

# Introduction to Many-Body Physics

Gonzalo Camacho Patricio

May 5, 2016

## Contents

<b>0</b>	<b>Introduction to the Many Body problem</b>	<b>2</b>
<b>1</b>	<b>Introduction to second quantization</b>	<b>4</b>
1.1	What does <i>second quantization</i> mean? . . . . .	4
1.2	Two types of particles . . . . .	5
1.3	The second quantization language . . . . .	7
1.4	The many-body state . . . . .	11
1.5	Exercises . . . . .	15
<b>2</b>	<b>Treating interacting systems</b>	<b>17</b>
2.1	A many-body problem . . . . .	17
2.2	The non-interacting Fermi gas . . . . .	19
2.3	Landau-Fermi liquid theory: concept of quasiparticle . . . . .	21
2.4	Finite temperature vs zero temperature . . . . .	23
2.5	Correlators . . . . .	24
2.6	Exercises . . . . .	27
<b>3</b>	<b>Approximation methods</b>	<b>29</b>
3.1	Failure of ordinary perturbation theory . . . . .	29
3.2	Three pictures of quantum mechanics . . . . .	29
3.2.1	Schrodinger picture . . . . .	29
3.2.2	Heisenberg picture . . . . .	30
3.2.3	Interaction picture . . . . .	32
3.3	Many Body Perturbation Theory . . . . .	33
3.4	Feynman diagrams: The world of interactions in pictures . . . . .	39
3.5	Exercises . . . . .	40
<b>4</b>	<b>Some important impurity models</b>	<b>41</b>
4.1	The Anderson Model . . . . .	41
4.2	The Kondo Model . . . . .	42
<b>5</b>	<b>References</b>	<b>45</b>

## 0 Introduction to the Many Body problem

The many-body problem is considered as one of the most difficult and challenging areas of physics. It was realised in the 17th century that a simple system of two interacting bodies can't be described easily if interactions between the constituents are taken into account. This is known as the Kepler problem or *two body* problem, where the motion between two gravitationally interacting bodies is described in the language of classical physics.

We can guess how the difficulty of the problem increases if, instead of considering two bodies, we want to describe the motion of three of them, interacting with each other. The three differential equations constitute an extremely complex problem from the classical point of view. When we have  $N$  ( $\sim 10^{23}$ ) particles interacting, there are  $N$  differential equations describing the motion of the particles. This adds an enormous complexity for the solution of the problem.

When quantum mechanics was developed, the theory of helium atom was the analog of a two body problem (the nucleus is considered fixed), in the quantum mechanical description. The wavefunction describes the system as a whole, in this case composed of two electrons. It is an example of a two body problem in quantum mechanics, where interactions between electrons are considered. The wavefunction of such a problem is built up by an Slater determinant. As we will see later, the  $N$  body wavefunction is considered as a Slater determinant only for one type of particles: fermions.

However, it became clear soon that the description of a quantum system by the many-body wavefunction is something unmanageable to do. In some areas like chemistry, when one is maybe interested in the wavefunction of a single molecule, solving the Schrodinger equation can be of interest. But, if one wants to describe fundamental properties of matter, for example, metallic behaviour or superconductivity, this approach is not suitable, since one has to find a wavefunction of  $3N$  coordinates and time, being  $N \sim 10^{23}$ . This can't be done even in a computer, so that a new theoretical approach for such big systems needed to be developed. This constitutes the basis of the *many-body theory*.

Why is many body interesting? The most important feature about many-body systems is that *collective behaviour between constituents give rise to emergent phenomena*. That is, if interactions weren't considered between particles, most of the properties in the system couldn't be observed. One example of this is the phenomenon of *superconductivity*, where the electron-phonon interaction is essential for the formation of Cooper pairs in the BCS theory. In this sense, many-body theory and statistical physics are equivalent, since both pretend to describe macroscopic phenomena in terms of microscopic behaviour of the constituents. In fact, many body theory englobes areas like statistical mechanics, quantum mechanics, quantum field theory, complex analysis... The field is very

extense and broad, another feature that makes it fascinating.

Finally, I want to say that two years ago, the field of many-body physics was totally unknown for me. After this year and a half of my PhD, I have had the privilege of study the subject and know just a tiny bit portion of it. In this small amount of knowledge, I have discovered the depth and beauty of the subject, and I hope to summarize this briefly in this notes. As a goal, I expect someone starting in the field to find them useful, or even if this isn't someone's field, to find them interesting.

# 1 Introduction to second quantization

## 1.1 What does *second quantization* mean?

The name *second quantization* is introduced in analogy with the *first quantization* in quantum mechanics. In first quantization, classical quantities are risen to the status of operators, and its a good tool to describe systems with one or a few number of particles. As the number of particles rises up, the first quantization description becomes unmanageable. When we are dealing with a huge number of particles in a system, lets say  $N$ , the wave function is now a function of  $N$  coordinates (and time):

$$\Psi(\vec{x}_1, \dots, \vec{x}_N, t) \tag{1.1}$$

In a solid, where the description of the system involves  $\sim 10^{23}$  atoms, this is a function we do not want to deal with.

The concept of second quantization is closely related to quantum field theory. In fact, what we are doing is to assume that all the degrees of freedom of the system are spreaded out in space and time continuously. This is the definition of a *field*. We are already familiar with classical fields such as the electric or magnetic fields, gravitatalinal field etc.... These classical fields are totally deterministic, and their values and contributions to a system can be known exactly.

On the other hand, a quantum field is a *highly fluctuating* object, that means that we have to take care of these fluctuations, since sometimes they are totally necessary for a good description of the system. When introducing second quantization, some quantities that where not considered operators before, are now risen to the status of operators as well. More concretely, a field in second quantization is represented by an operator, and therefore can be expressed in matrix notation.

The first example of second quantized quantity is the wave function<sup>1</sup>. When we were in first quantization,  $\psi(\vec{r}, t)$  was considered a complex number, representing the probability amplitude of finding the particle at position  $\vec{r}$  at time  $t$ . Now, we will consider this as a *field*, with infinite degrees of freedom and fluctuating in space and time. Doing that, some quantities such as the *density*:

$$\rho(\vec{r}) = \psi(\vec{r})^\dagger \psi(\vec{r}) \tag{1.2}$$

---

<sup>1</sup>Which should not be confused with the *many-body wavefunction*, since the later will continue to be a complex number (depending on each coordinate of the particles). Here, what we are rising to the status of operator is the *single particle wavefunction* from quantum mechanics.

are now considered operators as well. We will see this concepts much clearer in the following sections.

Just a final remark about this introduction. Since we will be dealing with systems where particle number is not *fixed*, we will be working in the *grand canonical* ensemble. That means that there are three quantities fixed in the system: volume, temperature (the system is in contact with a thermal bath), and the chemical potential  $\mu$ . This last quantity is extremely important, since it measures the amount of energy necessary to introduce or remove one particle from the system. In the grand canonical ensemble, the system can exchange particles with the reservoir, and in fact, the fluctuations of  $\langle N \rangle$  are important in some specific problems.

Lets make a summary about this brief introduction:

- Second quantization is used for systems where the number of particles  $N$  is large compared to the single particle description of quantum mechanics.
- The degrees of freedom of the system are the *fields*, which are now quantum fluctuating objects.
- Some quantities like the wavefunction  $\psi$  from quantum mechanics are risen to the status of operator.
- From a thermodynamical point of view, we will be working in the grand canonical ensemble, where particle number is not fixed (particles can be exchanged between the system and the reservoir).

## 1.2 Two types of particles

Imagine a box containing particles of the same type. If we make a classical description of the system, each particle is thought as a point moving in space and time, and we can follow its trajectory by solving Newton's equations in the system. That means we could in principle assign to each particle a label, and we could say where is particle  $A$  at time  $t$ , where is particle  $B$  at time  $t'$  etc...

This description is not valid in quantum mechanics. When we have an entire system of identical particles, we say they are *indistinguishable*, that is, we can't say which particle is which, since they are all exactly the same. The many-body wavefunction is an object depending on all coordinates of the particles, as we argued in (1.1). We can see what happens when we exchange two particles, lets say, particle at position  $\vec{r}_A$  and at  $\vec{r}_B$ . In that case, the wavefunction must only change by a phase factor:

$$\Psi(\vec{r}_1, \dots, \vec{r}_A, \dots, \vec{r}_B, \dots, \vec{r}_N) \rightarrow e^{i\theta} \Psi(\vec{r}_1, \dots, \vec{r}_B, \dots, \vec{r}_A, \dots, \vec{r}_N) \quad (1.3)$$

since the probability density must remain equal under the permutation:

$$|\Psi(\vec{r}_1, \dots, \vec{r}_A, \dots, \vec{r}_B, \dots, \vec{r}_N)|^2 = |\Psi(\vec{r}_1, \dots, \vec{r}_B, \dots, \vec{r}_A, \dots, \vec{r}_N)|^2 \quad (1.4)$$

If we now move the particles again, i.e, we make the inverse transformation as before, we should have the same wavefunction, and then:

$$e^{i\theta} \Psi(\vec{r}_1, \dots, \vec{r}_B, \dots, \vec{r}_A, \dots, \vec{r}_N) \rightarrow e^{i2\theta} \Psi(\vec{r}_1, \dots, \vec{r}_A, \dots, \vec{r}_B, \dots, \vec{r}_N) \quad (1.5)$$

Immediately we find:

$$e^{i2\theta} = 1 \rightarrow e^{i\theta} = \pm 1 \quad (1.6)$$

We see here two possible results under particle exchange for the wavefunction. One of them keeps the wavefunction unchanged under particle exchange, that is, the change is *symmetric* in this case. On the other hand, there is an *antisymmetric* case, where the exchange of two particles brings a change of sign in the wavefunction. This provides a sufficient argument to classify particles in two types: *bosons* and *fermions*.

When the wavefunction is invariant under an exchange of particles, that is, there is no change in sign, we say that the many-body wavefunction is *symmetric* under exchange, and this corresponds to bosons. Bosons are known by another property regarding their intrinsic angular momentum: their spin is always an integer number. This is the case of photons, with total spin  $S = 1$ . Other types of bosons are *phonons*, representing vibrational modes of the atoms in the solid around their equilibrium position.

On the other hand, *fermions* are particles with half integer spin, like the electron, with spin  $S = 1/2$ , and their many-body wavefunction must be *antisymmetric*. This antisymmetry of fermions is very important. Indeed, this change of sign in the wavefunction what makes *fermions* more special particles than bosons. Due to this antisymmetry, two fermions could never be in the same quantum state. This is known as the *Pauli exclusion principle*, and it is a purely quantum effect. When dealing with fermionic systems, this principle must always be taken into account.

There is another important remark about bosons and fermions, more concretely, we should distinguish between systems with conserved particle number and those who do not conserve them. In particular, it is in the case of phonons and photons where particle number is not conserved. Because both are collective modes of a medium (crystal and electromagnetic field, respectively), one can in

principle add or subtract as many excitations as one wishes. In that case, the chemical potential  $\mu$  is absent, since there is no energy cost about adding or subtracting a mode.<sup>2</sup>

On the other hand, for fermionic systems  $\mu$  must always be included in the description, since fermions always conserve particle number. If we recall the standard definition of  $\mu$  from thermodynamics:

$$\mu = -\left(\frac{\partial E}{\partial N}\right)_{T,V} \quad (1.7)$$

we see that it is a cost in the energy of the system associated with a change of the particle number<sup>3</sup>  $N$ . Photons and phonons are *excitations* of some bosonic fields, and one can add as many as one wishes without energy cost in the system, since two bosons can occupy the same energy state. On the other hand, fermions can't occupy the same energy state due to the Pauli exclusion principle. Therefore, an energy cost must be added to the system if there is a variation in the total number of constituents.

But that's all the qualitative description about these systems. What are the mathematics behind all this? We can figure out that as we are still using quantum mechanics, operators algebra will remain as the basic tool to study such systems. However, when second quantization arises, there is no classical analogy, as with ordinary quantum mechanics. That has to be with the concept of *particle field*. In classical physics, particles are considered point-like objects evolving in space and time with some coordinates. Here, in the second quantization language, particles can be *created* and *destroyed*, and they are represented by the field operator  $\psi$ .

In the next section, we will start learning the basics of second quantization, getting familiar with the notation.

### 1.3 The second quantization language

In second quantization, the single particle wavefunction doesn't exist anymore as a complex number: instead, now it is an operator. We will call this new operator the *field*:

$$\psi(\vec{r}, t) \quad (1.8)$$

---

<sup>2</sup>However, not all bosons follow that. For example, when treating a system of  $\alpha$  particles, the total particle number is conserved, and the chemical potential  $\mu$  must be included in the description.

<sup>3</sup>Which is not fixed in the grand canonical ensemble, as we said before.

and we will give to it the following interpretation: it destroys a particle at position  $\vec{r}$  at time  $t$ . Its hermitian conjugate  $\psi^\dagger(\vec{r}, t)$ , creates a particle at  $\vec{r}$  in  $t$ .

However, *and here is when everything starts*, these operators can't be treated in the same way if they are representing *bosons* or *fermions*. To distinguish between both, and make the notation more clear, lets identify:

$$\begin{aligned}\psi(\vec{r}, t) &\rightarrow \text{fermions (fermionic field)} \\ \varphi(\vec{r}, t) &\rightarrow \text{bosons (bosonic field)}\end{aligned}$$

For bosons, fields obey a *commutation algebra*, which means that they satisfy:

$$\begin{aligned}[\varphi(\vec{x}), \varphi^\dagger(\vec{y})] &= \delta(\vec{x} - \vec{y}) \\ [\varphi(\vec{x}), \varphi(\vec{y})] &= 0 \\ [\varphi^\dagger(\vec{x}), \varphi^\dagger(\vec{y})] &= 0\end{aligned}\tag{1.9}$$

Thus, when dealing with bosons, we must always use a commutation algebra and these relationships. The fields for bosons *commute*. This is not the case for *fermions*, where an *anticommutation algebra*<sup>4</sup> must be followed:

$$\begin{aligned}\{\psi(\vec{x}), \psi^\dagger(\vec{y})\} &= \delta(\vec{x} - \vec{y}) \\ \{\psi(\vec{x}), \psi(\vec{y})\} &= 0 \\ \{\psi^\dagger(\vec{x}), \psi^\dagger(\vec{y})\} &= 0\end{aligned}\tag{1.10}$$

One important remark here is that this commutation/anticommutation relations are valid *only at equal times*. We will see later that, when these objects are evaluated at different times, that has another physical interpretation, and it is in general a difficult many-body problem.

Our treatment now will follow fermionic fields, but the same can be applied to bosons, only taking the commutation relations into account. Lets get back to our first quantization scheme, where the single-particle wavefunction can be expressed as a linear combination of any basis of states:

$$\psi(\vec{r}) = \sum_{\lambda} c_{\lambda} \phi_{\lambda}(\vec{r})\tag{1.11}$$

The basis states  $\{\phi_{\lambda}\}$  must satisfy the completeness and orthogonality relations

---

<sup>4</sup>The commutation of two operators  $\hat{A}$  and  $\hat{B}$  is defined as  $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ . On the other hand, the anticommutator of two operators  $A$  and  $B$  is defined as  $\{A, B\} = AB + BA$



(see exercise), and  $\lambda$  is an index running through all possible values of the *spectrum*. Usually, this basis states are the single particle states for the Schrodinger equation. It may be useful for now (to keep the idea clear) to think about  $\lambda$  representing the crystal momentum of a lattice  $\vec{k}$ . Of course, the definition is more general, and  $\lambda$  doesn't need to represent a momentum label specifically. Lets choose the basis  $\{\phi_\lambda\}$  to be the eigenstates of a single particle hamiltonian:

$$\begin{aligned} H_{SP} &= -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \\ H_{SP}\phi_\lambda(\vec{r}) &= \varepsilon_\lambda\phi_\lambda(\vec{r}) \end{aligned} \quad (1.12)$$

In a non-interacting system, where particles don't see the others, the problem is as easy<sup>5</sup> as solving the single particle hamiltonian, and then summing up for all the particles. We can say that, a non-interacting system of particles doesn't really constitute a *many-body* problem, since it can always be reduced to a single particle problem.

Since in second quantization we are working with *fields*, equation (1.11) is a *linear combination of operators, where the single particle wavefunctions  $\phi_\lambda$  are the coefficients of the expansion*. Concretely, the operators  $c_\lambda$  represent new field operators, but instead of doing it in real space, they are representing operators in the  $\lambda$  space. The operator  $c_\lambda$  destroys a particle in the state  $\lambda$ , whereas its hermitian conjugate  $c_\lambda^\dagger$  creates a particle in the  $\lambda$  state. That is why they are called *annihilation* and *creation* operators, respectively. Because we are working with fermions, these operators must satisfy the anticommutation relations we were talking about before:

$$\begin{aligned} \{c_\lambda, c_\mu^\dagger\} &= \delta_{\mu\lambda} \\ \{c_\lambda, c_\mu\} &= 0 \\ \{c_\lambda^\dagger, c_\mu^\dagger\} &= 0 \end{aligned} \quad (1.13)$$

Note that the  $\delta_{\lambda\mu}$  is a Kronecker delta, since we are considering  $\lambda$  and  $\mu$  indices to be discrete. The treatment for bosons would just change anticommutation by commutation. A very nice picture to keep in mind is that we can always decompose the field by its *Fourier components*:

$$\psi(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \quad (1.14)$$

---

<sup>5</sup>In the *many body* sense; that doesn't mean that the single particle Schrodinger equation is easy to solve itself, at least analitically.

This is nothing but a linear combination of operators, each for a different mode  $\vec{k}$ , where the coefficients of the expansion are determined by the set of plane waves.

The non-interacting hamiltonian in second quantization can be expressed as:

$$H = \int d^3\vec{r} \hat{\psi}^\dagger(\vec{r}) H_{SP} \hat{\psi}(\vec{r}) \quad (1.15)$$

being  $H_{SP}$  the single particle hamiltonian. The expression is telling us how the total hamiltonian is determined by the energy of the field at every point in space.

Lets insert equation (1.10) here, and applying the properties of basis, we should find:

$$\boxed{H = \sum_{\lambda} \varepsilon_{\lambda} c_{\lambda}^{\dagger} c_{\lambda}} \quad (1.16)$$

That is the **non-interacting hamiltonian** expressed in the  $\lambda$  space, in terms of creation and annihilation operators for that space. If we follow our example, this will be:

$$H = \sum_{\vec{k}, \sigma} \varepsilon_{\vec{k}, \sigma} c_{\vec{k}, \sigma}^{\dagger} c_{\vec{k}, \sigma} \quad (1.17)$$

The same treatment could have been done for bosons, finding:

$$H = \sum_{\lambda} \varepsilon_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} \quad (1.18)$$

where the  $a$  operators must satisfy *commutation relations*. A hamiltonian of the form (1.15) looks very much like the one obtained in the single particle harmonic oscillator. The only thing changing here is that instead of only one kind of *raising* and *lowering* operators, we now have a family of them, one pair for each value of  $\lambda$ . So the interpretation of a second quantized hamiltonian (for non-interacting particles) is now clear: The system can be well described by a set of quantum harmonic oscillators, each of them with energy  $\varepsilon_{\lambda}$ .

The way of expressing hamiltonians in terms of these creation and annihilation operators constitutes the base for the many body theory. If we can always find a set of operators  $\xi_{\lambda}, \xi_{\lambda}^{\dagger}$  so that we can express our hamiltonian

like (1.15) for fermions and (1.17) for bosons, then the system is *diagonal* in that basis of operators, and the problem is solved. That implies that for a non-interacting system, there is not more complication than diagonalizing the hamiltonian, sometimes that implies to work in a different basis of operators, but it is still a diagonalization exercise. We will see later that the difficulty in many-body theory arises when interactions between the constituents of the system are considered.

Since now  $\psi(\vec{r})$  represents a field, the density is also an operator:

$$\hat{\rho}(\vec{r}) = \psi^\dagger(\vec{r})\psi(\vec{r}) \quad (1.19)$$

which becomes very relevant when interactions are introduced in the system.

Finally, and as a little summary, we have found that the field operators  $\psi, \varphi$  can always be expanded in another *basis* of operators, that, instead of acting over the real space, they act over a space  $\lambda$  that can represent momentum space or something else. The change of basis can also be inverted:

$$\begin{aligned} \psi(\vec{r}) &= \sum_{\lambda} c_{\lambda} \phi_{\lambda}(\vec{r}) \\ c_{\lambda} &= \int d^3\vec{r} \phi_{\lambda}^*(\vec{r}) \psi(\vec{r}) \end{aligned} \quad (1.20)$$

always keeping in mind that both  $c_{\lambda}, \psi(\vec{r})$  represent operators. We have given a nice interpretation of equation (1.15), but what is the meaning of the operator  $n_{\vec{k},\sigma} = c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma}$ ? We will discover it in the next section, where we introduce the quantum many-body state.

## 1.4 The many-body state

We have introduced before the creation and annihilation operators, both for fermions and bosons, and that's all well to express the hamiltonian in terms of them. However, when treating many-body systems, we will be interested in knowing the state. Moreover, we would like to see how our second quantized hamiltonian acts on it. For that, we need to introduce again a new notation.

The quantum mechanical state, in a system of  $N$  particles can be expressed as:

$$|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \dots \otimes |\psi_N\rangle \quad (1.21)$$

For second quantization, since we are dealing with creation and destruction operators, we can think about the many-body state like a state where we can label each site with  $\lambda_i$ , making  $i$  run over all possible values of  $\lambda$ , and insert or destroy particles on this site. To put this in mathematical notation, we want a state representing how many particles are in state  $\lambda_1$ , in  $\lambda_3$  or  $\lambda_{145}$ . This big ket we will express it by:

$$|MBS\rangle = |n_{\lambda_1} n_{\lambda_2} \dots n_{\lambda_j} \dots\rangle \quad (1.22)$$

where the  $n_{\lambda_i}$  represent the total number of particles in the state  $\lambda$ . One of the most important states we can define now is the vacuum, that *empty* state where there are no particles<sup>6</sup>:

$$|\text{vacuum}\rangle = |0\rangle = |000\dots 000\dots\rangle \quad (1.23)$$

That state has the property that gets annihilated if we want to remove a particle from it (since there are no particles). Thus, it doesnt matter if we have fermions or bosons since:

$$\begin{aligned} c_{\lambda_j} |0\rangle &= 0 \\ a_{\lambda_j} |0\rangle &= 0 \end{aligned} \quad (1.24)$$

and whatever the value  $j$  is. Lets start with the case of bosons. Imagine we want to insert two bosons, one of them in the  $\lambda_1$  state, and the other in the  $\lambda_3$ . The many-body ket then looks like:

$$a_{\lambda_1}^\dagger a_{\lambda_3}^\dagger |0\rangle = |10100\dots 00\dots\rangle = |\Psi\rangle \quad (1.25)$$

Also, because we are dealing with bosons, we can put as many particles as we want in the same quantum state. Therefore, we could add one more particle to the  $\lambda_1$  state, resulting in:

$$a_{\lambda_1}^\dagger a_{\lambda_1}^\dagger a_{\lambda_3}^\dagger |0\rangle = |20100\dots 00\dots\rangle = |\Psi\rangle \quad (1.26)$$

since now we have created two particles in that state. However, this is not

---

<sup>6</sup>The vacuum state doesnt contain any particles on it, but that doesnt mean necessarily that it doesnt have any energy associated. Remember the case of the single particle harmonic oscillator: even when we didnt have any excitation, there was a *vacuum* energy of  $\hbar\omega/2$

complete yet. The many-body ground state must be a *normalized* state, that means that:

$$\langle \Psi | \Psi \rangle = 1 \quad (1.27)$$

Since bosonic operators commute, the order of the operators doesn't matter at all when we are putting particles in different places. Also, for each value of  $\lambda$ , there are  $n!$  times we can proceed by acting with  $a_\lambda^\dagger$  in  $n$  times over the vacuum. Thus, the appropriate (and normalized) expression for the **many-body bosonic state** will be:

$$|BS\rangle = \frac{(a_{\lambda_1}^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(a_{\lambda_2}^\dagger)^{n_2}}{\sqrt{n_2!}} \dots \frac{(a_{\lambda_m}^\dagger)^{n_m}}{\sqrt{n_m!}} |0\rangle \quad (1.28)$$

Things are different for fermions. This is due to the anticommutation relations we introduced before. If we would like to insert two fermions in the same quantum state:

$$c_{\lambda_1}^\dagger c_{\lambda_1}^\dagger |0\rangle = 0 \quad (1.29)$$

the answer is 0 (looking at (2.12), can you see why?). This is a proof that anticommutation algebra for fermions is compatible with Pauli's exclusion principle, where not more than one fermion can occupy a quantum state. This *filling restriction* makes fermionic systems special compared to bosons. **For fermions, the occupation factors  $n_{\lambda_i}$  are restricted to be 0 or 1.** Then, no normalization factor is needed for the many body state. Also, one must take care about the order of the operators. One can construct the state:

$$c_{\lambda_1}^\dagger c_{\lambda_2}^\dagger |0\rangle = |1100\dots 000\dots\rangle \quad (1.30)$$

and naively think that:

$$c_{\lambda_2}^\dagger c_{\lambda_1}^\dagger |0\rangle = |1100\dots 000\dots\rangle \quad (1.31)$$

This is not true. Due to the anticommutation relations, we have:

$$c_\lambda^\dagger c_\mu^\dagger = -c_\mu^\dagger c_\lambda^\dagger \quad (1.32)$$

Therefore, states (2.27) and (2.28) differ by a minus sign, and these signs must always be taken into account when dealing with fermionic systems. When two fermionic operators are swapped (for different states), there is always a minus sign to carry.

This property of fermions lead us to calculate the *ground state* of a non-interacting fermionic system very easily. Lets now identify  $\lambda = \vec{k}, \sigma$ , where  $\sigma$  represents the spin index, and  $\vec{k}$  is the crystal momentum in the solid. To build up the lowest energy state, we create a fermion in the lowest  $\vec{k}$  value, with spin up, acting on the vacuum. We can create another fermion in the same  $\vec{k}$  state, but now the spin must be down. Then, we continue *filling* the  $\vec{k}$  states, till we have no particles left. Therefore we have:

$$|FS\rangle = \prod_{k \leq k_F} c_{\vec{k}\uparrow}^\dagger c_{\vec{k}\downarrow}^\dagger |0\rangle \quad (1.33)$$

This state represents the *Fermi sea*, where the highest energy level filled is called the *Fermi energy*. Therefore, a system of non-interacting electrons has a ground state formed by filling all energies below the Fermi level. We will see that in detail with the Fermi gas.

Remember that the energy states for the electrons in the solid are represented by a dispersion relation  $\xi_{\vec{k}} = \varepsilon_{\vec{k}} - \mu$  measured respect a chemical potential. Therefore, for the *Fermi momentum*  $k_F$  (that is, the highest value of  $\vec{k}$  when we fill the states), we have the Fermi energy  $\xi(k_F)$ .

We are now in position to understand the expression (1.15) for the non-interacting hamiltonian. First, lets see what does the operator  $c_\lambda^\dagger c_\lambda$  do to the many body state, for example, for a value of  $\lambda_k$ <sup>7</sup>

$$n_{\lambda_k} |\lambda_1 \lambda_2 \dots \lambda_k \dots\rangle = c_{\lambda_k}^\dagger c_{\lambda_k} |\lambda_1 \lambda_2 \dots \lambda_k \dots\rangle \quad (1.34)$$

We first act with the annihilation operator on the state, removing one particle from  $\lambda_k$ . After this, we create it again, obtaining the same many-body ground state. However, we know that for a fermionic many body state, the different  $\lambda$  states can only be 0 or 1. If the occupation of  $\lambda_k$  is 0, then the action of  $c_{\lambda_k}$  over the many body state gives 0, since there are no particles to annihilate. On the other hand, if the state is occupied, we remove the particle and we put it back again. In some sense, the operator  $n_{\lambda_k}$  is counting how many particles we have in that state. This operator is called the *number operator*, and it is very

<sup>7</sup>That  $k$  here should be confused with the crystal momentum. It is just an index, to represent one of the possible values of  $\lambda$ .

important in the many body description.

Now take a look at eq.(1.15). In the basis of creation and annihilation operators, the hamiltonian (total energy of the system) is the sum of the **energies of each state times the total number of particles in that state**. Remember that, for fermions, on each state we can only have zero or one particle.

Just a final note about bosons: for a bosonic hamiltonian, eq.(1.15) is also valid, we just need to substitute bosonic operators instead of fermionic ones. However, since bosons follow a commutation algebra, the occupation for each state can run from 0 particles to  $N$ . In other words, for bosons we can put as many particles as we want in a quantum state, and the number operator ( $a_\lambda^\dagger a_\lambda$  in that case) will give us how many particles are in one state  $\lambda_k$ .

For a (non-interacting) bosonic hamiltonian we will have:

$$H = \sum_{k\sigma} \varepsilon_{k,\sigma} a_{k,\sigma}^\dagger a_{k,\sigma} \quad (1.35)$$

Without taking into account the spin index  $\sigma$ , this looks a lot like the quantum harmonic oscillator. When we were working with one particle, the energy of the oscillator was determined by the level  $n$  where the particle was located. Here, in the second quantized picture, *each energy level*  $\varepsilon_k$  can have a different number of **excitations**, counted by the number operator  $n_{k,\sigma} = a_{k,\sigma}^\dagger a_{k,\sigma}$ . This gives a nice interpretation to the second quantised hamiltonian: a second quantised hamiltonian<sup>8</sup> is a set of quantum oscillators, each of them with different energy, and this energy is given by the number of particles in that mode  $k$ . For fermions, the case is easier, since every quantum oscillator can only have one or zero excitations for each mode. But for bosons, this restriction disappears.

## 1.5 Exercises

1) *Completeness and orthogonality* The completeness and orthogonality relations for a basis are:

$$\begin{aligned} \sum_{\lambda} \phi_{\lambda}^*(\vec{r}_i) \phi_{\lambda}(\vec{r}_j) &= \delta(\vec{r}_i - \vec{r}_j) \\ \int d\vec{r} \phi_{\lambda}^*(\vec{r}) \phi_{\mu}(\vec{r}) &= \delta_{\mu\lambda} \end{aligned} \quad (1.36)$$

where  $\lambda$  and  $\mu$  are discrete index. Using these relations, and equation (1.11),

---

<sup>8</sup>And again, non-interacting

obtain a second quantized expression for the density operator  $\hat{\rho}(\vec{r})$ .

2) Consider equations (1.9) and (1.10), for bosonic and fermionic fields. Making use of (1.11), and being  $\phi_\lambda(\vec{r})$  a *complete* and *orthogonal* set of functions, obtain both the commutation/anticommutation relations in  $\lambda$  space.

3) *Bogoliubov transformation*

a) Consider the following single-boson hamiltonian:

$$H = -\omega a^\dagger a + E_0(a^\dagger a^\dagger + aa) \quad (1.37)$$

where  $\omega, E_0$  are energy parameters. Check that the change:

$$b = ua + va^\dagger \quad (1.38)$$

leaves the commutation relations unchanged, provided that:

$$u^2 - v^2 = 1 \quad (1.39)$$

b) Identify  $u = \cosh(z)$  and  $v = \sinh(z)$ . Show that the hamiltonian can be diagonalized in the  $b$  operators, providing the condition:

$$\tanh(z) = -\frac{E_0}{\omega}(1 + \tanh^2(z)) \quad (1.40)$$

and express  $\Delta$  and  $K$  in:

$$H = \Delta b^\dagger b + K \quad (1.41)$$

in terms of  $E_0$  and  $\omega$ .



## 2 Treating interacting systems

### 2.1 A many-body problem

We have introduced before the second quantization language, focusing only on non interacting systems. The thing is that for such systems, a diagonalization of the hamiltonian is always possible, and expressing  $H$  in the form of (1.15) completely solves the problem.

However, we know that in reality, the constituents of a system do interact with each other. We can have interactions between electrons in a solid, or electrons interacting with phonons, electrons interacting with *spin* impurities in a material etc...

This terms add an additional complexity to the hamiltonian. In what follows, we will consider just the electron-electron interactions. Terms of this type can be written:

$$V_{\text{int}} = \frac{1}{2} \int d^3\vec{x} \int d^3\vec{y} \rho(\vec{x}) V(\vec{x} - \vec{y}) \rho(\vec{y}) \quad (2.1)$$

where the interaction term  $V(\vec{x} - \vec{y})$  depends only on the relative coordinates of the particles. In second quantization, this becomes an operator because the density  $\rho$  is an operator. However, with interacting terms **one always have to be careful with the order of the field operators**. The rule to follow is simple: *All creation operators must be to the left of all destruction operators in an interacting term*. The reason for that is to avoid terms where particles interact with themselves, something we know it doesnt make sense. The second quantized interaction is:

$$V_{\text{int}} = \frac{1}{2} \int d^3\vec{x} \int d^3\vec{y} : \rho(\vec{x}) \rho(\vec{y}) : V(\vec{x} - \vec{y}) \quad (2.2)$$

where  $: \rho(\vec{x}) \rho(\vec{y}) := \psi^\dagger(\vec{x}) \psi^\dagger(\vec{y}) \psi(\vec{x}) \psi(\vec{y})$  is the *normal ordered* product of the densities, expressed with the  $:$  symbol. The interaction term is the usual Coulomb potential:

$$V(\vec{x} - \vec{y}) = \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\vec{x} - \vec{y}|} \quad (2.3)$$

Now, we can use the plane waves basis to expand the field operators in  $\vec{k}$  space:

$$\psi_\sigma(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} c_{\vec{k},\sigma} e^{i\vec{k}\cdot\vec{r}} \quad (2.4)$$

Substituting that in (3.2), we are left with:

$$V_{\text{int}} = \frac{1}{2V^2} \sum_{\substack{k_1, k_2, k_3 \\ k_4, \sigma, \tau}} c_{k_1, \sigma}^\dagger c_{k_2, \tau}^\dagger c_{k_3, \sigma} c_{k_4, \tau} \int d^3 \vec{x} \int d^3 \vec{y} e^{-i(\vec{k}_1 - \vec{k}_3) \cdot \vec{x}} e^{-i(\vec{k}_2 - \vec{k}_4) \cdot \vec{y}} V(\vec{x} - \vec{y})$$

Lets now change variables:

$$\vec{r} = \vec{x} - \vec{y} \rightarrow \vec{x} = \vec{r} + \vec{y} \quad (2.5)$$

Then we have:

$$V_{\text{int}} = \frac{1}{2V^2} \sum_{\substack{k_1, k_2, k_3 \\ k_4, \sigma, \tau}} c_{k_1, \sigma}^\dagger c_{k_2, \tau}^\dagger c_{k_3, \sigma} c_{k_4, \tau} \int d^3 \vec{r} \int d^3 \vec{y} e^{-i(\vec{k}_1 - \vec{k}_3) \cdot \vec{r}} e^{-i(\vec{k}_2 - \vec{k}_4 + \vec{k}_1 - \vec{k}_3) \cdot \vec{y}} V(\vec{r})$$

Now lets call:

$$\vec{q} = \vec{k}_1 - \vec{k}_3 \quad (2.6)$$

so that we end up with:

$$V_{\text{int}} = \frac{1}{2V^2} \sum_{\substack{q, k_2, k_3 \\ k_4, \sigma, \tau}} c_{k_3+q, \sigma}^\dagger c_{k_2, \tau}^\dagger c_{k_3, \sigma} c_{k_4, \tau} \underbrace{\int d^3 \vec{r} e^{-i\vec{q} \cdot \vec{r}} V(\vec{r})}_{V(\vec{q})} \int d^3 \vec{y} e^{-i(\vec{k}_2 - \vec{k}_4 + \vec{q}) \cdot \vec{y}}$$

The integral in  $\vec{y}$  is a delta function, giving the condition<sup>9</sup>

$$\delta(\vec{k}_2 - \vec{k}_4 + \vec{q}) \rightarrow \vec{k}_2 = \vec{k}_4 - \vec{q} \quad (2.7)$$

The final expression for the interacting term becomes:

$$V_{\text{int}} = \frac{1}{2V} \sum_{\substack{q, k_3, k_4 \\ \sigma, \tau}} V(\vec{q}) c_{k_3+q, \sigma}^\dagger c_{k_4-\vec{q}, \tau}^\dagger c_{k_3, \sigma} c_{k_4, \tau} \quad (2.8)$$

---

<sup>9</sup>This is the conservation of momentum

This has a nice interpretation if we look at it. There are two annihilation operators for different value of the spin, and two creation operators. We can imagine this as a fermion with spin  $\tau$  and momentum  $\vec{k}_4$  meeting a particle with spin  $\sigma$  and momentum  $\vec{k}_3$ . At the same time, and when they interact, a momentum  $\vec{q}$  is transferred from one particle to the other, due to the interaction. The new *created* particles conserve the spin, but one of them has momentum  $\vec{k}_3 + \vec{q}$ , whereas the other has  $\vec{k}_4 - \vec{q}$  after the *scattering*. Also, the  $q = 0$  term is excluded in the sum (why is that the case?).

The scattering amplitude of the interaction is given by  $V(\vec{q})$ , which is nothing but the Fourier transform of the potential.<sup>10</sup> Therefore, we are left with a second quantised expression to add to our non-interacting hamiltonian, just by considering any kind of interaction between electrons.

## 2.2 The non-interacting Fermi gas

To start getting familiar with the many-body formalism, we apply it to the simplest case. Consider a gas, where electrons don't interact with each other. We have seen that for this case, the non-interacting hamiltonian can be obtained by just summing all the individual particle hamiltonians:

$$H = \sum_{i=1}^N \frac{p^2}{2m} \quad (2.9)$$

If the electrons don't interact, we know the dispersion relation as a function of  $\vec{k}$  (momentum crystal analogy):

$$\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m} \quad (2.10)$$

and therefore, there is rotational symmetry in the  $\vec{k}$  space. We have already seen what would the the second quantized hamiltonian look like, making use of creation and annihilation operators. Using them, the hamiltonian (3.9) is expressed as:

$$H = \sum_{\vec{k}, \sigma} \varepsilon_{\vec{k}, \sigma} c_{\vec{k}, \sigma}^\dagger c_{\vec{k}, \sigma} \quad (2.11)$$

---

<sup>10</sup>Though there might be some cases where the Fourier transform of a given potential doesn't exist, i.e the case of interactions by a Lennard-Jones potential.

At zero temperature, the only state of the system is the *ground state*<sup>11</sup>, which we have defined previously as the Fermi sea. We create it by filling the vacuum successively in  $\vec{k}$ :

$$|FS\rangle = \prod_{k \leq k_F} c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger |0\rangle \quad (2.12)$$

Doing that, and because the rotational symmetry in  $k$  from the dispersion relation, the Fermi energy is the *surface* of a **sphere of radius**  $k_F$  (Fermi wavevector). To calculate the Fermi wave-vector, the total number of particles (its average) must be equal to:

$$\langle N \rangle = 2 \sum_{k \leq k_F} \langle n_{\vec{k}} \rangle \quad (2.13)$$

where the 2 comes from summation over spin. At  $T = 0$ , we only average the number operator over the ground state. We already know that this is the Fermi-Dirac distribution, such that:

$$\langle n_k \rangle = \begin{cases} 1 & k \leq k_F \\ 0 & k > k_F \end{cases} \quad (2.14)$$

In the *thermodynamic limit*<sup>12</sup>, we can convert the summation into an integral:

$$\sum_k \rightarrow V \int \frac{d^3 \vec{k}}{(2\pi)^3} \quad (2.15)$$

Then we have:

$$\frac{\langle N \rangle}{V} = 2 \int \frac{d^3 \vec{k}}{(2\pi)^3} \cdot 1 = \frac{1}{\pi^2} \int_0^{k_F} dk k^2 = \frac{1}{3\pi^2} k_F^3 \quad (2.16)$$

which gives a direct relation between the Fermi wave-vector and the density of the system.

<sup>11</sup>State of minimum energy, the definition is the same as in ordinary quantum mechanics, although here we are considering a *macro-state* or ensemble.

<sup>12</sup>That limit is used commonly in many-body physics. It allows us to take the volume of the system  $V \rightarrow \infty$  to convert summations into integrals. Doing that, we are saying that the *low energy* physics of the system should not change as the volume is increased, and thus we have macroscopic properties. Another interesting limit is the *continuous limit*, where the lattice spacing  $a \rightarrow 0$ .

This simple model offers a poor approximation of a solid, we know that electrons interact with each other, and in fact, these interactions are not neglectable respect to the kinetic energy, but dominant!. However, when interactions are considered, there is a way to express the system in terms of some new *particles* with renormalized parameters, as if they were not interacting between them. That is the Landau-Fermi liquid theory.

### 2.3 Landau-Fermi liquid theory: concept of quasiparticle

What is the picture when we turn on the interactions? As we know, electrons are filling the Fermi sea till some energy level called the Fermi level ( $\varepsilon_F$ ) at  $T = 0$  when there are no interactions. However, the *bad news* is that when interactions are considered, they are dominant over the kinetic energy terms of the hamiltonian. Therefore, it seems like perturbative techniques are insufficient to describe such a system. Also, experimental evidence suggests that the non-interacting model of the previous section (the Fermi gas) describes considerably well most of the low energy properties of too many metals. If interactions are dominant in the hamiltonian, how can we explain that analogy between experimental evidence in real metals and the non-interacting picture?

Our total hamiltonian describing a Fermi liquid is:

$$H = \sum_{k,\sigma} \varepsilon_{\vec{k},\sigma} c_{k,\sigma}^\dagger c_{\vec{k},\sigma} + \frac{1}{2V} \sum_{q, k_3, k_4} V(\vec{q}) c_{k_3+q,\sigma}^\dagger c_{k_4-\vec{q},\tau}^\dagger c_{k_3,\sigma} c_{k_4,\tau} \quad (2.17)$$

where interactions between electrons are considered in the second term. This second term is a set of scattering events between electrons. As a result of this interaction, excitations appear above the Fermi surface. We will expect the electron **occupation** to change in the vicinity of the Fermi surface. Due to that interactions, we would have passed from the non-interacting ground state (the Fermi sea), to an interacting one, where the Fermi surface and the occupation number are changed. It seems a difficult problem then, since eq. (2.17) can't be diagonalised containing the interacting term.

However, there is another approach. Landau proposed the following: if interactions are turned on *smoothly* and *slow*, these excitations close to the Fermi surface can be considered *still* as electron excitations, *but with renormalized parameters*. Therefore, the picture becomes non-interacting again. This is called **adiabatic continuity**, which suggests a direct mapping between an interacting ground state to a non-interacting one, by only changing some parameters of the model.

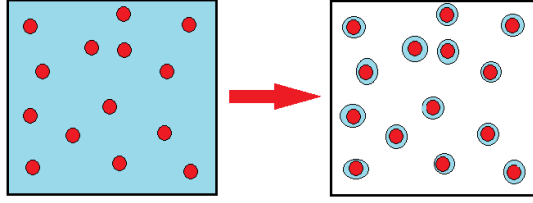


Figure 1: **Concept of quasiparticle:** Electrons inside a real material interact with each other. That can be thought as if in every point of space, each electron would be suffering the potential created there by other electrons (left). In the Landau-Fermi liquid theory, these interactions are considered as part of new *quasiparticles*, that move freely (non-interacting with each other) in the material. The effect of these quasiparticles on the electrons manifest in different values for the mass and energies.

These low energy excitations that now describe a non-interacting system are called *quasiparticles*. A quasiparticle can be thought as an electron surrounded by interactions with the other constituents. In other words, we can imagine a quasiparticle like an electron *dressed* by interactions, and therefore a bit *heavier*. These *quasiparticles* are only allowed to live in the vicinity of the Fermi surface. The fact that these new particles live close to the Fermi surface says something about their stability: they have a *long life*. Conceptually, just imagine that there is not too much energy cost if we perturb slightly an electron and we put it a bit above the Fermi surface. Since that doesn't cost too much energy, the system will be stable under such perturbations.

What is then the advantage of using such a picture? Well, the first thing is that working with quasiparticles, we don't have to deal with the second term of (2.17). The *effective* hamiltonian has now changed to:

$$H_{eff} = \sum_{k,\sigma} \xi_{\vec{k},\sigma} c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} \quad (2.18)$$

which is non-interacting. The occupation number associated with the quasiparticles follows the Fermi-Dirac statistics: then, at  $T = 0$ , this is just a step function. Now, the creation and annihilation operators create or destroy a quasiparticle of energy  $\xi_{\vec{k}}$ . The mass associated with these quasiparticles is called the *effective mass*, and usually denoted by  $m^* > m_e$ , where  $m_e$  is the mass of the electron ( $\sim 9.12 \cdot 10^{-31} \text{kg}$ ).

Therefore, the Landau-Fermi liquid theory provides a nice interpretation about why a big number of metals can be described by a non-interacting model.

## 2.4 Finite temperature vs zero temperature

Our treatment has concerned so far systems at zero temperature. In such systems, the only state occupied in the ensemble is the *ground state*. This is because as temperature is getting lower, some degrees of freedom of the system become irrelevant. According to statistical mechanics:

$$P(\varepsilon_n) \sim e^{-\beta\varepsilon_n} \quad (2.19)$$

is the probability of finding the system in a state of energy  $\varepsilon_n$ . In the limit<sup>13</sup>  $\beta \rightarrow \infty$ , the exponential with *highest* value is that with the lowest  $\varepsilon_n$ , and exactly the ground state is found.

However, we could ask ourselves what happens at  $T \neq 0$ . We will not go into detail here, but we only one to make a clear separation between the zero temperature case and finite temperature.

At finite temperature, there is no single state for the system, since it is in an ensemble, and each of the states has probability (3.19). Therefore, an expectation value:

$$\langle O \rangle = \frac{\text{Trace}(O\rho)}{\text{Trace}\rho} \quad (2.20)$$

involves the operator  $\hat{\rho} = e^{-\beta\hat{H}}$ . In general,  $\hat{H}$  can be expressed as a non-interacting part and an interacting one:

$$\hat{H} = \hat{H}_0 + \hat{V} \quad (2.21)$$

The exponential dependence on the temperature contrast with the Heisenberg picture<sup>14</sup> dependence for the operator  $O$ :

$$O(t) = e^{iHt/\hbar} O e^{-iHt/\hbar} \quad (2.22)$$

Both exponential operators involve  $H$  now, and then, the interaction of the hamiltonian  $\hat{V}$  needs in principle to be treated separately for both terms. This can be avoided if we consider  $\beta$  as an imaginary time, so that  $\beta = it = \tau$ . This is called the Matsubara formalism. In the Matsubara formalism, there are only

<sup>13</sup>Remember that  $\beta = 1/T$  ( $k_B = 1$ )

<sup>14</sup>To understand the Heisenberg picture, go to section 4.3

some allowed excitations  $\omega_n$  (called Matsubara frequencies), and the *correlators* (See next subsection) are expressed in terms of them as a infinite sum.

From now on, we will focus only in the  $T = 0$  case, where this mathematical trick is unnecessary. We will only say that there are different approaches to solve a many-body problem for a zero temperature case.

The first of them is to calculate all quantities (correlation functions) in terms of the ground state for the zero temperature case. More concretely, in perturbation theory only the ground state of the non-interacting system is considered in the expansion.

The other approach is to work out the problem for a general temperature  $T$ , and once we have the correlators, obtain the zero temperature ones by analytical continuation<sup>15</sup>. Which of the two approaches is better is something to choose depending on the problem under consideration.

## 2.5 Correlators

We have arrived perhaps at the most important part of this very brief introduction to the subject. *What is a correlator?* Correlation functions appear in two many branches of physics, from magnetism to a simulated hard disks fluid model. Lets remember from quantum mechanics what is the *probability* of passing from one state  $|n\rangle$  to a state  $|m\rangle$  under some perturbation  $V$  over the initial state. This is given by the Fermi golden rule:

$$P_{n \rightarrow m} \sim |\langle m|V|n\rangle|^2 \tag{2.23}$$

This is nothing but a number, that tells us how the state changes when a perturbation is added to it. In order to get a non-zero answer<sup>16</sup>, the action of the operator  $V$  over  $|n\rangle$  must transform the state into  $|m\rangle$ .

A *correlator* covers this idea (roughly speaking). It can be regarded as a *disturbance* in the system, and what is the probability amplitude of that disturbance taking place.

More concretely, in a quantum field theory, dynamical objects are the *fields*. We have seen before that, for each type of particle, we assign one scalar field (the *particle-field*), creating or annihilating a particle in space-time. We want to make use of that tools now, to calculate how the particle can move from one state *to the same one* after some action of an operator in the state.

---

<sup>15</sup>That is a rotation in the complex plane, passing from the imaginary time  $\tau$  to real time.

<sup>16</sup>Because we are supposing  $|n\rangle$  and  $|m\rangle$  to be orthogonal.



Imagine the following situation: a system of interacting particles in a box. Lets consider that the configuration of the system is some state <sup>17</sup> $|\Psi\rangle$ . Then, we select the particle at position  $\vec{r}_1$  at time  $t$ , and we *propagate* the particle from  $\vec{r}_1$  to  $\vec{r}_2$ , in an interval of time  $t' - t$ . In the process, the particle can change its spin projection from  $\sigma$  to  $\sigma'$ . The final state has to be  $|\Psi\rangle$  again, but we just want to see what is the *probability amplitude* of such a process.<sup>18</sup>. In our second quantised language, that is the same as saying that we *destroy* the particle in  $(\vec{r}_1, t)$  to create it at  $(\vec{r}_2, t')$ . In all the propagation process, there are interactions of this particle with the others. This situation we have described here is called the **single particle Green's function**<sup>19</sup> and we define it as:

$$G_{\sigma,\sigma'}(\vec{r}_1, \vec{r}_2, t, t') = -i\langle\Psi|\hat{T}\psi_\sigma(\vec{r}_1, t)\psi_{\sigma'}^\dagger(\vec{r}_2, t')|\Psi\rangle \quad (2.25)$$

Here,  $\hat{T}$  represents the time ordering operator, defined acting on two<sup>20</sup> operators  $\hat{A}$  and  $\hat{B}$ :

$$\hat{T}\hat{A}(t)\hat{B}(t') = \begin{cases} \hat{A}(t)\hat{B}(t') & t > t' \\ \pm\hat{B}(t')\hat{A}(t) & t' > t \end{cases} \quad (2.26)$$

the minus sign in the second case appearing for fermionic operators (remember that swapping two fermionic operators gives a minus sign always). Although we have written  $\psi$  for the field operator, the expression above is valid also for bosonic operators, just by taking into account the commutation properties. We have to choose one type of particles for the description, and we will keep going for fermions, since Pauli's exclusion principle simplifies things. We have to say that the expression above is only valid for *real time*, and *zero temperature* systems, therefore  $|\Psi\rangle = |GS\rangle$  is the ground state **of the whole interacting system**. In translationally invariant systems, and with a hamiltonian independent of time, this correlator is only a function of the relative position  $\vec{r}_1 - \vec{r}_2$  and the interval  $t - t'$ , as both momentum and energy are conserved.

<sup>17</sup>Which is not necessarily the ground state, it can in principle be any of the possible states of the ensemble

<sup>18</sup>Look at expression (2.23). Here, the probability amplitude won't be a number, but a function of the coordinates  $\vec{r}_1$  and  $\vec{r}_2$

<sup>19</sup>You can find the definition of a propagator in every QFT book. In more technical ways, the propagator is a solution of the equation:

$$-\hat{D}G(x - y) = \delta^N(x - y) \quad (2.24)$$

where  $\hat{D}$  is a differential operator and  $N$  the dimension of space. However, here we are talking about *response functions*, that is, how the system responds under external perturbations (for example, if we try to measure something)

<sup>20</sup>There is a generalisation of the time ordering operator, where all operators act in a *causalway*, starting from the right those operators appearing first in time.

Lets now Fourier transform the expression above. The result is, using the plane wave representation<sup>21</sup>:

$$G_{\sigma,\sigma'}(\vec{r}_1 - \vec{r}_2, t - t') = -i \frac{1}{N} \sum_{k,k'} e^{i\vec{k}\cdot\vec{r}_1} e^{-i\vec{k}'\cdot\vec{r}_2} \langle \hat{T} c_{k,\sigma}^\dagger(t) c_{k',\sigma'}(t') \rangle \quad (2.27)$$

where the average  $\langle \dots \rangle$  is over the interacting ground state  $|\Psi\rangle = |GS\rangle$ . For a fermionic system, we know already this state (the Fermi sea) because we discussed it before.

Lets work out this expression for the case of a Fermi gas. In the case of a Fermi gas, the hamiltonian is totally independent of the spin  $\sigma$ , therefore we don't expect any change in the spin projection. Also, it is clear that if we remove a particle from the Fermi sea (or alternatively, we create a *hole*) with momentum<sup>22</sup>  $\vec{k}$ , then the particle created again must have the same momentum  $\vec{k}$ , so that the correlator is non-zero. Explicitly:

$$G_{\sigma,\sigma'}(\vec{r}_1 - \vec{r}_2, t - t') = \frac{-i}{N} \sum_k e^{i\vec{k}(\vec{r}_1 - \vec{r}_2)} \langle \hat{T} c_{k,\sigma}^\dagger(t) c_{k,\sigma'}(t') \rangle \delta_{\sigma,\sigma'} \quad (2.28)$$

for the Fermi gas. Lets ommit the spin index. This can be written as:

$$G(\vec{r}_1 - \vec{r}_2, t - t') = \frac{1}{N} \sum_k e^{i\vec{k}(\vec{r}_1 - \vec{r}_2)} G(\vec{k}, t - t') \quad (2.29)$$

Since these are both wavefunctions for non-interacting systems, call them  $G_0(\vec{r}_1 - \vec{r}_2, t - t')$  and  $G_0(\vec{k}, t - t')$ . We are now left with the evaluation of the quantity:

$$G_0(\vec{k}, t - t') = -i \langle GS | T c_{\vec{k}}(t) c_{\vec{k}}^\dagger(t') | GS \rangle \quad (2.30)$$

which is left as an exercise in the problems. But lets give an interpretation of both Green's functions: In real space, it provides information about the probability amplitude of putting an electron in one position and time and let it propagate to another position and time. In momentum representation, as in eq.(2.30), we create a particle at time  $t'$  with some momentum and we let it propagate. We argued before that, because we are returning to the same state, the only possibility to conserve momentum is that the particle we remove in  $t$  has exactly the same value  $\vec{k}$  for it.

<sup>21</sup>Remember this is the usual choice for translational invariant systems.

<sup>22</sup>We have to say that notation here is a bit lazy. The sum in  $k$  is in fact a sum in  $\vec{k}$ , but we are just ommiting this keeping in mind that  $k$  represents a 3-dimensional vector.

Depending on the sign of  $t - t'$ , we distinguish between two types of correlators: *retarded* and *advanced*. We don't need to go into much detail here, however it is useful to know that this distinction between both has some justification. Moreover, the analytical properties of both functions are exactly opposite: the retarded correlator is always analytic in the complex upper half-plane of the excitation energies  $\omega$ , whereas the advanced one is analytic in the lower half plane.

Correlators are the most interesting quantities in many-body physics, since they provide direct information about measurable properties of the system. However, every measure taken in a lab has to be in relation with a retarded correlator, since otherwise, causality is violated<sup>23</sup>.

I want to make a final connection with the field theory for this very brief introduction of correlators. One of the nice features about them is that they can also be calculated by the *functional derivative* of the Feynman path integral  $Z$ . That is why sometimes  $Z$  is called the *generating functional*. Depending on the problem under study, a field theoretic approach may be more convenient<sup>24</sup> than the many-body description we were considering before, whereas sometimes it can be the other way around.<sup>25</sup>

## 2.6 Exercises

1) Evaluation of the non-interacting single particle Green's function at  $T = 0$ : Go back to equation (2.30). By making use of the Heisenberg representation for operators:

$$c_{\vec{k}}^- = e^{iHt} c_{\vec{k}}^- e^{-iHt} \quad (2.31)$$

calculate  $G_0(k, t - t')$ , being careful with the time ordering operator. (*Hint*: The action of the exponential operator  $e^{i\hat{H}t}$  over the ground state is an eigenvalue equation for a non-interacting system. More over, adding or removing an electron to  $|GS\rangle$  will only change the total energy by  $\varepsilon_k$ )

b) Sometimes is more convenient to express the non-interacting Green's function as a function of  $\vec{k}$  and  $\omega$  by just Fourier transforming:

$$G_0(\vec{k}, \omega) = \int d(t - t') e^{i\omega(t - t')} G_0(\vec{k}, t - t') \quad (2.32)$$

Use the previous result to evaluate this function. *Hint*: You have to be careful

<sup>23</sup>There are no experiments in which a cause precedes an action...

<sup>24</sup>That is, by treating the *fields* as dynamical objects, instead of the creation and annihilation operators.

<sup>25</sup>A functional is a map that associates a number with each function of one kind

about evaluating integrals of the type:

$$\lim_{\delta \rightarrow 0^+} \int_0^{+\infty} dz e^{izt - \delta t} = \lim_{\delta \rightarrow 0^+} \frac{1}{z + i\delta} \quad (2.33)$$

Verify that this integral is the definition of the Dirac delta when the limit is applied. Show that the limit differs depending on the sign of  $t - t'$ .

2) Electrons in a gas interact via Coulomb interaction, expressed in equation (2.3). Fourier transform this expression in 1D, 2D, and 3D. Is there any peculiarity in these cases? Verify that the Yukawa potential  $V(r) = K \frac{e^{-\lambda r}}{r}$  has a well defined Fourier transform in 3D. ( $K$  is a constant to provide correct units)

## 3 Approximation methods

### 3.1 Failure of ordinary perturbation theory

All is ok if we want to study non-interacting systems, since we have seen that we can compute some properties without too much effort. However, we know that real systems do include interactions between constituents. From a hamiltonian like (2.17), we can use ordinary perturbation techniques to see how the second term changes the ground state energy.

From quantum mechanics, the corrections to the ground state energy of a system can be expressed as:

$$E_{GS} = E_0 + \lambda \langle GS | \hat{V} | GS \rangle + \frac{\lambda^2}{2} \sum_n \frac{|\langle n | \hat{V} | GS \rangle|^2}{E_n - E_0} + \dots \quad (3.1)$$

However, the second term in perturbation already contains a sum over all many-body states  $|n\rangle$ , and, meanwhile the first term looks reasonable to calculate, the second term doesn't. This fact gives a reason why ordinary perturbation theory has to fail in treating many-body systems. Simply, the number of states we would need to include is huge even to reach a second order correction.

The solution to that problem has to be with the inclusion of a new parameter in the description, which we have already anticipated previously. The *time evolution* can give an idea about how a non-interacting ground state evolves to the interacting one.<sup>26</sup>

However, to go a bit further we need to say a few words about the different representations in quantum mechanics.

### 3.2 Three pictures of quantum mechanics

#### 3.2.1 Schrodinger picture

In ordinary quantum mechanics, the time evolution of the system is described by the Schrodinger equation ( $\hbar = 1$ ):

$$i\partial_t \psi(\vec{r}, t) = \hat{H} \psi(\vec{r}, t) \quad (3.2)$$

---

<sup>26</sup>Anticipating a bit, we will say that there is a theorem relating both ground states of the interacting system and the non-interacting one, known as the Gell-Mann and Low theorem.

where the wavefunction depends explicitly on time. Moreover, if the hamiltonian doesn't depend on time, then the spatial and time parts of the wavefunction factorize:

$$\psi(\vec{r}, t) = \phi(\vec{r})e^{-iEt} \quad (3.3)$$

In Dirac notation, equation (3.2) can be easily solved to give:

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle \quad (3.4)$$

That is, the operator  $e^{-i\hat{H}t}$  *evolves or propagates* the state  $|\psi(0)\rangle$  to a later time. Thus, we have seen that in the Schrodinger picture, operators do not depend on time, but states do.

### 3.2.2 Heisenberg picture

Let us now take the average value of some operator over the state  $|\psi(t)\rangle$ , that is:

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(0)|e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}|\psi(0)\rangle \quad (3.5)$$

Look at this expression. We can interpret it in two ways. The first is the usual Schrodinger picture we described above, where  $\hat{A}$  is an operator that doesn't depend on time explicitly. All the time dependence is found in the states.

But, there is another view we can take here. We can name our operator  $\hat{A} = \hat{A}(t)$  by identifying:

$$\hat{A}(t) = e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t} \quad (3.6)$$

and the state is taken as  $|\psi(0)\rangle$ . Having done that, the dynamical quantity is now the operator itself, and the states remain *frozen* in an initial time. This picture is known as the Heisenberg picture, and it provides exactly the same results as the Schrodinger picture.

However, if the states are no longer dynamical objects in this picture, what happens with Schrodinger equation (3.2)? There is indeed an Schrodinger equation analog for the Heisenberg case, however, its form differs from (3.2). We

have to remember that in this picture, the *objects* evolving in time are the operators. Since the Schrodinger equation involves a first time derivative for the states, let us calculate the time derivative for the operator  $\hat{A}(t)$ :

$$\begin{aligned}\frac{d\hat{A}}{dt}(t) &= (i\hat{H})e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t} + e^{i\hat{H}t}\hat{A}(-i\hat{H})e^{-i\hat{H}t} \\ \frac{d\hat{A}}{dt}(t) &= -i[\hat{A}(t), \hat{H}]\end{aligned}\tag{3.7}$$

This is the form of the Schrodinger equation in the Heisenberg picture, describing the time evolution of the operator  $\hat{A}$ . One important fact about this equation (and that makes the Heisenberg picture more useful in some cases) is that we can easily observe *conserved quantities* by just seeing how the operator commutes with  $H$ . If one operator commutes with the total hamiltonian, then:

$$\frac{d\hat{A}}{dt}(t) = 0\tag{3.8}$$

the quantity described by the operator  $\hat{A}$  is a conserved quantity, that is, it doesn't evolve in time. To describe many body systems, it is easy to convince oneself that the Heisenberg picture provides a better tool, since the time evolution of a whole many body state is something difficult to deal with. When calculating correlation functions, we will be working in the Heisenberg picture, and that is something we anticipated before.

We can justify equation (2.31) knowing this. Lets go even further, and calculate the time dependence of the annihilation operator in a non-interacting fermionic system, where:

$$\hat{H} = \sum_k \varepsilon_k c_k^\dagger(t) c_k(t)\tag{3.9}$$

To see that, we evaluate how this operator acts on the many-body state:

$$c_k(t)|FS\rangle = e^{i\hat{H}t} c_k e^{-i\hat{H}t} |FS\rangle\tag{3.10}$$

This state is the Fermi sea we have found before. Since it is an eigenstate of the hamiltonian, the exponential operator is changed in the argument by its eigenvalue:

$$e^{i\hat{H}t} c_k e^{-iE_F t} |FS\rangle\tag{3.11}$$

Now the first exponential is just a factor. When we act with  $c_k$  over the Fermi sea, the total energy is lowered by a factor  $\varepsilon_k$ , that is, we remove a single mode, but the remaining state is still an eigenvector of the operator  $\hat{H}$ . Then, when we act with the first exponential, we have:

$$e^{i(E_F - \varepsilon_k)t} c_k e^{-iE_F t} |FS\rangle = c_k e^{-i\varepsilon_k t} |FS\rangle \quad (3.12)$$

so we can deduce that the annihilation operator in Heisenberg picture is:

$$c_k(t) = e^{-i\varepsilon_k t} c_k \quad (3.13)$$

that is, it oscillates in time and destroys a mode of energy  $\varepsilon_k$ .

### 3.2.3 Interaction picture

Another way of expressing operators and states is the *interaction picture*. In fact, this picture is the most important one when all is about calculating Green functions perturbatively. There are two important comments to make about this picture: First, operators depend on time, but in a different way than in Heisenberg picture. Second, states depend on time too!

To see this dependence, consider the many-body hamiltonian in our problem divided into a non-interacting part  $H_0$  and the interacting part  $V$ :

$$H = H_0 + V \quad (3.14)$$

We have omitted the hats, but it should be clear we are working with operators. Usually,  $V$  will not commute with  $H_0$ , and that is assumed here. Coming back to (3.5):

$$\langle \psi(t) | \hat{A} | \psi(t) \rangle = \langle \psi(0) | e^{iHt} \hat{A} e^{-iHt} | \psi(0) \rangle \quad (3.15)$$

We can now multiply inside by  $I = e^{-iH_0 t} e^{iH_0 t}$ , the identity operator, so that:

$$\langle \psi(t) | \hat{A} | \psi(t) \rangle = \langle \psi(0) | e^{iHt} e^{-iH_0 t} (e^{iH_0 t} \hat{A} e^{-iH_0 t}) e^{iH_0 t} e^{-iHt} | \psi(0) \rangle \quad (3.16)$$



Now identify:

$$\begin{aligned}\hat{A}_I(t) &= e^{iH_0t}\hat{A}e^{-iH_0t} \\ |\psi(t)\rangle_I &= e^{iH_0t}e^{-iHt}|\psi(0)\rangle\end{aligned}\tag{3.17}$$

where the index  $I$  just reminds us that we are in the interaction representation. We see that, in this representation, the operators evolve in time as in the Heisenberg picture. But there is a slight difference: they evolve in time under a non-interacting hamiltonian (compare with equation (3.6)). Since now the states depend on time, we can calculate the variation in time to set up an analog of Schrodinger's equation in this picture. The result is left as an exercise at the end of the chapter, and gives:

$$\partial_t|\psi(t)\rangle_I = -i\hat{V}(t)|\psi(t)\rangle_I\tag{3.18}$$

where the operator  $\hat{V}(t)$  is defined as in (3.17). We see that, within this picture, the many-body states evolve only under the action of interactions, that is, interactions are responsible of the dynamics of the states.

Another great advantage is that, when dealing with operators, these evolve *free*, since according to (3.7), the dynamics would be governed by  $H_0$  in this case. Thus, if an operator commutes with the *non-interacting* part of the hamiltonian, that operator will be a conserved quantity in the interaction representation.

The interaction representation is very useful to establish a perturbation theory consistent with the many-body formalism. Our next subsection will just give brief tips about how perturbation theory works in many-body physics. For an extended version and detailed treatment, I refer the reader to G.Mahan, "*Many Particle Physics*", an excellent reference book for many body theory.

### 3.3 Many Body Perturbation Theory

There is an extensive and detailed way of introducing perturbation theory for many body systems (G.Mahan) that we won't enter here. Instead, we will focus on the main expressions and the meaning of building up such a technique, and why we may find it useful.

First of all, we have seen that there are three pictures of quantum mechanics. We can deduce now why the interaction picture provides a better way to work

out a perturbation theory: Since the operators only depend on  $H_0$ , their evolution is only given by the non-interacting part of the hamiltonian. Knowing that, we can act with that operators over the **non-interacting** states to build up terms higher and higher in perturbation. The recipe is the same as with ordinary perturbation theory, the difference lays in the many-body aspects of the problem.

How can we define the interacting ground state of a system? This question is answered in a theorem derived by Gell-Mann and Low, which states that the ground state of an interacting system is related to the non-interacting ground state by:

$$|\Psi(0)\rangle = S(0, -\infty)|\phi_0\rangle \quad (3.19)$$

Here,  $|\phi_0\rangle$  denotes the non-interacting ground state of the system, and  $S(0, -\infty)$  is an operator (called the  $S$  matrix), that drives the state to the interacting ground state at zero time  $|\Psi(0)\rangle$ .

There is an important comment to do here. This theorem only applies if interactions in the system are switched on *adiabatically* (remember the Landau-Fermi liquid theory), that is, in a sufficiently smooth way. Also, it only relates the zero temperature ground states.

What is the operator  $S$ ? It remind us a bit the operator  $e^{-iHt}$  we found previously in (3.4). It is not the same, but there exists some relationship between them. Consider the Schrodinger equation (3.18). Its solution can be expressed as:

$$|\psi(t)\rangle_I = \hat{U}(t)|\psi(0)\rangle_I \quad (3.20)$$

where we define:

$$\hat{U}(t) = T e^{-i \int_0^t dt_1 \hat{V}(t_1)} \quad (3.21)$$

This is a very poor way of deriving this operator, which in fact can be identified from (3.17) as:

$$\hat{U}(t) = e^{iH_0 t} e^{-iHt} \quad (3.22)$$

The equivalence of both expressions is derived in detail in Mahan. The appearance of the *time ordering* operator  $T$  comes out directly from the proof, and we

have seen previously the definition of that operator when we discussed Green functions. There are some nice properties about this operator. One of them is that it is unitary:

$$\hat{U}^\dagger(t)\hat{U}(t) = I \quad (3.23)$$

With that operator, we can define another called the  $S$  matrix:

$$S(t, t') = U(t)U^\dagger(t') \quad (3.24)$$

Then, this operator can be defined as:

$$S(t, t') = T e^{-i \int_{t'}^t dt_1 \hat{V}(t_1)} \quad (3.25)$$

This operator is in fact the one appearing in the theorem we described above. The  $S$  matrix operator evolves the state from two different times  $t'$  and  $t$ , whereas the time ordering operator  $T$  ensures correct order in the expression.

We can then define the operator in the far away past and far away future:

$$S(+\infty, -\infty) = T e^{-i \int_{-\infty}^{+\infty} dt_1 \hat{V}(t_1)} \quad (3.26)$$

which admits a series expansion characteristic of the exponential:

$$S(+\infty, -\infty) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{+\infty} dt_1 \dots \int_{-\infty}^{+\infty} dt_n \hat{T} \hat{V}(t_1) \dots \hat{V}(t_n) \quad (3.27)$$

This is in fact the important term appearing in perturbation theory in QFT. It can be proved (Mahan) how the following expression is found for the single particle Green function:

$$G(k, k', t, t') = -i \frac{{}_0\langle \hat{T} c_k(t) c_{k'}^\dagger(t') S(+\infty, -\infty) \rangle_0}{{}_0\langle \hat{T} S(+\infty, -\infty) \rangle_0} \quad (3.28)$$

The derivation of the expression is not as important as its understanding. Both numerator and denominator are taken in average respect to the non interacting ground state (as expected since it is the only thing we know before doing

perturbation theory). The  $S$  matrix can be expressed in series as in (3.27), therefore, the  $n^{\text{th}}$  term of the series represents the  $n^{\text{th}}$  order of perturbation. Also, in this expression, all operators are in the **interaction picture**, which means that they evolve freely with the non-interacting hamiltonian.

We will say here that the denominator is not important at all. In fact, it turns out that it cancels with some parts of the numerator<sup>27</sup>.

The best way to understand how this works is with an example. We come back to our known case of a non-interacting gas of fermions. Lets consider the interacting term in (2.17) as a perturbation. We know that the non-interacting ground state for this system is the Fermi sea, where all energy states below the Fermi level are occupied. Lets also forget about the spin index since the interaction doesn't depend on the spin.

The zeroth order of perturbation doesn't contain any interacting term, and therefore, for the single particle Green's function is just the non interacting part:

$$G_0(k, t) = -i \langle FS | T c_k(t) c_k^\dagger(0) | FS \rangle \quad (3.29)$$

We have directly changed the momentum to be only  $k$  since we know it has to be conserved, and time runs from 0 to  $t$ . All is known here, as this expression has been derived in the previous section.

Lets compute the first order term. From the expansion of the  $S$  matrix, this reads:

$$G^{(1)} = -i \sum_{q, k_1, k_2} (-i)V(q) \int_{-\infty}^{+\infty} dt_1 \langle FS | T c_k(t) c_{k_1+q}^\dagger(t_1) c_{k_2-q}^\dagger(t_1) \dots c_{k_1}(t_1) c_{k_2}(t_2) c_{k'}^\dagger(0) | FS \rangle \quad (3.30)$$

The issue here is to evaluate the bracket:

$$\langle FS | T c_k(t) c_{k_1+q}^\dagger(t_1) c_{k_2-q}^\dagger(t_1) c_{k_1}(t_1) c_{k_2}(t_2) c_{k'}^\dagger(0) | FS \rangle \quad (3.31)$$

To do that, there is another theorem that allows us to *split* the bracket into single particle Green functions (the non-interacting ones). It is known as Wick's

---

<sup>27</sup>This is called the *vacuum polarization*, and represents all non-connected diagrams of the expansion. It comes clearer when Feynmann diagrams are introduced, however, we will limit here to practical purposes and we will just omit this term in the following.

theorem: *Within a non-interacting system, the bracket written above is equivalent to the product of non-interacting Green function in all possible ways we can combine them.*

We have three creation and three annihilation operators, so we can divide the bracket in a product of three non-interacting Green functions. If we would have had three creation operators and a different number of annihilation operators, the theorem won't hold and we have to go to the appropriate order where the number of them is the same.

Take the first pairing without moving the operators. That is equivalent according to the theorem to:

$$\langle T c_k(t) c_{k_1+q}^\dagger(t_1) \rangle \langle T c_{k_2-q}^\dagger(t_1) c_{k_1}(t_1) \rangle \langle T c_{k_2}(t_1) c_{k'}^\dagger(0) \rangle \quad (3.32)$$

All averages are taken respect to the non-interacting ground state  $|FS\rangle$ , where only the theorem applies. If we swap the operators of the second bracket, a minus sign appear, so we have:

$$\langle T c_{k_2-q}^\dagger(t_1) c_{k_1}(t_1) \rangle = -\langle T c_{k_1}(t_1) c_{k_2-q}^\dagger(t_1) \rangle \quad (3.33)$$

Remember this can only be done for equal time operators. Momentum has to be conserved in all the brackets, which gives the conditions:

$$k = k_1 + q \quad k_2 - q = k_1 \quad k_2 = k' \quad (3.34)$$

Which is equivalent to say:

$$q = 0 \quad k = k' \quad (3.35)$$

Therefore, we have found the first term:

$$G^{(1)}(k, t) = -V(q=0) \int_{-\infty}^{+\infty} dt_1 \langle T c_k(t) c_k^\dagger(t_1) \rangle \langle T c_k(t_1) c_k^\dagger(t_1) \rangle \langle T c_k(t_1) c_k^\dagger(0) \rangle$$

Looking at the brackets, we see that this is a product of non-interacting Green functions, which are already known. The Green function evaluated at equal time:

$$G(t, 0^-) = -i \langle c_k^\dagger(t_1) c_k(t_1) \rangle = -i\theta(k_F - k) \quad (3.36)$$

removes the ambiguity by taking the normal order of the operators, so the result is the occupation factor or number operator  $n_k$ , which can be expressed as a step function for values of  $k \leq k_F$ .

The meaning of the above equation is the following: An intergration over intermediate times is performed to calculate the first order correction. What we are integrating is the probability amplitude of the particle with momentum  $k$  propagating towards time  $t$  from the origin of time. Our expression can be written:

$$G^{(1)}(k, t) = -V(q=0) \int_{-\infty}^{+\infty} dt_1 (i)^3 G_0(k, t-t_1) G_0(k, 0^-) G_0(k, t_1) \quad (3.37)$$

The  $i^3 = -i$  factor comes from the definition of the Green functions. In most cases, this expression is more useful if we Fourier transform it to frequency (energy) space:

$$G(k, \omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} G(k, t) \quad (3.38)$$

In this representation, the Green function is, in first order of perturbation:

$$G^{(1)}(k, \omega) = iV(q=0)\theta(k_F - k)G_0^2(k, \omega) \quad (3.39)$$

We have to say something about the term calculated here. Although being finite, it is of no interest, since the  $q=0$  case corresponds to the case where there is no momentum exchange. In other words, there is no direct interaction of the particle at later times. In terms of *Feynmann diagrams*, that means that this term of interaction is represented by a either non-connected diagram or a connected one but with zero contribution to the energy of the particle propagating.

It is time now to say another thing about the perturbation technique. In momentum-energy representation, as we have above, there exists an equation which gives the exact result for  $G$ , the total Green function of the interacting system. This is Dyson's equation:

$$G(k, \omega) = G_0(k, \omega) + G_0(k, \omega)\Sigma(k, \omega)G(k, \omega) \quad (3.40)$$

The quantity  $\Sigma$  is the *self-energy*, and it is unknown in principle. In fact, it is the only difficulty found in the expression, since the  $G_0$  are known from the

non-interacting case. One has to be careful with the order of terms in the above expression, since sometimes  $G, \Sigma$  and  $G_0$  are represented by matrices. The important bit here is to understand this equation: the self-energy is a quantity that can be calculated at any order of perturbation, that is:

$$\Sigma(k, \omega) = \Sigma(k, \omega)^{(1)} + \Sigma(k, \omega)^{(2)} + \dots + \Sigma(k, \omega)^{(n)} + \dots \quad (3.41)$$

So, at any order of perturbation, we can add more and more terms to the total self-energy.<sup>28</sup> We are starting to see that further comprehension of these concepts requires the introduction of Feynmann diagrams. That is something we will talk about in the next section.

### 3.4 Feynman diagrams: The world of interactions in pictures

One of the central techniques in quantum field theory is based on calculating how particles interact with each other on a microscopic level. The way these particles interact is the central aim of Feynmann diagrams, developed by the outstanding american physicist. He noticed that these fundamental interactions between particles could be represented by graphs or diagrams, were interactions are driven by particles like phonons, photons, gluons etc... depending on the problem in question.

The true power of using these diagrams is that they serve as a useful representation for perturbative methods like the ones described before. Each term of perturbation theory can be described by Feynmann diagrams. Concretely, for the non-interacting single particle Green's function, we represent the diagram as a single straight line, with momentum  $k$  and energy  $\omega$ . We remember that, for translationally invariant systems, **momentum has to be conserved**, and for time invariant systems, energy is conserved too.

To take a look at this Feynman diagrams technique, and to get introduced into them, please go to **THE ONLINE VIDEO ON FEYNMAN DIAGRAMS**.

---

<sup>28</sup>That doesn't mean in principle that we can solve the problem *exactly*. In fact, perturbation theory is only justified for small values of the coupling constant, where the interacting part is much smaller than the non-interacting part. However, there are some cases where this perturbative methods break down (which means the theory is *non-renormalizable*), giving rise to divergences in the terms. In that cases, an alternative route to solve the problem might be tried.

### 3.5 Exercises

1) Derive equation (3.18).

2) Using Wick's theorem, we have evaluated one of the terms of first order of perturbation. The term we derived is known as the *Hartree* term. By making the other possible pairing of operators, find the other term appearing in first order of perturbation, known as the *Fock* term. What is the value of  $q$  here?

3) *Non-connected contributions*: In the two possible pairings we have done before, we have missed more possibilities. Try to find them out and understand them in terms of Feynmann diagrams (next section). Convince yourself that this diagrams are not connected and therefore, don't contribute to Dyson's equation.



## 4 Some important impurity models

Impurity models are important in many body physics: their understanding took a lot of effort, and some of them remained unsolved for long time. Here we present two of the most important impurity problems: The Anderson model and the Kondo model. We will say that both are related to each other under certain limits of the parameters involved.<sup>29</sup>

### 4.1 The Anderson Model

The Anderson model appears as an explanation about why some metals develop a Curie susceptibility, that is:

$$\chi = A + \frac{B}{T} \quad (4.1)$$

This is different of what is found in most of metals: A Pauli magnetic susceptibility is found in a metal, where there is no  $T$  dependence and therefore,  $\chi = A$  in a metal (constant). The second term of (4.1) becomes important at low temperatures, and it is an indication that a localized magnet (single spin) has appeared in the material.

However, there was something not considered here: If there is an impurity of energy  $\varepsilon_0$ , there is no way to form a localized magnetic moment. Suppose  $\varepsilon_0 > \varepsilon_F$  (the Fermi energy): then the minimum energy (ground state) for the system should leave the impurity level empty. Therefore, in this case no local magnetic moment forms in the system.

For the case when  $\varepsilon_0 < \varepsilon_F$ , the minimum energy state will put two electrons in the impurity level. However, we know that the wavefunction there has to be antisymmetric. Since the spatial part is symmetric for a  $d$  orbital, it is the spin part the one who has to be antisymmetric:

$$|\Phi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (4.2)$$

therefore the impurity forms a singlet, so that the total spin is 0. In either case, it looks like a single impurity embedded in the material doesn't develop a Curie term in the susceptibility, that is, the impurity is always non-magnetic. The part missed here is that the double occupancy from the impurity also contains a Coulomb interaction  $U$  between electrons. This was first realised by Anderson,

---

<sup>29</sup>This was shown by Schrieffer and Wolff in a paper in 1966

and the model:

$$H = \sum_{k\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \varepsilon_0 d^\dagger d + \sum_{k,\sigma} V_k (c_{k,\sigma}^\dagger d + \text{h.c.}) + U n_{d,\uparrow} n_{d,\downarrow} \quad (4.3)$$

is known as the Anderson model. This model describes the interaction of surrounding electrons with an impurity site. When this impurity site is doubly occupied, there is a cost in energy  $U$ , since electrons in the impurity interact via Coulomb interactions. The term with  $V_k$  is known as the *hybridization* term. It allows *jumps* from the conduction band to the impurity, so that we remove one electron in the band ( $c_k$ ) to create it in the impurity ( $d^\dagger$ ), and the opposite (the h.c part represents the *hermitian conjugate*, which in this case is  $d^\dagger c_{k,\sigma}$ ). Usually, the parameter  $V_k$  can be considered as independent of momentum. This model is closely related to the Kondo problem, which will be introduced in the next part.

The relevant energy scale of the problem is described by the hybridization function:

$$\Delta(\omega) = \pi \sum_k V_k^2 \delta(\omega - \varepsilon_k) \quad (4.4)$$

For most calculations, the hopping parameter can be considered independent of  $k$ , and the density of states is approximated by a constant value at the Fermi level. Then we have  $\Delta = \pi \rho(\varepsilon_F) V^2$ . In the single impurity limit (that is, when the impurity can only be singly occupied), this function describes the broadening of the spectral function (density of states), described as a Lorentzian<sup>30</sup>:

$$\rho(\omega) = \frac{1}{\pi} \frac{\Delta}{\omega^2 + \Delta^2} \quad (4.5)$$

Due to the hybridization of electrons of the impurity with the conduction electrons, the density of states for the impurity broadens (there are more states available with energies ranging from  $[-\Delta, +\Delta]$ ).

## 4.2 The Kondo Model

We can ask ourselves what happens when we take the impurity of the Anderson model  $\varepsilon_0$  so high in energy that a double or empty state is unlikely to happen. In this case, the impurity can be only occupied with spin up or down. This is

---

<sup>30</sup>This is only in the single impurity limit, that is, when there is no interaction  $U$  present in the model.

the definition of a *localised magnet*. Therefore, the impurity becomes magnetic, with spin 1/2. However, is it that simple? What is the hamiltonian describing such a situation?

If we bring the impurity far enough from the Fermi sea, this localization happens, and the double and single states are now part of the *high-energy* manifold of the hamiltonian. On the other hand, the low energy manifold will be described by the up or down state in the impurity. We can't also forget about the conduction electrons surrounding the impurity. In fact, it is the *hybridization* term of equation (4.3) the one that allows a change from the impurity to the conduction sea, and viceversa. An effective **low energy** hamiltonian must then derive in order to account virtual processes, where particles from the impurity can virtually leave the state, to flip the spin state later or remain the same, by interaction with one electron of the bath. Schematically, we allow processes like:

$$\begin{aligned} |\uparrow\rangle &\rightarrow |0\rangle \rightarrow |\downarrow\rangle \\ |\uparrow\rangle &\rightarrow |\uparrow\downarrow\rangle \rightarrow |\uparrow\rangle \end{aligned} \quad (4.6)$$

Therefore, the high-energy manifold is always visited during these virtual processes. The aim is to transform the Anderson hamiltonian by using a canonical transformation:

$$e^{-S} \hat{H}_A e^S = \hat{H}_K \quad (4.7)$$

where  $\hat{H}_K$  is the low energy effective hamiltonian, taking into account processes like (4.4). The whole procedure can be followed through a paper in 1969 by Schrieffer and Wolff, and the transformation is known as the Schrieffer-Wolff transformation. The resulting hamiltonian is the **Kondo hamiltonian**:

$$H_K = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \sum_{k,k',\sigma\tau} c_{k\sigma}^\dagger c_{k'\tau} \vec{\sigma}_{\sigma,\tau}(0) \cdot \vec{S} \quad (4.8)$$

Here,  $\vec{S}$  represents the impurity spin operator, and  $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$  are the Pauli sigma matrices.  $J > 0$  is the coupling, proved to be antiferromagnetic by the transformation. The analysis of the Kondo problem will require long treatment (and of course, much more knowledge from myself!). The subject has lived for years, and has also occupied whole books topics<sup>31</sup>. We will limit ourselves here to explain that this hamiltonian has caught attention from the theoretical point of view, but intimately close to some experimental facts.

---

<sup>31</sup>see A.C.Hewson: *The Kondo problem to heavy fermions*

The first evidence of the role of magnetic impurities in metals was shown experimentally, when a drop to a minimum in the resistivity of some metals was found without any explanation. It was the hamiltonian (4.6), first proposed by Kondo, the one expected to explain this behaviour. Kondo showed that a third order of perturbation term was necessary to explain such an effect. However, this term contained a singularity:

$$\rho^{(3)} \sim J^3 \log\left(\frac{T}{T_k}\right) \quad (4.9)$$

For temperatures much smaller than  $T_k$ , the theory apparently breaks down, since the term diverges at zero temperature. This mysterious logarithm remained for over a decade without a good understanding, until Anderson, and later Wilson, will start to develop methods of *scaling* in the theory, which will lead later to the Renormalization Group technique. An exact solution of the model was found in the 80's by Wiegman. However, the Kondo problem is today still a corner stone to understand many-body impurity problems, when sometimes a direct way of tackling them passes by finding an analogy with the hamiltonian (4.6).

## 5 References

Here are some of the many good references that you can find for a deeper insight into the subject:

- Gerald D.Mahan: *Many-particle physics* is an excellent book for the subject, very complete and focused in Green functions formalism and Feynman diagrams. The many-body bible.
- Fetter and Walecka: *Quantum Theory of many-particle systems* A very nice book and complete for the many-body theory, with different applications in different chapters. Not suitable for quantum impurity problems.
- Piers Coleman: *Introduction to many-body physics*: An excellent reference with a good insight into the underlying physics of the many-body problem, good to study Renormalization Group concepts.
- Sam T. Carr: *Quantum Field Theory II: Introduction to Feynman diagrams*: Excellent lecture notes about Feynman diagrams and the connection with the theory of Green functions, focused on the Fermi liquid case.
- Alexander Altland and Ben Simons: *Condensed Matter Field Theory*: More oriented to the field theoretic approach (Feynman path integrals, bosonization...), but very nice to study condensed matter field theory, and with good solved exercises at the end of each chapter.