q},\lambda}a^\dagger_{\vec{p}-\vec{q},\mu}a_{\vec{p}\mu}a_{\vec{k}\lambda} \qquad (1.43)$$

where the first term corresponds to the kinetic energy term and the second one to the potential energy term where we have to remember that in the sum we should

consider only $q \neq 0$ terms. Hence, up to now we have not done nothing new: we have only rewritten the Hamiltonian in the second quantization form both for the kinetic and potential terms.

In order to proceed we need to do a further observation: this Jellium model is drastic approximation of a real metal and of course we have missed the information of some characteristic properties of a real metal such as the lattice parameter, the interatomic distance and so on and so forth. Essentially, our model is just characterized by two quantities, i.e. the two characteristic lengths of the system:

Characteristic lengths: r_0 and a_0

- the **interparticle distance** (electron-electron), which is called r_0. Imagine we assign a small spherical volume V_0 to each electron, the total volume can be written as (it is not possible to fill the whole space, but we have in mind only the order of magnitude of r_0):

$$V_0 = \frac{4\pi}{3} r_0^3 \quad \rightarrow V = N V_0 = \frac{4\pi}{3} r_0^3 N$$

where N is the total number of particles. Clearly, using this expression one can immediately write the expression of the r_0 parameter:

$$V_0 = \frac{V}{N} = \frac{1}{n} \quad \rightarrow r_0 = \left(\frac{3}{4\pi n} \right)^{1/3}$$

This distance is important because because even though we have no special property in our Jellium model, in order to mimic real metal behavior, what we can do is to define the density and thus we can define the interparticle distance r_0.

- the **Bohr radius** a_0 is a relevant distance because the kind of interaction between electron-electron and backgorund-electrons is a Coulomb one. In particular, the Bohr radius corresponds to the radius of the Hydrogen atom in its ground state in which there is a Coulomb interaction between the electron and the proton of the atom. Hence, the Bohr radius is another characteristic length which is related to the kind of interaction which acts in our system.

The dimensionless ratio between these two lengths results:

$$r_s \equiv \frac{r_0}{a_0}$$

which corresponds to the interparticle spacing in terms of the Bohr radius and characterizes the density of the system.

Remark. r_s is a common parameter to characterize the Jellium model, for instance by taking into account the density of real metals, the value of r_s is between 2 and 6.

Now, since we have introduce those two parameters r_0, a_0 and this dimensionless quantity r_s, we can also define other dimensionless quantities as:

$$\bar{V} \equiv \frac{V}{r_0^3}, \quad \bar{\vec{k}} \equiv r_0 \vec{k}, \quad \bar{\vec{p}} \equiv r_0 \vec{p}, \quad \bar{\vec{q}} \equiv r_0 \vec{q}$$

For example:

- for the *kinetic term*:

$$a_0 = \frac{\hbar^2}{me^2} \quad \rightarrow \frac{\hbar^2}{m} = a_0 e^2$$

- for the *potential term*:

$$\frac{e^2}{V} \frac{1}{q^2} = \frac{e^2}{\bar{V} r_0^3} \frac{r_0^2}{\bar{q}^2} = \frac{e^2}{\bar{V} \bar{q}^2} \frac{1}{r_s a_0} = \left(\frac{e^2}{2a_0} \right) \frac{2}{r_s^2} \frac{r_s}{\bar{V} \bar{q}^2}$$

Now, by taking into account this change in term of dimensionless variable, we can rewrite the Hamiltonian in second quantization in this way:

$$\hat{H} = \frac{e^2}{a_0 r_s^2} \left(\underbrace{\sum_{\vec{k}\lambda} \frac{1}{2} \bar{k}^2 a_{\vec{k}\lambda}^\dagger a_{\vec{k}\lambda}}_{\hat{H}_0} + \underbrace{\frac{r_s}{2\bar{V}} {\sum_{\vec{k}\vec{p}\vec{q}}}' \sum_{\lambda\mu} \frac{4\pi}{\bar{q}^2} a_{\vec{k}+\vec{q},\lambda}^\dagger a_{\vec{p}-\vec{q},\mu}^\dagger a_{\vec{p}\mu} a_{\vec{k},\lambda}}_{\hat{H}_1} \right) = \frac{e^2}{a_0 r_s^2} \left(\hat{H}_0 + \hat{H}_1 \right)$$

(1.44)

where we have inside the parenthesis the same quantities as before, with the only difference that we have replaced the quantities with their correspondent dimensionless one and we have the r_s parameter in the potential energy term. Note that the term in front of the parenthesis can be written also as:

$$\frac{e^2}{a_0 r_s^2} = \left(\frac{e^2}{2a_0} \right) \frac{2}{r_s^2} = (1 \text{ Ryd}) \cdot \frac{2}{r_s^2}$$

where $1 \text{ Ryd} = 13.6 \,\text{eV}$, the neutral unit for the energy (the ground state energy of the hydrogen atom).

Perturbative approach

The most important result is that we can rewrite schematically the Hamiltonian as the sum of $\hat{H}_0$ and $\hat{H}_1$ contributions, where the first term is just the kinetic term and the second term is the potential interaction term, which is multiplied by the r_s parameter. The latter, is the goal of this derivation because it implies that as $r_s \to 0$, the potential energy becomes a small perturbation. It is a contro-intuitive result, because it means that in high-density limit the electron-electron interaction becomes smaller with respect to the kinetic dominant contribution. In practice, in the so high-density limit, we expect that a perturbative approach, starting from a non interacting system, is possible even though the Coulomb potential is neither weak nor short-range.

Perturbative approach

One could expect that just considering few terms in the perturbative approach could give a good result. Unfortunately, while one can easily evaluate the *leading term* in the interaction energy (i.e. the 1st order perturbation theory), several problems appear considering higher-oders (for instance the 2nd order term diverges logarithmically!). The total energy can be rewritten as:

Total energy in perturbative form

$$E = \frac{Ne^2}{a_0 r_s^2} \left(a + br_s + cr_s^2 \ln r_s + \dots \right)$$

(1.45)

where the green term represents a constant, the yellow term the 1st order approximation term and the red term the 2nd order one, where we can see the exponential divergence in the limit $r_s \to 0$.

To summarize, we have shown that the potential energy of our Jellium model becomes a small perturbation as the density of the system becomes higher, i.e. in the limit $r_s \to 0$. We have also anticipated that unfortunately it is not trivial to perform a perturbative approach just considering few orders in the perturbative expansion, because yet in the second term one find problems. More specifically, we will see it will be necessary to consider an infinite number of terms in order to have convergence of the result.

Now we evaluate the a and b parameters, namely the first two terms in the perturbative series (the zero order correction and the first order one).

Unperturbed hamiltonian $\hat{H}_0$

Let us start considering

$$\hat{H}_0 = \sum_{\vec{\mathbf{k}}\lambda} \frac{\hbar^2 k^2}{2m} a_{\vec{\mathbf{k}}\lambda}^\dagger a_{\vec{\mathbf{k}}\lambda} = \sum_{\vec{\mathbf{k}}\lambda} \frac{\hbar^2 k^2}{2m} \hat{n}_{\vec{\mathbf{k}}\lambda}$$

that is the unperturbed Hamiltonian representing a *non-interacting* Fermi system (while $\hat{H}_1$ is the small perturbation). In practice, this is the zero order term in the perturbative approach, which as expected is easy to treat because in this term we describe only non-interacting particles. Now, the problem is what is our system when the particle are non interacting, the idea is simple: the system obeys the Pauli exclusion principle. Indeed, due to the Pauli exclusion principle each momentum (or wave vector) eigenstate (each single-particle state) can be occupied by only two electrons: one with spin-up and one with spin-down. Essentially, the *ground state* of the non-interacting degenerate electron gas is the so called **Fermi sphere** , a sphere in the momentum space (or in the reciprocal space), and the ground state is represented as $|F\rangle$. In particular, inside the sphere we have all the occupied states, while outside the empty ones. The Fermi sphere is thus obtained by filling it with single-particle states up to a *maximum value* (depending on the total number of particles), that is called the **Fermi momentum**:

$$p_F = \hbar k_F$$

that is the product of the **Fermi wave vector** per $\hbar$. Clearly, the occupied states are denoted by states where:

$$\left| \vec{\mathbf{k}} \right| \leq \left| \vec{\mathbf{k}}_F \right|$$

We have to respect also the boundary conditions:

$$\vec{\mathbf{k}} = \frac{2\pi}{L}\vec{\mathbf{n}}$$

Thus, the spacing between the $\vec{\mathbf{k}}$ value is:

$$\Delta k_\alpha = \frac{2\pi}{L} \quad \alpha = x, y, z \quad \rightarrow \left| \Delta \vec{\mathbf{k}} \right| = \frac{(2\pi)^3}{L^3}$$

it corresponds to a small cube assigned in the reciprocal space to every state $\left| \Delta \vec{\mathbf{k}} \right|$.
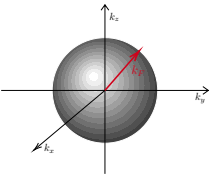
Now, lets try to make the sum over all these states::

$$\sum_{|\vec{\mathbf{k}}| \leq k_F} 1 = \frac{N}{2}$$

this must be equal to the total number of particle divided by a factor 2, because ,due to spin degeneracy, every single state characterized by a given value of the $\vec{\mathbf{k}}$ wave vector can be occupied by up to two electrons (spin-up and spin-down). Now, it is convenient to work in the thermodynamic limit $L \to \infty$ to replace the discrete sum with an integral over $\vec{\mathbf{k}}$ (it is convenient because in general we know better how to solve and integral than the corresponding sum). In practice we can transform the sum into an integral as follow:

$$\sum_{\vec{\mathbf{k}}} = \sum_{\vec{\mathbf{k}}} \frac{\left|\Delta\vec{\mathbf{k}}\right|}{\left|\Delta\vec{\mathbf{k}}\right|} = \frac{1}{\left|\Delta\vec{\mathbf{k}}\right|} \sum_{\vec{\mathbf{k}}} \left|\Delta\vec{\mathbf{k}}\right| \overset{L\to\infty}{\to} \frac{V}{(2\pi)^3} \int d\vec{\mathbf{k}} \qquad (1.46)$$

Fermi sphere

Figure 1.6: Fermi sphere.

In practice, in our specific case:

$$\sum_{|\vec{\mathbf{k}}|\leq k_F} \overset{L\to\infty}{\Rightarrow} \frac{V}{(2\pi)^3}\int_{|\vec{\mathbf{k}}|\leq k_F} \mathrm{d}\vec{\mathbf{k}} = \frac{V}{(2\pi)^3}\boxed{\frac{4\pi}{3}k_F^3} = \frac{N}{2}$$

where the green term is the volume of the Fermi sphere. With such a relation we can directly relate the Fermi wave vector k_F to the particle density (N/V):

$$k_F = \left(3\pi^2 n\right)^{1/3} \sim n^{1/3}$$

Let us evaluate the 0-order term in the perturbative approach, i.e. the energy for the non-interacting system:

$$E_0 = \langle F|\,\hat{H}_0\,|F\rangle = \sum_{\vec{k}\lambda} \frac{\hbar^2 k^2}{2m}\,\langle F|\,\hat{n}_{\vec{\mathbf{k}}\lambda}\,|F\rangle$$

which is just the kinetic energy contribution and it is estimated by taking the matrix element between the unperturbed ground state. Then, we have written it in second quantization and since by its definition the effect of the number operator multiplied to a state just gives the occupation of the state itself and since $\hat{n}_{\vec{\mathbf{k}}\lambda}$ refers to the wave vector $\vec{\mathbf{k}}$ with spin λ, this gives:

$$\begin{cases} \hat{n}_{\vec{\mathbf{k}}\lambda}\,|F\rangle = |F\rangle & \text{if } \left|\vec{\mathbf{k}}\right| \leq k_F \\ \hat{n}_{\vec{\mathbf{k}}\lambda}\,|F\rangle = 0 & \text{if } \left|\vec{\mathbf{k}}\right| > k_F \end{cases}$$

with the normalization condition on the ground state $\langle F|F\rangle = 1$.

Clearly, we can easily evaluate the matrix element in E_0:

$$E_0 = 2\sum_{|\vec{\mathbf{k}}|\leq k_F} \frac{\hbar^2 k^2}{2m}$$

where the 2 factor derives from the sum over the spins λ (for each state it can be occupied by two electrons with spin-up and spin-down). Now, we go to the thermodynamic limit and since the integral depends only on the modulus of $\vec{\mathbf{k}}$ we can immediately evaluate the spherical integral in the second step. Hence, the total energy the ground state of the non-interacting system results:

$$E_0 \overset{L\to\infty}{\Rightarrow} \frac{V}{(2\pi)^3}2\int_{|\vec{\mathbf{k}}|\leq k_F} \mathrm{d}\vec{\mathbf{k}}\,\frac{\hbar^2 k^2}{2m} = \frac{V}{(2\pi)^3}2\frac{4\pi\hbar^2}{2m}\int_0^{k_F} \mathrm{d}k\,k^4$$

$$= \frac{V\hbar^2}{2\pi^2 m}\frac{k_F^5}{5} \overset{k_F^3=3\pi^2\frac{N}{V}}{=} \frac{3}{5}\underbrace{\left(\frac{\hbar^2 k_F^2}{2m}\right)}_{\varepsilon_F}N = \frac{3}{5}\varepsilon_F N$$

where we have defined the **Fermi energy** as ε_F. Let us notice that: *Fermi energy*

$$\frac{E_0}{N} = \frac{3}{5}\varepsilon_F > 0$$

so if we compute the energy per particle, the result is positive (the Fermi energy is of order of few eV) and in particular, even at zero temperature (remind that we implictly assume that we are working at $T = 0$) the total energy of the system is not zero but finite and positive. As said, this is a consequence of the Pauli exclusion principle, because when we try to occupy the states in the Fermi sphere, with particle

different from bosons, we cannot put all the electrons in the lowest energy state but we should occupy also states at finite energy.

Now, let us manipulate a little the expression of k_F^3:

$$k_F^3 = 3\pi^2 n = \frac{3\pi^2}{V_0} = \frac{3\pi^2 3}{4\pi r_0^3} = \frac{9\pi}{4 r_0^3} = \frac{9\pi}{4 r_s^3 a_0^3}$$

where V_0 is the small volume associated to each electron. Hence, the Fermi energy can be expressed as:

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2 a_0^2} = \left(\frac{e^2}{2a_0}\right)\underbrace{\left(\frac{1}{e^2}\frac{\hbar^2}{ma_0}\right)}_{=1}\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2} = \left(\frac{e^2}{2a_0}\right)\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2}$$

where the yellow term is equal to 1 because is just the definition of the Bohr radius. Thus we can write:

$$E_0 = \frac{3}{5}\left(\frac{e^2}{2a_0}\right)\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2}N = 2.21\underbrace{\left(\frac{e^2}{2a_0}\right)}_{=1\text{Ryd}}\frac{1}{r_s^2}N = \frac{2.21}{r_s^2}N\,\text{Ryd}$$

where we have estimated the numerical value using the definition of Rydberg, namely the ground state energy of the Hydrogen atom. The energy is an extensive quantity and as expected it is proportional to the number of particle:

$$E_0 \sim N$$

Moreover, the energy E_0 goes as the inverse of the square of r_s:

$$E_0 \sim \frac{1}{r_s^2}$$

this is the zero order perturbative expansion of E (see Eq.(1.45)). It means that E_0 is larger if the density is high, so if $r_s \to 0$ (i.e. if the volume per particle is small). From a physical point of view this means that the kinetic energy contribution is larger for a more concentrated system. Clearly, we can also understand this behavior also on the basis of the *uncertainty principle*: if we force particles to be very close to each other (because of the high density), we constrain their position to be very close but the uncertainty principle has as a consequence that there is a large uncertainty on the momentum. Hence, the kinetic energy which is proportional to the square of momentum, is large.

To summarize, we have evaluated the ground state energy for non-interacting system and since non-interacting behavior its evaluation was relatively easy. Then we have seen that this term has a larger value, if the density of the system system is high. The next step is try to evaluate the first order correction, in particular we should try to compute the b parameter.

Lecture 6.
Friday 27th March, 2020.
Compiled: Friday 8th May, 2020.

First order correction

First order correction $\hat{H}_1$

Now, let us evaluate the first order correction term. Clearly, in the perturbative approach, the **first order correction** term is obtained just by taking the matrix element of the potential energy term between the non-interacting Fermi ground state:

$$E^{(1)} = \langle F|\,\hat{H}_1\,|F\rangle = \frac{e^2}{2V}\sideset{}{'}\sum_{\vec{k}\vec{p}\vec{q}}\sum_{\lambda\mu}\frac{4\pi}{q^2}\langle F|\,a^\dagger_{\vec{k}+\vec{q},\lambda}a^\dagger_{\vec{p}-\vec{q},\mu}a_{\vec{p}\mu}a_{\vec{k}\lambda}\,|F\rangle$$

where we have

$$a_{\vec{\mathbf{p}}\mu}a_{\vec{\mathbf{k}}\lambda}\left|F\right\rangle \neq 0 \quad \text{only if } \left|\vec{\mathbf{k}}\right| \leq k_F, |\vec{\mathbf{p}}| \leq k_F$$

and

$$\left\langle F\right| a_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}^{\dagger}a_{\vec{\mathbf{p}}-\vec{\mathbf{q}},\mu}^{\dagger} = \left(a_{\vec{\mathbf{p}}-\vec{\mathbf{q}},\mu}a_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}\left|F\right\rangle\right)^{\dagger} \neq 0 \quad \text{only if } \left|\vec{\mathbf{k}}+\vec{\mathbf{q}}\right| \leq k_F, |\vec{\mathbf{p}}-\vec{\mathbf{q}}| \leq k_F$$

where the condition is such that the wave vectors are inside the Fermi sphere. Hence the matrix element $\left\langle F\right|\hat{H}_1\left|F\right\rangle$ can be different from zero only if certain conditions apply. In particular, the first two destruction operators $a_{\vec{\mathbf{p}}\mu}a_{\vec{\mathbf{k}}\lambda}$ destroy two particles while the other two creation operators $a_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}^{\dagger}a_{\vec{\mathbf{p}}-\vec{\mathbf{q}},\mu}^{\dagger}$ create two particles and, in order that the action of these last two creation operators gives a result different from zero, they should act on an empty state. More specifically, the matrix element can be different from zero only if the two creation operators exactly fill up the holes made by the two destruction operators, namely two particles are destroyed and then two additional particles are created in exactly the same state inside the Fermi sphere. By considering the wave vector index of these operators, there are only two possibilities:

$$\begin{cases} \vec{\mathbf{k}}+\vec{\mathbf{q}} = \vec{\mathbf{k}} & (\lambda = \lambda) \\ \vec{\mathbf{p}}-\vec{\mathbf{q}} = \vec{\mathbf{p}} & (\mu = \mu) \end{cases} \qquad \begin{cases} \vec{\mathbf{k}}+\vec{\mathbf{q}} = \vec{\mathbf{p}} & (\lambda = \mu) \\ \vec{\mathbf{p}}-\vec{\mathbf{q}} = \vec{\mathbf{k}} & (\mu = \lambda) \end{cases}$$

where the the contribution on the left is called **direct term** while the one on the right **exchange term**. The direct term realizes only if $\vec{\mathbf{q}} = 0$, but in the sum $\sum'$ the $\vec{\mathbf{q}} = 0$ term is not considered. Hence, in our specific case, the condition in the direct term is not possible. On the contrary, the condition of the exchange term can be realized. It is called exchange term, because if we interpreted $\vec{\mathbf{q}}$ as a wave vector, or momentum, there is momentum transferred from one particle to another one. Moreover, this case is applicable if we consider interactions only between electrons with equal spins, $\delta_{\lambda,\mu}$. In practice, this means that the only possibility is:

$$E^{(1)} = \frac{e^2}{2V}\sum_{\vec{\mathbf{k}}\vec{\mathbf{q}},\lambda}'\frac{4\pi}{q^2}\left\langle F\right| a_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}^{\dagger}\boxed{a_{\vec{\mathbf{k}},\lambda}^{\dagger}a_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}}a_{\vec{\mathbf{k}}\lambda}\left|F\right\rangle$$

Figure 1.7: Direct interaction.

$$= \frac{e^2}{2V}\sum_{\vec{\mathbf{k}}\vec{\mathbf{q}},\lambda}'\frac{4\pi}{q^2}\left\langle F\right| a_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}^{\dagger}\boxed{\left(-a_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}a_{\vec{\mathbf{k}}\lambda}^{\dagger} + \underbrace{\delta_{\vec{\mathbf{k}},\vec{\mathbf{k}}+\vec{\mathbf{q}}}}_{=0\,(\vec{\mathbf{q}}\neq 0)}\right)}a_{\vec{\mathbf{k}}\lambda}\left|F\right\rangle$$

where the green transforms due to the anticommutation rule and where the δ is different from zero only if $\vec{\mathbf{q}} = 0$. Hence, since in our case the $\vec{\mathbf{q}} = 0$ term is not present, the δ gives no contribution (in practice, we can interchange these two operators by adding a minus sign). By replacing the destruction and creation operator with the number ones:

Figure 1.8: Exchange interaction.

$$E^{(1)} = -\frac{e^2}{2V}\sum_{\substack{\vec{\mathbf{k}}\vec{\mathbf{q}},\lambda \\ |\vec{\mathbf{k}}|\leq k_F, |\vec{\mathbf{k}}+\vec{\mathbf{q}}|\leq k_F}}'\frac{4\pi}{q^2}\left\langle F\right|\hat{n}_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda}\hat{n}_{\vec{\mathbf{k}}\lambda}\left|F\right\rangle < 0!$$

this exchange term results negative even though the electron-electron interaction is repulsing. It is called **Hartree-Fock** approximation, for a homogeneous system. Now, we should try to really evaluate this expression. First of all, we observe that:

$$\begin{cases} \hat{n}_{\vec{\mathbf{k}}\lambda} = \left|F\right\rangle & \text{if } \left|\vec{\mathbf{k}}\right| \leq k_F \\ \hat{n}_{\vec{\mathbf{k}}+\vec{\mathbf{q}},\lambda} = \left|F\right\rangle & \text{if } \left|\vec{\mathbf{k}}+\vec{\mathbf{q}}\right| \leq k_F \end{cases}$$

because by construction $\vec{\mathbf{k}}$ and $\vec{\mathbf{k}} + \vec{\mathbf{q}}$ are in the Fermi sphere. Therefore, we get:

$$E^{(1)} = -\frac{e^2}{2V} \underset{\substack{\vec{\mathbf{k}}\vec{\mathbf{q}},\lambda \\ |\vec{\mathbf{k}}| \le k_F, |\vec{\mathbf{k}}+\vec{\mathbf{q}}| \le k_F}}{\sum{}'} \frac{4\pi}{q^2} \xrightarrow[L\to\infty]{} -\frac{2\,e^2}{2V} \frac{V^2}{(2\pi)^6} \int \mathrm{d}\vec{\mathbf{k}} \int \mathrm{d}\vec{\mathbf{q}}\, \frac{4\pi}{q^2} \Theta(k_F - k)\Theta(k_F - |\vec{\mathbf{k}} + \vec{\mathbf{q}}|)$$

where by considering the thermodynamic limit we compute integrals instead of sums (it is simpler), going from a double sum to a double integral. In particular, we get the yellow term "2" by summing over λ and the θ functions are introduced to enforce the conditions in the sums. Moreover, $\vec{\mathbf{q}} \ne 0$ can be omitted since it effects the integrand at only a single point, so it is negligible compared to the rest of the contribution.

Now it is convenient to make the expression more symmetric. For that purpose, we introduce new variables:

$$\vec{\mathbf{p}} \equiv \vec{\mathbf{k}} + \frac{\vec{\mathbf{q}}}{2} \quad \Rightarrow \vec{\mathbf{k}} = \vec{\mathbf{p}} - \frac{\vec{\mathbf{q}}}{2}$$

Thus we obtain:

$$E^{(1)} = -\frac{4\pi e^2 V}{(2\pi)^6} \int \mathrm{d}\vec{\mathbf{q}}\, \frac{1}{q^2} \int \mathrm{d}\vec{\mathbf{p}}\, \Theta\left(k_F - \left|\vec{\mathbf{p}} - \frac{\vec{\mathbf{q}}}{2}\right|\right)\Theta\left(k_F - \left|\vec{\mathbf{p}} + \frac{\vec{\mathbf{q}}}{2}\right|\right)$$

and considering that $\left|\vec{\mathbf{p}} \pm \frac{\vec{\mathbf{q}}}{2}\right| \le k_F$, the region of integration over $\vec{\mathbf{p}}$ is the intersection between 2 spheres of radius k_F. Indeed, it is easy to demonstrate that you can have a non vanishing contribution only if $|\vec{\mathbf{q}}| \le 2k_F$. Hence, this integral is equal to compute the volume of the intersection between two spheres of radius k_F (see Fig.1.9) that are located in a such a way that the distance between their centers is exactly given by $\vec{\mathbf{q}}$. Thus we have reduced an integral to a geometrical problem by evaluating the intersection between two spheres at distance $\vec{\mathbf{q}}$.
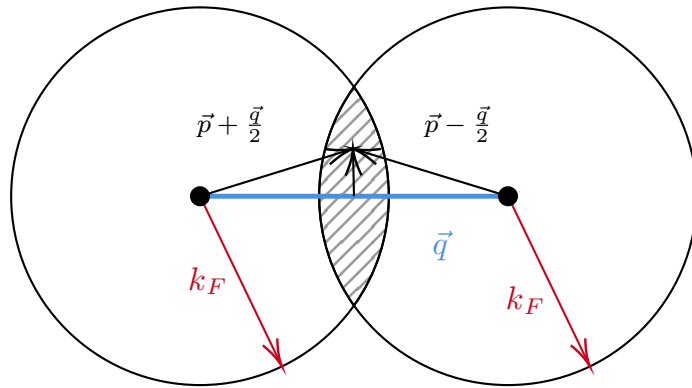
Figure 1.9: Intersection between two spheres of radius k_F at distance $|\vec{\mathbf{q}}| \le 2k_F$.

It is convenient to go to dimensionless variables:

$$x \equiv \frac{q}{2k_F}$$

Hence:

$$
\int \frac{\mathrm{d}\vec{q}}{q^2} \int \mathrm{d}\vec{p}\, \Theta\!\left(k_F - \left|\mathbf{p} - \frac{\vec{q}}{2}\right|\right) \Theta\!\left(k_F - \left|\mathbf{p} + \frac{\vec{q}}{2}\right|\right) = \int \frac{\mathrm{d}\vec{q}}{q^2} \frac{4\pi k_F^3}{3}\left(1 - \frac{3}{2}x + \frac{x^3}{2}\right)\Theta(1-x)
$$

$$
= 4\pi \int_0^\infty \mathrm{d}q\, \frac{q^2}{q^2}\left[\frac{4\pi k_F^3}{3}\left(1 - \frac{3}{2}x + \frac{x^3}{2}\right)\Theta(1-x)\right]
$$

$$
= 4\pi 2k_F \int_0^\infty \mathrm{d}q\, \frac{1}{2k_F}\left[\frac{4\pi k_F^3}{3}\left(1 - \frac{3}{2}x + \frac{x^3}{2}\right)\Theta(1-x)\right]
$$

$$
= 4\pi 2k_F \int_0^\infty \mathrm{d}x\, \left[\frac{4\pi k_F^3}{3}\left(1 - \frac{3}{2}x + \frac{x^3}{2}\right)\right]\Theta(1-x)
$$

$$
= 4\pi 2k_F \int_0^1 \mathrm{d}x\, \left[\frac{4\pi k_F^3}{3}\left(1 - \frac{3}{2}x + \frac{x^3}{2}\right)\right]
$$

The first correction term results:

$$
E^{(1)} = -\frac{4\pi e^2 V}{(2\pi)^6}(4\pi 2k_F)\frac{4\pi k_F^3}{3}\underbrace{\left[\int_0^1 \mathrm{d}x\left(1 - \frac{3}{2}x + \frac{x^3}{2}\right)\right]}_{=3/8}
$$

$$
= \frac{2}{3}\frac{e^2 V}{\pi^3}k_F^3 k_F\left(\frac{3}{8}\right) \overset{(a)}{=} \frac{2e^2 N}{\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s a_0}\left(\frac{3}{8}\right)
$$

$$
= -\left(\frac{e^2}{2a_0}\right)\frac{N}{r_s}\underbrace{\left[\left(\frac{9\pi}{4}\right)^{1/3}\frac{3}{2\pi}\right]}_{=0.916}
$$

where in the step (a) we have made the substitutions:

$$
k_F^3 = 3\pi^2 \frac{N}{V} \qquad k_F = \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s a_0}
$$

By substituting the numerical result we have:

$$
E^{(1)} = -\underbrace{\left(\frac{e^2}{2a_0}\right)}_{=1\mathrm{Ryd}}\frac{N}{r_s}\cdot 0.916 < 0 \tag{1.47}
$$

so the first order correction (exchange or Hartree-Fock term) is negative as antici-
pated.

Now, the question is how we can interpret this contro-intuitive fact from a physical
point of view, namely the reason why the electron-electron interaction gives a negative
contribution to the energy. Since mathematically the the minus sign rise due to
the antisymmetry of the wave functions, the physical origin is the Pauli exclusion
principle, which prevents two electrons with parallel spin from getting too close.
More specifically, we can visualize the situation as follow (see Fig.1.10): suppose that
we put an electron in the origin and we want to look at the probability of finding
another electron at a certain distance r. If we consider an independent particle
approach and suppose that electrons have parallel spins, since there is no interaction
term the probability of finding the electron at the distance r is uniform (i.e. the same
at all the distances). However, we are considering electrons with parallel spins hence,
even if there is no direct Coulomb interaction acting on the system, in any case there
is the Pauli exlusion principle: we cannot have the two electrons with parallel spins
occupy the same position or even very close to each other. This produced the so
called **exchange-hole** concept, which means that the probability of finding another
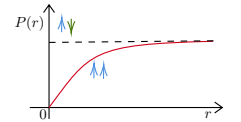
Figure 1.10: Probability of finding an electron at the distance r, for parallel and antiparallel spins.

Exchange-hole

electron with same spin very close to the given electron is reduced with respect to the situation where the Pauli principle where not active.

In other words, the electrons are forced somehow to avoid each other since only one electron at a time can be at a given point in space: the "direct" classical Coulomb interaction ($\vec{q} = 0$) does not take this into account (it was just used to cancel divergences) and overstimates the energy while the "exchange" part correct for this by being negative. In other words, while a direct classical term does not take Pauli exclusion principle into account and tend to overstimate the energy, the exchange part corrects for this and gives a negative contribution. This is the reason why we really get a minus sign for this contribution to the energy.

In Fig.1.11 are shown some pictures to have a better idea of what is happening. In particular, on the right there is the Fermi sphere, on the left it is projected just along one dimension and the states are occupied up to the Fermi level.
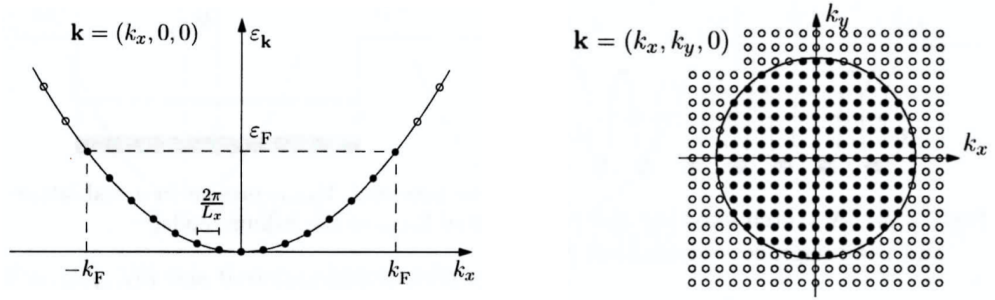
Figure 1.11: Two aspects of $|F\rangle$ in $\vec{k}$-space. To the left the disperion relation $\varepsilon_{\vec{k}}$ is plotted along the line $\vec{k} = (k_x, 0, 0)$ and ε_F and k_F are indicated. To the right the occupation of the states is shown in the plane $\vec{k} = (k_x, k_y, 0)$. The Fermi sphere is shown as a circle with radius k_F. Filled and empy circles represent occupied and unoccupied states, respectively.

Jellium model: final results and comments

To summarize, we have seen that in the high density limit ($r_s \to 0$), the total energy of the Jellium system is given by:

$$E = E_0 + E^{(1)} + \dots$$

Thus, the energy per particle is:

$$\frac{E}{N} \underset{r_s \to 0}{=} \left(\frac{e^2}{2a_0} \right) \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \dots \right]$$

where the yellow term correspond to the kinetic energy term, while the green one the Hartree-Fock exchange energy term. Of course, in principle, we have an infinite series of terms; all the remaining terms are denoted by the definition of Wigner (1933) as **correlation energy**. This historical definition is misleading, because in principle also the Hartree-Fock exchange energy has to do with some sort of correlations between the electrons. Another definition is given by Feymann (1972) that called all the remaining terms **stupidity energy**, because of the difficulty to go beyond the Hartree-Fock term in order of expansion.

Correlation energy

Let us consider only the first two terms; hence, the energy per particle at the first order in the high density limit results:

$$\frac{E}{N} \underset{r_s \to 0}{\simeq} \left(\frac{e^2}{2a_0} \right) \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} \right]$$

It is interesting to consider E/N as a function of r_s as in Fig.1.12. We can note that the dominant term as $r_s \to 0$ is the kinetic energy term, while the exchange term is the dominant one if r_s is large. The combination of the two contribution is the solid line in orange. In particular, this curve has a *minimum* for a negative value of the energy and for a given value of r_s. Physically, it means that the system is stable system and bounded which explains why the metals are stable. One should remember that while in the vanishing $r_s \to 0$ region the exact solution is the one founded, we cannot say the same for relatively large value of the r_s parameter. Indeed, even around the minimum the result is just an approximation because we stopped at the first order term.
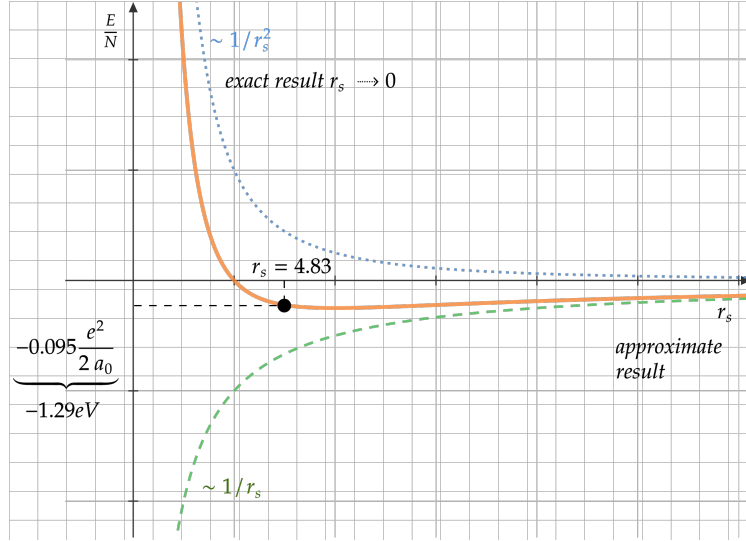
Figure 1.12: Energy per particle at the first order.

For resuming, as $r_s \to 0$, high density limit, this is the exact solution, while for larger values of r_s the solution is only approximate. However, by using the **variational principle**:

$$\langle F | \hat{H} | F \rangle = \langle F | \hat{H}_0 + \hat{H}_1 | F \rangle \geq \langle O | \hat{H} | O \rangle$$

it states that if we compute the Hamiltonian in the non-interacting ground state, by stopping at the first term of the perturbative expansion, the energy that we find is in any case higher or at most equal to the true ground state. Hence, our solution at the first order is an upperbound of the true solution! Thus since already our solution gives a bound state, the true solution is even more bounded.

The exact solution certainly represents a bound system with energy lying below the approximated curve. As said, this explains why a metal is stable and this very simple model is able to explain the largest part of the binding energy of metals in a semi-quantitative way. For instance, let us consider Table 1.2 in which we compare our results with the one obtained experimentally for the coesive energy of sodium. The correspondence is quite nice and the error is really small. Therefore, the very important result is that we have a semi-quantitative agreement with experiments.

	r_s	$E/N \, (eV)$
Na	3.96	-1.13
Jellium model	4.83	-1.29

Table 1.2: Experimental results vs Jellium model.

However, one should make some observation that in some sense reduce this good agreement:

- First of all, in our model there is nothing that has to do with the crystal lattice, so with the specific metallic system. One can show that for instance by comparing the results with experimental values for other metals the agreement is less good, so sodium is the best case that we can compare with.

- Despite of the variational principle our extimated binding energy is lower than the experimental one $E_{\text{Na}} > E_{jellium}$, due to the fact that we are neglecting a positive contribution to the kinetic energy due to the localized ions in real metals.

To make the situation clear, let us see the picture in Fig.1.13 where the dashed line is the exchange contribution, the dotted line the kinetic contribution and the solid line the combination of the two. We can see that the binding energy of sodium is higher than our estimate, while from the variational principle we have expected the opposite. Of course we are neglecting some crucial features of real metals, that are characterized by not a smeared positive background, but by distribution of localized ions. Since this ions are surrounded by core electrons, the valence electrons, that form the dynamical particles of the Jellium model, cannot go too close to these ions, so this means that they have roughly speaking less space to move in the system. Since this means that they should be a little more localized than in the Jellium model, more localization due to uncertainty principle means higher momentum. In conclusion, in our model we are neglecting a positive contribution to the kinetic energy, which would make our solution higher in energy than our estimate.

Free electron gas
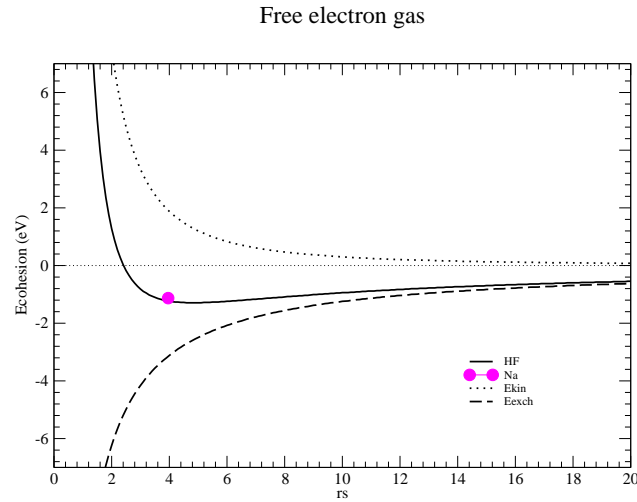
Figure 1.13: Hartree-Fock energy.

Despite these observations, the one obtained is a very nice conclusion! Our very simple model is able to explain the most important contributions to the binding energy of real metals.

One could also think to go further improving the first order result by addition terms in the perturbative approach. Unfortunately, if one tries to improve the 1st order result by going to, for instance, 2nd order perturbation theory, the result is disastrous: it diverges. It happens similarly for additionally terms. Hence, it is necessary some sort of **regularization** of the divergent behavior by taking higher

order perturbation terms into account; the wrong idea is that by taking into account many terms in the perturbative approach, we are able to regularize these divergences. Actually, it is not enough even take a large number of perturbative terms and one has to consider perturbation theory to **infinite order** (i.e. an infinite number of terms), which is not possible using standard perturbative approach, but we have to exploit all the possibilities of the quantum field theory. First of all, we will need to introduce some technical tools to be able to afford such a problem.

Wigner solid

Up to now we have estimated the basic properties, as equilibrium density and energy, of the Jellium model considering in particular the high density limit, where the kinetic energy is the dominant term. One can also wonder what happens considering the opposite limit: the low density case $r_s \to \infty$. One can show (Wigner, 1938) that a lower energy (than that of the Jellium model) can be obtained by allowing the electrons to "crystallize" in a so called **Wigner solid**. Hence, instead of being free to move above the homogeneous background, electrons are localized in a crystal of negative charges.

Low density limit

In fact, if the density is low there is a lot of space available for electrons and the zero-point kinetic energy associated with localizing the electrons becomes negligible in comparison with the electrostatic energy of a classical lattice of charges. Since essentially the electrons are very far from each other and are localized around lattice site, actually the quantum mechanical description is no longer essential because we can treat the particles as classical charged particles in a lattice. Then, for instance the energy can be evaluated, despite of the long-range nature of the Coulomb interaction, by using methods used in solid state theory as for instance the Madelung-Ewald method in ionic solid.

Remark. Since from the variational principle we know that the true energy has a energy lower than the Jellium model energy and since in this case we get for large r_s a solution which is lower in energy than that obtained for the Jellium model, the Wigner solution is better than the Jellium one.

The details of the derivation has been done by Wigner and we illustrate only the final conclusion. Thus, in the limit of low density, the energy per particle is given by:

$$\frac{E}{N} \underset{r_s \to \infty}{=} \left(\frac{e^2}{2a_0} \right) \left[-\frac{1.79}{r_s} + \frac{2.66}{r_s^{3/2}} + \dots \right]$$

where the yellow term is obtained as the difference between the potential of the electrons on fixed lattice sites and the exchange energy[4], while the green term is the zero-point oscillation of electrons about their equilibrium positions (i.e. electrons are forces to remain close to their lattice positions, but they can oscillate around these positions).

Summarizing, we have obtained two estimates of energy per particle in such a model, one for high density and one for low density. To be more precise:

- in the Jellium model the kinetic term dominates and it is valid for very high density: $r_s < 1$.

- in the Wigner-solid model the electrostatic potential energy term dominates and it is valid for very low density: $r_s > 20$.

Unfortunately, the region which is more interesting from a physical point of view is the one which corresponds to the densities of real metals and it is intermediate

---

[4]Remember that also for the Jellium model the exchange energy goes as the inverse of r_s.

between these two cases: $2 < r_s < 6$. In particular, in this region the kinetic and potential energy are comparable. This is clear from Fig.1.13, in which in the region from 2 to 6 both the kinetic energy and the exchange energy really are comparable.

In practice, it means that, as we will see better in the future, one needs to interpolate between high and low density to try to reproduce the behavior of real metals.

In conclusion, despite of the simplicity of the Jellium model, this is an interesting example in which we can apply the second quantization formalism and it is also interesting from a physical point of view for describing real metals.

Now, we skip to chapter 4 of the [1] to try to develop the important formalism and tools that are required to go further in the perturbative approach. Hence, we do not deal with chapter 2, which is a summary of the basic notions of quantum statistical mechanics but we strongly suggest to read this chapter, because we will need some basic concepts of quantum statistical mechanics in the future.

Chapter 2

Green's function

In most cases of interest, the first few orders of perturbation theory cannot provide an adequate description of an interacting many-particle system. For this reason, it becomes essential to develop systematic methods for solving the Schrödinger equation to all orders in perturbation theory. In this chapter, first of all we present the Green's function concept and then the formalism of the different picture of quantum mechanics.

2.1   Green's function

As said, we need more sophisticated tools of quantum field theory for instance to find the correlation energy of degenerate electron gas due to the presence of divergences. One of such tools is represented by the **Green's function** (or *wave function propagator*, as it is sometimes called).

The Green's function method has many variants and a lot of application as for instance in solving differential equation. Here, we are interested in the fact that this concept is useful when we apply perturbative approaches.

Let us rewrite the Hamiltonian in second quantization in terms of field operators:

$$\hat{H} = \sum_{\alpha} \int \mathrm{d}^3\vec{\mathbf{x}}\, \hat{\psi}_{\alpha}^{\dagger}(\vec{\mathbf{x}})T(\vec{\mathbf{x}})\hat{\psi}_{\alpha}(\vec{\mathbf{x}}) + \frac{1}{2}\sum_{\alpha\beta} \int \mathrm{d}^3\vec{\mathbf{x}} \int \mathrm{d}^3\vec{\mathbf{x}}'\, \hat{\psi}_{\alpha}^{\dagger}(\vec{\mathbf{x}})\hat{\psi}_{\beta}^{\dagger}(\vec{\mathbf{x}}')V(\vec{\mathbf{x}},\vec{\mathbf{x}}')\hat{\psi}_{\beta}(\vec{\mathbf{x}}')\hat{\psi}_{\alpha}(\vec{\mathbf{x}})$$

where we assume that the ground state $|\psi_0\rangle$ is normalized and the standard time independent Schrödinger equation is:

$$\hat{H}\,|\psi_0\rangle = E\,|\psi_0\rangle\,, \quad \langle\psi_0|\psi_0\rangle = 1$$

Now, we define new *time dependent* **Heisenberg field operators**. We will present the Heisenberg picture in the future, but for the moment we give just the definition of these new operators. For instance, for the destruction operator:

$$\hat{\psi}_{H\alpha}(\vec{\mathbf{x}}, t) \equiv e^{\frac{i\hat{H}t}{\hbar}}\,\hat{\psi}_{\alpha}(\vec{\mathbf{x}})e^{\frac{-i\hat{H}t}{\hbar}} \tag{2.1}$$

where we have introduced the time dependent by applying the new operator $e^{i\hat{H}t/\hbar}$ both on the left and on the right. Of course, a similar definition is valid for the creation operator.

Now, we define the **single-particle Green's function** (or the two points Green's function) as follow:

$$iG_{\alpha\beta}(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') \equiv \frac{\langle\psi_0|\, T\left[\hat{\psi}_{H\alpha}(\vec{\mathbf{x}}, t)\hat{\psi}_{H_{\beta}}^{\dagger}(\vec{\mathbf{x}}', t')\right]|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} \tag{2.2}$$

where α, β are spin indexes, the denominator is just the normalization and the numerator is essentially the expectation value on the ground state of two operators. In particular, T is a **time-ordered** product of operators (the operator containing the latest time stands farthest to the left): it orders the operators from *right* to *left* in *ascending* time order with a $(-1)^p$ factor, where p is the number of interchanges of fermions operators from the original given order (for bosons nothing special happens)

In practice, if we consider the action of this time order operator to two field operators, we essentially obtain:

$$T\left[\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t)\hat{\psi}^\dagger_{H_\beta}(\vec{\mathbf{x}}', t')\right] = \begin{cases} \hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t)\hat{\psi}^\dagger_{H_\beta}(\vec{\mathbf{x}}', t') & \text{if } t > t' \\ \pm\hat{\psi}_{H_\beta}(\vec{\mathbf{x}}', t')\hat{\psi}^\dagger_{H_\alpha}(\vec{\mathbf{x}}, t) & \text{if } t < t' \end{cases}$$

where the plus sign refers to bosons, while the minus sign to fermions.

Let us note that the Green's function is a matrix element, namely the expectation value of field operators in the ground state, and it is essentially a function of the coordinate variables $\vec{\mathbf{x}}, t, \vec{\mathbf{x}}', t'$. It means that GF contains only part of the full information carried by the wave functions of the systems, however it includes the most relevant information:

1. the expectation value of any single-particle operator in the ground state of the system;

2. the ground state (total) energy of the system;

3. the excitation spectrum of the system.

The first two points are demonstrated below, while the third follows from the Lehmann representation, which is discussed later in this section. Moreover, in the spirit of the perturbative approach, one can demonstrate that the Feynman rules for finding the contribution of the n-th order perturbation theory are simpler for G than for other combinations of field operators.

> **Property 1: Homogeneity in time**
>
> If $\hat{H}$ is time independent, the Green's function is homogeneous in time, i.e. it depends only on $t - t'$ and not separately from t and t'.

Proof of propty.(2.1). We can always assume that the ground state is normalized and that the Schrödinger is the following:

$$\hat{H}\ket{\psi_0} = E\ket{\psi_0}, \quad \braket{\psi_0|\psi_0} = 1$$

Let us consider the case $t > t'$, i.e. we assume a specific time ordering in the definition of the Green's function:

$$\begin{aligned} iG_{\alpha\beta}(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') &= \bra{\psi_0}\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t)\hat{\psi}^\dagger_{H_\beta}(\vec{\mathbf{x}}', t')\ket{\psi_0} \\ &= \bra{\psi_0}e^{\frac{i\hat{H}t}{\hbar}}\hat{\psi}_\alpha(\vec{\mathbf{x}})\underbrace{e^{-\frac{i\hat{H}t}{\hbar}}e^{\frac{i\hat{H}t'}{\hbar}}}_{e^{-\frac{i\hat{H}(t-t')}{\hbar}}}\hat{\psi}^\dagger_\beta(\vec{\mathbf{x}}')e^{-\frac{i\hat{H}t'}{\hbar}}\ket{\psi_0} \\ &\stackrel{(a)}{=} e^{\frac{iE(t-t')}{\hbar}}\bra{\psi_0}\hat{\psi}_\alpha(\vec{\mathbf{x}})e^{-\frac{i\hat{H}(t-t')}{\hbar}}\hat{\psi}^\dagger_\beta(\vec{\mathbf{x}}')\ket{\psi_0} \\ &= iG_{\alpha\beta}(\vec{\mathbf{x}}, \vec{\mathbf{x}}', (t-t')) \end{aligned}$$

where in step (a) we had put togheter the middle exponential operators (since they commute) and we had put outside the term $e^{iE(t-t')/\hbar}$ because it is a c-number. In particular, the latter was derived by considering the action of the exponential

operators both to the state on the left and on the right (since the property $H \left| \psi_0 \right\rangle = E \left| \psi_0 \right\rangle$ is valid also for an exponential of the hamiltonian).

If we consider the case $t < t'$ and we repeat the entire computation, ww end up that the Green's function only depend on $t - t'$ (i.e. it is homogeneous in time).

∎

1 - Expectation value of single particle operators

Now, let us demonstrate that from the GF we obtain the expectation value of any single-particle operator in the ground state: Let us assume to have a general single-particle operator in second quantization:

Expectation value of single particle operators

$$\hat{J} = \int \mathrm{d}x \, \hat{j}(\vec{\mathbf{x}})$$

which is the integral of the density operator in second quantization, which corresponds in first quantization to a generic operator $J_{\beta\alpha}(\vec{\mathbf{x}})$:

$$\hat{j}(\vec{\mathbf{x}}) = \sum_{\alpha\beta} \hat{\psi}_\beta^\dagger(\vec{\mathbf{x}}) J_{\beta\alpha}(\vec{\mathbf{x}}) \hat{\psi}_\alpha(\vec{\mathbf{x}})$$

where we have written $\beta\alpha$ order instead of $\alpha\beta$, because it will be more convenient ant this is not relevant.

Again considering that the ground state is normalized ($\langle \psi_0 | \psi_0 \rangle$), if we take the matrix element over the ground state of the last operator, we obtain:

$$\langle \psi_0 | \hat{j}(\vec{\mathbf{x}}) | \psi_0 \rangle \overset{(a)}{=} \lim_{\vec{\mathbf{x}}' \to \vec{\mathbf{x}}} \sum_{\alpha\beta} J_{\beta\alpha}(\vec{\mathbf{x}}) \langle \psi_0 | \hat{\psi}_\beta^\dagger(\vec{\mathbf{x}}') \hat{\psi}_\alpha(\vec{\mathbf{x}}) | \psi_0 \rangle$$

$$\overset{(b)}{=} \lim_{\substack{\vec{\mathbf{x}}' \to \vec{\mathbf{x}} \\ t' \to t}} \sum_{\alpha\beta} J_{\beta\alpha}(\vec{\mathbf{x}}) \langle \psi_0 | \hat{\psi}_{H_\beta}^\dagger(\vec{\mathbf{x}}', t') \hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t) | \psi_0 \rangle$$

$$\overset{(c)}{=} \pm \lim_{\substack{\vec{\mathbf{x}}' \to \vec{\mathbf{x}} \\ t' \to t}} \sum_{\alpha\beta} J_{\beta\alpha}(\vec{\mathbf{x}}) \langle \psi_0 | T \left[\hat{\psi}_{H_\beta}^\dagger(\vec{\mathbf{x}}', t') \hat{\psi}_{H_\alpha} \right] (\vec{\mathbf{x}}, t) | \psi_0 \rangle$$

$$= \pm i \lim_{\substack{\vec{\mathbf{x}}' \to \vec{\mathbf{x}} \\ t' \to t}} \sum_{\alpha\beta} \left[J_{\beta\alpha} G_{\alpha\beta}(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') \right]$$

$$= \pm i \lim_{\substack{\vec{\mathbf{x}}' \to \vec{\mathbf{x}} \\ t' \to t}} \mathrm{Tr} \left[J_{\beta\alpha} G_{\alpha\beta}(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') \right]$$

where in the step (a) formally we can write x' by taking the limit $x' \to x$. In the step (b) we have multiplied the operators inside by the factor $e^{\frac{i\hat{H}t}{\hbar}}$ in such a way to introduce the Heisenberg field operators (it is allowed if we take the limit $t' \to t$, as you can see from the previous proof). In the step (c), we have introduced the T product, provided that $t' \to t$ from above (t' is infinitesimally later than t), because in that case the action of the two operators change the order and we recover the $\alpha\beta$ order in the definition of the Green function (2.2) and from the normalization condition we recover the original definition of the Green's function. Then, we have interpreted the $\sum_{\alpha\beta}$, as a trace of the matrix product between J and the Green's function. Remember that the + sign stands for bosons, while the - sign for fermions.

Remark. If we have:

$$C = A \cdot B \quad \Rightarrow C_{ij} = \sum_l A_{il} B_{lj}$$

The trace is:

$$\mathrm{Tr}(AB) = \mathrm{Tr}(C) = \sum_i C_i i = \sum_{il} A_{il} B_{li}$$

Example 10: Total kinetic energy

For instance, the total kinetic energy of the system ($\hat{H} = \hat{T} + \hat{V}$) is the integral over the kinetic energy density in second quantization:

$$\hat{T} = \int d\vec{x}\,\tau(\vec{x}), \quad \tau(\vec{x}) \equiv \sum_{\alpha\beta} \hat{\psi}_\beta(\vec{x})\left(-\frac{\hbar^2 \boldsymbol{\nabla}_x^2}{2m}\right)\hat{\psi}_\alpha(\vec{x})\delta_{\alpha\beta}$$

In particular, the kinetic energy density in first quantization is:

$$\tau_{\beta\alpha}(\vec{x}) = -\frac{\hbar^2 \boldsymbol{\nabla}_x^2}{2m}\delta_{\alpha\beta}$$

which is diagonal in the spin indexes.
Now let us write the expectation value on the ground state of the kinetic energy as a function of the Green's function:

$$\langle\psi_0|\,\hat{T}\,|\psi_0\rangle = \pm i \int d\vec{x}\,\lim_{\vec{x}'\to\vec{x}}\left(-\frac{\hbar^2 \boldsymbol{\nabla}_x^2}{2m}\sum_{\alpha\beta}\delta_{\alpha\beta}G_{\alpha\beta}(\vec{x}t,\vec{x}'t')\right)$$

$$= \pm i \int d\vec{x}\,\lim_{\vec{x}'\to\vec{x}}\left(-\frac{\hbar^2 \boldsymbol{\nabla}_x^2}{2m}\,\text{Tr}\big[G(\vec{x}t,\vec{x}'t')\big]\right)$$

where we should apply the kinetic energy differential term, depending just on $\vec{x}$, before taking the limit $x' \to x$.
In conclusion, it is essentially the expression of the kinetic energy term as a function of the Green's function and as we will see it is really useful.

2 - Ground state energy of the system

Total ground state energy

In order to determine the ground state energy:

$$E = \langle\psi_0|\,\hat{H}\,|\psi_0\rangle = \langle\psi_0|\,\hat{T}\,|\psi_0\rangle + \langle\psi_0|\,\hat{V}\,|\psi_0\rangle$$

One should evaluate also the expectation value of the potential energy as a function of the Green's function.

The potential energy in second quantization as a function of field operators can be written as:

$$\hat{V} = \frac{1}{2}\sum_{\substack{\alpha\alpha'\\\beta\beta'}}\int d^3\vec{x}\int d^3\vec{x}'\,\hat{\psi}_\alpha^\dagger(\vec{x})\hat{\psi}_\beta^\dagger(\vec{x}')V(\vec{x},\vec{x}')_{\substack{\alpha\alpha'\\\beta\beta'}}\hat{\psi}_{\beta'}(\vec{x}')\hat{\psi}_{\alpha'}(\vec{x})$$

Now we want to evaluate the expectation value $\langle\psi_0|\,\hat{V}\,|\psi_0\rangle$. Since it involves 4 field operators, while in the definition of the Green's function we have involved only 2 operators, one could expect to need a two-particle Green's function (that is more complicated and it is expressed as a function of 4 operators)[1]. However, actually the standard single-particle Green's function is sufficient to evaluate this expectation value, because we can use the Schrödinger equation, which contains the potential energy.

First of all, let us consider the equation of motion for the Heisenberg field operator:

Heisenberg equation of motion

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[1]See Prob. 3.3., page 116 [1].

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}},t) = \frac{i^2\hat{H}\cancel{\hbar}}{\cancel{\hbar}}e^{\frac{i\hat{H}t}{\hbar}}\hat{\psi}_\alpha(\vec{\mathbf{x}})e^{-\frac{i\hat{H}t}{\hbar}} + e^{\frac{i\hat{H}t}{\hbar}}\hat{\psi}_\alpha(\vec{\mathbf{x}})\left(-\frac{i^2\hat{H}\cancel{\hbar}}{\cancel{\hbar}}\right)e^{-\frac{i\hat{H}t}{\hbar}}$$

$$= -\hat{H}\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}},t) + \hat{\psi}_{H_\alpha}(\vec{\mathbf{x}},t)\hat{H}$$

$$= \left[\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}},t),\hat{H}\right] \tag{2.3}$$

$$= e^{\frac{i\hat{H}t}{\hbar}}\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{H}\right]e^{-\frac{i\hat{H}t}{\hbar}}$$

$$= e^{\frac{i\hat{H}t}{\hbar}}\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{T}\right]e^{-\frac{i\hat{H}t}{\hbar}} + e^{\frac{i\hat{H}t}{\hbar}}\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{V}\right]e^{-\frac{i\hat{H}t}{\hbar}}$$

where we have used the fact that the exponential term commutes with the hamiltonian.

Now let us focus on the commutator between the standard field operator and the kinetic energy operator:

Commutator between field and kinetic energy operators

$$\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{T}\right] = \lim_{\vec{y}'\to\vec{y}}\sum_\beta\int \mathrm{d}\vec{y}\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{\psi}_\beta^\dagger(\vec{y}')\left(-\frac{\hbar^2\boldsymbol{\nabla}_y^2}{2m}\right)\hat{\psi}_\beta(\vec{y})\right]$$

$$= \sum_\beta\int \mathrm{d}\vec{y}\lim_{\vec{y}'\to\vec{y}}\left(-\frac{\hbar^2\boldsymbol{\nabla}_y^2}{2m}\right)\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{\psi}_\beta^\dagger(\vec{y}')\hat{\psi}_\beta(\vec{y})\right]$$

where we have used the definition of the kinetic energy operator in terms of the field operators and where it is convenient to use the dummy variable $\vec{y}$. The important thing is that we should take the limit $y' \to y$ after the action of the kinetic energy term $\boldsymbol{\nabla}_y$, and because this term only acts on $\vec{y}$, not on $\vec{y}'$, in the second step we can take formally this term in front of the commutator.

Now we introduce the important relations:

Commuation relation

$$[A,BC] = \begin{cases} [A,B]C - B[C,A] \\ \{A,B\}C - B\{C,A\} \end{cases} \tag{2.4}$$

Proof. For instance:

$$[A,BC] = ABC - BCA$$

$$= ABC - \boxed{BAC} + \boxed{BAC} - BCA$$

$$= [A,B]C - B[C,A]$$

∎

Now, let us focus on fermions, however the final results will be valid for both fermions and bosons. Using the property of the commutator (2.4), we can write:

$$[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{\psi}_\beta^\dagger(\vec{y}')\hat{\psi}_\beta(\vec{y})] = \underbrace{\{\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{\psi}_\beta^\dagger(\vec{y}')\}}_{\delta_{\alpha\beta}\delta(\vec{\mathbf{x}}-\vec{y}')}\hat{\psi}_\beta(\vec{y}) - \hat{\psi}_\beta^\dagger(\vec{y}')\underbrace{\{\hat{\psi}_\beta(\vec{y}),\hat{\psi}_\alpha(\vec{\mathbf{x}})\}}_{=0}$$

Hence, for the kinetic energy term we obtain:

$$[\hat{\psi}_\alpha(\vec{\mathbf{x}}),\hat{T}] = \sum_\beta\int \mathrm{d}\vec{y}\lim_{\vec{y}'\to\vec{y}}\left(-\frac{\hbar^2\boldsymbol{\nabla}_y^2}{2m}\right)\delta_{\alpha\beta}\delta_{\vec{\mathbf{x}}-\vec{y}}\hat{\psi}_\beta(\vec{y})$$

$$= \sum_\beta\delta_{\alpha\beta}\int \mathrm{d}\vec{y}\lim_{\vec{y}'\to\vec{y}}\delta(\vec{\mathbf{x}}-\vec{y})\left(-\frac{\hbar^2\boldsymbol{\nabla}_y^2}{2m}\right)\hat{\psi}_\beta(\vec{y}) \tag{2.5}$$

$$= -\frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\hat{\psi}_\alpha(\vec{\mathbf{x}})$$

where the differential operator only acts on $\vec{y}$ if we take the limit on the proper order.

Now, let us focus on the potential energy term:

$$[\hat{\psi}_\alpha(\vec{x}), \hat{V}] = \frac{1}{2} \sum_{\substack{\beta\beta' \\ \gamma\gamma'}} \int d\vec{y} \int d\vec{y}' \left[\underbrace{\hat{\psi}_\alpha(\vec{x})}_{A}, \underbrace{\hat{\psi}^\dagger_\beta(\vec{y})\hat{\psi}^\dagger_\gamma(\vec{y}')}_{B} V(\vec{y},\vec{y}')_{\beta\beta'}_{\gamma\gamma'} \underbrace{\hat{\psi}_{\gamma'}(\vec{y}')\hat{\psi}_{\beta'}(\vec{y})}_{C} \right]$$

where V is just a function (i.e, not an operator). Then we can exploit using the relation of commutators (2.4):

$$[A, BC] = [A, B]C - B[C, A]$$
$$= \left[\hat{\psi}_\alpha(\vec{x}), \hat{\psi}^\dagger_\beta(\vec{y})\hat{\psi}^\dagger_\gamma(\vec{y}') \right] \hat{\psi}_{\gamma'}(\vec{y}')\hat{\psi}_{\beta'}(\vec{y}) - \hat{\psi}^\dagger_\beta(\vec{y})\hat{\psi}^\dagger_\gamma(\vec{y}') \underbrace{\left[\hat{\psi}_{\gamma'}(\vec{y}')\hat{\psi}_{\beta'}(\vec{y}), \hat{\psi}_\alpha(\vec{x}) \right]}_{=0}$$

where the last term is zero because they are all destruction field operators. Hence, remains just the term $[A, B]C$:

$$\left[\hat{\psi}_\alpha(\vec{x}), \hat{V} \right] = \frac{1}{2} \sum_{\substack{\beta\beta' \\ \gamma\gamma'}} \int d\vec{y} \int d\vec{y}' \left[\underbrace{\hat{\psi}_\alpha(\vec{x})}_{a}, \underbrace{\hat{\psi}^\dagger_\beta(\vec{y})}_{b}\underbrace{\hat{\psi}^\dagger_\gamma(\vec{y}')}_{c} \right] V(\vec{y},\vec{y}')_{\beta\beta'}_{\gamma\gamma'} \hat{\psi}_{\gamma'}(\vec{y}')\hat{\psi}_{\beta'}(\vec{y})$$

Thus:

$$[a, bc] = \{a, b\}c - b\underbrace{\{c, a\}}_{=\{a,c\}}$$

$$\implies \left[\hat{\psi}_\alpha(\vec{x}), \hat{\psi}^\dagger_\beta(\vec{y})\hat{\psi}^\dagger_\gamma(\vec{y}') \right] = \delta_{\alpha\beta}\delta(\vec{x}-\vec{y})\hat{\psi}^\dagger_\gamma(\vec{y}') - \hat{\psi}^\dagger_\beta(\vec{y})\delta_{\alpha\gamma}\delta(\vec{x}-\vec{y}')$$

The commutator between the potential energy and the field operator becomes:

$$\left[\hat{\psi}_\alpha(\vec{x}), \hat{V} \right] = \frac{1}{2} \sum_{\substack{\beta' \\ \gamma\gamma'}} \int d\vec{y}'\, \hat{\psi}^\dagger_\gamma(\vec{y}')\hat{\psi}_{\gamma'}(\vec{y}')\hat{\psi}_{\beta'}(\vec{x}) V(\vec{x},\vec{y}')_{\alpha\beta'}_{\gamma\gamma'}$$

$$- \frac{1}{2} \sum_{\substack{\beta\beta' \\ \gamma'}} \int d\vec{y}\, \hat{\psi}^\dagger_\beta(\vec{y}) \underbrace{\hat{\psi}_{\gamma'}(\vec{x})\hat{\psi}_{\beta'}(\vec{y})}_{-\hat{\psi}_{\beta'}(\vec{y})\hat{\psi}_{\gamma'}(\vec{x})} V(\vec{y},\vec{x})_{\beta\beta'}_{\alpha\gamma'}$$

$$\overset{(a)}{=} \frac{1}{2} \sum_{\substack{\beta' \\ \gamma\gamma'}} \int d\vec{y}'\, \hat{\psi}^\dagger_\gamma(\vec{y}')\hat{\psi}_{\gamma'}(\vec{y}')\hat{\psi}_{\beta'}(\vec{x}) V(\vec{x},\vec{y}')_{\alpha\beta'}_{\gamma\gamma'}$$

$$+ \frac{1}{2} \sum_{\substack{\beta\beta' \\ \gamma'}} \int d\vec{y}\, \hat{\psi}^\dagger_\beta(\vec{y})\hat{\psi}_{\beta'}(\vec{y})\hat{\psi}_{\gamma'}(\vec{x}) V(\vec{y},\vec{x})_{\beta\beta'}_{\alpha\gamma'}$$

where (a) we have interchanged the destruction operators just by introducing a minus sign in front.

Since the particles are *identical* the interaction potential is unchanged under particle interchange:

$$V(\vec{x},\vec{x}')_{\substack{\alpha\alpha' \\ \beta\beta'}} = V(\vec{x}',\vec{x})_{\substack{\beta\beta' \\ \alpha\alpha'}} \tag{2.6}$$

it means that the potential is symmetric.

Remark. Typically the potential will be the standard Coulomb interaction:

$$V(\vec{x},\vec{x}') = \frac{e^2}{|\vec{x}-\vec{x}'|}\delta_{\substack{\alpha\alpha' \\ \beta\beta'}}$$

By changing the dummy variables in the first (yellow) term above:

$$\gamma \to \beta, \quad \gamma' \to \beta', \quad \beta' \to \gamma', \quad \vec{\mathbf{y}}' \to \vec{\mathbf{y}}, \quad \vec{\mathbf{y}} \to \vec{\mathbf{y}}'$$

and by considering the symmetry of the potential, we see that the first term is equal to the second one. This means that in practice we can multiply the first term by a factor 2 and neglect the second one. The final commutator result:

$$\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{V}\right] = \sum_{\substack{\beta' \\ \gamma\gamma'}} \int d\vec{\mathbf{y}}' \, \hat{\psi}_\gamma^\dagger(\vec{\mathbf{y}}')\hat{\psi}_{\gamma'}(\vec{\mathbf{y}}')\hat{\psi}_{\beta'}(\vec{\mathbf{x}})V(\vec{\mathbf{x}},\vec{\mathbf{y}}')_{\substack{\alpha\beta' \\ \gamma\gamma'}} \tag{2.7}$$

where we have three field operators and the potential function.

In conclusion, the total commutator between the field operator and the Hamiltonian is:

$$\begin{aligned}\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{H}\right] &= \left[\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{T}\right] + \left[\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{V}\right] \\ &= -\frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\hat{\psi}_\alpha(\vec{\mathbf{x}}) + \sum_{\substack{\beta' \\ \gamma\gamma'}} \int d\vec{\mathbf{y}}' \, \hat{\psi}_\gamma^\dagger(\vec{\mathbf{y}}')\hat{\psi}_{\gamma'}(\vec{\mathbf{y}}')\hat{\psi}_{\beta'}(\vec{\mathbf{x}})V(\vec{\mathbf{x}},\vec{\mathbf{y}}')_{\substack{\alpha\beta' \\ \gamma\gamma'}}\end{aligned} \tag{2.8}$$

Recalling the equation of motion for the Heisenberg field oeprator $\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t)$ (Eq.(2.3)):

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t) = e^{\frac{i\hat{H}t}{\hbar}}\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{H}\right]e^{-\frac{i\hat{H}t}{\hbar}}$$

Now we can substitute the commutator $\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{H}\right]$ with its explicit expression previously obtained and, since we have the exponential operators both on left and right, we can easily transform standard field operators into the Heisenberg field operators and also put on the left the kinetic energy part. The result is:

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right]\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t) = \sum_{\beta'\gamma\gamma'} \int d\vec{\mathbf{y}} \, \hat{\psi}_{H_\gamma}^\dagger(\vec{\mathbf{y}}, t)\hat{\psi}_{H_{\gamma'}}(\vec{\mathbf{y}}, t)\hat{\psi}_{H_{\beta'}}(\vec{\mathbf{x}}, t)V(\vec{\mathbf{x}},\vec{\mathbf{y}})_{\substack{\alpha\beta' \\ \gamma\gamma'}}$$

where we have also make the substitution $\vec{\mathbf{y}}' \to \vec{\mathbf{y}}$. Then, multiplying by $\hat{\psi}_{H_\alpha}^\dagger(\vec{\mathbf{y}}, t)$ on the left and taking the ground state expectation value of all the equation:

$$\begin{aligned}&\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right]\frac{\langle\psi_0|\hat{\psi}_{H_\alpha}^\dagger(\vec{\mathbf{x}}', t')\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t)|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} = \\ &= \sum_{\beta'\gamma\gamma'} \int d\vec{\mathbf{y}} \, \frac{\langle\psi_0|\hat{\psi}_{H_\alpha}^\dagger(\vec{\mathbf{x}}', t')\hat{\psi}_{H_\gamma}^\dagger(\vec{\mathbf{y}}, t)\hat{\psi}_{H_{\gamma'}}(\vec{\mathbf{y}}, t)\hat{\psi}_{H_{\beta'}}(\vec{\mathbf{x}}, t)|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}V(\vec{\mathbf{x}},\vec{\mathbf{y}})_{\substack{\alpha\beta' \\ \gamma\gamma'}}\end{aligned}$$

Let us focus on the left-side term which has an expression reminiscent of the Green's function definition (2.2) if $t' \to t^+$ and $\vec{\mathbf{x}}' \to \vec{\mathbf{x}}$ (remember that the Green's function definition involves the $\psi^\dagger$ in the right, so we should reorder in a proper way):

$$\pm i \lim_{\substack{\vec{\mathbf{x}}' \to \vec{\mathbf{x}} \\ t' \to t^+}} \left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right)G_{\alpha\alpha}(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t')$$

where the $\pm$ sign refers to bosons/fermions. Then we complete the derivation by summing over the spin index α and integrating over the $\vec{\mathbf{x}}$ variable. This means that on the left we get:

$$\pm i \int d\vec{\mathbf{x}} \lim_{\substack{\vec{\mathbf{x}}' \to \vec{\mathbf{x}} \\ t' \to t^+}} \sum_\alpha \left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right)G_{\alpha\alpha}(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t')$$

Repeating all these operations for the right-side of the equation we get:

$$\sum_{\substack{\alpha\beta' \\ \gamma\gamma'}} \int d\vec{\mathbf{x}} \int d\vec{\mathbf{y}} \lim_{\substack{\vec{\mathbf{x}}'\to\vec{\mathbf{x}} \\ t'\to t^+}} \frac{\langle\psi_0|\hat{\psi}^\dagger_{H_\alpha}(\vec{\mathbf{x}}',t')\hat{\psi}^\dagger_{H_\gamma}(\vec{\mathbf{y}},t)\hat{\psi}_{H_{\gamma'}}(\vec{\mathbf{y}},t)\hat{\psi}_{H_{\beta'}}(\vec{\mathbf{x}},t)|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} V(\vec{\mathbf{x}},\vec{\mathbf{y}})_{\substack{\alpha\beta' \\ \gamma\gamma'}}$$

$$\stackrel{(a)}{=} \sum_{\substack{\alpha\beta' \\ \gamma\gamma'}} \int d\vec{\mathbf{x}} \int d\vec{\mathbf{y}} \frac{\langle\psi_0|\hat{\psi}^\dagger_\alpha(\vec{\mathbf{x}})\hat{\psi}^\dagger_\gamma(\vec{\mathbf{y}})\hat{\psi}_{\gamma'}(\vec{\mathbf{y}})\hat{\psi}_{\beta'}(\vec{\mathbf{x}})|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} V(\vec{\mathbf{x}},\vec{\mathbf{y}})_{\substack{\alpha\beta' \\ \gamma\gamma'}}$$

$$\stackrel{(b)}{=} 2\frac{\langle\psi_0|\frac{1}{2}\int d\vec{\mathbf{x}}\int d\vec{\mathbf{y}}\,\hat{\psi}^\dagger_\alpha(\vec{\mathbf{x}})\hat{\psi}^\dagger_\gamma(\vec{\mathbf{y}})\hat{\psi}_{\gamma'}(\vec{\mathbf{y}})\hat{\psi}_{\beta'}(\vec{\mathbf{x}})V(\vec{\mathbf{x}},\vec{\mathbf{y}})_{\substack{\alpha\beta' \\ \gamma\gamma'}}|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}$$

$$\stackrel{(c)}{=} 2\underbrace{\frac{\langle\psi_0|\hat{V}|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}}_{=1}$$

where in step (a) we should let $\vec{\mathbf{x}}' \to \vec{\mathbf{x}}$ and $t' \to t^+$. It means that in the Heisnberg field operators, the exponential terms are relative to the same times, thus we obtain the standard field operators without time dependence. In step (b) we divide by a factor 2 and in step (c) we recognize the expression in second quantization of the potential energy term in terms of field operators.

Expectation value for the potential energy operator

Now, if we compare the right-hand side with the left-hand side, it is easy to arrive at:

$$\langle\psi_0|\hat{V}|\psi_0\rangle = \pm\frac{i}{2}\int d\vec{\mathbf{x}} \lim_{\substack{\vec{\mathbf{x}}'\to\vec{\mathbf{x}} \\ t'\to t^+}} \sum_\alpha \left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right)G_{\alpha\alpha}(\vec{\mathbf{x}}t,\vec{\mathbf{x}}'t')$$

The conclusion is that the expectation value of the potential energy operator in the ground state is given by an integral of the Green's function. In particular, the most important result is that thanks to this trick (the potential energy is inside the Schrödinger equation) we were able to express the potential energy expectation value as a function of a single-particle Green's function, despite of the potential energy operator depends on four field operators.

Recalling the expression for the expectation value of the kinetic energy operator in terms of the single-particle Green's function (Eq.(2.1)):

$$\langle\psi_0|\hat{T}|\psi_0\rangle = \pm i\int d\vec{\mathbf{x}} \lim_{\substack{\vec{\mathbf{x}}'\to\vec{\mathbf{x}} \\ t'\to t^+}} \sum_\alpha \left(-\frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right)G_{\alpha\alpha}(\vec{\mathbf{x}}t,\vec{\mathbf{x}}'t')$$

the total energy of our system is the sum of expectation value of kinetic energy operator and potential energy operator:

$$E = \langle\psi_0|\hat{H}|\psi_0\rangle = \langle\psi_0|\hat{T}|\psi_0\rangle + \langle\psi_0|\hat{V}|\psi_0\rangle$$

Now it is clear that the potential energy expectation value can be expressed as:

$$\langle\psi_0|\hat{V}|\psi_0\rangle = \frac{i}{2}\int d\vec{\mathbf{x}} \lim_{\substack{\vec{\mathbf{x}}'\to\vec{\mathbf{x}} \\ t'\to t^+}} \sum_\alpha \left(i\hbar\frac{\partial}{\partial t}\right)G_{\alpha\alpha}(\vec{\mathbf{x}}t,\vec{\mathbf{x}}'t') - \frac{i}{2}\int d\vec{\mathbf{x}} \lim_{\substack{\vec{\mathbf{x}}'\to\vec{\mathbf{x}} \\ t'\to t^+}} \sum_\alpha \left(-\frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right)G_{\alpha\alpha}(\vec{\mathbf{x}}t,\vec{\mathbf{x}}'t')$$

$$= \frac{1}{2}(\dots) - \frac{1}{2}\langle\psi_0|\hat{T}|\psi_0\rangle$$

Total energy

By taking togheter these terms, the total energy results:

$$E = \langle\psi_0|\hat{H}|\psi_0\rangle = \pm\frac{i}{2}\int d\vec{\mathbf{x}} \lim_{\substack{\vec{\mathbf{x}}'\to\vec{\mathbf{x}} \\ t'\to t^+}} \left[i\hbar\frac{\partial}{\partial t} - \frac{\hbar^2\boldsymbol{\nabla}_x^2}{2m}\right]\text{Tr}\,G(\vec{\mathbf{x}}t,\vec{\mathbf{x}}'t') \qquad (2.9)$$

and as promised the total energy is expressed as a function of a single-particle Green's function. We have essentially derived this for fermions, but if you repeat the derivation for bosons the result is the same (the + sign holds for bosons, while the − sign for fermions).

2.1.1 Fourier transform of Green's functions

Property 2: Homogeneity in space

If the system is homogeneous in space, i.e. the total momentum commute with the Hamiltonian ($[\hat{\vec{p}}, \hat{H}] = 0$), the Green's function is homogeneous in space, i.e. it depends only on $\vec{x} - \vec{x}'$ and not separately from $\vec{x}$ and $\vec{x}'$.

Moreover, for a system confined in a large box of volume V, this means that it is more convenient to work not in the real space but in the reciprocal one. Hence, it is convenient to take the Fourier transform of the Green's function.

Let us suppose that our system is homogeneous in time and space:

$$G_{\alpha\beta}(\vec{x}t, \vec{x}'t') = G_{\alpha\beta}(\vec{x} - \vec{x}', t - t') \equiv \sum_{\vec{k}} \frac{1}{V} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{i\vec{k}\cdot(\vec{x}-\vec{x}')} e^{-i\omega(t-t')} \boxed{G_{\alpha\beta}(\vec{k}, \omega)}$$

$$(2.10)$$

where the red term is the Fourier transform of the Green's function, which depends on the wave vector and on the frequency. Now, since typically we work in a very large box of infinite volume, we can go from the sum over $\vec{k}$ wave vector to an integral over $\vec{k}$ (we already know the recipt for going from sum to integral derived in Eq.(1.46)). Thus we can write:

$$G_{\alpha\beta} \underset{\Delta\vec{k}=(2\pi)^3/V}{\overset{V \to \infty}{=}} \frac{1}{(2\pi)^4} \int d\vec{k} \int_{-\infty}^{+\infty} d\omega \, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')} e^{-i\omega(t-t')} G_{\alpha\beta}(\vec{k}, \omega)$$

Example 11: Total energy in the Fourier space

Let us express the formula of the total energy, derived above in Eq.(2.9), in terms of the Fouerier transformed Green's function, by replacing the Green's function with the expansion in term of Fourier components.

$$E = \pm\frac{i}{2} \int d\vec{x} \lim_{\substack{\vec{x}' \to \vec{x} \\ t' \to t^+}} \frac{1}{(2\pi)^4} \int d\vec{k} \int_{-\infty}^{+\infty} d\omega \left(\hbar\omega + \frac{\hbar^2 k^2}{2m} \right) e^{i\vec{k}\cdot(\vec{x}-\vec{x}')} e^{-i\omega(t-t')} \operatorname{Tr} G(\vec{k}, \omega)$$

where of course the yellow term in (2.9) involving the time derivative, produces the factor $\hbar\omega$ and the green term, the second order derivative in spatial coordinates, produces $\frac{\hbar^2 k^2}{2m}$. In this way, we have expressed the total energy in terms of the trace of the Fourier trandformed Green's function.

At this point, we can immeadiatly take the limit $\vec{x}' \to \vec{x}$ because only one term contains the dependence on $\vec{x}$:

$$\int d\vec{x} \, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')} \overset{\vec{x}' \to \vec{x}}{\longrightarrow} V$$

Concerning the time dependence, considering that t' slightly larger than t, we can define the new variable η as:

$$\eta \equiv t' - t \quad \Rightarrow e^{-i\omega(t-t')} \to e^{i\omega\eta} \quad \text{with } \eta > 0, \, t' \to t^+$$

In conclusion, the alternative expression for the total energy of the system in

terms of the Fourier transformed Green's function is:

$$E = \pm \frac{i}{2} \frac{V}{(2\pi)^4} \lim_{\eta \to 0^+} \int \mathrm{d}\vec{\mathbf{k}} \int_{-\infty}^{+\infty} \mathrm{d}\omega \; e^{i\omega\eta} \left(\hbar\omega + \frac{\hbar^2 k^2}{2m} \right) \mathrm{Tr}\, G(\vec{\mathbf{k}}, \omega) \qquad (2.11)$$

The presence of the expoential factor in yellow, which depends on the imaginary contribution, means that if we want to make a computation we have to work in the complex frequency plane ω and in particular this exponential will define the appropriate contour in this space.

This complete our derivation of the basic property of Green's function. However, we have still to demonstrate that we can obtain the excitation spectrum of the system as a function of the Green's function. Before proceeding, we make a small exercise in order to compute the Green's function for a simple case: non interacting free fermions.

2.2 Green's function for free fermions

Now, we make an exercise to really look at the explicit expression for Green's functions in the simple case of free fermions (for a non interacting homogeneous system of fermions). In practice, we consider a degenerate electron gas model but neglecting the electron-electron interaction (**non-interacting system**). The ground state is represented by the Fermi sphere, also called **filled Fermi sea**.

In order to evaluate the Green's function it is convenient to perform a **canonical transformation** to **particles** and **holes**.

The latter consists in redefining the fermion operator $c_{\vec{\mathbf{k}}\lambda}$ as follow:

$$c_{\vec{\mathbf{k}}\lambda} = \begin{cases} a_{\vec{\mathbf{k}}\lambda} & |\vec{k}| > k_F \quad \text{for } \textbf{Particles} \\ b^{\dagger}_{-\vec{\mathbf{k}}\lambda} & |\vec{k}| \leq k_F \quad \text{for } \textbf{Holes} \end{cases} \qquad (2.12)$$

where holes indicate the absence of particles (if we create a hole, we destroy a particle). In particular, the minus sign in the $\vec{\mathbf{k}}$ wave vector is explained as follow: if we consider the Fermi sphere and we create an hole inside, the total momentum is reduced by a factor $\vec{\mathbf{k}}$ because we have destroyed a particle with momentum $\vec{\mathbf{k}}$. Of course, the same trasnformation can be applied to the costruction operator.

As defined,

- $a_{\vec{\mathbf{k}}\lambda}$ destroys a **particle** *above* the Fermi sea.

- $b^{\dagger}_{-\vec{\mathbf{k}}\lambda}$ creates a **hole** (absence of a particle) *inside* the Fermi sea.

Remark. This transformation is "canonical" because preserves the anticommuation rules, which implies that the physics is unchanged. Indeed, it is easy to demonstrate:

$$\{a_{\vec{\mathbf{k}}}, a^{\dagger}_{\vec{\mathbf{k}}'}\} = \{b_{\vec{\mathbf{k}}}, b^{\dagger}_{\vec{\mathbf{k}}'}\} = \delta_{\vec{\mathbf{k}}\vec{\mathbf{k}}'}$$
$$\{a_{\vec{\mathbf{k}}}, b^{\dagger}_{\vec{\mathbf{k}}'}\} = 0$$

In particular $a_{\vec{\mathbf{k}}}$ and $b^{\dagger}_{\vec{\mathbf{k}}'}$ commute because they refer to different $\vec{\mathbf{k}}$ vectors (above or below the Fermi wave vector).

Now, it is interesting to rewrite the Hamiltonian for the non-interacting system using this canconical trasformation. Using the well known form of the Hamiltonian

in second quantization:

$$
\begin{aligned}
\hat{H}_0 &= \sum_{\vec{\mathbf{k}}\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{\vec{\mathbf{k}}\lambda} c_{\vec{\mathbf{k}}\lambda} = \sum_{\vec{\mathbf{k}}\lambda} \varepsilon_{\vec{\mathbf{k}}} c^\dagger_{\vec{\mathbf{k}}\lambda} c_{\vec{\mathbf{k}}\lambda} \\
&= \sum_{|\vec{\mathbf{k}}|\leq k_F,\lambda} \varepsilon_{\vec{\mathbf{k}}} b_{-\vec{\mathbf{k}}\lambda} b^\dagger_{-\vec{\mathbf{k}}\lambda} + \sum_{|\vec{\mathbf{k}}|> k_F,\lambda} \varepsilon_{\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}
\end{aligned}
$$

where we have rewritten by exploiting the canconical transformation, thanks to we obtain two contributions. Now, let us focus on the first contribution and since this term is symmetric in $\vec{\mathbf{k}}$, we can change the wave vector $-\vec{\mathbf{k}}' \to \vec{\mathbf{k}}$, obtaining:

$$
\hat{H}_0 = \sum_{|\vec{\mathbf{k}}|\leq k_F,\lambda} \varepsilon_{\vec{\mathbf{k}}} b_{\vec{\mathbf{k}}\lambda} b^\dagger_{\vec{\mathbf{k}}\lambda} + \sum_{|\vec{\mathbf{k}}|> k_F,\lambda} \varepsilon_{\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}
$$

Then, using the anticommuation rule $b_{\vec{\mathbf{k}}\lambda} b^\dagger_{\vec{\mathbf{k}}\lambda} = (1 - b^\dagger_{\vec{\mathbf{k}}\lambda} b_{\vec{\mathbf{k}}\lambda})$ we obtain:

$$
\hat{H}_0 = \boxed{\sum_{|\vec{\mathbf{k}}|\leq k_F,\lambda} \varepsilon_{\vec{\mathbf{k}}}} + \boxed{\sum_{|\vec{\mathbf{k}}|> k_F,\lambda} \varepsilon_{\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}\lambda} a_{\vec{\mathbf{k}}\lambda}} - \boxed{\sum_{|\vec{\mathbf{k}}|\leq k_F,\lambda} b^\dagger_{\vec{\mathbf{k}}\lambda} b_{\vec{\mathbf{k}}\lambda}}
$$

where the yellow term refers to particles (creating a particle raised the energy), while the green term to holes (creating a hole lowers the energy). Eventually, the pink term is just the same of the kinetic energy contribution for $\left|\vec{\mathbf{k}}\right| \leq k_F$ which corresponds to E_0, the ground state energy of the filled Fermi sea (in the absence of particles or holes, the energy is that of the filled Fermi sea).

How can we interpret physically this canonical trasformation? Let us consider a filled Fermi sea (ground state of the non-interacting system), then we excite the system obtaining a particle that goes outside the Fermi sphere and that creates an hole inside it. Instead, using the canonical transformation we start with a system which has no particles inside (empty state) and after we have excited the system we get a particle, the hole. This is possible because the pink term is just a constant contribution which corresponds to E_0. Hence, the canonical transformation is equivalent to a *shift* in energy (change the "zero" level: $E_0 \to 0$). Actually, with the canonical transformation we only consider particle outside the Fermi sphere and holes inside.

Let us note that:

- If the total number of fermions is fixed, particles and holes necessarily occur in pairs.

- since each particle-hole pair has a net positive energy, the filled Fermi sea is really the ground state (so when we consider a particle outside the fermi sphere we are increasing the energy). The net positive energy is due to the fact that in the second term we have $|\vec{k}| > k_F$, while in the third term $|\vec{k}| \leq k_F$, thus the third contribution is smaller in absolute value with respect to the second one. The effect is a positive contribution.

In order to evaluate the Green's function for the free fermion system, we come back to Heisenberg field operators. In our specific case the Hamiltonian reduces to that of non-interacting particle $\hat{H} \to \hat{H}_0$, this will correspond to the "interaction" picture operators but we will see this later.

Let us consider the expression for the Heisenberg field operator (Eq.(2.1)):

$$
\hat{\psi}_{H\alpha}(\vec{\mathbf{x}}, t) \equiv e^{\frac{i\hat{H}_0 t}{\hbar}} \hat{\psi}_\alpha(\vec{\mathbf{x}}) e^{\frac{-i\hat{H}_0 t}{\hbar}} = e^{\frac{i\hat{H}_0 t}{\hbar}} \left(\sum_{\vec{\mathbf{k}}} \frac{e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}}{\sqrt{V}} \eta_\alpha c_{\vec{\mathbf{k}}\alpha} \right) e^{\frac{-i\hat{H}_0 t}{\hbar}}
$$

where the standard field operator is made by combination of plane waves multiplied by a spin function. The difficulty is that this formula relate the two operators $\hat{H}_0$ and $c_{\vec{\mathbf{k}}\alpha}$.

One can easily show that the last expression can be written with a sequence of commutators. In particular:

$$e^{\frac{i\hat{H}_0 t}{\hbar}} c_{\vec{\mathbf{k}}\alpha} e^{\frac{-i\hat{H}_0 t}{\hbar}} = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{i}{\hbar}\hat{H}_0 t, \left[\frac{i}{\hbar}\hat{H}_0 t, \dots \left[\frac{i}{\hbar}\hat{H}_0 t, c_{\vec{\mathbf{k}}\alpha} \right] \dots \right] \right]$$

as can be verified by expanding the exponential operators and checking that the left-hand and the right-hand terms are the same. Moreover, since the $\frac{it}{\hbar}$ are just numbers they can be putted outside of the commutators, obtaining:

$$e^{\frac{i\hat{H}_0 t}{\hbar}} c_{\vec{\mathbf{k}}\alpha} e^{\frac{-i\hat{H}_0 t}{\hbar}} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{it}{\hbar} \right)^n \left[\hat{H}_0, \left[\hat{H}_0, \dots \left[\hat{H}_0, c_{\vec{\mathbf{k}}\alpha} \right] \dots \right] \right]$$

Now, let us focus on the inner commutator $[\hat{H}_0, c_{\vec{\mathbf{k}}\alpha}]$. By writing it explicitely (using the expression in second quantization for $\hat{H}_0$) we have:

$$[\hat{H}_0, c_{\vec{\mathbf{k}}\alpha}] = \sum_{\vec{\mathbf{k}}'\alpha'} \varepsilon_{\vec{\mathbf{k}}'} \left[c_{\vec{\mathbf{k}}'\alpha'}^{\dagger} c_{\vec{\mathbf{k}}'\alpha'}, c_{\vec{\mathbf{k}}\alpha} \right] = \sum_{\vec{\mathbf{k}}'\alpha'} \varepsilon_{\vec{\mathbf{k}}'} \left(- \left[c_{\vec{\mathbf{k}}\alpha}, c_{\vec{\mathbf{k}}'\alpha'}^{\dagger} c_{\vec{\mathbf{k}}'\alpha'} \right] \right)$$

$$= \sum_{\vec{\mathbf{k}}'\alpha'} \varepsilon_{\vec{\mathbf{k}}'} \left(- \underbrace{\left\{ c_{\vec{\mathbf{k}}\alpha}, c_{\vec{\mathbf{k}}'\alpha'}^{\dagger} \right\}}_{=\delta_{\vec{\mathbf{k}}\vec{\mathbf{k}}'}\delta_{\alpha\alpha'}} c_{\vec{\mathbf{k}}'\alpha'} + c_{\vec{\mathbf{k}}'\alpha'}^{\dagger} \underbrace{\left\{ c_{\vec{\mathbf{k}}'\alpha'}, c_{\vec{\mathbf{k}}\alpha} \right\}}_{=0} \right)$$

$$= -\varepsilon_{\vec{\mathbf{k}}} c_{\vec{\mathbf{k}}\alpha}$$

where we have used the relation Eq.(2.4).

Then, by repeating this procedure n times for n commutators, we can rewrite the sequence of operators as follow:

$$e^{\frac{i\hat{H}_0 t}{\hbar}} c_{\vec{\mathbf{k}}\alpha} e^{\frac{-i\hat{H}_0 t}{\hbar}} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{it}{\hbar} \right)^n (-\varepsilon_{\vec{\mathbf{k}}})^n c_{\vec{\mathbf{k}}\alpha} = e^{-\frac{i\varepsilon_{\vec{\mathbf{k}}} t}{\hbar}} c_{\vec{\mathbf{k}}\alpha}$$

the nice thing is that we were able to put in evidence the explicit time dependence of the Fermi sea operator in the Heisenberg picture. The nice thing is that we were able to put in evidence to elucidate the explicit time dependence of the sea operator in the Heisenberg picture. Let us come back to the original expression of the Heisenberg field operator:

$$\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t) = e^{\frac{i\hat{H}_0 t}{\hbar}} \left(\sum_{\vec{\mathbf{k}}} \frac{e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}}}{\sqrt{V}} \eta_\alpha c_{\vec{\mathbf{k}}\alpha} \right) e^{\frac{-i\hat{H}_0 t}{\hbar}}$$

$$= \sum_{\vec{\mathbf{k}}} \frac{e^{(i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}} - \omega_{\vec{\mathbf{k}}} t)}}{\sqrt{V}} \eta_\alpha c_{\vec{\mathbf{k}}\alpha}$$

where for simplicity we have defined $\omega_{\vec{\mathbf{k}}} \equiv \varepsilon_{\vec{\mathbf{k}}}/\hbar$ and we have written explicitly the space and time dependence of the Heisenberg field operator.

Using the canonical transformation we get:

$$\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}}, t) = \sum_{\substack{\vec{\mathbf{k}} \\ |\vec{\mathbf{k}}| \leq k_F}} \frac{e^{(i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}} - \omega_{\vec{\mathbf{k}}} t)}}{\sqrt{V}} \eta_\alpha b_{-\vec{\mathbf{k}}\alpha} + \sum_{\substack{\vec{\mathbf{k}} \\ |\vec{\mathbf{k}}| > k_F}} \frac{e^{(i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}} - \omega_{\vec{\mathbf{k}}} t)}}{\sqrt{V}} \eta_\alpha a_{\vec{\mathbf{k}}\alpha}$$

Let us focus on the first term, clearly here we can replace $-\vec{\mathbf{k}} \to \vec{\mathbf{k}}$ and so we get:

$$\hat{\psi}_{H\alpha}(\vec{\mathbf{x}}, t) = \sum_{\substack{\vec{\mathbf{k}} \\ |\vec{\mathbf{k}}| \le k_F}} \frac{e^{-(i\vec{\mathbf{k}} \cdot \vec{\mathbf{x}} + \omega_{\vec{\mathbf{k}}} t)}}{\sqrt{V}} \eta_\alpha b_{\vec{\mathbf{k}}\alpha} + \sum_{\substack{\vec{\mathbf{k}} \\ |\vec{\mathbf{k}}| > k_F}} \frac{e^{(i\vec{\mathbf{k}} \cdot \vec{\mathbf{x}} - \omega_{\vec{\mathbf{k}}} t)}}{\sqrt{V}} \eta_\alpha a_{\vec{\mathbf{k}}\alpha}$$

Now, in order to compute the Green's function we need to use $\hat{\psi}_{H\alpha}$ and $\hat{\psi}_{H\alpha}^\dagger$ expressed in term of b and a operators. We can use the fact that the particle and hole destruction operators both annihilate the ground state:

$$\begin{cases} a_{\vec{\mathbf{k}}\alpha} |0\rangle = 0 & \text{(there are no particles above the Fermi sea)} \\ b_{\vec{\mathbf{k}}\alpha} |0\rangle = 0 & \text{(there are no holes below the Fermi sea)} \end{cases}$$

since there are no particles above or holes below the Fermi sea in the state $|0\rangle$. For instance the first relation gives zero because it would destroy a particle outside the Fermi sphere, but in the non-interacting state there are no particles. Similarly, the second relation means that the operator would destroy a hole inside the Fermi sphere but destroying a hole inside the Fermi sphere would correspond in creating a particle inside. It is not possible, because inside the Fermi sphere, in the non-interacting ground state, the state is already filled and so we cannot create an additional particle. Hence, we get zero.

By considering the expression for the Green's function we get:

$$iG_{\alpha\beta}^0(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') = \langle 0| T\left[\hat{\psi}_{H\alpha}(\vec{\mathbf{x}}t)\hat{\psi}_{H\beta}^\dagger(\vec{\mathbf{x}}'t')\right]|0\rangle$$

It is easy to check that by replacing the Heisenber field operators, in principle we should get 4 terms, but in practice only 2 non-vanishing contributions survive (usefulness of the particle-hole notation):

$$iG_{\alpha\beta}^0(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') \begin{cases} \frac{1}{V} \sum_{\substack{|\vec{\mathbf{k}}| > k_F \\ |\vec{\mathbf{k}}'| > k_F}} e^{i(\vec{\mathbf{k}} \cdot \vec{\mathbf{x}} - \omega_{\vec{\mathbf{k}}} t)} e^{-i(\vec{\mathbf{k}}' \cdot \vec{\mathbf{x}}' - \omega_{\vec{\mathbf{k}}'} t')} \eta_\alpha \eta_\beta^\dagger + \langle 0| a_{\vec{\mathbf{k}}\alpha} a_{\vec{\mathbf{k}}'\beta}^\dagger |0\rangle & t > t' \\ -\frac{1}{V} \sum_{\substack{|\vec{\mathbf{k}}| \le k_F \\ |\vec{\mathbf{k}}'| \le k_F}} e^{i(\vec{\mathbf{k}}' \cdot \vec{\mathbf{x}}' + \omega_{\vec{\mathbf{k}}'} t')} e^{-i(\vec{\mathbf{k}} \cdot \vec{\mathbf{x}} + \omega_{\vec{\mathbf{k}}} t)} \eta_\beta^\dagger \eta_\alpha + \langle 0| b_{\vec{\mathbf{k}}'\beta} b_{\vec{\mathbf{k}}\alpha}^\dagger |0\rangle & t < t' \end{cases}$$

Then by replacing $-\vec{\mathbf{k}} \to \vec{\mathbf{k}}$ and considering that

$$\langle 0| a_{\vec{\mathbf{k}}\alpha} a_{\vec{\mathbf{k}}'\beta}^\dagger |0\rangle = \langle 0| b_{\vec{\mathbf{k}}'\beta} b_{\vec{\mathbf{k}}\alpha}^\dagger |0\rangle = \delta_{\vec{\mathbf{k}}\vec{\mathbf{k}}'}\delta_{\alpha\beta}$$

which means that for instance if we create a particle outside the Fermi sphere with $a_{\vec{\mathbf{k}}'\beta}^\dagger$, the only possibility to get a non vanishing contribution is that this destroy exactly the same particle. Similarly for the b operator.

The final result is

$$iG_{\alpha\beta}^0(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') = \frac{\delta_{\alpha\beta}}{V} \sum_{\vec{\mathbf{k}}} e^{i\vec{\mathbf{k}} \cdot (\vec{\mathbf{x}} - \vec{\mathbf{x}}')} e^{-i\omega_{\vec{\mathbf{k}}}(t - t')} \times$$
$$\times \left[\Theta(t - t')\Theta(|\vec{k}| - k_F) - \Theta(t' - t)\Theta(k_F - |\vec{k}|)\right] \tag{2.13}$$

this is the explicit form of the Green's function in the case of free fermions (non interacting system).

Now, considering that the system is homogeneous in space and in time (the hamiltonian is time independent), G^0 only depends on the difference between the spatial coordinates and times. Thus it is convenient to consider the Fourier transform of the Green's function:

$$G_{\alpha\beta}^0(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') = G_{\alpha\beta}^0(\vec{\mathbf{x}} - \vec{\mathbf{x}}', t - t') \equiv \frac{1}{2\pi V} \sum_{\vec{\mathbf{k}}} \int_{-\infty}^{+\infty} d\omega \, e^{i\vec{\mathbf{k}} \cdot (\vec{\mathbf{x}} - \vec{\mathbf{x}}')} e^{-i\omega(t - t')} G_{\alpha\beta}^0(\vec{\mathbf{k}}, \omega)$$

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Tuesday 7th April, 2020.
Compiled: Friday 8th May, 2020.

Let us focus on the time-dependent of $G^0_{\alpha\beta}$ and consider only the first time dependent term of Eq.(2.13):

$$\Theta(t - t')e^{-i\omega(t-t')} \equiv \frac{1}{2\pi} \int d\omega\, f(\omega)e^{-i\omega(t-t')}$$

where we have performed of course the Fourier transform with respect to the time variable. The $f(\omega)$ can be obtained by a reverse integral over time of the left-hand side of the previous equation where we consider $\tau \equiv t - t'$:

$$f(\omega) = \int_{-\infty}^{+\infty} d\tau\, e^{i\omega\tau} \left[\Theta(\tau)e^{-i\omega_k\tau}\right] = \int_0^\infty d\tau\, e^{i(\omega-\omega_k)\tau} =$$

$$= \frac{e^{i(\omega-\omega_k)\tau}}{i(\omega - \omega_k)}\bigg|_0^\infty \overset{(a)}{=} \lim_{\eta\to 0^+} \frac{e^{i(\omega-\omega_k+i\eta)\tau}}{i(\omega - \omega_k + i\eta)}\bigg|_0^\infty =$$

$$= \lim_{\eta\to 0^+} -\frac{1}{i}\frac{1}{(\omega - \omega_k + i\eta)} = \lim_{\eta\to 0^+} \frac{i}{(\omega - \omega_k + i\eta)}$$

where in step (a) in order to make the integral convergent we have introduced a small positive quantity $\eta > 0$. Then, we repeat the same analysis for the second term of Eq.(2.13), obtaining a similar result:

$$\Theta(t' - t)e^{-i\omega(t'-t)} \longrightarrow \lim_{\eta\to 0^+} -\frac{i}{(\omega - \omega_k - i\eta)}$$

By replacing the time dependent part with the Fourier expansion, one can rewrite the original non interacting Green's function as follow:

$$iG^0_{\alpha\beta}(\vec{\mathbf{x}}t, \vec{\mathbf{x}}'t') = \frac{\delta_{\alpha\beta}}{2\pi V} \sum_{\vec{\mathbf{k}}} e^{i\vec{\mathbf{k}}\cdot(\vec{\mathbf{x}}-\vec{\mathbf{x}}')} \left[\Theta(|\vec{k}| - k_f) \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega(t-t')} \frac{i}{\omega - \omega_k + i\eta}\right.$$

$$\left. + \Theta(k_f - |\vec{k}|) \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega(t-t')} \frac{i}{\omega - \omega_k - i\eta}\right]$$

and we notice that in the original Green's function (Eq.(2.13)) we have a minus sign between the two terms, while in the Fourier transformed one there is a plus sign. By using Eq.(2.10), we recover the explicit expression for the non-interacting Green's function in reciprocal space (in terms of the wave vector and of the frequency). Hence, we arrive at the expression of the Fourier transform of the non-interacting Green's funciton:

$$G^0_{\alpha\beta}(\vec{\mathbf{k}}, \omega) = \delta_{\alpha\beta} \left[\frac{\Theta(|\vec{k}| - k_F)}{\omega - \omega_k + i\eta} + \frac{\Theta(k_F - |\vec{k}|)}{\omega - \omega_k - i\eta}\right] \tag{2.14}$$

where the green term is valid for $\vec{\mathbf{k}}$ vectors larger than the Fermi wave vector k_F, which means for electrons that are created and destoryed outside the Fermi sphere. The second term is due to holes that are created or destroyed inside the Fermi sphere.

Now, let us consider $G^0_{\alpha\beta}$ as a function in the complex ω plane in Fig.2.1 (by also taking into account that of course the frequency is releated to energy with $\omega_k = \varepsilon_k/\hbar = \hbar k^2/(2m)$).

- For a given $\vec{\mathbf{k}}$ with $|\vec{k}| > k_F$ there is a larger contribution whenever the denominator approaches zero. Exactly when the denominator is zero there is a single *pole* and the frequency is that is equal to $\omega_p = \omega_k - i\eta$ which is just below the real axis in Fig.2.1.

- For a given $\vec{\mathbf{k}}$ with $|\vec{k}| \leq k_F$ a single *pole* is when $\omega_p = \omega_k + i\eta$ which is just above the real axis in Fig.2.1.
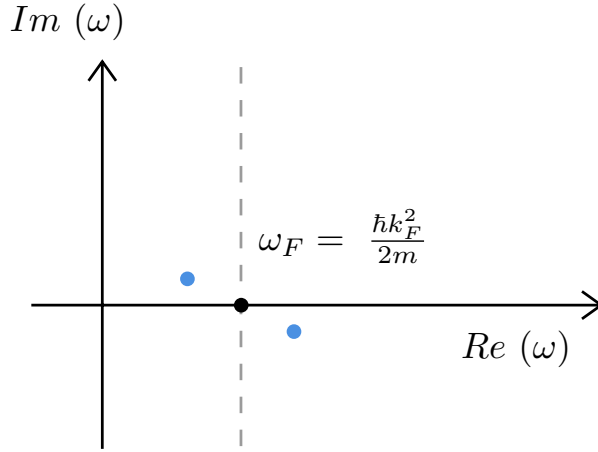
Figure 2.1: Complex plane ω, where ω_F is the Fermi frequency.

This is an interesting result because we will see that something similar happen for a general interacting system Green's function.

To summarize, we have written explicitly the non-interacting Green's function both in the real space (Eq.(2.13)) and reciprocal space (Eq.(2.14)). Using the Green's function we can compute the most interesting property of the system, as the ground state energy of the system E_0. We have already derived E_0 by using the second quantization approach, but it could be interesting to try to recover the ground state energy using the Green's function G_0.

2.3   The Lehmann representation

Now let us come back to the general Green's function by considering the case of **interacting** particles and let us try to show some other general properties of the Green's function. In particular, we are considering fermions but similar properties hold for bosons.

Let us rewrite the exact general Green's function as in Eq.(2.2) (with $\langle\psi_0|\psi_0\rangle = 1$):

$$iG_{\alpha\beta}(\vec{x}t, \vec{x}'t') \equiv \langle\psi_0| T\left[\hat{\psi}_{H\alpha}(\vec{x}, t)\hat{\psi}^\dagger_{H_\beta}(\vec{x}', t')\right]|\psi_0\rangle$$

$$= \Theta(t - t') \langle\psi_0| \hat{\psi}_{H\alpha}(\vec{x}, t)\hat{\psi}^\dagger_{H_\beta}(\vec{x}', t')|\psi_0\rangle$$

$$- \Theta(t' - t) \langle\psi_0| \hat{\psi}^\dagger_{H_\beta}(\vec{x}', t')\hat{\psi}_{H\alpha}(\vec{x}, t)|\psi_0\rangle$$

where due to the effect of the time order operator, we have the sum of two contribution depending on the order of t with respect of t'. Let us focus only on the matrix element of the first term and we rewrite it by explicitly writing the Heisenberg field operators in terms of the ordinary field operators:

$$\langle\psi_0| \hat{\psi}_{H\alpha}(\vec{x}, t)\hat{\psi}^\dagger_{H_\beta}(\vec{x}', t')|\psi_0\rangle = \langle\psi_0| e^{i\frac{\hat{H}t}{\hbar}} \hat{\psi}_\alpha(\vec{x})e^{-i\frac{\hat{H}t}{\hbar}} e^{i\frac{\hat{H}t'}{\hbar}} \hat{\psi}^\dagger_\beta(\vec{x}')e^{-i\frac{\hat{H}t'}{\hbar}}|\psi_0\rangle$$

If we assume that $\hat{H}|\psi_0\rangle = E_0|\psi_0\rangle$, we have already shown in the case of the demonstration that the Green function is uniform in time if the hamiltonian is time independent, that we can extract the exponential term from the matrix:

$$\langle\psi_0| \hat{\psi}_{H\alpha}(\vec{x}, t)\hat{\psi}^\dagger_{H_\beta}(\vec{x}', t')|\psi_0\rangle = e^{i\frac{E_0(t-t')}{\hbar}} \langle\psi_0| \hat{\psi}_\alpha(\vec{x})e^{-i\frac{\hat{H}(t-t')}{\hbar}} \hat{\psi}^\dagger_\beta(\vec{x}')|\psi_0\rangle$$

Now let us consider the *complete* set of all eigenstates of the system

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \qquad \sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{1}$$

If we insert this complete set of states between the field operators we obtain:

$$\Theta(t-t') \langle\psi_0| \hat{\psi}_{H\alpha}(\vec{\mathbf{x}},t)\hat{\psi}^\dagger_{H_\beta}(\vec{\mathbf{x}}',t') |\psi_0\rangle = \sum_n e^{i\frac{E_0(t-t')}{\hbar}} \langle\psi_0| \hat{\psi}_\alpha(\vec{\mathbf{x}})e^{-i\frac{\hat{H}(t-t')}{\hbar}} |\psi_n\rangle \langle\psi_n| \hat{\psi}^\dagger_\beta(\vec{\mathbf{x}}') |\psi_0\rangle$$

$$= \sum_n e^{-i\frac{(E_n-E_0)(t-t')}{\hbar}} \langle\psi_0| \hat{\psi}_\alpha(\vec{\mathbf{x}}) |\psi_n\rangle \langle\psi_n| \hat{\psi}^\dagger_\beta(\vec{\mathbf{x}}') |\psi_0\rangle$$

and similarly for the second term corresponding to $\Theta(t'-t)$. Hence, essentially the Lehman representation means using this trick.

Since the Green's function G is homogeneous in time (because the hamiltonian is time independent) it is convenient to take the *partial* Fourier transform:

$$G_{\alpha\beta}(\vec{\mathbf{x}},\vec{\mathbf{x}}',t-t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega\tau}\widetilde{G}_{\alpha\beta}(\vec{\mathbf{x}},\vec{\mathbf{x}}',\omega)$$

with the Fourier transform instead of depending on two times, the Green's function depends only on one single frequency. In particular, it is a partial Fourier transform in the sense that it is the Fourier transform of the original Green's function only in terms of the time variable, while the space dependence remains the same.

One can compute this partial Fourier transform $\widetilde{G}$ by repeating a similar approach that we have used for the non-interacting Green's function. It is not necessary to repeat all the procedure, because actually we can exploit the similarity between this general case case and the previous non-interacting case. Hence, in the Green's function in Eq.(2.13) we have an exponential term related to time dependence and now for the general Green's function (Eq.(2.3)) we have a similar term (of course by considering that the frequency is proportional to the energy):

$$\underbrace{e^{-i\omega_{\vec{\mathbf{k}}}(t-t')}}_{\text{in } G_0} = e^{-i\frac{\varepsilon_k(t-t')}{\hbar}} \longrightarrow \underbrace{e^{-i\frac{(E_n-E_0)(t-t')}{\hbar}}}_{\text{in } G}$$

indeed we can again an exponential factor with the only difference that instead of ω_k (or $\varepsilon_k/\hbar$) we get this energy difference. Thus, by using the same result obtained in the case of the non-interacting Green's function (Eq.(2.14)) we obtain:

$$\widetilde{G}_{\alpha\beta}(\vec{\mathbf{x}},\vec{\mathbf{x}}',\omega) = \sum_n \left[\frac{\langle\psi_0| \hat{\psi}_\alpha(\vec{\mathbf{x}}) |\psi_n\rangle \langle\psi_n| \hat{\psi}^\dagger_\beta(\vec{\mathbf{x}}') |\psi_0\rangle}{\omega - \frac{(E_n-E_0)}{\hbar} + i\eta} + \frac{\langle\psi_0| \hat{\psi}^\dagger_\beta(\vec{\mathbf{x}}') |\psi_n\rangle \langle\psi_n| \hat{\psi}_\alpha(\vec{\mathbf{x}}) |\psi_0\rangle}{\omega + \frac{(E_n-E_0)}{\hbar} - i\eta} \right]$$

$$(2.15)$$

where we in particular note the presence of the poles. As said, the denominators are just obtained by a similar approach as the corresponding denominators in the non-interacting Green's function. The frequency dependence is just trough those two denominators.

The last equation represent a **"meromorphic"** function, which is an analytic function over all the complex ω (frequency) plane, with the exception of a set of *isolated* points (**poles**). This is a generalization of the poles obtained in the non interacting case. In particular, those poles (singularities) are of course found whenever the denominators are closed to zero and so we have poles when the frequency is given by this expression:

$$\omega = \pm\frac{(E_n-E_0)}{\hbar} \mp i\eta$$

This is a very interesting result because it generalizes what we have obtained in the case of the non-interacting Green's function. The idea is that, as we will see in more details, while in the case of the non-interacting Green's function we had a single pole for a given $\vec{\mathbf{k}}$ wave vector, in the case of the general full interacting Green's function

we have a *discrete* set of poles that are obtained by considering the situation when the denominators in Eq.(2.15) vanishes.

Now, we try to understand better the meaning of the poles that we have seen looking at the denominator of this function. First we recall the expression of the total number of particle operator in second quantization:

$$\hat{N} = \sum_{\alpha'} \int \mathrm{d}\vec{\mathbf{x}}\, \hat{\psi}_{\alpha'}^{\dagger}(\vec{\mathbf{x}}) \hat{\psi}_{\alpha'}(\vec{\mathbf{x}})$$

Taking the commutator with the destruction field operator we obtain:

$$[\hat{N}, \hat{\psi}_{\alpha}(\vec{\mathbf{x}})] = -\hat{\psi}_{\alpha}(\vec{\mathbf{x}}) \quad \Rightarrow \hat{N}\hat{\psi}_{\alpha}(\vec{\mathbf{x}}) = \hat{\psi}_{\alpha}(\vec{\mathbf{x}})(\hat{N}-1)$$

Then, if we apply apply this sequnce of operators to the exact ground state of our system (which is a system made by N particles):

$$\hat{N}\left(\hat{\psi}_{\alpha}(\vec{\mathbf{x}})\,|\psi_0\rangle\right) = (N-1)\left(\hat{\psi}_{\alpha}(\vec{\mathbf{x}})\,|\psi_0\rangle\right)$$

This simply means that if ψ_0 is an eigenstate of the system with N particles, the application of the destruction field operator gives an eigenstate of $\hat{N}$ with eigenvalue $(N-1)$.

Now consider that in the Lehmann representation we have introduced the complete basis set: $\{|\psi_0\rangle\}$ are eigenstates of the *full* hamiltonian and in principle include *all possible numbers* of particles. Let us consider again the Eq.(2.15) and in particular the first matrix element. The latter must be different from zero in order to not have a vanishing contribution when there is a pole:

$$\langle\psi_0|\,\hat{\psi}_{\alpha}(\vec{\mathbf{x}})\,|\psi_n\rangle \neq 0 \quad \text{only if } M-1 = N \Rightarrow M = N+1$$

where $|\psi_n\rangle$ is an eigenstate of the system with M particles (where M is not necessarly equal to N), while $|\psi_0\rangle$ is an eigenstate of the system with N particles. In the last formula we have obtained that in order to not have a vanishing contribution we must have states with the same number of particle both on the left and right; this is only possible if $|\psi_n\rangle$ is an eigenstate of the system with $(N+1)$ particles. The important conclusion is that in order to have a non vanishing matrix element, the eignestate $|\psi_n\rangle$ must be an egeinstate of the system with one more particle! This is a peculiar effect different from the ordinary Schrödinger equation where we must consider systems with the number of particles constant somehow.

Now, let us examine the corresponding denominator (of the latter matrix element) $\omega - (E_n - E_0)/\hbar + i\eta$ and according to our observation, here the E_n energy is an eigenvalue of the system with $(N+1)$ particles. In the pole (singularity), hence whenever this denominator vanishes, we have the following situation:

$$\omega = \frac{(E_n - E_0)}{\hbar} - i\eta = \frac{E_n(N+1)}{\hbar} - \frac{E_0(N)}{\hbar} - i\eta$$
$$= \frac{1}{\hbar}\left[E_n(N+1) - E_0(N+1)\right] + \frac{1}{\hbar}\left[E_0(N+1) - E_0(N)\right] - i\eta \tag{2.16}$$

where we have added and substracted the same quantity $E_0(N+1)$. The last expression is very interesting:

- if we look at the first term in green, clearly this is the difference between the energy corresponding to the n level and the energy corresponding to the ground state, for the system with $(N+1)$ particles. In particular, this is the **excitation** energy of the system with $(N+1)$ particles which can be written as:

$$\frac{1}{\hbar}[E_n(N+1) - E_0(N+1)] \equiv \frac{\varepsilon_n(N+1)}{\hbar} \geq 0$$

indeed by definition of excitation energy is greater or equal than zero.

- If we look at the second term in red, this is the difference between the ground states energy of the system with $(N+1)$ and that with N particles. In physics this is a well known quantity called chemical potential[2]. The chemical potential is equivalent to the change in energy (at constant volume) of the ground states as one extra particle is added to the system. Thus we have:

$$\frac{1}{\hbar}[E_0(N+1) - E_0(N)] \equiv \frac{\mu}{\hbar}$$

Eventually, in the pole:

$$\omega = \frac{\varepsilon_n(N+1)}{\hbar} + \frac{\mu}{\hbar} - i\eta \tag{2.17}$$

indeed in this pole the frequency is equal to the exictation energy plus the chemical potential and minus a small imaginary correction. The latter makes this pole frequency slightly below the real ω frequency axes.

Similarly considering the matrix element of the second term in Eq.(2.15), we can repeat the same procedure as above. Firstly, we check whenever this matrix element does not vanish:

$$\langle \psi_0 | \hat{\psi}_\beta^\dagger(\vec{\mathbf{x}}') | \psi_n \rangle \neq 0 \quad \text{only if } M + 1 = N \Rightarrow M = N - 1$$

where again $|\psi_n\rangle$ is an eigenstate of the system with M particles, while $|\psi_0\rangle$ is an eigenstate of the system with N. In order to have a non vanishing contribution $|\psi_n\rangle$ must be an eigenstate of the system with $(N-1)$ particles, hence with one less particle. Then, we can focus again on the corresponding denominator $\omega + (E_n - E_0)/\hbar - i\eta$ where E_n is an eigenvalue of the system with $(N-1)$ particles. In the pole:

$$\begin{aligned} \omega &= -\frac{(E_n - E_0)}{\hbar} + i\eta = -\frac{E_n(N-1)}{\hbar} + \frac{E_0(N)}{\hbar} + i\eta \\ &= -\frac{1}{\hbar}\left[E_n(N-1) - E_0(N-1) \right] + \frac{1}{\hbar}\left[E_0(N) - E_0(N-1) \right] + i\eta \end{aligned} \tag{2.18}$$

where again:

- the first green quantity is the **excitation** energy of the system with $(N-1)$ particles and we can write

$$\frac{1}{\hbar}[E_n(N-1) - E_0(N-1)] \equiv \frac{\varepsilon_n(N-1)}{\hbar} \geq 0$$

- the second red term is the difference between the ground states energy of the system with N and that with $N-1$ particles, which again is the chemical potential:

$$\frac{1}{\hbar}[E_0(N) - E_0(N-1)] \equiv \frac{\mu}{\hbar}$$

Remark. In the chemical potential of Eq.(2.16) we had the difference $E_0(N+1) - E_0(N)$, while in Eq.(2.18) we had $E_0(N) - E_0(N-1)$. In the thermodynamic limit $(N \to \infty)$, the difference between the chemical potential of a system with $N+1$ particles and one with N is small because:

$$\mu(N+1) = \mu(N) + O\left(\frac{1}{N}\right)$$

---

[2] Read Chapter 2. of [?] for a review of this thermodynamic concept

Eventually, in the pole:

$$\omega = -\frac{\varepsilon_n(N-1)}{\hbar} + \frac{\mu}{\hbar} + i\eta \tag{2.19}$$

where we have have minus the excitation energy of the system with $N-1$ particles plus the chemical potential and plus a small imaginary positive correction, which makes this frequency slightly above the real frequency ω axes.

Finally, we can rewrite the Green's function in (2.15) by explicitly reformulating the denominators using Eq.(2.17) and Eq.(2.19):

$$\widetilde{G}_{\alpha\beta}(\vec{\mathbf{x}}, \vec{\mathbf{x}}', \omega) = \sum_n \left[\underbrace{\frac{\langle\psi_0|\,\hat{\psi}_\alpha(\vec{\mathbf{x}})\,|\psi_n\rangle\,\langle\psi_n|\,\hat{\psi}_\beta^\dagger(\vec{\mathbf{x}}')\,|\psi_0\rangle}{\omega - \frac{\varepsilon_n(N+1)}{\hbar} - \frac{\mu}{\hbar} + i\eta}}_{I} + \underbrace{\frac{\langle\psi_0|\,\hat{\psi}_\beta^\dagger(\vec{\mathbf{x}}')\,|\psi_n\rangle\,\langle\psi_n|\,\hat{\psi}_\alpha(\vec{\mathbf{x}})\,|\psi_0\rangle}{\omega + \frac{\varepsilon_n(N-1)}{\hbar} - \frac{\mu}{\hbar} - i\eta}}_{II} \right]$$

$$\tag{2.20}$$

It is interesting to look at the behaviour of this function in the frequency plane (or in the $\hbar\omega$ frequency plane, so in the energy plane which is the same) as in Fig.2.2, where the poles are represented as crosses (the singularities are of course obtained letting the denominators of Eq.(2.20) to go to zero). Note that there is a change of behaviour in correspondence of the chemical potential which distinguishes the part I of Eq.(2.20) with the part II. Clearly, we have that the poles are slightly above the real axes (red ones) if the energy is smaller than the chemical potential and slighly below the real axes (blue ones) if the energy is larger. This is a generalization for what we have found for non-interacting Green's function as in Fig.2.1. In this case we had only a single pole, just below or above the real axes, for given value of the $\vec{\mathbf{k}}$ wave vector).
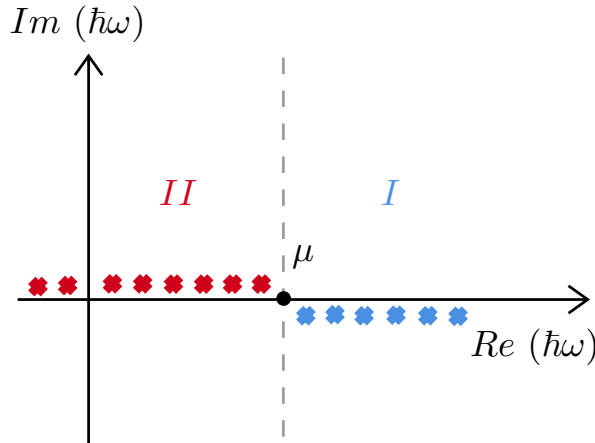
Figure 2.2: Complex energy plane $\hbar\omega$. The blue crosses represent the poles of the part I of Eq.(2.20), while the red crosses represent the poles of the part II. We note that there is a change of behaviour in correspondence of the chemical potential.

In conclusion, we have found the dependence on the frequency of the general, exact Green's function! This ia a general Green's function, not an approximating one, appropiate for the interacting system. To summarize, the poles go from above to below the real axis in the correspondence to the chemical potential of the system μ.

The excitation energies of those excited states, for which the numerators do not vanish, are given by the singularities of the Green's function (Eq.(2.20)). In particular they are:

- For the part I:
$$\varepsilon_n(N+1) = \hbar \operatorname{Re}(\omega_{pole}) - \mu \tag{2.21}$$

- For the part II:
$$\varepsilon_n(N-1) = -\hbar \operatorname{Re}(\omega_{pole}) + \mu \tag{2.22}$$

Thus the Green's function gives information on the **excitation spectrum** of the system with $N \pm 1$ particles. Hence, we essentially have satisfied the promised property (anticipated in Sec.2.1) of the Green's function which states that it is able to describe the excitation spectrum of the system! Summarizing, to get the excitation energies of the system we can just consider the singularities (poles) of the Green's funciton. To be more precise, of course we can get the excitation energies of those excited states for which the numerators do not vanish, otherwise it does not make any sense (if both the numerator and the denominator vanish at the same time, there are no more singularities).

The results obtained are of great importance to connect with experimental results. To ber more precise the Green's function can give informations on the excitation spectrum of the system with one more or one less particles. Clearly, this is essentially a formal difference because we should still remember that in our case we are considering always the theromydynamic limit ($N \to \infty$), so $N \pm 1$ differ very little from N.

2.3.1 Case: translational invariance

As previously supposed, our hamiltonian does not depend on time, hence the system is homogeneous in time. Now, let us consider a more particular case of also translational invariance, namely the total momentum of the system commutes with the total hamiltonian: $[\hat{\vec{\mathbf{p}}}, \hat{H}] = 0$. Thus, the Green's function is expected to be **homogeneous** both in **time** and **space**.

In second quantization, the total momentum can be expressed in terms of the field operators (or in terms of the creation and destruction operators) as:

$$\hat{\vec{\mathbf{p}}} = \sum_\alpha \int \mathrm{d}^3\vec{\mathbf{x}}\, \hat{\psi}_\alpha^\dagger(\vec{\mathbf{x}})\left(-i\hbar\vec{\boldsymbol{\nabla}}\right)\hat{\psi}_\alpha(\vec{\mathbf{x}}) = \sum_{\vec{\mathbf{k}},\alpha} \hbar\vec{\mathbf{k}}\, c_{\vec{\mathbf{k}}\alpha}^\dagger c_{\vec{\mathbf{k}}\alpha}$$

It is easy to demonstrate that:

$$\left[\hat{\psi}_\alpha(\vec{\mathbf{x}}), \hat{\vec{\mathbf{p}}}\right] = -i\hbar\vec{\boldsymbol{\nabla}}\hat{\psi}_\alpha(\vec{\mathbf{x}})$$

and that the integral form of the last relation is the following

$$\hat{\psi}_\alpha(\vec{\mathbf{x}}) = e^{-i\frac{\hat{\vec{\mathbf{p}}}\cdot\vec{\mathbf{x}}}{\hbar}}\hat{\psi}_\alpha(0)e^{i\frac{\hat{\vec{\mathbf{p}}}\cdot\vec{\mathbf{x}}}{\hbar}}$$

where $\hat{\psi}_\alpha(0)$ is the field operator acting on the origin of our system. This allowed us to extract the explicit space dependence from the field operator.

Now, we rewrite the Heisenberg field operator by explicitly writing the dependence on time and space:

$$\hat{\psi}_{H\alpha}(\vec{\mathbf{x}}, t) = e^{i\frac{(\hat{H}t - \hat{\vec{\mathbf{p}}}\cdot\vec{\mathbf{x}})}{\hbar}}\hat{\psi}_\alpha(0)e^{-i\frac{(\hat{H}t - \hat{\vec{\mathbf{p}}}\cdot\vec{\mathbf{x}})}{\hbar}}$$

The complete set of states $\{|\psi_n\rangle\}$, that we use in the Lehmann representation, can be taken as a set of eigenstates of momentum and, at the same time, as eigenstates of the total hamiltonian. For example, this means that if we apply the total momentum operator on the states $|\psi_n\rangle$ and $|\psi_0\rangle$, we get:

$$\hat{\vec{\mathbf{p}}}|\psi_n\rangle = \vec{\mathbf{p}}_n|\psi_n\rangle, \qquad \hat{\vec{\mathbf{p}}}|\psi_0\rangle = 0$$

where clearly in the ground state the total momentum is zero, because otherwise it would not be the ground state. Using those relations we can rewrite the first matrix element of Eq.(2.20) in this way:

$$\langle \psi_0 | \hat{\psi}_\alpha(\vec{\mathbf{x}}) | \psi_n \rangle = \langle \psi_0 | e^{-i\frac{\hat{\mathbf{P}} \cdot \vec{\mathbf{x}}}{\hbar}} \hat{\psi}_\alpha(0) e^{i\frac{\hat{\mathbf{P}} \cdot \vec{\mathbf{x}}}{\hbar}} | \psi_n \rangle = \langle \psi_0 | \hat{\psi}_\alpha(0) | \psi_n \rangle \, e^{i\frac{\vec{\mathbf{p}}_n \cdot \vec{\mathbf{x}}}{\hbar}}$$

and similarly for the second matrix element

$$\langle \psi_n | \hat{\psi}_\beta^\dagger(\vec{\mathbf{x}}') | \psi_0 \rangle = \langle \psi_n | e^{i\frac{\hat{\mathbf{P}} \cdot \vec{\mathbf{x}}}{\hbar}} \hat{\psi}_\beta^\dagger(0) e^{-i\frac{\hat{\mathbf{P}} \cdot \vec{\mathbf{x}}}{\hbar}} | \psi_0 \rangle = e^{i\frac{\vec{\mathbf{p}}_n \cdot \vec{\mathbf{x}}}{\hbar}} \langle \psi_n | \hat{\psi}_\beta^\dagger(0) | \psi_0 \rangle$$

In this way we have extracted the space dependence from the matrix elements.

Now, we can rewrite the mixed green function in Eq.(2.20) by explicitly writing the space dependence. Moreover, since the system is homogeneous in space we note that actually this function depends just on $z \equiv \vec{\mathbf{x}} - \vec{\mathbf{x}}'$:

$$\widetilde{G}_{\alpha\beta}(\vec{\mathbf{x}}, \vec{\mathbf{x}}', \omega) = \widetilde{G}_{\alpha\beta}(\underbrace{\vec{\mathbf{x}} - \vec{\mathbf{x}}'}_{\vec{\mathbf{z}}}, \omega) = \sum_n \Big[e^{i\frac{\vec{\mathbf{p}}_n \cdot (\vec{\mathbf{x}} - \vec{\mathbf{x}}')}{\hbar}} \frac{\langle \psi_0 | \hat{\psi}_\alpha(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}_\beta^\dagger(0) | \psi_0 \rangle}{\omega - \frac{\varepsilon_n(N+1)}{\hbar} - \frac{\mu}{\hbar} + i\eta} + $$
$$ + e^{i\frac{\vec{\mathbf{p}}_n \cdot (\vec{\mathbf{x}} - \vec{\mathbf{x}}')}{\hbar}} \frac{\langle \psi_0 | \hat{\psi}_\beta^\dagger(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}_\alpha(0) | \psi_0 \rangle}{\omega + \frac{\varepsilon_n(N-1)}{\hbar} - \frac{\mu}{\hbar} - i\eta} \Big]$$

Now, it it is convenient to shift to the complete fourier transform of the Green's function using the usual relation used to go from real space to reciprocal space:

$$\widetilde{G}_{\alpha\beta}(\vec{\mathbf{x}}, \vec{\mathbf{x}}', \omega) = \widetilde{G}_{\alpha\beta}(\underbrace{\vec{\mathbf{x}} - \vec{\mathbf{x}}'}_{\vec{\mathbf{z}}}, \omega) = \frac{1}{(2\pi)^3} \int d\vec{\mathbf{k}} \, e^{i\vec{\mathbf{k}} \cdot \vec{\mathbf{z}}} G_{\alpha\beta}(\vec{\mathbf{k}}, \omega)$$

The Fourier transform is:

$$G_{\alpha\beta}(\vec{\mathbf{k}}, \omega) = \int d\vec{\mathbf{z}} \, e^{-i\vec{\mathbf{k}} \cdot \vec{\mathbf{z}}} \widetilde{G}_{\alpha\beta}(\vec{\mathbf{z}}, \omega)$$

If we substitute the explicit form of $\widetilde{G}_{\alpha\beta}(\vec{\mathbf{z}}, \omega)$, we obtain:

$$G_{\alpha\beta}(\vec{\mathbf{k}}, \omega) = \int d\vec{\mathbf{z}} \sum_n \Big[e^{i\left(\frac{\vec{\mathbf{p}}_n}{\hbar} - \vec{\mathbf{k}}\right) \cdot \vec{\mathbf{z}}} \frac{\langle \psi_0 | \hat{\psi}_\alpha(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}_\beta^\dagger(0) | \psi_0 \rangle}{\omega - \frac{\varepsilon_n(N+1)}{\hbar} - \frac{\mu}{\hbar} + i\eta} + $$
$$ + e^{-i\left(\frac{\vec{\mathbf{p}}_n}{\hbar} + \vec{\mathbf{k}}\right) \cdot \vec{\mathbf{z}}} \frac{\langle \psi_0 | \hat{\psi}_\beta^\dagger(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}_\alpha(0) | \psi_0 \rangle}{\omega + \frac{\varepsilon_n(N-1)}{\hbar} - \frac{\mu}{\hbar} - i\eta} \Big] \qquad (2.23)$$

where we highlighted the most important parts which depend on $\vec{\mathbf{z}}$. Let us focus on this integral over the space, we can exploit the usual properties:

$$\int d\vec{\mathbf{z}} \, e^{i\left(\frac{\vec{\mathbf{p}}_n}{\hbar} - \vec{\mathbf{k}}\right) \cdot \vec{\mathbf{z}}} = V \delta_{\frac{\vec{\mathbf{p}}_n}{\hbar}, \vec{\mathbf{k}}}$$

$$\int d\vec{\mathbf{z}} \, e^{-i\left(\frac{\vec{\mathbf{p}}_n}{\hbar} + \vec{\mathbf{k}}\right) \cdot \vec{\mathbf{z}}} = V \delta_{\frac{\vec{\mathbf{p}}_n}{\hbar}, -\vec{\mathbf{k}}}$$

Using the last properties and dividing and multiplying by $\hbar$ Eq.(2.23) we obtain:

$$G_{\alpha\beta}(\vec{\mathbf{k}}, \omega) = \hbar V \sum_n \left[\frac{\langle \psi_0 | \hat{\psi}_\alpha(0) | n\vec{\mathbf{k}} \rangle \langle n\vec{\mathbf{k}} | \hat{\psi}_\beta^\dagger(0) | \psi_0 \rangle}{\hbar\omega - \left(\mu + \varepsilon_n^{(N+1)}(\vec{\mathbf{k}})\right) + i\eta} + \frac{\langle \psi_0 | \hat{\psi}_\beta^\dagger(0) | n, -\vec{\mathbf{k}} \rangle \langle n, -\vec{\mathbf{k}} | \hat{\psi}_\alpha(0) | \psi_0 \rangle}{\hbar\omega - \left(\mu - \varepsilon_n^{(N-1)}(-\vec{\mathbf{k}})\right) - i\eta} \right]$$
$$(2.25)$$

where $\left| n\vec{\mathbf{k}} \right\rangle$, $\left| n, -\vec{\mathbf{k}} \right\rangle$ indicate that the momentum of the intermediate state $|\psi_n\rangle$ must correspond to the wave number $\vec{\mathbf{k}}, -\vec{\mathbf{k}}$ as dictating by the two delta functions. In this way, also $G(\vec{\mathbf{k}}, \omega)$ has poles and these correspond to the exact excitation energy of the system with $N \pm 1$ particles with momentum $\pm\hbar\vec{\mathbf{k}}$ (since we have specified the $\vec{\mathbf{k}}$ wave vector).

2.3.2 Case: spin 1/2

Now let us consider a more specific case of a system of particles with spin 1/2 (it is the most interesting situation of electrons). In the Green's function definition α, β are spin indexes, hence if the spin is 1/2 the α, β can take two values (the only two possible orientations are up an down) and so $G_{\alpha\beta}$ is a 2×2 matrix. The $G_{\alpha\beta}$ spin matrix can be expanded in the complete set consisting of the unit matrix and the 3 Pauli spin matrices $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ where the components are:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.26}$$

Now, let us make not a rigorous demonstration but just a plausibility argument to show that the Green's function must be diagonal in the spin indexes. First of all, since our system is homogeneous we also expected that there is no preferred direction, so G must be scalar under spatial rotations. The directions can be determined just by $\vec{\mathbf{k}}$, vector made by wave numbers which appear in the definition of the Fourier transformed Green's function, and $\vec{\sigma}$, vector of spin matrices. This means that the only possibility is to combine them. To summarize, if there is no preferred direction G must be *scalar* under *spatial rotations*, and since $\vec{\mathbf{k}}$ is the only vector available to combine with σ, we have:

$$G(\vec{\mathbf{k}}, \omega) = a\mathbb{1} + b\vec{\sigma} \cdot \vec{\mathbf{k}} \tag{2.27}$$

with a and b parameters function of $|\vec{k}|^2$ and ω.

Invariance under spatial reflections

However, if the Hamiltonian $\hat{H}$ is also *invariant* under **spatial reflections** (as in case of Coulomb interaction), one can easily show that $b = 0$ because $\vec{\sigma} \cdot \vec{\mathbf{k}}$ is a "**pseudo-scalar**" (changes sign under spatial reflection). Indeed, if the Hamiltonian is invariant under spatial reflection also the Green's function should be, so the only possibility is that $b = 0$. Hence, basically the Green's function is just a diagonal object and in practice we can write:

$$G_{\alpha\beta}(\vec{\mathbf{k}}, \omega) = \delta_{\alpha\beta} G(|\vec{k}|, \omega) \tag{2.28}$$

where the delta makes the Green's function diagonal. We can also introduce a more compact notation where G without any index means the trace over the spin indexes divided by a factor:

$$G \equiv \frac{\sum_\alpha G_{\alpha\alpha}}{(2\delta + 1)} = \frac{G_{\alpha\alpha}}{(2\delta + 1)} \tag{2.29}$$

where in the last step we have simplified the notation by using the Einstein convention that the repeated indices are considered to be summed.

Now if $\beta = \alpha$, actually in Eq.(2.25) we have that the second matrix element of the first term can be written as:

$$(\beta = \alpha) \quad \Rightarrow \left\langle n\vec{\mathbf{k}} \right| \hat{\psi}_\beta^\dagger(0) \left| \psi_0 \right\rangle = \left(\left\langle \psi_0 \right| \hat{\psi}_\alpha(0) \left| n\vec{\mathbf{k}} \right\rangle \right)^\dagger$$

If we multiply the two matrix elements of the first term considering this relation, we get just the square modulus of this matrix element. Similarly for the second term. Thus we can rewrite Eq.(2.25) as:

$$G(\vec{\mathbf{k}}, \omega) = \frac{\hbar V}{2\delta + 1} \sum_n \left[\frac{\left| \langle \psi_0 | \hat{\psi}_\alpha(0) \left| n\vec{\mathbf{k}} \right\rangle \right|^2}{\hbar\omega - \left(\mu + \varepsilon_n^{(N+1)}(\vec{\mathbf{k}}) \right) + i\eta} + \frac{\left| \langle \psi_0 | \hat{\psi}_\alpha^\dagger(0) \left| n, -\vec{\mathbf{k}} \right\rangle \right|^2}{\hbar\omega - \left(\mu - \varepsilon_n^{(N-1)}(-\vec{\mathbf{k}}) \right) - i\eta} \right] \tag{2.30}$$

where we omit the indexes writing just $G(\vec{\mathbf{k}}, \omega)$ because of Eq.(2.29). Indeed, in the square modulus we have two α indexes, so implicitly we have a sum.

In the thermodynamic limit $V \to \infty$ and $N \to \infty$, hence $\vec{\mathbf{k}}$ wave vector becomes a continuous variable and the same for the variable n. In particular, the sum over a discrete set $\sum_n$ tends to become a sum over a continuous set of states, or in other words becomes an integral. So it is convenient to introduce $\mathrm{d}n$ which denotes the number of energy levels inside the small energy interval:

Thermodynamic limit

$$\varepsilon < \varepsilon_{n\vec{\mathbf{k}}} < \varepsilon + \mathrm{d}\varepsilon$$

where $\mathrm{d}\varepsilon$ is an infinitesimal quantity. This means that the sum over n, can be replaced by an integral that we can formally write as:

$$\sum_n \cdots \longrightarrow \int \mathrm{d}n \cdots = \int \frac{\mathrm{d}n(\varepsilon)}{\mathrm{d}\varepsilon} \, \mathrm{d}\varepsilon \cdots$$

where the yellow term as a form of a typical *density of levels*.

Let us define the positive-definite **weigth functions**:

Weigth functions

$$A(\vec{\mathbf{k}}, \omega) \equiv \lim_{V \to \infty} \frac{\hbar V}{(2\delta + 1)} \left| \langle \psi_0 | \hat{\psi}_\alpha(0) \left| n\vec{\mathbf{k}} \right\rangle \right|^2 \frac{\mathrm{d}n(\varepsilon)}{\mathrm{d}\varepsilon} \geq 0 \qquad (2.31\mathrm{a})$$

$$B(\vec{\mathbf{k}}, \omega) \equiv \lim_{V \to \infty} \frac{\hbar V}{(2\delta + 1)} \left| \langle \psi_0 | \hat{\psi}_\alpha^\dagger(0) \left| n\vec{\mathbf{k}} \right\rangle \right|^2 \frac{\mathrm{d}n(\varepsilon)}{\mathrm{d}\varepsilon} \geq 0 \qquad (2.31\mathrm{b})$$

that are in the thermodynamic limit. They are defined in such a way to have the square modulus of the matrix elements that appear in the definition of the Green's function and to be expressed as a function of the density levels.

Now, let us consider for instance the first term of the Green's function in Eq.(2.30) and let us take the thermodynamic limit, substituting the sum with an integral:

$$\frac{V}{(2\delta + 1)} \sum_n \left| \langle \psi_0 | \hat{\psi}_\alpha(0) \left| n\vec{\mathbf{k}} \right\rangle \right|^2 = \frac{V}{(2\delta + 1)} \int \mathrm{d}\varepsilon \left| \langle \psi_0 | \hat{\psi}_\alpha(0) \left| n\vec{\mathbf{k}} \right\rangle \right|^2 \frac{\mathrm{d}n}{\mathrm{d}\varepsilon}$$

If we consider that $\varepsilon = \hbar\omega$ and the definition of the weigth function Eq.(2.31a), we can easily rewrite the last quantity as an integral over the energy and then over the frequency, as:

$$\frac{V}{(2\delta + 1)} \int \mathrm{d}\varepsilon \left| \langle \psi_0 | \hat{\psi}_\alpha(0) \left| n\vec{\mathbf{k}} \right\rangle \right|^2 \frac{\mathrm{d}n}{\mathrm{d}\varepsilon} = \frac{1}{\hbar} \int \mathrm{d}\varepsilon \, A\left(\vec{\mathbf{k}}, \frac{\varepsilon}{\hbar}\right) = \int_0^\infty \mathrm{d}\omega \, A\left(\vec{\mathbf{k}}, \omega\right)$$

Similarly for the other term of the Green's function in Eq.(2.30), but now using Eq.(2.31b).

Eventually, we can rewrite Eq.(2.30) as:

Spectral representation

$$G(\vec{\mathbf{k}}, \omega) = \int_0^\infty \mathrm{d}\omega' \left[\frac{A(\vec{\mathbf{k}}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega' + i\eta} + \frac{B(\vec{\mathbf{k}}, \omega')}{\omega - \frac{\mu}{\hbar} + \omega' - i\eta} \right] \qquad (2.32)$$

that is called **spectral representation**. In particular, in the infinite volume limit the discrete the analytical properties of the Green's function are changed: the discrete poles have merged into a continuum branch line (because the frequency changes continuously).

Moreover, it is easy to show that:

$$\int_0^\infty \mathrm{d}\omega \left[A(\vec{\mathbf{k}}, \omega) + B(\vec{\mathbf{k}}, \omega) \right] = 1 \qquad (2.33)$$

which is consistent with the definition of these quantities as weight functions.

In conclusion, we have written the Green's function also in the spectral representation. However, we get a problem: both in the original and in spectral representation

the Green's function is analytic in neither the upper nor the lower ω frequency plane, because it has poles both below and above the real frequency axis. This is not convenient for practical calculations where you have to choose suitable contour of integration, so it is useful to define new functions that are similar to the original Green's function but that are analytic in one half plane or the other.

2.3.3 Retarded and Advanced Green's function

Assuming that the ground state is normalized ($\langle\psi_0|\psi_0\rangle$), we define a new pair of functions called **retarded** and **advanced** Green's functions:

$$iG^R(\vec{\mathbf{x}}t,\vec{\mathbf{x}}'t') \equiv \langle\psi_0|\,\{\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}},t),\hat{\psi}^\dagger_{H_\beta}(\vec{\mathbf{x}}',t')\}\,|\psi_0\rangle\,\Theta(t-t') \tag{2.34a}$$

$$iG^A(\vec{\mathbf{x}}t,\vec{\mathbf{x}}'t') \equiv -\,\langle\psi_0|\,\{\hat{\psi}_{H_\alpha}(\vec{\mathbf{x}},t),\hat{\psi}^\dagger_{H_\beta}(\vec{\mathbf{x}}',t')\}\,|\psi_0\rangle\,\Theta(t'-t) \tag{2.34b}$$

Let us note that they are similar to the definition of the original Green's function (Eq.(2.2)), but with important differences:

- first of all, in place of the time order operator we have the anticommutator;

- there is also the Θ function which means that the first term does not vanish only for $t > t'$ while the second for $t > t'$;

- the advanced Green's function has a minus sign.

By applying the same procedure as for the original Green's function, one obtains, for a homogeneous system, the Lehmann representation of G^R and G^A:

$$G^{R,A}_{\alpha\beta}(\vec{\mathbf{k}},\omega) = \hbar V \sum_n \left[\frac{\langle\psi_0|\,\hat{\psi}_\alpha(0)\,\left|n\vec{\mathbf{k}}\right\rangle \left\langle n\vec{\mathbf{k}}\right|\,\hat{\psi}^\dagger_\beta(0)\,|\psi_0\rangle}{\hbar\omega - \left(\mu + \varepsilon_n^{(N+1)}(\vec{\mathbf{k}})\right) \pm i\eta} + \frac{\langle\psi_0|\,\hat{\psi}^\dagger_\beta(0)\,\left|n,-\vec{\mathbf{k}}\right\rangle \left\langle n,-\vec{\mathbf{k}}\right|\,\hat{\psi}_\alpha(0)\,|\psi_0\rangle}{\hbar\omega - \left(\mu - \varepsilon_n^{(N-1)}(-\vec{\mathbf{k}})\right) \pm i\eta} \right]$$
$$\tag{2.35}$$

where the upper sign referes to the retarded Green's function while the minus sign to the advanced one. In particular:

- G^R has poles all in the *lower* half plane (since here there are only plus sign, while in the original Green's function both plus and minus)[3]. We can conclude that G^R is analytic for $\text{Im}\,\omega > 0$.

- G^A has poles in the *upper* half plane. It is analytic for $\text{Im}\,\omega < 0$.

Moreover, since the difference between retarded and advanced Green's function is just in the sign of the imaginary part, it is easy to conclude that for *real* ω:

$$\left[G^R_{\alpha\beta}(\vec{\mathbf{k}},\omega)\right]^* = G^A_{\alpha\beta}(\vec{\mathbf{k}},\omega)$$

Then, supposing again to have *real* ω, if we compare Eq.(2.35) with the original Green's function in Eq.(2.25) it is easy to conclude that:

- The retarded Green's function coincides with the original one for real frequencies larger than the chemical potential (divided by hbar):

$$G^R_{\alpha\beta}(\vec{\mathbf{k}},\omega) = G_{\alpha\beta}(\vec{\mathbf{k}},\omega) \quad \omega > \mu/\hbar$$

- The advanced Green's function coincides with the original one for real frequencies smaller than the chemical potential (divided by hbar):

$$G^A_{\alpha\beta}(\vec{\mathbf{k}},\omega) = G_{\alpha\beta}(\vec{\mathbf{k}},\omega) \quad \omega < \mu/\hbar$$

---

[3] When you take the pole you have to take the denominator equal to zero, so we have $+i\eta \to -i\eta$

In the thermodynamic limit we can also obtain the spectral representation of the retarded and advanced Green's functions (repeating the same step as for the original Green's function):

$$G^{R,A}(\vec{k}, \omega) = \int_0^\infty \mathrm{d}\omega' \left[\frac{A(\vec{k}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega' \pm i\eta} + \frac{B(\vec{k}, \omega')}{\omega - \frac{\mu}{\hbar} + \omega' \pm i\eta} \right] \qquad (2.36)$$

which is of course quite similar to the original spectral representation (Eq.(2.32)) with the clear difference in the signs of these imaginary corrections.

Let us consider the symbolic identity (for *real* ω):

Cauchy Principal Value

$$\frac{1}{\omega \pm i\eta} = \mathcal{P}\frac{1}{\omega} \mp i\pi\delta(\omega) \qquad (2.37)$$

where $\mathcal{P}$ is the Cauchy Principal Value. In particular, the **Cauchy Principal Value** is a "generalized function" that makes sense only if it is included in an integral, under an integration operation. In practice, it means:

$$\mathcal{P} \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{\omega} = \lim_{\varepsilon \to 0} \left[\int_{-\infty}^{-\varepsilon} \frac{\mathrm{d}\omega}{\omega} + \int_{\varepsilon}^{+\infty} \frac{\mathrm{d}\omega}{\omega} \right]$$

if the limit exists.

Remark. Let us recall that the weight functions (Eq.(2.31a) and Eq.(2.31b)) make sense only for positive frequencies, because because ω' correspond to the excitation energies (which are positive by definition).

Now, we apply the symbolic identity of Eq.(2.37) in the spectral representation in Eq.(2.36):

$$G^{R,A}(\vec{k}, \omega) = \mathcal{P} \int_0^\infty \mathrm{d}\omega' \frac{A(\vec{k}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega'} \mp i\pi \int_0^\infty \mathrm{d}\omega' \delta\left(\omega - \frac{\mu}{\hbar} - \omega'\right) A(\vec{k}, \omega') +$$

$$+ \mathcal{P} \int_0^\infty \mathrm{d}\omega' \frac{B(\vec{k}, \omega')}{\omega - \frac{\mu}{\hbar} + \omega'} \mp i\pi \int_0^\infty \mathrm{d}\omega' \delta\left(\omega - \frac{\mu}{\hbar} + \omega'\right) B(\vec{k}, \omega')$$

By exploiting the property of the delta function, we get:

$$G^{R,A}(\vec{k}, \omega) = \mathcal{P} \int_0^\infty \mathrm{d}\omega' \frac{A(\vec{k}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega'} \mp i\pi A(\vec{k}, \omega' - \frac{\mu}{\hbar}) +$$

$$+ \mathcal{P} \int_0^\infty \mathrm{d}\omega' \frac{B(\vec{k}, \omega')}{\omega - \frac{\mu}{\hbar} + \omega'} \mp i\pi B(\vec{k}, \frac{\mu}{\hbar} - \omega')$$

The imaginary part of the last expression is given just by:

$$\operatorname{Im} G^{R,A}(\vec{k}, \omega') = \mp\pi A(\vec{k}, \omega' - \frac{\mu}{\hbar}) \mp \pi B(\vec{k}, \frac{\mu}{\hbar} - \omega')$$

By taking the principal value of this imaginary part :

$$\mp\mathcal{P} \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega'}{\pi} \frac{\operatorname{Im} G^{R,A}(\vec{k}, \omega')}{\omega - \omega'} = \mathcal{P} \int_{-\infty}^{+\infty} \mathrm{d}\omega' \left[\frac{A(\vec{k}, \omega' - \frac{\mu}{\hbar})}{\omega - \omega'} + \frac{B(\vec{k}, \frac{\mu}{\hbar} - \omega')}{\omega - \omega'} \right]$$

$$\overset{\omega'' = \omega' - \frac{\mu}{\hbar}}{=} \mathcal{P} \int_0^{+\infty} \mathrm{d}\omega'' \left[\frac{A(\vec{k}, \omega'')}{\omega - \omega'' - \frac{\mu}{\hbar}} + \frac{B(\vec{k}, \omega'')}{\omega + \omega'' - \frac{\mu}{\hbar}} \right]$$

$$\overset{\omega'' \to \omega'}{=} \mathcal{P} \int_0^{+\infty} \mathrm{d}\omega' \left[\frac{A(\vec{k}, \omega')}{\omega - \omega' - \frac{\mu}{\hbar}} + \frac{B(\vec{k}, \omega')}{\omega + \omega' - \frac{\mu}{\hbar}} \right]$$

where ω'' is just a dummy variable, then we have changed again it in $\omega'' \to \omega'$. Finally we note that:

$$\mp \mathcal{P} \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\operatorname{Im} G^{R,A}(\vec{\mathbf{k}}, \omega')}{\omega - \omega'} = \operatorname{Re} G^{R,A}(\vec{\mathbf{k}}, \omega) \tag{2.38}$$

This expression is important because it means that G^R and G^A satisfy the **dispersion relations** (or Kramers-Kronig relations). Thus, if we know $\operatorname{Im} G^{R,A}(\vec{\mathbf{k}}, \omega)$ for *all* ω values, we know also $\operatorname{Re} G^{R,A}(\vec{\mathbf{k}}, \omega)$ and therefore the whole $G^{R,A}$ and from it the original Green's function the G function.

In summary, in order to know the other quantities we must know the imaginary part for all the possible frequencies. In practice, the imaginary part is often connected to experiments : for instance it is related with the absobtion spectrum in experiments.

Moreover:

$$\frac{A(\vec{\mathbf{k}}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega' \pm i\eta} = \frac{A(\vec{\mathbf{k}}, \omega')}{\omega \left(1 - \frac{\mu/\hbar + \omega' \mp i\eta}{\omega}\right)} \overset{\omega \to \infty}{=} \frac{A(\vec{\mathbf{k}}, \omega')}{\omega} \left(1 + \frac{\mu/\hbar + \omega' \mp i\eta}{\omega} + \dots\right)$$

where in the last step we have taken the expansion of the denominator for large frequencies. If we come back to the spectral reperesentation of the Green's function in Eq.(2.32), in the high freuqnecy limit we have:

$$G(\vec{\mathbf{k}}, \omega) = \int_0^\infty d\omega' \left[\frac{A(\vec{\mathbf{k}}, \omega')}{\omega - \frac{\mu}{\hbar} - \omega' + i\eta} + \frac{B(\vec{\mathbf{k}}, \omega')}{\omega - \frac{\mu}{\hbar} + \omega' - i\eta}\right]$$

$$\overset{\omega \to \infty}{=} \frac{1}{\omega} \underbrace{\left[\int_0^\infty d\omega' \left(A(\vec{\mathbf{k}}, \omega') + B(\vec{\mathbf{k}}, \omega')\right)\right]}_{=1} + O\left(\frac{1}{\omega^2}\right)$$

$$\overset{\omega \to \infty}{\sim} \frac{1}{\omega} + O\left(\frac{1}{\omega^2}\right)$$

where in the last step we used Eq.(2.33). Thus, we know the behaviour of the Green's function in the high frequency limit. This is a general result for every interacting system (we have considered a general system). This relation is valid both for the original Green's function and for the retarded G^R and advanced G^A ones (one can easily demonstrate it).

Chapter 3

Perturbation theory

The preceding section described the single-particle Green's function. Unfortunately it is very difficult to know the exact Green's function because it is equivalent to know the exact solution of the Schrödinger equation and we have to make approximations if we want to deal with the many-body problem. To address the many-body problem we should try to evaluate the Green's function approximately by a *perturbative approach*:

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

where we have assumed that our Hamiltonian is constituted by a non-interacting term $\hat{H}_0$ (supposed known) and a difficult interacting term $\hat{H}_1$[1]. The next chapter will be devoted to present such a possible perturbative approach for evaluating in an approximate way the Green's function.

To be more precise, now we will introduce the so called **adiabatic "switching on"** approach. The idea is that even though H is tipically time independent, we can introduce an Hamiltonian which is formally time dependent as follow:

$$\hat{H}(t) = \hat{H}_0 + +e^{-\varepsilon|t|}\hat{H}_1$$

where $\varepsilon \to 0^+$ is a small positive quantity. In particular, results should not depend on the specific value of this parameter. Hence, at time zero we will recover the full interacting system, while for very large times (both in the past and in the future) the hamiltonian tends to the simpler non-interacting hamiltonian:

$$\hat{H}(0) = \hat{H}_0 + \hat{H}_1, \qquad \hat{H}(t \to \pm\infty) = \hat{H}_0$$

Let us consider the usual Schrödinger equation:

$$\hat{H}(t)\,|\psi_E(t)\rangle = E(t)\,|\psi_E(t)\rangle$$

The adiabatic "switching on" approach means that the full interacting eigenstate tends to the non interacting state for $t \to \pm\infty$, by assuming that it is the eigenstate for the non interacting system:

$$\lim_{t\to\pm\infty} |\psi_E(t)\rangle = |\Phi_E\rangle, \qquad \hat{H}_0\,|\Phi_E\rangle = E_0\,|\Phi_E\rangle$$

Schematically, we can say that the eigenvalue goes from the non-interacting value in the past $(t \to -\infty)$, at $t = 0$ becomes the eigenvalue of the full interacting system and finally for very large positive times $(t \to +\infty)$ it returns to the non-interacting system.

For a more convenient perturbative evaluation of the Green's function it is useful to consider different "pictures" of quantum mechanics. Indeed, in order to perform this perturbative approach it is more convenient to use a picture called "interaction picture" rather than the standard Schrödinger one.

---

[1] In the case of free fermions we have derived both the basic properties and also the non-interacting Green's function.

3.0.1   Pictures of quantum mechanics

Schrödinger picture

The usual elementary description of quantum mechanics assumes that the state vectors are time dependent, wherears the operators are time independent and are constructed by the familiar rules from the corresponding classical quantities. The Schrödinger equation therefore takes the form

$$i\hbar\frac{\partial}{\partial t}\left|\psi_S(t)\right\rangle = \hat{H}\left|\psi_S(t)\right\rangle, \qquad \hat{H} = \hat{H}_0 + \hat{H}_1 \tag{3.1}$$

where $\hat{H}$ is assumed to have no explicit time dependence. Since Eq.(3.1) is a first-order differential equation, the initial state at t_0 determines the subsequent behaviour, and a formal solution is readily obtained by writing

$$\left|\psi_S(t)\right\rangle = e^{-i\hat{H}(t-t_0)/\hbar}\left|\psi_S(t_0)\right\rangle \tag{3.2}$$

Here the exponential of an operator is defined in terms of its power series expansion. Furthermore, $\hat{H}$ is hermitian so that the exponential represents a unitary operator. Given the solution to the Schrödinger equation at the time t_0, the unitary transformation in Eq.(3.2) generates the solution at time t.

Heisenberg picture

The state vector in the Heisenberg picture is defined as

$$\left|\psi_H(t)\right\rangle = e^{i\hat{H}t/\hbar}\left|\psi_S(t)\right\rangle = \left|\psi_S(0)\right\rangle \tag{3.3}$$

where in the second step we used Eq.(3.2) (at $t_0 = 0$) obtaining that the state vector is time independent. The generic operator in the Heisenberg picture can be written as:

$$\hat{O}_H(t) = e^{i\hat{H}t/\hbar}\hat{O}_S e^{-i\hat{H}t/\hbar} \tag{3.4}$$

which instead depends on time.

Interaction picture

Let us suppose[2] to have a general time independent operator $\hat{O}_S$, as in the usual Schrödinger picture. In the interaction picture we define a generic operator as follow:

$$\hat{O}_I(t) \equiv e^{i\hat{H}_0t/\hbar}\hat{O}_S e^{-i\hat{H}_0t/\hbar} \tag{3.5}$$

where the time dependence is essentially driven by the exponential factor, while H_0 is the non-interacting hamiltonian.

Clearly, different "pictures" of quantum mechanics must be physically equivalent. It means that the matrix element that we compute by using for instance the interaction picture, must be equal to the corresponding matrix element obtained using the Schrödinger picture:

$$\left\langle\psi_I(t)\right|\hat{O}_I\left|\psi_I(t)\right\rangle = \left\langle\psi_I(t)\right|e^{i\hat{H}_0t/\hbar}\hat{O}_S e^{-i\hat{H}_0t/\hbar}\left|\psi_I(t)\right\rangle = \left\langle\psi_S(t)\right|\hat{O}_S\left|\psi_S(t)\right\rangle$$

It must be:
$$e^{-i\hat{H}_0t/\hbar}\left|\psi_I(t)\right\rangle = \left|\psi_S(t)\right\rangle$$

---

[2]The interaction picture has been implicitly used when we have played with the non-interacting Green's function G_0, even if we have not called that as interaction picture.

which relate the state vector in the interaction picture with the state vector in the Schrödinger picture. Clearly, if we invert this relation we get the state vector in the interaction picture:

$$|\psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar} |\psi_S(t)\rangle \tag{3.6}$$

and since $\hat{H}_0$ is an hermitian operator, this is a unitary transformation. In particular, we note that in the interaction picture the operators and the state vectors both depend on time, but the time-dependence of the operators is particularly simple.

Picture	State vector	Operator
Schrödinger	$\|\psi_S(t)\rangle = e^{-i\hat{H}t/\hbar}\|\psi_S(0)\rangle$ depends on time	$\hat{O}_S$ time-independent
Heisenberg	$\|\psi_H(t)\rangle = e^{i\hat{H}t/\hbar}\|\psi_S(t)\rangle = \|\psi_S(0)\rangle$ time-independent	$\hat{O}_H(t) = e^{i\hat{H}t/\hbar}\hat{O}_S e^{-i\hat{H}t/\hbar}$ depends on time
Interaction	$\|\psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar}\|\psi_S(t)\rangle$ depends on time	$\hat{O}_I(t) \equiv e^{i\hat{H}_0 t/\hbar}\hat{O}_S e^{-i\hat{H}_0 t/\hbar}$ depends on time but the time dependence is simple

Table 3.1: Summary of the different pictures for the quantum mechanical description of the system. Let us note that the time-dependence of the interaction operator is very simple, because it does not depend on the full hamiltnonian but just on the easy non-interacting part $\hat{H}_0$. The general operator in the Heisenberg picture as a complicated time-dependence in terms of the full interacting hamiltonian.

In addition, it is easy to show that the three different pictures coincide at $t = 0$:

$$|\psi_H\rangle = |\psi_S(0)\rangle = |\psi_I(0)\rangle \tag{3.7a}$$

$$\hat{O}_S = \hat{O}_H(0) = \hat{O}_I(0) \tag{3.7b}$$

Let us find the equation of motion of the state vector in the interaction picture:

Interaction picture: equation of motion

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = -\hat{H}_0 e^{i\hat{H}_0 t/\hbar}|\psi_S(t)\rangle + e^{i\hat{H}_0 t/\hbar}\,i\hbar\frac{\partial}{\partial t}|\psi_S(t)\rangle$$

$$\overset{(3.1)}{=} -\hat{H}_0 e^{i\hat{H}_0 t/\hbar}|\psi_S(t)\rangle + e^{i\hat{H}_0 t/\hbar}\left[\hat{H}_0 + \hat{H}_1\right]|\psi_S(t)\rangle$$

where we can delete the terms because $\hat{H}_0$ and $e^{i\hat{H}_0 t/\hbar}$ commute. Thus we obtain:

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar}\hat{H}_1|\psi_S(t)\rangle = \left(e^{i\hat{H}_0 t/\hbar}\hat{H}_1 e^{-i\hat{H}_0 t/\hbar}\right)\left(e^{i\hat{H}_0 t/\hbar}|\psi_S(t)\rangle\right)$$

$$= \hat{H}_{I_1}(t)|\psi_I(t)\rangle$$

We can conclude that the time dependent state vector in the interaction picture satisfies a Schrödinger like equation with the difference that with respect to the ordinary Schrödinger equation there is *only* the interaction part of the hamiltonian $\hat{H}$:[3]

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \hat{H}_{I_1}(t)|\psi_I(t)\rangle \tag{3.8}$$

In order to solve in practice the equation of motion in the interaction picture it is convenient to define a unitary operator $\hat{U}(t, t_0)$ such that it determines the time-evolution from t_0 to t of a state vector:

$$|\psi_I(t)\rangle = \hat{U}(t, t_0)|\psi_I(t_0)\rangle \tag{3.9}$$

---

[3]More or less this is the reason of the name, because we obtain an equation of motion with only the difficult perturbation part.

Formally we can write $\hat{U}(t, t_0)$ as follows:

$$
\begin{aligned}
|\psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar} |\psi_S(t)\rangle &\stackrel{(3.2)}{=} e^{i\hat{H}_0 t/\hbar} e^{-i\hat{H}(t-t_0)/\hbar} |\psi_S(t_0)\rangle \\
&= \left(e^{i\hat{H}_0 t/\hbar} e^{-i\hat{H}(t-t_0)/\hbar} e^{-i\hat{H}_0 t_0/\hbar} \right) |\psi_I(t_0)\rangle \\
&= \hat{U}(t, t_0) |\psi_I(t_0)\rangle
\end{aligned}
\tag{3.10}
$$

We can easily demonstrate that:

- $\hat{U}(t, t_0)$ is an **unitary operator**:

$$
\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0) = \mathbb{1} \quad \Rightarrow \hat{U}^\dagger(t, t_0) = \hat{U}^{-1}(t, t_0)
$$

- $\hat{U}(t, t_0)$ has the **group property**:

$$
\hat{U}(t, t_0) = \hat{U}(t, t_1)\hat{U}(t_1, t_0)
$$

- $\hat{U}(t, t_0)$ is coherent with the notion of **evolution operator**:

$$
\hat{U}(t_0, t_0) = \mathbb{1} \quad \Rightarrow \hat{U}(t_0, t)\hat{U}(t, t_0) = \mathbb{1}
$$

  which implies that

$$
\hat{U}^\dagger(t, t_0) = \hat{U}(t_0, t)
$$

Altough Eq.(3.10) is the formal solution to the problem posed by Eq.(3.9), it is not very useful for computational purposes because it is very complicated. Indeed, $\hat{H}$ and $\hat{H}_0$ do not commute and the total order of these operators must be preserved.

It is more convenient to construct an integral equation for $\hat{U}$ (of course involving the interaction part of the interaction picture, $\hat{H}_{I_1}$), which can then be solved by iteration. This integral equation can be easily obtained by remembering the equation of motion for the state vector in the interaction picture:

$$
i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = \hat{H}_{I_1}(t) |\psi_I(t)\rangle
$$

$$
\Rightarrow i\hbar \frac{\partial}{\partial t} \left(\hat{U}(t, t_0) |\psi_I(t_0)\rangle \right) = \hat{H}_{I_1}(t)\hat{U}(t, t_0) |\psi_I(t_0)\rangle
$$

Since this differential equation must hold for any (time-independent) $|\psi_I(t_0)\rangle$ factor, as a consequence the time evolution operator $\hat{U}$ must satisfies itself this differential equation:

$$
i\hbar \frac{\partial}{\partial t} \hat{U}(t, t_0) = \hat{H}_{I_1}(t)\hat{U}(t, t_0)
$$

Changing $t \to t'$ and integrating the equation from t_0 to t:

$$
\int_{t_0}^{t} dt' \, i\hbar \frac{\partial}{\partial t'} \hat{U}(t', t_0) = \int_{t_0}^{t} dt' \, \hat{H}_{I_1}(t')\hat{U}(t', t_0)
$$

Clearly the left hand integral is quite easy:

$$
i\hbar \left[\hat{U}(t, t_0) - \underbrace{\hat{U}(t_0, t_0)}_{=\mathbb{1}} \right] = \int_{t_0}^{t} dt' \, \hat{H}_{I_1}(t')\hat{U}(t', t_0)
$$

$$
\hat{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, \hat{H}_{I_1}(t')\hat{U}(t', t_0)
\tag{3.11}
$$

The last integral is complicated because it contains the $\hat{U}$ operator both outside and inside the integral. Clearly, the time independent variable t appears as the *upper limit* in the integral. Thus, if in place of the $\hat{U}$ operator (inside the integral) we had a c-number, it would be a "**Volterra integral equation**" which may be solved by *iteration* (and the solution is guaranteed to converge); in our case $\hat{U}$ is an operator, but we try to solve the equation by iteration always mantaining the *proper order* of the operators during all the derivation. At the end we should check that we found a reasonable result, because there is no assurance that the present operator equation has the same properties.

By iteration means that we can interpret the interaction part $\hat{H}_{I_1}$ as a small perturbation:

- at order 0: $\hat{U}^{(0)}(t, t_0) = \mathbb{1}$[4];

- at order 1: $\hat{U}^{(1)}(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^{t} \mathrm{d}t_1 \, \hat{H}_{I_1}(t_1)\mathbb{1}$;

- at order 2:

$$\hat{U}^{(2)}(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^{t} \mathrm{d}t_1 \, \hat{H}_{I_1}(t_1)\hat{U}^{(1)}(t_1, t_0)$$

$$= \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^{t} \mathrm{d}t_1 \, \hat{H}_{I_1}(t_1) - \frac{1}{\hbar^2} \int_{t_0}^{t} \mathrm{d}t_1 \, \hat{H}_{I_1}(t_1) \int_{t_0}^{t_1} \mathrm{d}t_2 \, \hat{H}_{I_1}(t_2)$$

- at order n:

$$\hat{U}^{(n)}(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^{t} \mathrm{d}t_1 \, \hat{H}_{I_1}(t_1)\hat{U}^{(n-1)}(t_1, t_0) \tag{3.12}$$

In order to proceed, let us focus on the double integral inside the expansion at order 2. This term can be rweritten as:

$$\int_{t_0}^{t} \mathrm{d}t_1 \, \hat{H}_{I_1}(t_1) \int_{t_0}^{t_1} \mathrm{d}t_2 \, \hat{H}_{I_1}(t_2) = \frac{1}{2} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \, \hat{H}_{I_1}(t_1)\hat{H}_{I_1}(t_2) + $$

$$+ \frac{1}{2} \int_{t_0}^{t} \mathrm{d}t_2 \int_{t_2}^{t} \mathrm{d}t_1 \, \hat{H}_{I_1}(t_1)\hat{H}_{I_1}(t_2) \tag{3.13}$$

since the last term on the right is just obtained by reversing the order of the integrations, as illustrated in Fig.3.1.

- The first integration order in red (Eq.(3.13)) means that first we fix t_1; then t_2 goes from t_0 to t_1. After that t_1 goes from t_0 to t.

- In the second integral, for a given t_2, t_1 goes from t_2 to t; then t_2 goes from t_0 to t.
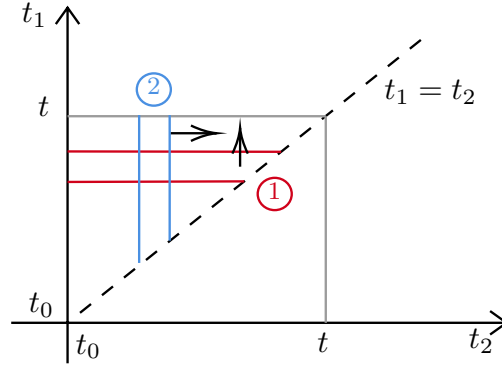
So you cover exactly the same integration region, what is changed is just the order of integration.

By interchanging the integration dummy variables in the second integral ($t_1 \rightarrow t_2, t_2 \rightarrow t_1$) we have:

$$\frac{1}{2} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_1}^{t} \mathrm{d}t_2 \, \hat{H}_{I_1}(t_2)\hat{H}_{I_1}(t_1)$$

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[4]Because if we neglect the term containing the $\hat{H}_{I_1}$ in the integral equation, we have left with just $\mathbb{1}$)

Figure 3.1: Integration regions for second order-term $\hat{U}(t, t_0)$. The integration regions are the same, just the order of the integrations is reversed. In particular, the region 1, in red, corresponds to the red integral in Eq.(3.13), while the region 2 to the second integral.

and recombining it with the first integral

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \, \hat{H}_{I_1}(t_1) \hat{H}_{I_1}(t_2) = \frac{1}{2} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \Big[\hat{H}_{I_1}(t_1) \hat{H}_{I_1}(t_2) \Theta(t_1 - t_2) + $$
$$+ \hat{H}_{I_1}(t_2) \hat{H}_{I_1}(t_1) \Theta(t_2 - t_1) \Big]$$

Now (this is the exciting conclusion) we can replace the expression on the square parenthesis with just a time ordered product of the sequence of the two hamiltonian:

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \, \hat{H}_{I_1}(t_1) \hat{H}_{I_1}(t_2) = \frac{1}{2!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \, T\Big[\hat{H}_{I_1}(t_1) \hat{H}_{I_1}(t_2) \Big] \qquad (3.14)$$

Note that the $\hat{H}_{I_1}$ do not necessarily commute at different times thus the proper order of the operators must be mantained. Furthermore, having introduced the time-ordered product, we have some hope that we there is a connection with the Green's function. It is a consistent definition also for fermions, because of course we can remember that typically this interaction part $\hat{H}_{I_1}$ vcontains four field operator, so we can interachange these terms which are made by an even number of field operators without introducing a minus sign. Moreover, it is more convenient to generalize that formula by introducing a $\frac{1}{2!}$, because in that way we can generalize easily this procedure to the n-th order. By recovering the constant factors:

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n \, T\Big[\hat{H}_{I_1}(t_1) \ldots \hat{H}_{I_1}(t_n) \Big] \qquad (3.15)$$

In practice, at order n there are $n!$ possible time ordering of the labels $t_1, \ldots, t_n$, and any time ordering gives the *same* contribution. So the basic idea that we have explicitly checked at the second order is that by choosing such a time ordering, if we select a different time ordering, it gives exactly the same contribution to the final result. We can also formally write:

$$\hat{U}(t, t_0) = T\Big[e^{\frac{i}{\hbar} \int_{t_0}^{t} dt' \hat{H}_{I_1}(t')} \Big] \qquad (3.16)$$

by considering the power-series expansion of the expontential function. This is a very important result, because from this we will start to build a perturbative approach in terms of the Green's function.

Bibliography

[1] Fetter A.L., Walecka J.D., *Quantum Theory of Many-Particle Systems"*. (1971,2003)