Concepts in Quantum Many-Body Theories

Giampaolo Co'

Dipartimento di Matematica e Fisica, "Ennio De Giorgi"
Università del Salento
and
INFN, Sezione di Lecce

Foreword

These notes are conceived to present the problem of describing many-body systems in Quantum Mechanics. The public to which these notes are addressed is that of the graduate students of the Physics course. I give for granted a basic knowledge of non-relativistic Quantum Mechanics and its simple applications such as the solution of the Schrödinger equation of a particle in a potential, the quantization of the angular momenta and the rules to sum them, the treatment of the identical particles, their classification in fermions and bosons, and the related quantum statistics.

Many of the calculations are presented with a certain detail in order to allow the reader to verify the results and to show how to apply techniques acquired in the basic mathematics and physics courses in the undergraduate studies.

Despite the formal aspect of the presentation, no ambition of mathematical rigor is attempted in the proofs, in particular, questions of convergence have been treated very lightly. In this presentation I have been more interested in clarifying the physics behind the heavy mathematical apparatus than in the mathematical rigor. I excuse myself in advance for these gaps.

The attention is focused to the description of the various many-body theories, while I limited the presentation of the results of the applications to realistic cases. This because these last ones are in continuous evolution and they are better acquired by consulting updated review articles. On the contrary, the formulation of the theories is, now, well grounded and can be the subject of a handbook presentation.

Few words on the notation adopted. The operators are identified with a hat to distinguish them from the functions. This rules is not adopted when the form of the operator is made explicit, for example when it written as product or sum of derivatives. We use a relatively small number of acronyms whose meanings are listed in Table E of the Appendix. The symbols which maintain the same meaning all through the notes are listed in Table F of the Appendix.

Giampaolo Co'
Lecce Sept. 2022

Contents

Chapter 1

Defining the many-body problem

The modern description that physicists gives of the universe reduces every natural phenomenon to the interaction of six leptons and six quarks mediated by four fundamental interactions: gravitation, electromagnetic, strong and weak nuclear forces. This picture, so concise and powerful, is the result of studies inspired to the most extreme reductionism: the understanding of a complex system goes through the identification of its components and of their interactions. Decomposing a complex system in its parts is a much simpler task than that of reconstructing, or building from scratch, the system starting from its components.

This last job is the goal of the many-body theories. The necessary preconditions to carry out this work are:
a) definition of the theoretical framework,
b) choice of the fundamental degrees of freedom, or in other words the basic components of the system,
c) definition of their interaction.
These preconditions are not necessary independent of each other.

The theoretical framework can be, for example, that of the Classical Physics, of the non-relativistic quantum Mechanics or of the Quantum Field Theory. Evidently, the choice is strictly related to the kind of system under investigation. The description of a planetary system in terms of Quantum Field Theory is not at all convenient. On the other hand, it would be very difficult to use Classical Physics for the description of a barion in terms of quarks and antiquarks. In the present tradition of the physics, when the words many-body theories are used, the speaker refers to theories developed in the framework of non-relativistic Quantum Mechanics. From the pragmatical point of view, this means that the many-body problem consists in solving the Schrödinger equation for a system of identical, and interacting, particles. The validity of the non-relativistic Quantum Mechanics is limited to those microscopic phenomena where the energies into play are much smaller than the rest masses of the components of the system. These are atoms, molecules, quantum liquids, metals, crystals and also atomic nuclei, which we shall call simply nuclei henceforth.

The second precondition requires the definition of the fundamental degrees of freedom, which are, in other words, the particles composing the system. Also in this case, the choice is related to an economy principle in the description of the problem. As it has been already point out, at present, the fundamental bricks of the matter are leptons, quarks, the bosons mediating the four fundamental interactions and the Higgs boson. Even though it is correct from the fundamental point of view, the use of these physical entities to describe every microscopic many-body system is not convenient. For each system it is necessary to identify the physical entities of which it is possible to ignore the internal structure in the description of the many-body system which does not disregard the essential phenomenology. For example, the structure of the nucleus is studied by considering the nucleons, protons and neutrons, as basic degrees of freedom. The description of the liquid helium is carried out by using the helium atoms as fundamental particles.

The third precondition to be defined, the interaction between the basic degrees of freedom, is, clearly, related to the second precondition. The choice of the particle defines what is the interaction to be used, which is not directly one of the four fundamental forces quoted above. The relation between particles and their interaction is the topic of the Chapter 3.

After having chosen theoretical framework, fundamental degrees of freedom and their interaction, the many-body problem is well defined and it is only matter of solving the differential, or better to say the integro-differential, equations which describe the system. In the case of our interest it is matter of solving the many-body Schrödinger equation. Formally, it is a purely technical problem, but, in reality, the problem can be solved without making approximation, only for a limited number of cases. For more general treatments it is necessary to formulate approximations which simplify the problem. The development of these approximations, their validity, the possibility of controlling, and to improve, them at will are the topics of the many-body theories. To make this work it is necessary to investigate deeply the problem, one has to understand the relations between the various theoretical and physical quantities in order to identify what is relevant and, if it possible, to separate it from what is negligible. A problem which, formally, is only technical, leads to the investigation of the physical characteristics of the many-body system in terms of its components.

In the study of the many-body systems of different nature, it comes out the remarkable fact that the interactions between the different particles show some common features, which are analogous for the interaction between nucleons, and between atoms or molecules. For this reason, the approximated techniques aimed to solve the many-body Schrödinger equation are, in fact, independent of the system under study. These techniques are universal in the sense that they can be applied without using other assumptions concerning the system. The only differences are the characteristics of the particles and the interactions which are external inputs of the theories. There is an important discriminating fact in the structure of the particles and this is related to their bosonic or fermionic structure. Apart from this important feature, the theories developed have validity ranges which span on 6 orders of magnitude for what concerns the distances, from the nano to the femto meter, and about 12 orders of magnitudes for what the energy is concerned, from the meV up to the GeV.

There is not a unique way of tackling the many-body problem. In these notes, the variety of approaches are divided in two main groups. The first group is that of the theories inspired to the Quantum Field Theory. The theories of this group are the most commonly used, for both the techniques, but especially for having defined a specific language. The second group is that of the theories inspired to the Statistical Mechanics. The two groups of theories focus their attentions on different aspects of the many-body problem. As usual, studying a problem from different perspectives allows a better understanding the various aspects pointed out with different emphasis by the each specific perspective.

The last part of these notes presents the phenomenological approaches where the physical properties of the particles forming the systems and, consequently, their interactions are modified in order to reformulate the many-body problem in an manner which is technically more easy to solve.

Part I

Basic information

Chapter 2

Mean-field models

2.1 General properties

The mean-field (MF) model is the starting point from where all the many-body theories evolve. This is also the easiest approach to the problem, since it makes an approximation which tranforms the many-body problem in many one-body problems.

In the framework of the non-relativistic Quantum Mechanics, a very general expression of the hamiltonian describing the many-body system is

$$\hat{H} = \sum_{i=1}^{A} \left(-\frac{\hbar^2}{2m_i} \nabla_i^2 + \hat{V}_0(i) \right) + \frac{1}{2} \sum_{i,j=1}^{A} \hat{V}(i,j) + \cdots \ , \tag{2.1}$$

where A is the number of particles, each of them with mass m_i. In the expression (2.1), the term containing the laplacian operator ∇_i^2 represents the kinetic energy, $\hat{V}_0(i)$ is a generic potential acting on each particle, and $\hat{V}(i,j)$ is the interaction between two particles. The dots indicate the presence of more complex terms of the interaction, a point discussed in Chapter 3. These terms are not considered at the moment.

The use of potential terms implies an instantaneous action between the two particles, a concept valid only a non-relativistic framework. Let's consider, for example, the case of the electrons of an atomic system. In this case, the potential term $\hat{V}_0(i)$ of the hamiltonian (2.1) is the electrostatic potential generated by the nucleus

$$\hat{V}_0(i) = -\frac{e^2}{4\pi\epsilon_0} \frac{Z}{r_i} \ , \tag{2.2}$$

where e and ϵ_0 are respectively the unitary charge and the vacuum permittivity, r_i the distance between the position of the electron and that of the nucleus which is at the center of the coordinate system, and Z represents the number of the protons of the nucleus, i.e. the atomic number which, obviously, is the same as the number of electrons. The interaction potential between two electron is

$$\hat{V}(i,j) = \frac{e^2}{4\pi\epsilon_0} \frac{1}{r_{ij}} \ , \tag{2.3}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between the two electrons. Obviously, in the atomic case in the expression (2.1) one has $Z = A$.

In the case of an atomic nucleus, the basic degrees of freedom are the nucleons and in the hamitonian (2.1)

$$\hat{V}_0(i) = 0 \ , \tag{2.4}$$

with $\hat{V}(i,j)$ representing the strong interaction potential between two nucleons.

By adding and subtracting to the expression (2.1) an average potential $\hat{U}(i)$ acting on a single particle at the time we obtain:

$$\hat{H} = \underbrace{\sum_i^A \left(-\frac{\hbar^2}{2m_i}\nabla_i^2 + \hat{V}_0(i) + \hat{U}(i) \right)}_{\hat{H}_0} + \underbrace{\frac{1}{2}\sum_{i,j}^A \hat{V}(i,j) - \sum_i^A \hat{U}(i)}_{\hat{H}_1} \ . \tag{2.5}$$

The term in parenthesis, $\hat{H}_0$, is a sum of terms acting on a single particle, the i-th particle, at the time. I can define each term of this sum as single-particle hamiltonian $\hat{h}(i)$,

$$\hat{H}_0 = \sum_i \hat{h}(i) = \sum_i^A \left(-\frac{\hbar^2}{2m_i}\nabla_i^2 + \hat{V}_0(i) + \hat{U}(i) \right) \ . \tag{2.6}$$

The basic approximation of the mean-field model consists in neglecting in the expression (2.5) the term $\hat{H}_1$ called residual interaction. In this way the many-body problem is transformed in a sum of one-body problems. The model is also called Independent Particle Model (IPM) since the particles described by $\hat{H}_0$ do not interact among them.

The fact that the hamiltonian $\hat{H}_0$ is a sum of independent terms implies that its eigenstates can be built as a product of the eigenstates of $\hat{h}(i)$

$$\hat{h}(i)|\phi_i\rangle = \epsilon_i|\phi_i\rangle \ , \tag{2.7}$$

therefore

$$\hat{H}_0|\Phi\rangle = \left(\sum_i \hat{h}(i) \right) |\Phi\rangle = \mathcal{E}|\Phi\rangle \ , \tag{2.8}$$

where

$$|\Phi\rangle = |\phi_1\rangle|\phi_2\rangle \cdots |\phi_A\rangle \ . \tag{2.9}$$

For fermions, the antisymmetry of the global wave function under the exchange of two particles implies that the wave function $|\Phi\rangle$ has to be described as sum of antisymmetrized products of one-particle wave functions. This solution is known in the literature as Slater determinant [Sla29]

$$|\Phi\rangle = \frac{1}{\sqrt{A!}} \det\{|\phi_i\rangle\} \ . \tag{2.10}$$

The mean-field potential $\hat{U}$ inserted in $\hat{H}_0$ is usually phenomenologically selected. For example, in the many electron atoms $\hat{U}(i)$ is a potential which consider the screening generated by the more internal electrons on the motion of the more external ones. In the case of atomic nuclei the most commonly used expression of $\hat{U}(i)$ are the harmonic oscillator and the Woods-Saxon potential

$$\hat{U}(r) = \frac{-U_0}{1 + \exp(\frac{r-R}{a})} \tag{2.11}$$

where U_0, R and a are real and positive constants whose values are selected with a procedure implying a comparison with empirical data.

In the following we present the solution of the mean field problem for some specific expressions of $\hat{U}$. We consider separately systems with spherical and translational symmetries.

2.2 Spherical symmetry

In the MF model the solution of the many-body problem consists in solving the one-body Schrödinger equation (2.7) for each particle.

Atoms and nuclei are systems which are well described by considering a set of spherical coordinates, and a MF potential which is symmetric with respect rotations of the coordinate system. The spherical symmetry of the potential implies $\hat{U}(\mathbf{r}) = \hat{U}(r)$, where I used $r = |\mathbf{r}|$. It is convenient search for solutions of the one-body Schrödinger equation of the type

$$\phi(\mathbf{r}) = \sum_{n,l,\mu,\sigma} R_{nl}(r) Y_{l\mu}(\Omega)\chi_\sigma \ , \tag{2.12}$$

where n, l, μ, σ are the quantum numbers identifying the various terms of the wave function: n is the principal quantum number, l is the quantum number indicating the orbital angular momentum, μ its projection on the quantization axis and σ the spin projection on this axis. We indicated with $Y_{l\mu}$ the spherical harmonics and with $\Omega \equiv (\theta, \phi)$ the angular part of the polar spherical coordinates. The Pauli spinor of the fermion, electron or nucleon, is indicated as

$$\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ ; \ \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ . \tag{2.13}$$

The techniques used to solve the one-body Schrödinger equation with a spherically symmetric potential are well known, see for example [Mes61]. The Laplace operator is expressed in spherical polar coordinates. In this way it is possible to separate the terms related to r, the distance from the center of coordinates, from those related to the angular coordinates Ω. Eigenstates of the angular part are the spherical harmonics $Y_{l,\mu}(\Omega)$, and the eigenvalues are $l(l+1)\hbar^2$. By inserting these eigenstates and the relative eigenvalues in the in the Schrödinger equation we obtain an expression that, from the operator point of view, depends only on r,

$$\left[\frac{\hat{p}_r^2}{2m} + \frac{l(l+1)\,\hbar^2}{2mr^2} + \hat{U}(r) - \epsilon_{nl}\right] [R_{nl}(r)Y_{l\mu}(\Omega)\chi_\sigma] = 0 \ , \tag{2.14}$$

where the explicit expression of the $\hat{p}_r^2$ operator is

$$\hat{p}_r^2 R_{nl}(r) = -\hbar^2 \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr} R_{nl}(r)\right) = -\hbar^2 \left(\frac{d^2}{dr^2} R_{nl}(r) + \frac{2}{r}\frac{d}{dr} R_{nl}(r)\right) \ . \tag{2.15}$$

By using a potential $\hat{U}$ depending only on r, and not on the particle spin, we obtain the expression

$$\frac{d^2}{dr^2} R_{nl}(r) + \frac{2}{r}\frac{d}{dr} R_{nl}(r) + \left[\frac{2m}{\hbar^2}(\epsilon_{nl} - U(r)) - \frac{l(l+1)}{r^2}\right] R_{nl}(r) = 0 \ . \tag{2.16}$$

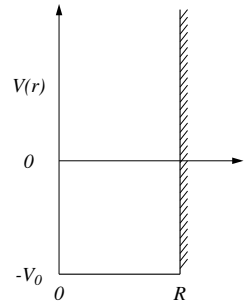

Figure 2.1: Infinite well potential.

This technique, which expands the wave function in spherical harmonics, is useful for every potential depending only on r. The results of its application is the reduction of a three-dimensional differential equation to a one-dimensional differential equation. Only after having obtained the expression (2.16) one has to specify the specific dependence on r of the potential. I consider here below the cases of potentials interesting for the many-body systems which will be considered in the next chapters.

A. Constant Potential

The constant potential is typical of systems having translational symmetry, such as the infinite Fermi gas or the free particle. In these cases

the value of the constant can be set equal to zero. The treatment of this problem by using the spherical symmetry technique outlined above is rather useful since the eigenstates can be used as basis to expand more complex situations.

Let's consider a spherical system whose dimensions are defined by R. The potential is

$$\hat{U}(r) = -V_0 \text{ for } r \leq R \text{ e } \hat{U}(r) = \infty \text{ for } r > R \tag{2.17}$$

as it is shown in Fig. 2.1. The equation (2.16) is defined in the range $0 \leq r \leq R$.

By dividing Eq. (2.16) by k^2 defined as

$$k^2 = \frac{2m}{\hbar^2}(\epsilon_{nl} + V_0) \tag{2.18}$$

we obtain the following equation which depends on the dimensionless variable $\rho = kr$

$$\frac{d^2}{d\rho^2}R_{nl}(\rho) + \frac{2}{\rho}\frac{d}{d\rho}R_{nl}(\rho) + \left[1 - \frac{l(l+1)}{\rho^2}\right]R_{nl}(\rho) = 0 \ . \tag{2.19}$$

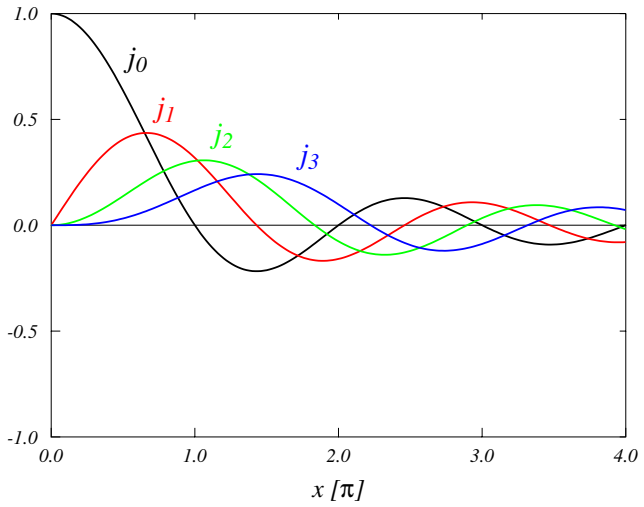

Figure 2.2: The first four spherical Bessel functions.

This differential equation is well known in the literature. Two types of independent solutions are the spherical Bessel functions $j_l(\rho)$, and the spherical Neumann functions $n_l(\rho)$. The former ones are regular at the origin, and the latter ones are irregular. Because of the physical meaning of the wave function, only the spherical Bessel functions must be considered.

The analytical expressions of the first two spherical Bessel functions are

$$j_0(\rho) = \frac{\sin\rho}{\rho} \ ; \ j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \ , \tag{2.20}$$

and, for $l > 0$, the following recurrence relation is valid

$$(2l+1)j_l(\rho) = \rho\left[j_{l+1}(\rho) + j_{l-1}(\rho)\right] \ . \tag{2.21}$$

From the physics point of view, since the potential goes to infinity for $r \geq R$, it is required that j_l is zero at the point $r = R$ and, obviously, for $r > R$. This means $j_l(kR) = j_l(X_{nl}) = 0$, and, because of the definition of k,

$$\frac{2m}{\hbar^2}(\epsilon_{nl} + V_0)R^2 = X_{nl}^2 \ ; \ \epsilon_{nl} = \frac{\hbar^2}{2m}\frac{X_{nl}^2}{R^2} - V_0 \ . \tag{2.22}$$

The zeros of the wave function depend on the principal quantum number n and on the orbital one l. For example, for j_0 the zeros are integer multiple of π. Eq. (2.22) clearly indicates that, in this case, all the eigenvalues are discrete.

B. Three-dimensional Harmonic Oscillator
In this case the potential is

$$\hat{U}(r) = \frac{1}{2}m\omega^2 r^2 \ . \tag{2.23}$$

Since $r^2 = x^2 + y^2 + z^2$ it is possible to solve the problem by rewriting the Schrödinger equation in cartesian coordinates. In this way the differential equation becomes separable in the tree coordinates and the eigenvalues can be built as product of eigenfunctions of one-dimensional Harmonic Oscillator obtained for each of the three coordinates. The eigenvalue is given by the sum of the single eigenvalues in the three directions.

Obviously, the Harmonic Oscillator potential is of central type, therefore it is possible to use the expansion in spherical harmonics. In this case the radial part of the wave function is proportional to the Laguerre polynomials [Mes61]. The energy eigenvalues can be expressed by using the quantum numbers identifying the single particle basis in spherical coordinates (2.12) as

$$\epsilon_{nl} = \hbar\omega\left(N + \frac{3}{2}\right) = \hbar\omega\left(N_x + N_y + N_z + \frac{3}{2}\right) = \hbar\omega\left(2(n-1) + l + \frac{3}{2}\right) \ . \tag{2.24}$$

The first two terms express the eigenvalues in terms of the quantum numbers of the solution obtained in cartesian coordinates, while the last expression uses the quantum numbers of the solution in spherical coordinates. In this latter case, $n - 1$ indicates the number of nodes of the wave function (the minimal value of n is 1), and l is the quantum number related to the orbital angular momentum. The value of the energy depends on N a number which can be obtained by changing both n and l. States with the same energy, even though characterized by different quantum numbers, are called degenerate. A degeneracy is called casual, or accidental, when is produced by a specific choice of the potential and not by global symmetry properties of the problem. A degeneracy of this latter type is related to the μ quantum number of the spherical harmonics, and it is present in all the problems with spherical symmetry.

N	n	l		n	l		Π
0	1	0	$1s$				+1
1	1	1	$1p$				-1
2	2	0	$2s$	1	2	$1d$	+1
3	2	1	$2p$	1	3	$1f$	-1

Table 2.1: Examples of combinations of quantum numbers producing the same energy values for the Harmonic Oscillator potential, Eq. (2.24). The various energy levels are identified with the traditional spectroscopic symbology. The last coloumn indicates the parity of the states obtained as $(-1)^l$.

A list of values of quantum numbers producing the same value of the energy (2.24) is shown in Tab. 2.1. It is evident that the Harmonic Oscillator produces sequences of eigenstates accidentally degenerated. It is interesting to notice that all the states with the same energy have the same parity, whose value changes when the energy eigenvalue is increased by one $\hbar\omega$ step.

C. Coulomb Potential
In the description of an atomic system with many electrons, the mean-field model intervenes when the interaction between electrons is neglected and only the interaction of every electron with the nucleus is considered. Eventually, the potential generated by the nucleus can be corrected by the presence of a mean-field potential describing the screening effect generated by the presence of other electrons. For distances very close to the origin of the coordinates the potential felts by the electron is that generated by the nucleus

$$\lim_{r_i \to 0} \hat{V}_0(i) + \hat{U}(i) = -\frac{e^2}{4\pi\epsilon_0}\frac{Z}{r_i} \ , \tag{2.25}$$

while at distances far from nucleus the electron is sensitive to a potential screened by the presence of N electrons

$$\lim_{r_i \to \infty} \hat{V}_0(i) + \hat{U}(i) = -\frac{e^2}{4\pi\epsilon_0}\frac{Z-(N-1)}{r_i} \ . \tag{2.26}$$

The bare Coulomb potential

$$\hat{V}(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{Z}{r} \ , \tag{2.27}$$

generates eigenvalues of the energy which are independent of l, accidental degeneracy, and of μ, degeneracy produced by the spherical symmetry od the potential

$$\epsilon_n = -\frac{1}{2}mc^2\frac{(Z\alpha)^2}{n^2} \ , \tag{2.28}$$

where α is the fine structure constant

$$\alpha = \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar c} \simeq \frac{1}{137} \ , \tag{2.29}$$

and n is the principal quantum number. For a given value of n the angular momentum quantum number l can assume the values $0, 1, \cdots, n-1$.

	n	l		n	l		n	l	
ϵ_1	1	0	$1s$						
ϵ_2	2	0	$2s$	2	1	$2p$			
ϵ_3	3	0	$3s$	3	1	$3p$	3	2	$3d$

Table 2.2: Level scheme generated by the Coulomb potential. The energies are identified by the quantum number n, therefore there is an accidental degeneracy for different values of l.

In table 2.2 levels with accidental degeneracy are shown. Every level has a degeneracy related to the values of the third component of angular momentum characterized by the quantum number μ which can assume $2l+1$ values. By considering also the fact that the potential does not depend on the direction of the electron spin, the global degeneracy is $2(2l+1)$. On this ground, by considering the Pauli exclusion principle, the periodic table of elements is built.

2.2.1 Spin-orbit potential

At the end of this section dedicated to the solution of the one-body Schrödinger equation with central potentials, we present the treatment related to the presence of a spin-orbit term in the potential. It is now established that the source of the effects generated by the presence of the interaction between orbital angular momentum and the half-integer spin of the fermion whose motion is described by the Schrödinger

equation is the relativity. This fact has always been accepted in atomic physics, but, in nuclear physics, it has been quantitatively understood only at the beginning of the '80s of the last century.

For our purposes, the idea is to describe the spin-orbit effects in the framework of the non-relativistic Quantum Mechanics. We add to one of the spherical potentials presented so far a new term proportional to the spin-orbit coupling

$$\hat{V}(r) = \hat{V}_c(r) - \frac{2\alpha}{\hbar^2}\hat{\mathbf{l}}\cdot\hat{\boldsymbol{\sigma}} \ , \tag{2.30}$$

where α is a real and positive constant. The scalar product between $\hat{\mathbf{l}}$ and the spin $\hat{\mathbf{s}} = \hat{\boldsymbol{\sigma}}/2$ is due the fact that the hamiltonian is a scalar operator, and this is the simplest type of coupling between the two vector operators describing the orbital angular momentum and the spin.

The presence of a spin-dependent term in the hamiltonian requires a change in the procedure used to solve the Schrödinger equation. We used so far an expansion of the wave functions (2.12) in terms of the spherical harmonics, eigenstates of the $\hat{\mathbf{l}}^2$ operator present in the hamiltonian. The Pauli spinors χ, eigenstates of $\hat{\mathbf{s}}^2$, were factorised. So far, the presence of these latter terms was irrelevant since the potentials adopted did not contain terms dependent on the spin. The present situation is more complicated due to the presence of a spin-dependent term in the hamiltonian.

Let's considers the total angular momentum of the fermion obtained as a sum of the orbital angular momentum and of the spin $\hat{\mathbf{j}} = \hat{\mathbf{l}} + \hat{\mathbf{s}}$. This definition implies

$$\hat{\mathbf{j}}^2 = (\mathbf{l}+\mathbf{s})^2 = \mathbf{l}^2 + \mathbf{s}^2 + 2\mathbf{l}\cdot\mathbf{s} \ , \tag{2.31}$$

from which one obtains an expression for $\hat{\mathbf{l}}\cdot\hat{\mathbf{s}}$ depending on the squares of the three angular momenta under consideration

$$\hat{\mathbf{l}}\cdot\hat{\mathbf{s}} = \frac{1}{2}\left(\hat{\mathbf{j}}^2 - \hat{\mathbf{l}}^2 - \hat{\mathbf{s}}^2\right) \ . \tag{2.32}$$

At this point, it is convenient to consider expressions of the eigenfunction of the hamiltonian of the form

$$\phi_{nljm}(\mathbf{r}) = R_{nlj}(r)\sum_{\mu\sigma}\langle l\,\mu\,\frac{1}{2}\,\sigma|j\,m\rangle Y_{l\mu}(\Omega)\chi_\sigma = R_{nlj}(r)\mathcal{Y}_{ljm}(\Omega) \ , \tag{2.33}$$

where spherical harmonics and Pauli spinors are connected by the Clebsch-Gordan coefficients and form the so-called the spin spherical harmonics [Edm57] which are eigenstates of the following operators

$$\hat{\mathbf{j}}^2\mathcal{Y}_{ljm}(\Omega) = j(j+1)\,\hbar^2\,\mathcal{Y}_{ljm}(\Omega) \quad ; \quad \hat{j}_z\mathcal{Y}_{ljm}(\Omega) = m\,\hbar\,\mathcal{Y}_{ljm}(\Omega) \ , \tag{2.34}$$

$$\hat{\mathbf{l}}^2\mathcal{Y}_{ljm}(\Omega) = l(l+1)\,\hbar^2\,\mathcal{Y}_{ljm}(\Omega) \quad ; \quad \hat{\mathbf{s}}^2\mathcal{Y}_{ljm}(\Omega) = \frac{3}{4}\,\hbar^2\,\mathcal{Y}_{ljm}(\Omega) \ , \tag{2.35}$$

The spin-orbit term inserted in the hamiltonian gives the result

$$\hat{\mathbf{l}}\cdot\hat{\mathbf{s}}\,\mathcal{Y}_{ljm}(\Omega) = \frac{1}{2}\left[\hat{\mathbf{j}}^2 - \hat{\mathbf{l}}^2 - \hat{\mathbf{s}}^2\right]\mathcal{Y}_{ljm}(\Omega) = \frac{1}{2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right]\hbar^2\mathcal{Y}_{ljm}(\Omega) \ , \tag{2.36}$$

and since $j = l \pm 1/2$ we obtain

$$\begin{aligned} &\text{for } \ j = l + \frac{1}{2} \qquad \left[(l+\frac{1}{2})(l+\frac{3}{2}) - l^2 - l - \frac{3}{4}\right] = l \\ &\text{for } \ j = l - \frac{1}{2} \qquad \left[(l-\frac{1}{2})(l+\frac{1}{2}) - l^2 - l - \frac{3}{4}\right] = -(l+1) \ , \end{aligned} \tag{2.37}$$

This means that ϵ^c_{nl}, the energy obtained by considering only the term $\hat{V}_c$ in Eq. (2.30), is modified as

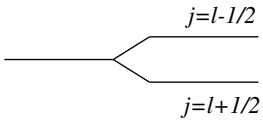

Figure 2.3: Splitting of the single particle level because of the action of the spin-orbit term in the potential.

$$\begin{aligned} \epsilon_{nlj} &= \epsilon^c_{nl} + \alpha(l+1) \text{ for } j = l - \frac{1}{2} \\ \epsilon_{nlj} &= \epsilon^c_{nl} - \alpha l \text{ for } j = l + \frac{1}{2} \end{aligned} \tag{2.38}$$

In Eq. (2.30) I defined the constants such as for $\alpha > 0$ the energy with $l - 1/2$ is smaller than ϵ^c_{nl}, and the contrary for $l + 1/2$. This is what happens in nuclear physics. In atomic physics the effect of the spin-orbit term is inverted.

2.3 Translational symmetry

Barions, nuclei, atoms and molecules are many-body systems well described by using a rotational symmetry. In these systems, even though they are deformed, it is possible to find a point around which the system develop and this can be considered the center of the mean-field. In the condensed matter conglomerates the translational symmetry dominates. A basic structure of the system is periodically repeated in three cartesian directions and it is not possible to find a central point.

The basic mean-field model for this type of systems consider the potential $\hat{U}$ to be constant. This fermionic system is commonly called *Fermi gas*. It is a toy model, homogeneous, with infinite volume, composed by an infinite number of fermions which do not interact with each other. Since the energy scale is arbitrary, it possibile to select $\hat{U} = 0$, without loosing generality. In this case, the one-body Schrödinger equation is

$$-\frac{\hbar^2}{2m_i}\nabla^2_i \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}) \ , \tag{2.39}$$

with

$$\phi_i(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}}\, e^{i(\mathbf{k}_i \cdot \mathbf{r})} \chi_\sigma \chi_\tau \ , \tag{2.40}$$

where $\mathcal{V}$ is the volume, and χ are the Pauli spinors related to the spin of the fermion and, eventually, to its isospin. The third components of spin and isopin are indicated as σ e τ, respectively. The physical quantities of interest are those independent of $\mathcal{V}$ whose value, at the of the calculations, is taken to be infinite.

The symmetry of the problem induces to consider the system contained in a cubic box of side $\mathrm{L} = \mathcal{V}^{1/3}$ with periodic boundary conditions

$$\phi_i(x + \mathrm{L}, y, z) = \phi_i(x, y + \mathrm{L}, z) = \phi_i(x, y, z + \mathrm{L}) = \phi_i(x, y, z) \ . \tag{2.41}$$

Since

$$\phi_i(\mathbf{r} = 0) = \frac{1}{\sqrt{\mathcal{V}}} \chi_\sigma \chi_\tau \ , \tag{2.42}$$

in order to satisfy the periodic conditions we have to impose

$$e^{ik_x \mathrm{L}} = e^{ik_y \mathrm{L}} = e^{ik_z \mathrm{L}} = 1 \ , \tag{2.43}$$

and this implies

$$k_x = \frac{2\pi}{\mathrm{L}} n_x \ ; \ k_y = \frac{2\pi}{\mathrm{L}} n_y \ ; \ k_z = \frac{2\pi}{\mathrm{L}} n_z \ , \tag{2.44}$$

where n_x, n_y, n_z are integer numbers. By defining $\mathbf{n} \equiv (n_x, n_y, n_z)$, we can write

$$d^3\,\mathbf{n} = \frac{\mathrm{L}^3}{(2\pi)^3} d^3\,\mathbf{k} = \frac{\mathrm{L}^3}{(2\pi\hbar)^3} d^3\,\mathbf{p} \ . \tag{2.45}$$

The evaluation of the density of states starts by considering the expression of the energy of the systems in a infinitesimally small energy interval, i.e. the energy between the value ϵ and $\epsilon + d\epsilon$. In non-relativistic mechanics, the momentum is related to the wave number by the relation $\mathbf{p} = m\mathbf{v} = \hbar\mathbf{k}$, therefore, $\epsilon = m\mathbf{v}^2/2 = \mathbf{p}^2/2m = \hbar^2\mathbf{k}^2/2m$. The energy differential is

$$d\epsilon = d\left(\frac{1}{2}m\mathbf{v}^2\right) = \frac{1}{2}m\,2\,v dv = v\,m\,dv = v\,dp \ , \tag{2.46}$$

with $v = |\mathbf{v}|$ and $p = |\mathbf{p}|$. The density of states is

$$\rho_\epsilon = \frac{d^3\mathbf{n}}{d\epsilon} = \frac{\mathrm{L}^3}{(2\pi\hbar)^3}\,d^3\mathbf{p}\frac{1}{v\,dp} = \frac{\mathcal{V}}{(2\pi\hbar)^3}\,p^2 d\Omega_p dp\frac{1}{v\,dp} = \frac{\mathcal{V}}{(2\pi\hbar)^3}\frac{p^2}{v}d\Omega_p \ , \tag{2.47}$$

where Ω_p indicates the spherical coordinates identifying the direction of $\mathbf{p}$. This is the expression of the density of states commonly adopted in the calculations of the scattering cross sections.

Let's calculate the density and the kinetic energy per particle of the Fermi gas. The normalization to 1 of the single particle wave functions (2.40) implies that each integral involving wave functions must be multiplied by the factor $\mathcal{V}/(2\pi)^3$. In effect,

$$\langle\phi_a|\phi_b\rangle = \frac{\mathcal{V}}{(2\pi)^3}\int d^3\,r\frac{1}{\sqrt{\mathcal{V}}}\,e^{-i(\mathbf{k}_a\cdot\mathbf{r})}\frac{1}{\sqrt{\mathcal{V}}}\,e^{i(\mathbf{k}_b\cdot\mathbf{r})} = \frac{\mathcal{V}}{(2\pi)^3}\frac{(2\pi)^3\delta(\mathbf{k}_a - \mathbf{k}_b)}{\mathcal{V}} = 1 \ . \tag{2.48}$$

The particle density, or number density, in the Fermi gas can be evaluated as

$$\rho(\mathbf{r}) = \sum_a^A |\phi_a(\mathbf{r})|^2 \ , \tag{2.49}$$

where A is the number of fermions composing the system. This expression is valid only within the the MF model. It can be obtained by calculating the mean value of the density operator between two Slater determinants. A more intuitive way of understanding its validity can be acheived by considering that the interpretation of $|\phi_a(\mathbf{r})|^2$ is the probability of finding a particle, characterized by the a quantum numbers, in an infinitesimal volume around $\mathbf{r}$. In a situation where the individual particles do not interact, the individual probabilities are independent of each other and, therefore, the global probability of finding a particle, independently of its quantum numbers, in the infinitesimal volume around $\mathbf{r}$, is the sum of the individual probabilities.

Each single particle state is characterized by energy and spin and isospin components and it is occupied by a single fermion. At zero temperature, when the system is in its ground state, all the single particle states below a certain value of the energy ϵ_F, called Fermi energy, are occupied. All the states with energy larger than ϵ_F are empty. In our case each state is characterised by a wave number directly related to its energy. The above statements can be repeated by considering a maximum momentum value, called Fermi momentum $\mathbf{p}_\mathrm{F}$, and the relative wave number $\mathbf{k}_\mathrm{F}$. The relation between Fermi energy and wave number is

$$\epsilon_\mathrm{F} = \frac{\hbar^2}{2m}\mathbf{k}_\mathrm{F}^2 \ . \tag{2.50}$$

As consequence of the considerations the particle density is calculated as

$$\rho(\mathbf{r}) = \sum_{a\le k_\mathrm{F}} |\phi_a(\mathbf{r})|^2 = \frac{\mathcal{V}}{(2\pi)^3}\,\mathscr{D}\int_0^{k_\mathrm{F}} d^3\,k\frac{1}{\sqrt{\mathcal{V}}}\,e^{-i(\mathbf{k}\cdot\mathbf{r})}\frac{1}{\sqrt{\mathcal{V}}}\,e^{i(\mathbf{k}\cdot\mathbf{r})} = \frac{\mathscr{D}}{(2\pi)^3}\int_0^{k_\mathrm{F}} d^3\,k \ . \tag{2.51}$$

In this expression $\mathscr{D}$ indicates the degeneracy factor related to the characteristics of the fermions forming the system. In the case of an electron gas, the wave function of each particle is characterised by its

momentum and by the orientation of the spin. In the case of nuclear matter there is an additional quantum number related to the third component of the isospin distinguishing protons from neutrons. Therefore, for electrons we have

$$\mathcal{D} = \sum_{\sigma=\pm 1/2} \chi_\sigma^\dagger \chi_\sigma = 2 \ , \tag{2.52}$$

and for the nucleons

$$\mathcal{D} = \sum_{\sigma=\pm 1/2} \chi_\sigma^\dagger \chi_\sigma \sum_{\tau=\pm 1/2} \chi_\tau^\dagger \chi_\tau = 4 \ , \tag{2.53}$$

The integral of Eq. (2.51) is given by

$$\rho(\mathbf{r}) = \frac{\mathcal{D}}{(2\pi)^3} \int_0^{k_{\rm F}} d^3\, k = \frac{\mathcal{D}}{(2\pi)^3} \int_0^{k_{\rm F}} k^2 dk \int d\,\Omega_k = \frac{\mathcal{D}}{(2\pi)^3}\, \frac{4}{3}\pi k_{\rm F}^3 = \frac{\mathcal{D}}{2\pi^2}\, \frac{k_{\rm F}^3}{3} \ . \tag{2.54}$$

The density is independent of $\mathbf{r}$, as expected, since we have considered that the system is homogeneous. In other words, since we have chosen the plane waves (2.39) as single particle basis, the homogeneity of the system is implicit. More interesting it is the dependence of the particle density on the third power of the Fermi momentum.

Let's calculate the mean kinetic energy of one particle

$$\langle \phi_{a'} | \frac{-\hbar^2}{2m} \nabla^2 | \phi_a \rangle = \frac{\mathcal{V}}{(2\pi)^3} \int d^3\, r \frac{1}{\sqrt{\mathcal{V}}}\, e^{-i(\mathbf{k}_{a'}\cdot\mathbf{r})} \left(\frac{-\hbar^2}{2m} \nabla^2 \right) \frac{1}{\sqrt{\mathcal{V}}}\, e^{i(\mathbf{k}_a\cdot\mathbf{r})} = \frac{\hbar^2 k_a^2}{2m} \ , \tag{2.55}$$

This expression confirms the validity of the non-relativistic relation between energy and momentum $\epsilon_a = p_a^2/2m$. The total kinetic energy of the system is

$$\begin{aligned} \mathcal{K} &= \sum_{k\le k_{\rm F}} \langle \phi_a | \frac{-\hbar^2}{2m} \nabla^2 | \phi_a \rangle = \mathcal{D} \frac{\mathcal{V}}{(2\pi)^3} \int_0^{k_{\rm F}} d^3\, k\, \frac{\hbar^2 k^2}{2m} = \mathcal{D} \frac{\mathcal{V}}{(2\pi)^3}\, \frac{\hbar^2}{2m}\, 4\pi \int_0^{k_{\rm F}} k^2\, k^2\, dk \\ &= \mathcal{D} \frac{\mathcal{V}}{(2\pi)^3}\, \frac{\hbar^2 4\pi}{2m}\, \frac{k_{\rm F}^5}{5} = \mathcal{D} \frac{\mathcal{V}}{(2\pi)^3}\, \frac{\hbar^2 4\pi}{2m}\, \frac{k_{\rm F}^2}{5} \left(\frac{2\pi^2 3\rho}{\mathcal{D}} \right) = \frac{3}{5} \mathcal{V} \rho \frac{\hbar^2 k_{\rm F}^2}{2m} = \frac{3}{5} A \epsilon_{\rm F} \ , \end{aligned} \tag{2.56}$$

therefore, the kinetic energy per particle is

$$\frac{\mathcal{K}}{A} = \frac{3}{5} \epsilon_{\rm F} \ . \tag{2.57}$$

	ρ [10^{22} cm^{-3}]	$k_{\rm F}$ [10^8 cm^{-1}]	$\epsilon_{\rm F}$ [eV]	B [dyne / cm^2]	$B_{\rm exp}$ [dyne/ cm^2]
Li	4.70	1.11	4.75	23.84	11.5
Na	2.65	0.92	3.24	9.17	6.42
K	1.40	0.75	2.12	3.17	2.81
Rb	1.15	0.70	1.86	2.28	1.92
Cs	0.91	0.65	1.59	1.54	1.43
Cu	8.45	1.36	7.02	63.37	134.3
Ag	5.85	1.20	5.50	34.34	99.9
Al	18.06	1.75	11.65	224.74	76.0

Table 2.3: The electron densities are empirical data used to obtain the values of $k_{\rm F}$, Eq. (2.54), $\epsilon_{\rm F}$, Eq. (2.50), and B, Eq. (2.60). This latter quantity is compared with measured values $B_{\rm exp}$. The empirical data are taken from Refs. [Ash76, Kit86].

Let's calculate the system pressure by considering that the total energy of a Fermi gas is given by the kinetic energy, the potential $\hat{U}$ is a constant renormalizing the total value,

$$E = \mathcal{K} = \frac{3}{5} A \epsilon_{\rm F} = \frac{3}{5} A \frac{\hbar^2 k_{\rm F}^2}{2m} = \frac{3}{5} A \frac{\hbar^2}{2m} \left(\frac{2\pi^2 3}{\mathcal{D}} \frac{A}{\mathcal{V}} \right)^{2/3} = \mathcal{S}\ \mathcal{V}^{-2/3} \ , \tag{2.58}$$

where we have identified with $\mathcal{S}$ the part multiplying the volume $\mathcal{V}$. The pressure can be expressed as

$$P = -\left(\frac{\partial E}{\partial \mathcal{V}} \right)_A = -\mathcal{S}\ \left(-\frac{2}{3} \right) \mathcal{V}^{-2/3} \mathcal{V}^{-1} = \frac{2}{3} \frac{E}{\mathcal{V}} = \frac{2}{3} \frac{1}{\mathcal{V}} \frac{3}{5} A \epsilon_{\rm F} = \frac{2}{5} \epsilon_{\rm F} \rho \tag{2.59}$$

The compressibility K is the inverse of the compression module B whose expression in the Fermi gas is

$$B = \frac{1}{K} = -\mathcal{V} \frac{\partial P}{\partial \mathcal{V}} = -\mathcal{V}\ \frac{2}{3}\ \mathcal{S}\ \mathcal{V}^{-5/3} \left(\frac{-5}{3} \right) \mathcal{V}^{-1} = \frac{10}{9} \frac{E}{\mathcal{V}} = \frac{2}{3} \epsilon_{\rm F} \rho \tag{2.60}$$

In Table 2.3 shows the values of $k_{\rm F}$, $\epsilon_{\rm F}$ and B calculated for the electron gases of different crystals. These results have been obtained by inserting in the equations (2.54) (2.50) e (2.60) empirical values of the electron densities. The comparison with measured values of the compression module clearly shows the limits of the mean-field model.

The MF models, or even better the IPM, provide a description of the many-body systems where each particle moves independently of the presence of the other particles. This fact is particularly evident in the case of translationally invariant systems where the total hamiltonian is the sum of hamiltonians describing the free particle motion Eq. (2.39). In this simple model is, however, inserted a physics ingredient which limits the free particle motion: the Pauli exclusion principle. This is enough to explain some phenomena appearing at macroscopic level. For example, the stability of a white dwarf star is understood in terms of Fermi gas model. We discuss here below another example: the case of the specific heat in metals.

The classical, non quantum, description of a gas of A pointlike non-interacting particles predicts for the specific heat the value $\frac{3}{2} A {\rm k_B}$, where $\rm k_B$ is the Boltzman constant [Kit80]. The measured values of the electronic contribution to the specific heat at room temperature are hundred times smaller. The explanation of this observation is related to the Pauli exclusion principle. In the classical description all the electrons of the system contribute to the specific heat, even at low temperature, i.e. when the excitation energies of the system are very small with respect to the total ground state energy. In the quantum case, at low temperatures, only those electrons close to the Fermi surface can change their state moving from a state below the Fermi surface, called hole state, to occupy a state above it, called particle state. For relatively small excitation energies, the electrons with energy much smaller than the Fermi energy cannot change their states since they would occupy states already occupied by other electrons.

Let's derive here below the expression of the specific heat of a gas of free electrons, i.e. for a Fermi gas. By using the expression (2.54) of the particle density, we obtain

$$k_{\rm F}{}^3 = \frac{2\pi^2}{\mathcal{D}} 3\,\rho \ , \tag{2.61}$$

$$\epsilon_{\rm F} = \frac{\hbar^2}{2m} k_{\rm F}{}^2 = \left(\frac{2\pi^2}{\mathcal{D}} 3\,\rho \right)^{2/3} \ , \tag{2.62}$$

$$A = \mathcal{V}\rho = \frac{\mathcal{V}\mathcal{D}}{2\pi^2 3} \left(\frac{2m}{\hbar^2} \epsilon_{\rm F} \right)^{3/2} \ , \tag{2.63}$$

therefore, the density of states can be expressed as

$$\rho_\epsilon(\epsilon_{\rm F}) \equiv \left(\frac{dA}{d\epsilon} \right)_{\epsilon=\epsilon_{\rm F}} = \frac{\mathcal{V}\mathcal{D}}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon_{\rm F}^{1/2} \tag{2.64}$$

The increase of internal energy E of an electron gas when the value of the temperature changes from 0 to T is given by

$$\Delta E \equiv E(T) - E(0) = \int_0^\infty d\epsilon\, \epsilon\, \rho_\epsilon(\epsilon) f(\epsilon, T) - \int_0^\infty d\epsilon\, \epsilon\, \rho_\epsilon(\epsilon) f(\epsilon, 0)\ . \tag{2.65}$$

In the traditional thermodynamics books, for example [Kit80, Blu06], the energy of the system E is indicated by the symbol U. In the above equation $f(\epsilon, T)$ is the Fermi-Dirac distribution

$$f(\epsilon, T) \equiv \frac{1}{\exp\left[(\epsilon - \mu)/\mathrm{k_B}T\right] + 1}\ , \tag{2.66}$$

where μ is the chemical potential

$$\mu = \frac{\partial E}{\partial A}\ , \tag{2.67}$$

whose value is ϵ_F at $T = 0$. The Fermi-Dirac distribution in the limit $T \to 0$ is $\Theta(\epsilon_\mathrm{F} - \epsilon)$, where $\Theta(x)$ is the step function equal to 1 for $x > 0$ and to 0 for $x < 0$. The equation (2.65) becomes

$$\Delta E \equiv E(T) - E(0) = \int_0^\infty d\epsilon\, \epsilon\, \rho_\epsilon(\epsilon) f(\epsilon, T) - \int_0^{\epsilon_\mathrm{F}} d\epsilon\, \epsilon\, \rho_\epsilon(\epsilon)\ . \tag{2.68}$$

By using the Fermi-Dirac distribution the number of particles can be expressed as

$$A = \int_0^\infty d\epsilon\, \frac{dA}{d\epsilon} = \int_0^\infty d\epsilon\, \rho_\epsilon(\epsilon) f(\epsilon, T)\ . \tag{2.69}$$

By multiplying this expression by ϵ_F we obtain

$$\epsilon_\mathrm{F} A = \left(\int_0^{\epsilon_\mathrm{F}} + \int_{\epsilon_\mathrm{F}}^\infty\right) d\epsilon\, \epsilon_\mathrm{F} \rho_\epsilon(\epsilon) f(\epsilon, T) = \int_0^{\epsilon_\mathrm{F}} d\epsilon\, \epsilon_\mathrm{F} \rho_\epsilon(\epsilon)\ . \tag{2.70}$$

where the last equality indicates that the number of particle does not change when the temperature changes from 0 to T. By adding and subtracting $\epsilon_\mathrm{F} A$ in the expression (2.68) of ΔE we obtain

$$\begin{aligned}
\Delta E &= \int_0^\infty d\epsilon\, \epsilon\, \rho_\epsilon(\epsilon) f(\epsilon, T) - \left(\int_0^{\epsilon_\mathrm{F}} + \int_{\epsilon_\mathrm{F}}^\infty\right) d\epsilon\, \epsilon_\mathrm{F} \rho_\epsilon(\epsilon) f(\epsilon, T) \\
&- \int_0^{\epsilon_\mathrm{F}} d\epsilon\, \epsilon\, \rho_\epsilon(\epsilon) + \int_0^{\epsilon_\mathrm{F}} d\epsilon\, \epsilon_\mathrm{F} \rho_\epsilon(\epsilon) \\
&= \int_{\epsilon_\mathrm{F}}^\infty d\epsilon\, (\epsilon - \epsilon_\mathrm{F})\, \rho_\epsilon(\epsilon) f(\epsilon, T) + \int_0^{\epsilon_\mathrm{F}} d\epsilon\, (\epsilon_\mathrm{F} - \epsilon) \rho_\epsilon(\epsilon)\left[1 - f(\epsilon, T)\right]\ .
\end{aligned} \tag{2.71}$$

The term $\rho_\epsilon(\epsilon) f(\epsilon, T) d\epsilon$ represents the number of electrons passing from levels with energy ϵ to levels of energy $\epsilon + d\epsilon$. In the second integral the term $1 - f(\epsilon, T)$ is the probability that an electron is removed from a level with energy ϵ.

The specific heat for an electron gas is given by

$$C_\mathrm{el} \equiv \frac{dE}{dT} = \int_0^\infty d\epsilon\, (\epsilon - \epsilon_\mathrm{F}) \rho_\epsilon(\epsilon) \frac{df(\epsilon, T)}{dT}\ , \tag{2.72}$$

where we have assumed that only term dependent on the temperature T is f. For temperatures much smaller than the Fermi temperature, i.e. $\mathrm{k_B}T \ll \epsilon_\mathrm{F}$, it is plausible to consider the density of states almost constant, therefore

$$C_\mathrm{el} \simeq \rho_\epsilon(\epsilon_\mathrm{F}) \int_0^\infty d\epsilon\, (\epsilon - \epsilon_\mathrm{F}) \frac{df(\epsilon, T)}{dT}\ . \tag{2.73}$$

This approximation is well verified if we consider that the typical values of the Fermi temperatures are of the order of $\sim 5 \times 10^4$K. The evaluation of the integral is presented in the box and it gives the result

$$C_{\rm el} \simeq {\rm k_B^2} T \rho_\epsilon(\epsilon_{\rm F}) \frac{\pi^2}{3} \tag{2.74}$$

In the following expressions we use the new variables defined as $\tau = {\rm k_B}T$ e $x = (\epsilon - \mu)/({\rm k_B}T)$.

$$\frac{1}{{\rm k_B}} \frac{df(\epsilon,T)}{dT} = \frac{df}{d\tau} = \frac{\exp(\frac{\epsilon-\mu}{{\rm k_B}T}) \frac{\epsilon-\mu}{({\rm k_B}T)^2}}{\left[\exp\left(\frac{\epsilon-\mu}{{\rm k_B}T}\right)+1\right]^2} = \frac{1}{[e^x+1]^2} e^x \frac{x}{\tau} \ . \tag{2.75}$$

For the definition of x one has $dx = d\epsilon/\tau$, therefore

$$\begin{aligned} C_{\rm el} &= {\rm k_B}\rho_\epsilon(\epsilon_{\rm F}) \int_{-\epsilon_{\rm F}/\tau}^{\infty} (dx\,\tau)(\tau x) \frac{1}{[e^x+1]^2} e^x \frac{x}{\tau} \\ &\simeq {\rm k_B}\tau\rho_\epsilon(\epsilon_{\rm F}) \int_{-\infty}^{\infty} dx\, x^2 \frac{e^x}{[e^x+1]^2} = {\rm k_B}\tau\rho_\epsilon(\epsilon_{\rm F}) \frac{\pi^2}{3} \ . \end{aligned} \tag{2.76}$$

In the last equation the lower integration limit has been extended to $-\infty$ since the term e^x is already very small for $x = -\epsilon_{\rm F}/\tau$ when we consider room temperatures. It only remains to calculate an integral which is well known in the literature.

From the equation (2.64) I obtain

$$\rho_\epsilon(\epsilon_{\rm F}) = \frac{1}{2}\frac{\mathcal{V}\mathcal{D}}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon_{\rm F}^{1/2} = \frac{1}{2}3\frac{1}{3}\frac{\mathcal{V}\mathcal{D}}{2\pi^2}\left(\frac{2m}{\hbar^2}\epsilon_{\rm F}\right)^{3/2} \frac{1}{\epsilon_{\rm F}} = \frac{3}{2}\frac{A}{\epsilon_{\rm F}} \ , \tag{2.77}$$

where I used the expression (2.63) for the electron number. By considering that $\epsilon_{\rm F} = {\rm k_B}T_{\rm F}$, the expression of the specific heat becomes

$$C_{\rm el} = \frac{\pi^2}{3}\frac{3}{2}\frac{A}{{\rm k_B}T_{\rm F}} {\rm k_B^2} T = \frac{\pi^2}{2} A {\rm k_B} \frac{T}{T_{\rm F}} \ . \tag{2.78}$$

This result indicates how, contrary to the prediction of the classical statistical mechanics, only a fraction of electrons, proportional to $T/T_{\rm F}$ is excited at the temperature T. These are the electrons close to the Fermi surface.

Element	Theory	Experiment
Cu	5.3	5.8
Ag	1.2	1.6
Au	1.5	1.6
Fe	1.5	12.0
Mn	1.5	40.0
Bi	4.3	0.2

Table 2.4: Values of the linear coefficient γ of the specific heats of some metals, Eq. (2.79). The values are expressed in units of 10^{-4} cal mole^{-1} K^{-2}. The empirical data are taken from Ref. [Ash76].

The prediction of the linear relation between temperature and specific heat in the metals is one of the most important consequences of the Fermi-Dirac statistics or, in other words, of the Pauli exclusion

principle for the electrons. The above result is valid if only the conduction electrons contribute to the specific heat. In the real situation, for temperatures above the room temperatures, the value of specific heat is dominated by the contributions of the ions forming the metal. Below room temperatures this contribution has a behaviour proportional to T^3, and at even lower temperatures it becomes even smaller than that of the electrons, which, as it is indicated by Eq. (2.78), is linearly dependent on T.

It is common practice to separate the two contributions as

$$c_v = \gamma T + KT^3 \quad . \tag{2.79}$$

where γ and K are two real constants. The experimental value of the γ coefficient is obtained by extrapolating the experimental values for $T \to 0$.

Table 2.4 compares some values of the γ coefficient calculated by using Eq. (2.78) with values taken from measurements. The alkaline metals (Cu, Ag, Au) are relatively well described by the Fermi gas model. This model makes completely wrong predictions for Fe and Mn giving values much smaller than the measured ones. On the contrary, the prediction for the Bi is remarkably larger than the observed value.

Chapter 3

Interactions

3.1 Introduction

In the MF models, the interactions between the particles composing the many-body system is not considered. In other words, in these models the interaction term of the hamiltonian in Eq. (2.1) is set to zero. In the previous chapter, we have shown how, by using this approximation, the total hamiltonian of the system becomes a sum of single particle hamiltonians. The many-body theories go beyond the mean-field models and also consider the interaction between the particles.

We have chosen to describe the many-body systems within the framework the non-relativistic Quantum Mechanics. The validity of this choice is restricted to situations where the values of the energies of the phenomena under study are much smaller than those of the rest masses of the particles forming the system. In the non relativistic framework the interaction between the particles is well described in terms of potential. The concept of potential implies an instantaneous transmission of the interaction, independently of the distance between the particles. This assumption is not valid in general because there is a limiting velocity of the signal transmission, the speed of light in vacuum. Despite of that, in the energetic conditions described above, the relativistic effects are negligible or, in case, they can be treated as perturbations.

In this chapter three different types of many-body systems are considered. They are electron gas, atomic nuclei and, quantum fluids, i.e. liquids and strongly interacting gases, whose basic particles are molecules. These systems are well described by non-relativistic quantum mechanics. They are also characterized by the fact that for for each particle, the interaction energy is comparable with the kinetic energy.

3.2 Electron gas

A good description of the metals is given by a model where the valence electrons of the atoms of the metal become conduction electrons and they move almost freely through the metal volume. The free electron model is the Fermi gas described in Sec. 2.3.

A more realistic description of a metal requires to consider the mutual interaction between the electrons and also that between the electrons and the ionized atoms composing the crystal lattice. The situation is very complicated, but, for temperature rather close to the absolute zero, the model called Jellium, or uniform electron gas, describes rather well the propertis of the many-body system. In this model, the positive charges forms a homogeneous background uniformly distributed in the space. This model emphasizes those effects that in the solids are generated by the quantum features of the electrons, the Pauli exclusion principle and their interaction, independently of the crystal structure.

In this model, the system hamiltonian is

$$\hat{H} = \sum_{i=1}^{A} \frac{-\hbar^2}{2m_i} \nabla_i^2 + \frac{1}{2} \sum_{i,j=1}^{A} \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \hat{U} \tag{3.1}$$

where e is the elementary charge and ϵ_0 the vacuum permittivity. We indicated with $|\mathbf{r}_i - \mathbf{r}_j|$ the distance between two interacting electrons and with $\hat{U}$ a constant potential which renormalizes the energy values.

3.3 Nuclei

The description of nuclear systems is based on the interaction between nucleons. Nucleons are not elementary entities of the nature, such as the electrons, but they are composite systems formed by quarks, antiquarks and gluons. At present, the most accredited theory describing the nuclear strong interaction, whose gluon and quarks are sensitive, but not leptons, is the Quantum Chromodynamics (QCD). This theory is non-perturbative in the energy range of interest for nuclear phenomena, from few keV to about 150 MeV, the pion emission threshold. For this reason, the well settled techiques used to solve Quantum Electrodynamics (QED), which is perturbative, cannot be used.

The QCD field equations are solved mainly numerically by discretizing the space and time in a set of points with the aim to bring this lattice more dense in order to describe a space-time continuum. Despite the great development of the computational devices, at present, we are still far from achieving this limit. From practical purposes QCD cannot be used even to describe mesons, barions and their interaction. Even more difficult is the description of atomic nuclei.

For the above mentioned reasons, the basic degrees of freedom used to describe nuclear systems are mesons and barions, mainly protons and neutrons, generically called nucleons. Clearly, QCD remains in the background as asymptotic limit, but it is never used to generate realistic interaction between nucleons.

3.3.1 Two-body forces

The nucleon-nucleon interaction is tailored to describe the experimental data related to the two-nucleon systems. This means the deuteron, the only bound state, and few thousand of elastic scattering data.

The deuteron has the following characteristics.

1. It is the only bound state of two nucleons.
2. It is composed by one proton and one neutron.
3. It has a binding anergy of abut 2.22 MeV.
4. It does not have excited states.
5. It has total spin $S = 1$.
6. It has a dipole magnetic moment whose value in, nuclear magnetons, is

   $$\mu_D = 0.8574 = \mu_p + \mu_n - 0.0222 \ ,$$

   where μ_p and μ_n are the dipole magnetic moments of the proton and of the neutron, respectively.
7. It has an electric quadrupole moment of Q=2.82 mb.

In the selection of the two-nucleon interaction, the main source of information comes from the scattering data. Since the internal structure of the nucleons is not considered, only elastic scattering processes are considered, where there is not exchange of energy between the nucleons to modify their internal structure. Elastic processes are the only ones permitted below the pion production threshold, about 145 MeV. This is roughly the maximum relative kinetic energy of the data used to determine the nucleon-nucleon interaction.

Experimental data have been taken in different laboratories. A big effort has been done in order to make homogeneous and coherent this set of data, and this work is in continuous evolution. At present the data base used to select the two-nucleon interaction is composed by about 3000 data of proton-proton scattering and about 4700 data of proton-neutron scattering.

The elastic cross sections are decomposed by using a partial wave expansion. Each partial wave depends on the relative angular momentum of the interacting nucleon pair. From these expanded cross sections it is possible the extraction of the phase shifts. The relation between the total cross section σ and the phase shifts is given by

$$\sigma = \frac{4\pi}{k^2} \sum_{L=0}^{\infty} (2L+1) \sin^2 \delta_L \ ,$$

where L is the relative angular momentum of the two-interacting nucleons and δ_L is the related phase shift. Nowadays nuclear potentials able to describe these data with a χ^2 per datum of about 1 are called *realistic*.

From the analysis of the two-nucleon data, it is possible to determine some general characteristics of the nucleon-nucleon potential.

- *Actraction.*
  Nuclei are bound systems of nucleons. This means that the nucleon-nucleon potential contains an attractive part able to bind the system.

- *Short-range.*
  There are quite a few observations indicating that the two-nucleon interaction is active up to distances of the order of 2 fm. For larger distances the interaction is not active. This is an essential difference with respect to the gravitational and electromagnetic interactions which have infinite interacting ranges.

- *Dependence on spin and isospin.*
  The only bound state of two nucleons is the deuteron formed by one proton and one neutron with total spin 1. The latter observation indicates a dependence on the spin orientation of the nuclear force. If the force would independent of the spin we would observe deuterons with spin 0 with abundancy of 1/3 with respect to those with spin 1. In analogy, if the interaction would be independent of the isospin we would observe also bound systems composed by two protons and two-neutrons.

- *Non centrality.*
  The deuteron has a non zero electric quadrupole moment. This is possible only if the charge distribution does not have spherical symmetry. For central potential the two-particle ground state is that with relative angular momentum zero, i.e. spherical symmetry. A deformation is possible only if the interaction contains a term which, even though the distance between two nucleons remains the same, behaves differently if the spins of the two nucleons have different orientation with respect to the direction of the line joining the two nucleons, for example if they parallel or orthogonal. This term, called tensor term, has a dependence of the type $(\hat{\boldsymbol{\sigma}}_1 \cdot \mathbf{r})(\hat{\boldsymbol{\sigma}}_2 \cdot \mathbf{r})$, where $\hat{\boldsymbol{\sigma}}$ indicates the nucleon spin and $\mathbf{r}$ is the vector joining the two nucleons.

- *Repulsive core.*
  The analysis of the elastic scattering phase shifts indicates that there is a change of sign with the increasing of the scattering energy. This means that, by increasing he resolution power of the probe, it is possibile to observe that the potential at short relative distances, smaller than 0.5 fm, becomes strongly repulsive.

The modelling of the nucleon-nucleon interaction must consider the following features related to general symmetry properties.

1. *Hermiticity.*
   Globally the hamiltonian is hermitian since its eigenvalues are observables, the energies of the system. Since the kinetic energy term is hermitian, also the potential term must be hermitian.

2. *Scalar expression*
   The hamiltonian is a scalar operator, therefore also the potential term must be a scalar operator.

3. *Invariance for coordinate exchange* $\Rightarrow \hat{V}(1,2) = \hat{V}(2,1)$.
   The interaction is active between identical particles.

4. *Translational invariance* $\Rightarrow \hat{V}(\mathbf{r}_1, \mathbf{r}_2) = \hat{V}(\mathbf{r}_1 - \mathbf{r}_2) \equiv \hat{V}(\mathbf{r}_{12})$.
   The interaction depends only on the distance between the two particles.

5. *Galilean invariance*
   The interaction depends only on the relative momentum between the two particles and it is independent of the motion of the observer.

6. *Invariance under space inversions* $\Rightarrow \hat{V}(\mathbf{r}, \mathbf{p}) = \hat{V}(-\mathbf{r}, -\mathbf{p})$.
   The strong interaction conserve parity, contrary to the weak interaction.

7. *Time reversal invariance* $\Rightarrow \hat{V}(\mathbf{p}, \mathbf{S}) = \hat{V}(-\mathbf{p}, -\mathbf{S})$,
   where $\hat{\mathbf{S}} = \hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2$ is the total spin of the nuclear pair.

8. *Invariance under space rotations*
   The total angular momentum of the system is conserved in presence of interaction between the particles.

9. *Invariance under isospin rotations*
   This property indicates that the nucleon-nucleon interaction is the same for proton-proton, neutron-neutron and proton-neutron scattering each time that the final states of this processes are comparable. This last statement is due to the fact that the nucleons, since are fermions, are subject to the Pauli exclusion principle, which is expressed by imposing that the global wave function describing a system composed by fermions must be antisymmetric under the exchange of two of them. Since proton and neutron are different particles, or in the isospin formalism they have different isospin third components, in the collisions they have access to all the possible final states. This is not possible for nucleons of the same type, where only specific combinations of partial waves and couplings of the spins are allowed. Modern experiments show small violations of this isospin symmetry, and in the updated potential there are terms taking care of these effects.

The procedure to construct a nucleon-nucleon potential consists in assuming a functional dependence of the potential containing various parameters. Clearly, this functional dependence must satisfy the properties indicated above. The values of the parameters are chosen to reproduce at best the experimental data. I indicate here below the three types of approaches used to generate nucleon-nucleon potentials

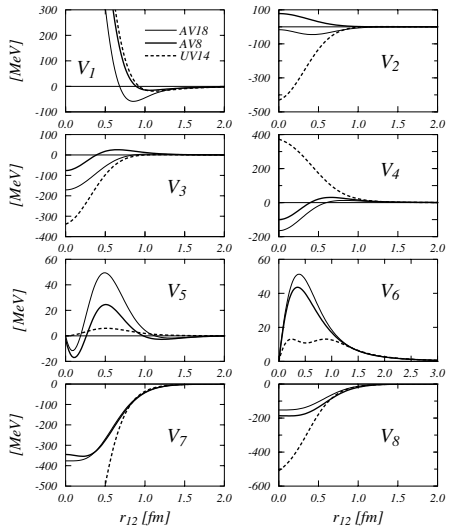

Figure 3.1: The first 8 terms defined in (3.2) for the Urbana V14 (UV14), Argonne V8 (AV8), and Argonne V18 (AV18) potentials.

Phenomenological potentials.

The goal of constructing these potentials is their use in nuclear structure calculations, without any ambition in understanding the physics providing their characteristics. It is a pure fit to the experimental data.

The most direct of these approaches consists in adopting an expression of the potential which is a sum of terms dependent on operators which respect the symmetries of the hamiltonian. If one neglects terms depending on derivatives of the position, the most commonly used expression is

$$\hat{V}(i,j) = \sum_{p=1,18} v_p(r_{ij}) \hat{O}^p_{ij} \tag{3.2}$$

where $v_p(r_{ij})$ are scalar functions whose dependence on the distance between the two interacting nucleons is expressed in terms of analytic functions containing the free parameters whose values are chosen to reproduce the experimental data.

In this representation, the so-called central terms are

$$\hat{O}^{p=1,4} = \hat{\mathbb{I}}, \quad \hat{\boldsymbol{\tau}}_i \cdot \hat{\boldsymbol{\tau}}_j, \quad \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j, \quad \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j \hat{\boldsymbol{\tau}}_i \cdot \hat{\boldsymbol{\tau}}_j \ , \tag{3.3}$$

and the tensor terms are

$$\hat{O}^{p=5,6} = \hat{S}_{ij}, \quad \hat{S}_{ij} \hat{\boldsymbol{\tau}}_i \cdot \hat{\boldsymbol{\tau}}_j \ , \tag{3.4}$$

where the tensor term is defined as

$$\hat{S}_{ij} = 3 \frac{\hat{\boldsymbol{\sigma}}_i \cdot \mathbf{r}_{ij} \hat{\boldsymbol{\sigma}}_j \cdot \mathbf{r}_{ij}}{\mathbf{r}^2_{ij}} - \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j \ . \tag{3.5}$$

Obviously, the tensor part is represented by the first term of this expression, the second one is added in order to set equal to zero the angular integral of S_{ij}. In the potential also spin-orbit terms are considered

$$\hat{O}^{p=7,8} = \hat{\mathbf{L}} \cdot \hat{\mathbf{S}} \, , \ \hat{\mathbf{L}} \cdot \hat{\mathbf{S}} \hat{\boldsymbol{\tau}}_i \cdot \hat{\boldsymbol{\tau}}_j \ , \tag{3.6}$$

where $\mathbf{L}$ is the relative angular momentum of the nucleon pair. Also quadratic terms of the angular momentum are considered

$$\hat{O}^{p=9,14} = \hat{\mathbf{L}}^2 \, , \hat{\mathbf{L}}^2 \hat{\boldsymbol{\tau}}_i \cdot \hat{\boldsymbol{\tau}}_j \, , \hat{\mathbf{L}}^2 \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j, \, , \hat{\mathbf{L}}^2 \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j \hat{\boldsymbol{\tau}}_i \cdot \hat{\boldsymbol{\tau}}_j \ . \tag{3.7}$$

The terms violating the rotational isospin invariance are

$$\hat{O}^{p=15,18} = \left[\hat{1},\, \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j\, \hat{S}_{ij}\right] \otimes [\hat{\tau}_{z,i} + \hat{\tau}_{z,j}] \tag{3.8}$$

This is the typical structure of potential called of Urbana and Argonne type. The $v_p(r_{ij})$ are constructed in order to have three different interacting ranges, a short range, up to about 0.5 fm, a medium range, up to about 1 fm, and a long range up to about 2 fm. Each of these parts has a special functional expression, for example sum of Yukawa functions (see below), and contains the parameters whose values are chosen for the fit to the experimental data.

In the figure 3.1 we show the first 8 terms for the Urbana U14, Argonne V8 e Argonne V18 potential as a function of the two-nucleon distance. Two comments are in order. The first one is that, even though the number of data to be reproduced is large, and all the potentials have similar performances in the fit procedure, $\chi^2 \sim 1$ per datum, the functions are quite different. This indicate that the data do not imply restrictions so severe to uniquely define the potential. The data are correlated and they can be reproduced by suitable combinations of the various terms.

The second observation is that all the parametrizations, in the scalar channel V_1, show a strongly repulsive core at small distances, an attractive pocket at intermediate distances and they go rapidly to zero at about 2 fm. The presence of the repulsive core makes inapplicable the traditional perturbative techniques.

Meson exchange potentials.

A more ambitious approach to the construction of the nucleon-nucleon potential starts from the Yukawa idea and shapes the potential in terms of exchange of mesons. The basic point is that the interaction range is determined by the mass of the meson exchanged by the two nucleons. The motion of the meson exchanged is a Yukawa function and it has the expression

$$\hat{V}(r) = \frac{e^{-\frac{m}{\hbar c}r}}{r} \quad ,$$

where m is the mass of the exchanged meson and r the distance between the two interacting nucleons. Evidently, $\hat{V}(r)$ goes more rapidly to zero the heavier is the exchanged meson.

The first nucleon-nucleon potentials constituted by a sum of terms summing contributions of exchanged mesons have been built at the beginning of the 80s of the past century. Table 3.1 present the characteristics of the mesons considered in the construction of these potentials. In addition to its mass, each meson is characterized by its spin and intrinsic parity. These characteristics identify the type of coupling with the nucleon. While the mass sets the interaction ranges, the type of meson-nucleon coupling selects operator dependence which, in the phenomenological potentials, is described by the O^p operators.

Type	J^π	coupling	meson	mass [MeV]
Pseudoscalar	0^-	γ_5	π	139.578
			η	548
			η'	958
Vector	1^-	γ_μ	ρ	765
			ω	783
			ϕ	1019
Scalar	0^+	1	σ	500

Table 3.1: Mesons used to construct the nucleon-nucleon potential.

The goal of this research project is to identify the mesons responsible for the various parts of the nucleon-nucleon interaction, both in terms of interaction range and also in terms of operator dependence. For example, the pion, the π meson, is the lightest meson and it is responsible of the long-range

part of the interaction, Furthermore, its pseudoscalar coupling is related, in a non-relativistic reduction, to the tensor-isospin channel $O^6_{ij} = S_{ij}\,\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$ of the interaction. In effect, in Fig. 3.1 the term with the longest interaction range is the tensor-isospin one, V_6.

This ambitious project has to face the limits of our knowledge of meson physics. We know mass, type of nucleon-meson coupling and the value of the coupling constant only for the π meson. This knowledge comes from the large amount of pion-nucleon scattering data available. For the other mesons the situation is not so well defined. The short life times of these other mesons do not allow to perform scattering experiments. Therefore, while we have information on their masses, spin and parity, and this means we know the type of coupling, we do not know the values of their coupling constants. In the construction of the potential, these experimentally unknown coupling constants are considered free parameters whose values are selected to fit the nucleon-nucleon data. The number of free parameters is almost the same used in the phenomenological approach. With this number of free parameters it is possibile to obtain fits to the experimental data of accuracy comparable to that obtained in the phenomenological approach.

At this point it is worth to emphasize that, in order to reproduce the two-nucleon experimental data, it is necessary to include a fake meson, never identified experimentally, the σ meson, which has a scalar coupling type and with a mass of, exactly, 500 MeV. This meson describe the attractive poket around the distances of about 1 fm. The need of including this fake meson is clearly a failure of this ambitious approach. In reality, the model has been constructed by considering the exchange of a single meson between the two interacting nucleons. Calculations considering also the exchange of two pions indicates that the fake meson σ simulates, at least in part, the exchange of two mesons in relative s wave.

This does not mean that the meson exchange potentials do not show differences, and advantages, with respect to the phenomenological potentials. The formulation is fully relativistic, therefore invariant for Lorentz transformations. This means that, by applying the charge conjugation operators, it is possible to obtain the nucleon-antinucleon potential and also that between two antinucleons. The comparison with the relatively few experimental data of these systems confirms the success of this approach in building the process.

The use of these potentials in standard nuclear structure calculations is not straightforward. This type of calculations require potentials which are non-relativistic and local, i.e. do not contain terms related to the derivative of the particle position. The meson exchange potentials are relativistic and they are usually expressed in momentum space with an explicit dependence on the momentum of each particle, in other words they are non-local. Before using these potential in nuclear structure calculations a non-relativistic reduction is required, and also the elimination of the non local terms.

Potentials from chiral effective field theories.
The most modern, and ambitious, method of modelling the two-nucleon potential is obtained from the so-called *chiral effective field theories*. The idea is to construct an effective theory of the QCD which is valid at energies of the order of the MeV. In the effective lagrangian the symmetry properties of the QCD are respected, especially the chiral symmetry. The lagrangian is built by considering pion exchanged at different orders. Each expansion order contains contact terms inserted to satisfy the chiral symmetry. The modern potentials include terms up the third perturbative order to obtain a fit of the two-nucleon data with $\chi^2 \simeq 1$. Also this model requires about 20 free parameters to generate this high-quality fit of the data. This is about the same number of free parameters used in the other two approaches.

3.3.2 Three-body forces

The fundamental assumption on which is based the construction of the nucleon-nucleon potential is that the nucleons are pointlike particles, in other words their internal structure is neglected. This is obviously

an approximation which is supposed to be valid in the energy range of interest for the nuclear physics. The data used to select the two-nucleon potential are only elastic scattering data, and those related to the deuteron.

Potential	2N	2N+3N
CD Bonn	7.953	8.483
Nijm II	7.709	8.477
Nijm I	7.731	8.480
Nijm 93	7.664	8.480
Reid 93	7.648	8.480
AV14	7.683	8.480
AV18	7.567	8.479

Table 3.2: Binding energies of ^{3}H, in MeV, calculated with different two-nucleon potentials and then obtained by inserting a proper three-body force. The experimental value of the ^{3}H binding energy is 8.481 MeV.

Since the two-nucleon systems are used to build the interaction, the simplest system where we can test the prediction power of the potential is the triton. The ^{3}H is formed by one proton and two neutrons. In this system the electromagnetic interaction is absent and, therefore, it is the ideal system to test the quality of the nucleon-nucleon potentials.

The techniques to solve the Schrödinger equations for a tree-body system are standardised as those of the two-body case. It is possible to solve the problem without approximations. Recently, ^{3}H binding energies obtained with seven different techniques have been compared. Given the same nucleon-nucleon potential all the results correspond, within the numerical accuracy of the calculations. This clearly indicates that the solution of the three-body problem, without approximation is well controlled.

Table 3.2 shows the ^{3}H binding energies obtained by using different nucleon-nucleon potentials, each of them describing the two-nucleon data with the same accuracy. The differences of the results are due only to the input of the potential, since the Schrödinger equation is solved without approximations. This results confirm what has been previously stated: the fit the two-nucleons data is not sufficiently restrictive on the construction of the potential. The main, and more general, results is that none of the two-body potential is able to reproduce the experimental value of the triton binding energy.

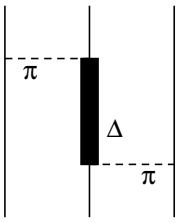

Figure 3.2: Fujita-Miyazawa three-body interaction.

Since all the computational techniques generate the same results and by using two-body potential one obtains binding energies smaller than the experimental one, it only remains to attribute to the hamiltonian the source of the discrepancy with the experiment, and more precisely to the assumption that nucleons are pointlike particles.

In Fig. 3.2 an example of a phenomenon not considered in the two-nucleon potential is shown. The diagram describes the system of three-nucleons, indicated by the three thin vertical lines. The nucleon in the middle interacts with the nucleon to its right, by exchanging a π meson, and it is transformed in a Δ resonance. While it is a Δ, the barion in the middle interacts with the nucleon to its left and it is transformed back into a nucleon. The initial and final states of this process involves only nucleons but there is a transformation of one nucleon in another barion. This is possibile only because the nucleon has an internal structure which can be modified by the interaction. Effects of nucleons changing their structure and in this state interact with another nucleon before turning back to its original nucleonic state are present also in the two-body interaction. These phenomena are automatically considered during the fit procedure. The process shown in Fig. 3.2 is not included in the construction of the two-body potential, and it has to be considered separately.

With the insertion of a three-body term, the hamiltonian becomes

$$\hat{H} = \sum_{i=1}^{A} \frac{-\hbar^2}{2m_i}\nabla_i^2 + \sum_{i<j}^{A} \hat{V}(i,j) + \sum_{i<j<k}^{A} \hat{W}(i,j,k) \ , \tag{3.9}$$

where the first term represents the kinetic energy, the second one is the two-body potential, selected to fit the two-body data, and the third one is the three-body potential. This latter contains the contribution of the process described in Fig. 3.2, called Fujita-Miyazawa, and, in addition, a phenomenological term whose parameters are selected to reproduce the experimental value of the triton binding energy. This procedure implies that each two-body potential has its own three-body force.

Since the hamiltonian containing only two-body terms of the interaction is not able to reproduce the simplest three-body system, and it requires the insertion of an *ad hoc* three-body interaction, it is reasonable to ask whether this procedure has to continue. To describe more more complicated systems, do we have to include four-, five-, ... A-body terms in the hamiltonian? Fortunately, the hamiltonian (3.9) is able to describe well also nuclear system containing more than three nucleons, as we discuss in Chapter 4.

The importance of the many-body forces increases with the probability of finding a certain number of particles sufficiently closed to interact. We remember that the nuclear interaction is short-ranged, therefore the particles must be within the interaction range in order to interact. For nuclear density of ordinary nuclei four-body forces are negligible with respect to the strength of two-, and three-, body forces.

3.4 Liquids and strongly interacting gases

The fundamental interaction forming liquids or strongly interacting gases is the electromagnetic interaction which is well described by the QED. The QED are solved with high accuracy by using perturbation techniques. In principle, it is possibile to use the QED equations to describe the interaction between atoms or molecules by considering the electromagnetic interaction between the basic elements forming these systems, i.e. electrons and nuclei.

This microscopic description of the interaction between atoms or between molecules is obtained by using a hamiltonian which describes the motion of the electrons, that of the nuclei forming the molecules and their mutual interactions of Coulomb type. The electrons do not have internal structure, and in this approach we would neglect the internal structure of the nuclei. This latter approximation is well justified by considering that the energies under study are of the order of eV, while those related to the nuclear system are of the order of MeV.

Molecular structure calculations are normally carried out by keeping fixed the distance between the nuclei of the atoms composing the molecule and by solving the Schrödinger equation which describe the electron motion. This is the essentially the so-called Born-Oppenheimer approximation. The calculations are repeated for different values of the distance between the nuclei to search for the minimum energy value. From this calculations it is possible to obtain the interacting potential between atoms, or molecules.

The description of a many atoms, or molecules, system starting from the electromagnetic interaction between its components is a program feasible, in principle. From the pragmatic point of view, it is very difficult to carry out, and, probably, excessively ambitious with respect to the purpose of describing the properties of many-atoms, many-molecules, systems.

A most pragmatical approach uses a strategy analogous to that used to define the nucleon-nucleon interaction. The basic interaction used to describe liquids and strongly interacting gases is obtained by neglecting the internal structure of what are considered the basic degrees of freedom, in this case, atoms or molecules. The interest is focused on the two atoms, or two molecules, interaction, which is quite different from the basic Coulomb interaction which generate them.

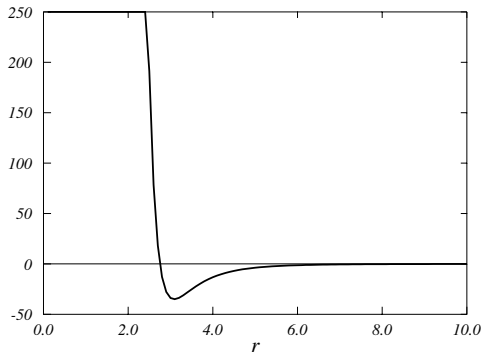

Figure 3.3: Lennard-Jones potential between two atoms of Ne expressed in K. The distances are expressed in Å.

In molecular physics, the forces acting among atoms are classified as (a) valence binding, (b) ionic binging, (c) metallic binding, (d) van der Waals binding. The forces (a) and (b), active for example in the diamonds or in NaCl, are so strong that at room temperature the systems form solid structures, therefore we do not consider them. The metal link forms the electron gas discussed in 3.1. We focus our attention on the van der Waals forces which are responsible of these substances that at room temperatures are in fluid state. These are the interactions active also in quantum liquids such as the superfluid helium, both in bosonic case, composed by atoms with ^{4}He nuclei, and in fermionic case, composed by atoms with ^{3}He nuclei.

The system we consider is formed by well structured molecules which do not share electrons with other molecules. In the case the molecules are composed by atoms of different type, or by atoms with a strong asymmetry of the electronic cloud, there is a polarization of the positive and negative charges in the space. These molecules have permanent electric multipoles, for example dipoles, quadrupoles etc. . The van der Waals interaction between molecule can be seen as interaction between different electric multipoles.

Also the case where the center of mass of positive and negative charges coincide, and this happens normally for molecules composed by identical atoms, can be described in terms of interaction among electric multipoles. This because the approaching of two molecules generates a distortion, a polarization, of the electon clouds.

The interaction between the two atoms or two molecules is zero at distances much larger than the atomic, or molecular dimensions. This because non-ionized atoms and molecules are neutral. At large distances, the centres of their positive and negative charge distributions are seen as overlapping. This feature puts these interactions in the class of the finite-range interactions, analogously to the nucleon-nucleon interaction. At intermediate distances, the interaction is, in first approximation, that between two electric dipoles, therefore essentially attractive. Finally, at short distances, the electron clouds start to overlap, and therefore there is repulsion. Fig. 3.3 shows the interaction potential between two neon atoms, calculated by using the Lennard-Jones potential discussed below. The behaviour is analogous to that of the scalar part of the nucleon-nucleon potential: zero at large distances, attractive at intermediate distances and with a strongly repulsive core at short distances.

The approach used to obtain this potential consists in using an analytic expression containing free parameters whose values are chosen to reproduce empirical data describing systems of two atoms or two molecules.

Probably the most used potential is the *Lennard-Jones* which is usually expressed as

$$V(r) = 4\epsilon \left\{ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right\} \tag{3.10}$$

where r is the distance between the two interacting particles wihch are assumed to be point-like, and ϵ and σ are the two free parameters.

The interaction between two molecules is much simpler than that between two nucleons: it is purely scalar, therefore independent of the spin of the two molecules and of their relative angular momenta. The expression (3.10) is extremely simple, but it contains all the relevant physics required to describe these many-body systems.

While in the nuclear case the interaction selected as indicated in Sect. 3.3 is used to describe every nucleus, in the case of fluids it is necessary to set the values of the interaction for every type of atom or

	Ne	Ar	Kr	Xe	N_2	CH
σ (Å)	2.75	3.405	3.60	4.10	3.70	3.82
ϵ(K)	35.6	119.8	171	221	95.1	148.2

Table 3.3: Parameters of the Lennard-Jones potential for some atoms and molecules, from [Pry66].

molecule which composes the system. As example, we show in Table 3.3 the values of the parameters selected for some molecules.

We have considered so far that the hamiltonian contains only two-body interaction terms. This description of the interaction is working until the assumption that the interacting particles do not have internal structure remains valid. We have shown that in the nucleonic case this assumption is not so reliable and it is necessary to include a three-body force in the nuclear hamiltonian. The assumption that the hamiltonians in molecular physics require only two-body interaction terms is usually called *pairwise additivity*. The validity of this assumption is widely analyzed in statistical and molecular physics (see for example the discussion in the Sect. 4.3.b of [Goo85]).

To evaluate the relevance of the many-body forces it is necessary to consider two physical quantities. The first one is the excitation energy of the basic particle which is considered point-like. The second quantity is the relative density of the system. The first quantity has to be compared with energy of the system. For example, the empirical value of binding energy of nuclear matter in the stability point is about 16 MeV per nucleon. The first resonance of the nucleon is the Δ which has a mass about 300 MeV larger than that of the nucleon. This means that the nucleonic internal structure starts to be important at energies about 18 times the energy of the system. The typical energies of superfluid helium are about 2μeV, while the energy of the first excited state of He atom is about 20 eV. There are 7 orders of magnitude of difference. By comparing these numbers, evidently the assumption of neglecting the internal structure of the basic degrees of freedom of the system is much more valid in liquid helium than un nuclear matter.

The second quantity to be considered is the probability that the particle get sufficiently close to interact, which is strictly related to the density of the system. The particles must be in the interaction range of the force which is short-ranged. An estimate of this probability can be obtained by considering how many particle stay in the volume defined by the repulsive short-range core of the interaction. Here below we calculate these numbers for both liquid helium and nuclear matter. The results indicate that, at the equilibrium density, there are 0.084 nucleons in volume of interest, to be compared with 2.317 helium atoms in the liquid helium case. From the relative densities point of view liquid helium is much denser than nuclear matter. The probability to find three helium atoms interacting is certainly larger than that to find three nucleons interacting. On the other hands, has discussed above, the energetics indicate that exciting helium atoms in liquid helium is much less probable than exciting a nucleon in nuclear matter. For this reason three-body forces are seldom used in the description of liquid helium.

Relative densities

In the framework of the many-body theories, the relative densities are important. These densities are related to the number of particles, whose internal structure is not considered, which are in the volume characterized by repulsive short-range core of the interaction.

1. *Nuclear matter.*
   In this case the range of the repulsive core is $\sigma \simeq 0.5$ fm. The value of the reference volume is then
   $$\mathcal{V} = \frac{4}{3}\pi\sigma^3 = 0.524\,\mathrm{fm}^3$$

The empirical value of the nuclear matter density at equilibrium is 0.16 nucleons per fm^3. The number of nucleons in the volume of interest is

$$N = \rho\mathcal{V} = (0.16)\frac{\text{nucleons}}{\mathrm{fm}^3}(0.524)\,\mathrm{fm}^3 = 0.084\,\text{nucleons}$$

2. *Liquid Helium.*
The mass density of liquid helium is $1.47 \cdot 10^5$ g m^{-3}. The molecular weight is 4 g mole^{-1}, which is the weight of an Avogadro number of helium atoms. The number density of helium atoms in liquid helium is

$$\rho = \frac{1.47 \cdot 10^5 \mathrm{g}}{\mathrm{m}^3}\frac{6.2 \cdot 10^{23}}{4\mathrm{g}} = \frac{2.263 \cdot 10^{28}\mathrm{atoms}}{\mathrm{m}^3}$$

In liquid helium the range of the repulsive core of the interaction i s σ=2.9 Å= 2.9 10^{-10} m. The volume of the sphere of radius σ is $\mathcal{V} = 1.024 \cdot 10^{-28}\mathrm{m}^3$. The number of atoms in this volume is $(\mathcal{V}\rho) = 2.317$.

Part II

Solutions without approximations

Chapter 4

Monte Carlo Techniques

After having defined the theoretical framework, the degrees of freedom (the particles) and the hamiltonian (the interaction), the remaining task is the solution of the Schrödinger equation. Since the two-body systems, and eventually also the three-body systems, have been used to define the interaction, see Chapter 3, the first, and easiest, application of theory is done on four-body systems. This allows a pragmatical definition of many-body system, which is composed by more than three particles.

There are techniques which consider the solution of the Schrödinger equation for 4, 5, and even 6 body systems without approximations. Usually, these techniques have been tailored to treat this specific number of particles, and it is difficult to extend them to handle systems with larger numbers of particles.

In this chapter, we present a technique which solves the many-body Schrödinger equation without approximation, and it is formulated independently of the number of particles to be considered. As we shall discuss, the only limitations are of pragmatical type, related to the technological limits of computational resources.

The development of the electronic technology has strongly increased the possibility of performing numerical calculations. These technological advances allowed the use of Monte Carlo calculations. The name Monte Carlo indicates a way of using the computer based on its capacity to generate sequences of random numbers. This feature is used in different manners, for example to simulate the behaviour of complex systems such as the time evolution of the population or the performances of particle detectors.

In these notes we discuss how Monte Carlo techniques are used in the framework of the many-body physics. As I have already stated above, these techniques allows the solution of the Schrödinger equation without approximation. The only assumptions, and approximations, are of numerical type, related to the algorithm used in the calculations.

The application of the Monte Carlo techniques in this contest is related to the possibility to carry out multidimensional integrals in reasonable execution times. We first present the basic idea behind the numerical integration with the Monte Carlo techniques, and then the implementations related to the many-body problems.

4.1 Numerical integrations

If we neglect the presence of spin and, eventually, isospin, the many-body wave function $|\Psi\rangle$ is characterized by the $3A$ variables identifying the position of each particle. This means that the calculation of the energy of the system

$$E = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \ , \tag{4.1}$$

involves $3A$ dimensional integrals. If we consider a uniform grid of cartesian coordinates, and indicate with N the number of points of each dimension of the grid, the number of these $3A$ dimensional integrals to be calculate is $N^{3A-1}+1$. The number of integration points, N in this example, commonly used in the ordinary integration techniques, Simpson, etc. , is of the order of 100. Even assuming very short times to execute each integral, let's say 10^{-6} s, it is evident the difficulty of using these integration techniques to describe a many-body system. The calculation of a system with $A = 4$ would require 10^6 s, about four months, with $A = 5$ about 400 years.

The computation of integrals with Monte Carlo techniques is not convenient for one, two-dimensional integrals since it requires much more time machine than that use by the usual integration methods to obtain similar numerical accuracy. On the other hand, this is the only techniques which allows us to make estimates of multidimensional integrals in reasonable times. We present here below the basic idea of the Monte Carlo integration by using a one-dimensional example. The generalization to more dimension is straightforward.

Any definite integral can be expressed as

$$\int_a^b f(u)\,du = (b-a)\int_0^1 f(x)\,dx\ , \tag{4.2}$$

where we used a new integration variable

$$x = \frac{u-a}{b-a}\ . \tag{4.3}$$

This indicates that the problem to be tackled is an integration in the dominion between 0 and 1, where the computer generates random numbers.

From the numerical point of view the value of the integral is obtained by summing the values of f calculated for N random values of the integration variable x,

$$I = \int_0^1 f(x)\,dx \simeq \frac{1}{N}\sum_{i=1}^{N} f(x_i)\ . \tag{4.4}$$

The estimate of I improves by increasing the number N. The value of N good enough to obtain an accurate estimate of the integral depends on the behaviour of f in the integration domain. If f is rather flat, few points would be sufficient. In the limit when f is a constant, one point is enough.

A useful strategy to make flat the behaviour of the function to integrate consists in multiplying it, and also dividing it, by a weight function P, defined always positive in the integration interval, and behaving as a probability density

$$\int_0^1 P(x)\,dx = 1\ , \tag{4.5}$$

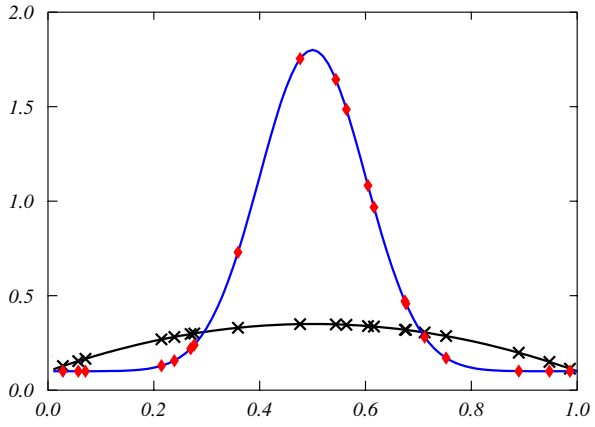

Figure 4.1: Functions to be integrated with the Monte Carlo method. The red points and the black crosses indicate the points of the two functions selected by the same random choice of the variable x.

therefore

$$I = \int_0^1 f(x)\,dx = \int_0^1 \frac{f(x)}{P(x)}P(x)\,dx = \int_0^1 F(x)P(x)\,dx\ . \tag{4.6}$$

We define a new variable

$$y(x) = \int_0^x P(x')\,dx'\ \ ;\ \ \frac{dy(x)}{dx} = P(x)\ \ ;\ \ y(0) = 0\ \ ;\ \ y(1) = 1\ , \tag{4.7}$$

and then

$$I = \int_0^1 f(x)\,dx = \int_0^1 F(x)P(x)\,dx = \int_0^1 F(x(y))\,dy \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x(y_i))}{P(x(y_i))}\ . \tag{4.8}$$

The better choices of P are those able to make almost constant the ratio f/P. The problematic point of the procedure is the inversion of the relation (4.7), which could not be trivial.

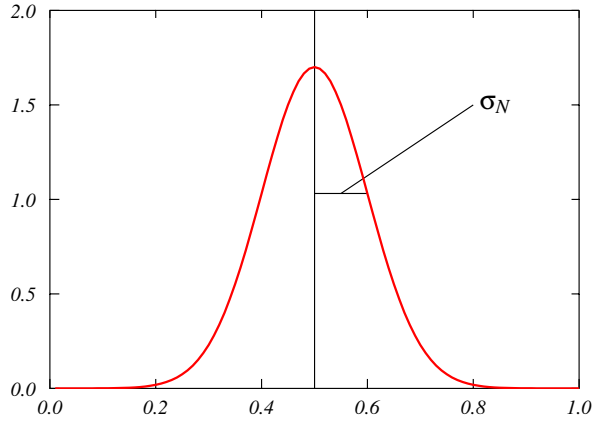

Figure 4.2: Gaussian distribution around the central value.

At this point, a theorem, called Theorem of the central limit, describes the distribution of the approximated values of I. The theorem states that, for a function $F(x)$, the probability distribution $\mathcal{P}(I_N)$ of the values I_N, defined as

$$I_N = \frac{1}{N}\sum_{i=1}^{N} F(x_i)\ , \tag{4.9}$$

has a gaussian form

$$\lim_{N\to\infty}\mathcal{P}(I_N) = \frac{1}{\sqrt{2\pi\sigma_N^2}}\exp\left(\frac{(I_N-\langle F\rangle)^2}{2\sigma_N^2}\right)\ . \tag{4.10}$$

In the above expression, we used the quantities defined as

$$\begin{aligned}\langle F\rangle &= \int_0^1 F(x)P(x)dx \quad ;\\ \langle F^2\rangle &= \int_0^1 F^2(x)P(x)dx \quad ;\\ \sigma_N^2 &= \frac{1}{N}\left(\langle F^2\rangle - \langle F\rangle^2\right)\ .\end{aligned}$$

The theorem is based on the ansatz that the values of x_i are independent of each other and have the same probability of being selected. The theorem indicates that the value of I has, for N sufficiently large, a gaussian distribution around the expected value. The width of the amplitude is σ_N, and scales as $N^{-1/2}$. Therefore,

$$I = \int_0^1 f(x)\,dx = \int_0^1 F(x)P(x)\,dx = \int_0^1 F(x(y))\,dy \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x(y_i))}{P(x(y_i))} \pm \sigma_N \tag{4.11}$$

This technique can be extended to multidimensional integrals. The gaussian uncertainty is independent of the number of dimension. The idea is to apply this technique to evaluate the energy (4.1), or, more in general, to calculate the expectation value of a generic operator $\hat{\mathcal{O}}$ between two many-body states.

4.2 Variational Monte Carlo

A first application of the Monte Carlo techniques, called Variational Monte Carlo (VMC), for the evaluation of the energy of the ground state of a many-body system is based on the variational principle.

Searching for the minimum of the energy functional (4.1) is equivalent of solving the Schrödinger equation (see Appendix A). In practical applications, the search for the energy minimum is done by

considering only wave functions with precise functional form. This limitation restricts the search within a Hilbert sub-space. For this reason, the solution of the Schrödinger equation is approximated, and the obtained energy value is always larger than those obtained without approximations.

In the case of the VMC calculations, the trial wave function is built in analogy to what it is done in the Correlated Basis Function theory, which will be presented in Chapter 13,

$$|\Psi_T\rangle = F|\Phi\rangle \tag{4.12}$$

where $|\Phi\rangle$ is a Slater determinant, and $\hat{F}$ is called correlation function. This function is defined the Jastrow's ansatz, i.e. as a product of two-body correlation functions f

$$F = \prod_{i<j}^{A} f(r_{ij}) \ . \tag{4.13}$$

We have pointed out in Chapter 3, that a typical feature of the interactions in many-body systems is the presence of a strongly repulsive core at short distance between interacting particles. The goal of the correlation f is to prohibit two particles to approach in the range of the repulsive core. For this reason, f is essentially zero at short relative distances, and becomes 1 at distances larger than the interaction range.

The complexity of the nucleon-nucleon interaction, requires, in nuclear physics, the use of correlation expressions depending on various operator terms, in analogy with the expression of the interaction presented in Chapter 3.3.1

$$\hat{F} = \mathcal{S} \prod_{i<j}^{A} \left(\sum_{p} f^p(r_{ij}) \hat{O}^p_{ij} \right) \ , \tag{4.14}$$

where $\mathcal{S}$ is an operator which makes symmetric $\hat{F}$ for the exchange of two fermions, i.e. the two indexes i, j. This is necessary since the Slater determinant Φ is already antisymmetrized for two-fermions exchange, and, in general, the $\hat{O}^p$ operators do not commute with each other. The explicit expressions of the operators are those presented in Sect. 3.3.1.

The wave functions used in VMC calculations are expressed as:

$$|\Psi(\mathbf{r}), S, T\rangle \equiv \sum_{s=1,2^A} \sum_{t=1,2^A} \mathcal{R}_{s,t}(\boldsymbol{R}) \mathcal{X}_s(S) \mathcal{X}_t(T) \ , \tag{4.15}$$

where $\mathcal{R}$ indicates the radial part of the wave function, $\boldsymbol{R}$ is the set of all the space coordinates describing the fermions of the system, and $\mathcal{X}_s$ and $\mathcal{X}_t$ are the parts of the wave function describing the spin S, and eventually, isospin T terms. This part of the wave function describes all the possible spin and isospin combinations in the system formed by A fermions. If we consider a nucleus with Z protons and $A - Z$ neutrons, the number of these combinations is given by

$$N_{\rm conf} = 2^A \frac{A!}{Z!(A-Z)!} \ . \tag{4.16}$$

The values of $N_{\rm conf}$ for some nuclei of interest are given in Table 4.1.

As we discussed in Chapter 3.3.1, in nuclear physics the interaction between two nucleons can be expressed by using an expression of the type

$$\hat{V}(i,j) = \sum_{p} v_p(r_{ij}) \hat{O}^{(p)}_{ij} \ , \tag{4.17}$$

where v^p are scalar functions of the relative distance between the two interacting particles. The matrix elements of the interaction (4.17) can be directly evaluated for states in the representation (4.15), as it is shown in the box for the case of 3 particles.

Nucleo	Z	N=A-Z	N_{conf}
^{3}H	1	2	24
^{3}He	2	1	24
^{4}He	2	2	96
^{6}He	2	4	960
^{6}Li	3	3	1280
^{8}He	2	6	7168
^{12}C	6	6	3784704
^{16}O	8	8	$8.4 \cdot 10^{8}$
^{40}Ca	20	20	$1.5 \cdot 10^{23}$
^{48}Ca	20	28	$4.7 \cdot 10^{27}$

Table 4.1: Number of spin and isospin configurations for some nuclei.

Let's consider, for example, the term depending on the spin $p = 3$ in (4.14). By using the traditional Pauli matrices we obtain

$$\hat{\sigma}_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \ \hat{\sigma}_y \equiv \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \ , \ \hat{\sigma}_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ . \tag{4.18}$$

We define rising and lowering operators as

$$\hat{\sigma}_+ \equiv \frac{1}{2}\left(\hat{\sigma}_x + i\hat{\sigma}_y\right) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \ , \ \hat{\sigma}_- \equiv \frac{1}{2}\left(\hat{\sigma}_x - i\hat{\sigma}_y\right) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{4.19}$$

whose action on the spin eigenstates is

$$\hat{\sigma}_+|\downarrow\rangle = |\uparrow\rangle \ ; \ \hat{\sigma}_+|\uparrow\rangle = 0 \ ; \ \hat{\sigma}_-|\downarrow\rangle = 0 \ ; \ \hat{\sigma}_-|\uparrow\rangle = |\downarrow\rangle \ ; \ \hat{\sigma}_z|\uparrow\rangle = |\uparrow\rangle \ ; \ \hat{\sigma}_z|\downarrow\rangle = -|\downarrow\rangle \ . \tag{4.20}$$

To simplify the writing we indicated with $|\uparrow\rangle$ the spin wave function with $1/2$ projection on the quantization, z, axis, and with $|\downarrow\rangle$ that with $-1/2$ components.
We express the scalar product between two spin operators as sum of lowering and rising operators

$$\hat{\boldsymbol{\sigma}}(1)\cdot\hat{\boldsymbol{\sigma}}(2) = 2\left[\hat{\sigma}_+(1)\hat{\sigma}_-(2) + \hat{\sigma}_+(2)\hat{\sigma}_-(1)\right] + \hat{\sigma}_z(1)\hat{\sigma}_z(2) \ . \tag{4.21}$$

By considering, for example, the case of three fermions we obtain

$$\hat{\boldsymbol{\sigma}}(1)\cdot\hat{\boldsymbol{\sigma}}(2) \begin{pmatrix} (\downarrow_1\downarrow_2\downarrow_3) \\ (\uparrow_1\downarrow_2\downarrow_3) \\ (\downarrow_1\uparrow_2\downarrow_3) \\ (\uparrow_1\uparrow_2\downarrow_3) \\ (\downarrow_1\downarrow_2\uparrow_3) \\ (\uparrow_1\downarrow_2\uparrow_3) \\ (\downarrow_1\uparrow_2\uparrow_3) \\ (\uparrow_1\uparrow_2\uparrow_3) \end{pmatrix} = \begin{pmatrix} (\downarrow_1\downarrow_2\downarrow_3) \\ 2(\downarrow_1\uparrow_2\downarrow_3) - (\uparrow_1\downarrow_2\downarrow_3) \\ 2(\uparrow_1\downarrow_2\downarrow_3) - (\downarrow_1\uparrow_2\downarrow_3) \\ (\uparrow_1\uparrow_2\downarrow_3) \\ (\downarrow_1\downarrow_2\uparrow_3) \\ 2(\downarrow_1\uparrow_2\uparrow_3) - (\uparrow_1\downarrow_2\uparrow_3) \\ 2(\uparrow_1\downarrow_2\uparrow_3) - (\downarrow_1\uparrow_2\uparrow_3) \\ (\uparrow_1\uparrow_2\uparrow_3) \end{pmatrix} \ , \tag{4.22}$$

where we used the subindexes to identify the particle, and in the round parentheses we put the product of three spin eigenstates.

The calculation of the energy does not present formal problems and consists in evaluating the expectation value of the hamiltonian

$$E = \langle\hat{H}\rangle = \frac{\langle\Psi_{\rm T}|\hat{H}|\Psi_{\rm T}\rangle}{\langle\Psi_{\rm T}|\Psi_{\rm T}\rangle} \ . \tag{4.23}$$

The variational principle is applied by searching for the minimum of this energy functional. The parts of the the many-body wave function which can variate are the single particle wave functions ϕ_i forming the Slater determinant and the scalar functions f of the correlation.

In the calculation of the energy (4.23), or more in general of the expectation value of any operator $\hat{\mathcal{O}}$, the module of the wave function $|\Psi|^2$ plays the role of the weight function $P(x)$ introduced in the previous section. The wave function Ψ of a fermionic system is antisymmetric for the exchange of two particles. This means that the by exchanging two particles the wave function changes sign. Since Ψ is a continuous function of the space coordinates, there are values of $\mathbf{R}$ for which the wave function is zero, and, obviously, also its square modulus is zero. Evidently, these points, where $P(x)$ is zero, create problems in the calculation of the integral (4.11). This problem, know in the literature as sign problem, is tackled by using approximate techniques. This includes in the calculation of fermionic systems some assumptions absent in the bosonic case.

4.3 Green Function Monte Carlo (GFMC)

The theoretical limitations of the VMC calculations are related to the need of choosing specific expression of the trial wave function. In the case above discussed this is the expression (4.12) proposing a trial wave function formed by a single Slater determinant multiplied by a correlation function which also has a peculiar expression. The GFMC technique solves the Schrödinger equation without making any assumption on the expression of the many-body wave function. This technique is independent of parameters or assumptions on he form of the wave function, it depends only on the hamiltonian, i.e. on the interaction.

A trial wave function can be expressed as linear combination of eigenstates of the hamitonian $\hat{H}$

$$|\Psi_{\mathrm{T}}\rangle = \sum_n D_n |\Psi_n\rangle \ , \tag{4.24}$$

wehre the D_n coefficients are numbers. We construct an operator which applied to the trial wave function isolates the $|\Psi_n\rangle$ with the smallest energy eigenvalue. We use an evolution operator whose evolution parameter τ has the dimension of an imaginary time. We apply this operator to the trial wave function, and we carry out the asymptotic limit of τ. We obtain

$$\lim_{\tau\to\infty} e^{-\frac{\hat{H}-E_0}{\hbar}\tau}|\Psi_{\mathrm{T}}\rangle = \lim_{\tau\to\infty} e^{-\frac{\hat{H}-E_0}{\hbar}\tau}\sum_n D_n|\Psi_n\rangle = \lim_{\tau\to\infty}\sum_n e^{-\frac{E_n-E_0}{\hbar}\tau} D_n|\Psi_n\rangle = D_0|\Psi_0\rangle \ , \tag{4.25}$$

this because for $n \neq 0$ $E_n > E_0$, where E_0 is the smallest eigenvalue. If the set of quantum numbers characterising the $|\Psi_n\rangle$ states is the same of those which describe the ground state of the system, then E_0 is the ground state energy.

The evolution of a state in coordinates representation $|\boldsymbol{R}\rangle$ for small increments, $d\tau$, of the imaginary time an be expressed as

$$\Psi(\boldsymbol{R},\tau+d\tau) \equiv \langle \boldsymbol{R}|\Psi(\tau+d\tau)\rangle = \langle \boldsymbol{R}|e^{-(H-E_0)\frac{d\tau}{\hbar}}|\Psi(\tau)\rangle = \int d\boldsymbol{R}' \underbrace{\langle \boldsymbol{R}|e^{-(H-E_0)\frac{d\tau}{\hbar}}|\boldsymbol{R}'\rangle}_{\text{propagator}}\langle \boldsymbol{R}'|\Psi(\tau)\rangle \ , \tag{4.26}$$

where we used the completeness

$$\int d\boldsymbol{R}'|\boldsymbol{R}'\rangle\langle\boldsymbol{R}'| = 1 \ .$$

We consider the hamiltonian $\hat{H} = \hat{T}+\hat{V}$, and we make the assumption that the potential $\hat{V}$ is diagonal in $\boldsymbol{R}$, in other words that the potential is local. This means that the operator terms forming the potential do not contain derivatives with respect to $\boldsymbol{R}$. This is one of the essential requirements of the Monte Carlo

calculations. In order to simplify the calculations it is convenient to use an approximated expression, named Trotter-Suzuki formula, of the evolution operator.

$$e^{-(\hat{T}+\hat{V}-E_0)\frac{d\tau}{\hbar}} = e^{-\frac{1}{2}(\hat{V}-E_0)\frac{d\tau}{\hbar}} e^{-\hat{T}\frac{d\tau}{\hbar}} e^{-\frac{1}{2}(\hat{V}-E_0)\frac{d\tau}{\hbar}} + O(d\tau^3) \ , \tag{4.27}$$

which is valid when

$$|d\tau^3(\hat{T}\hat{V} - \hat{V}\hat{T})| \ll 1 \ . \tag{4.28}$$

By using the Trotter-Suzuki formula, and neglecting the terms in $d\tau^3$, we obtain

$$\begin{aligned}\Psi(\boldsymbol{R}, \tau + d\tau) &\simeq \int \langle \boldsymbol{R}|e^{-\frac{1}{2}(\hat{V}-E_0)\frac{d\tau}{\hbar}}|\boldsymbol{R}\rangle\langle \boldsymbol{R}|e^{-\hat{T}\frac{d\tau}{\hbar}}|\boldsymbol{R}'\rangle\langle \boldsymbol{R}'|e^{-\frac{1}{2}(\hat{V}-E_0)\frac{d\tau}{\hbar}}|\boldsymbol{R}'\rangle\Psi(\boldsymbol{R}', \tau)d\boldsymbol{R}' \\ &= \int e^{-\left[\frac{1}{2}(\hat{V}(\mathbf{R})+\hat{V}(\mathbf{R}'))-E_0\right]\frac{d\tau}{\hbar}} \langle \boldsymbol{R}|e^{-\hat{T}\frac{d\tau}{\hbar}}|\boldsymbol{R}'\rangle\Psi(\boldsymbol{R}', \tau)\, d\boldsymbol{R}' \ . \end{aligned} \tag{4.29}$$

The calculation of the evolution propagator defined in Eq. (4.25) is presented in the box here below.

We define the propagators

$$G_{\rm V}(\boldsymbol{R} \leftarrow \boldsymbol{R}') = e^{-\left[\frac{1}{2}(\hat{V}(\mathbf{R})+\hat{V}(\mathbf{R}'))-E_0\right]\frac{d\tau}{\hbar}} \ , \tag{4.30}$$

$$G_0(\boldsymbol{R} \leftarrow \boldsymbol{R}') = \langle \boldsymbol{R}|e^{-\hat{T}\frac{d\tau}{\hbar}}|\boldsymbol{R}'\rangle \ . \tag{4.31}$$

We obtain the expression of the free propagator G_0 by using a Schrödinger-like equation depending on the imaginary time τ,

$$\hbar\frac{\partial}{\partial\tau}\Phi(\boldsymbol{R}, \tau) - \frac{\hbar^2}{2m}\nabla^2\Phi(\boldsymbol{R}, \tau) = 0 \ . \tag{4.32}$$

Let's formally solve this equation by using the Fourier transform of Φ in $n = 3A$ dimensions

$$\tilde{\Phi}(\boldsymbol{K}, \tau) = \int d\boldsymbol{R}\, e^{-i\mathbf{K}\cdot\mathbf{R}}\Phi(\boldsymbol{R}, \tau) \ , \tag{4.33}$$

which satisfies the equation

$$\hbar\frac{\partial}{\partial\tau}\tilde{\Phi}(\boldsymbol{K}, \tau) + \frac{\hbar^2\boldsymbol{K}^2}{2m}\tilde{\Phi}(\boldsymbol{K}, \tau) = 0 \ , \tag{4.34}$$

with

$$\tilde{\Phi}(\boldsymbol{K}, \tau) = \tilde{\Phi}(\boldsymbol{K}, 0)\exp\left(-\frac{\hbar^2K^2}{2m}\frac{\tau}{\hbar}\right) = \tilde{\Phi}(\boldsymbol{K}, 0)\tilde{g}(\boldsymbol{K}, \tau) \ , \tag{4.35}$$

where we defined

$$\tilde{g}(\boldsymbol{K}, \tau) = \exp\left(-\frac{\hbar K^2}{2m}\tau\right) \ . \tag{4.36}$$

For the folding theorem of the Fourier transforms, Eq. (4.35) can be considered as the result of the folding product between Φ and g expressed in coordinates space, therefore, we can write

$$\Phi(\boldsymbol{R}, \tau) = \int \Phi(\boldsymbol{R}', 0)g(\boldsymbol{R}' - \boldsymbol{R}, \tau)d\boldsymbol{R}' \ , \tag{4.37}$$

This expression allows us to obtain g in coordinates space as anti-transform

$$g(\boldsymbol{R}, \tau) = \frac{1}{(2\pi)^n}\int d\boldsymbol{K}e^{i\mathbf{K}\cdot\mathbf{R}}e^{-\frac{\hbar\tau}{2m}K^2} = \frac{\exp\left(-2mR^2/4\hbar\tau\right)}{(2\frac{\hbar\tau}{2m})^{n/2}} \ , \tag{4.38}$$

therefore

$$\Phi(\boldsymbol{R}, \tau) = \frac{1}{(\hbar\tau/m)^{n/2}}\int d\boldsymbol{R}' \exp\left[-\frac{m}{2\hbar\tau}(\boldsymbol{R} - \boldsymbol{R}')^2\right]\Phi(\boldsymbol{R}', 0) \ , \tag{4.39}$$

The free propagator can be expressed as

$$G_0(\boldsymbol{R} \leftarrow \boldsymbol{R}', \tau) = \left(\frac{\hbar\tau}{m}\right)^{-n/2}\exp\left[-\frac{m}{2\hbar\tau}(\boldsymbol{R} - \boldsymbol{R}')^2\right] \ . \tag{4.40}$$

By using the expressions of the free and interacting propagators, the evolution of the wave function given in Eq. (4.29) can be expressed as

$$\Psi(\boldsymbol{R},\tau+\Delta\tau) \simeq \int d\boldsymbol{R}' \exp\left\{\left[-\frac{1}{2}\left(\hat{V}(\boldsymbol{R}')+\hat{V}(\boldsymbol{R})\right)-E_0\right]\frac{\Delta\tau}{\hbar}\right\} \times\left(\frac{\hbar}{m}\Delta\tau\right)^{-n/2}\exp\left[-\frac{m}{2\hbar\Delta\tau}(\boldsymbol{R}-\boldsymbol{R}')^2\right]\Psi(\boldsymbol{R}',\tau)\ . \quad (4.41)$$

To calculate the expectation value of an operator it is common use to adopt a mixed representation where both the trial and the time evolved states are present. By naming $\boldsymbol{R}_n$ the set of space coordinates at the time τ_n and

$$\mathbf{P}_n = \boldsymbol{R}_n\boldsymbol{R}_{n-1}\boldsymbol{R}_{n-2}\cdots\boldsymbol{R}_0\ , \quad (4.42)$$

we express the expectation values of the operator $\hat{\mathcal{O}}$ in the mixed representation as

$$\langle\hat{\mathcal{O}}\rangle_{\rm mix} = \frac{\langle\Psi_{\rm T}|\hat{\mathcal{O}}|\Psi(\tau)\rangle}{\langle\Psi_{\rm T}|\Psi(\tau)\rangle} = \frac{\int d\mathbf{P}_n\Psi_{\rm T}^\dagger(\boldsymbol{R}_n)\,\hat{\mathcal{O}}\,G(\boldsymbol{R}_n,\boldsymbol{R}_{n-1})\cdots G(\boldsymbol{R}_1,\boldsymbol{R}_0)\Psi_{\rm T}(\boldsymbol{R}_0)}{\int d\mathbf{P}_n\Psi_{\rm T}^\dagger(\boldsymbol{R}_n)G(\boldsymbol{R}_n,\boldsymbol{R}_{n-1})\cdots G(\boldsymbol{R}_1,\boldsymbol{R}_0)\Psi_{\rm T}(\boldsymbol{R}_0)}\ , \quad (4.43)$$

where the propagator G is given by the product of G_V and G_0. With good approximation the expectation value of $\hat{\mathcal{O}}$ is given by

$$\langle\hat{\mathcal{O}}\rangle \simeq \langle\hat{\mathcal{O}}\rangle_{\rm mix} + \left[\langle\hat{\mathcal{O}}\rangle_{\rm mix} - \langle\hat{\mathcal{O}}\rangle_{\rm T}\right]\ . \quad (4.44)$$

Method	Trial wave function	Energy (K)
VMC	McMillan	-5.72(2)
VMC	PPA	-5.93(1)
VMC	Shadow	-6.24(4)
VMC	McMillan + 3B	-6.65(2)
VMC	OPT + 3B	-6.79(1)
GFMC	McMillan	-7.12(3)
Exp.	-	-7.14

Table 4.2: Energies, expressed in K, of liquid He^4 calculated with VMC and GFMC by using different types of trial wave functions. Exp. inidicates the experimental value of the energy. Data taken from Ref. [Sch92].

As examples of Monte Carlo calculations, we compare in Tables 4.2 and 4.3 the binding energies of liquid helium systems obtained in VMC and GFMC calculations by using different types of trial wave functions. The results show a great sensitivity of the VMC results to the choice of the trial wave function $\Psi_{\rm T}$. The GFMC results are independent of this choice and they produce smaller energies than those obtained by VMC calculations. This is a quantitive confirmation of the limitation of the use of the variational principle. The bosonic liquid, He^4 is more bound than the fermionic one, He^3. The agreement between the GFMC results and the experimental value is spectacular.

Similar calculations have been done for light nuclei. We summarize the GFMC results for the ground states of some light nuclei of Ref. [Car15]. The blue points have been obtained by considering only a two-body nucleon-nucleon interaction, the Argonne V18. The red points show the results obtained when three-body terms of the interaction are included in the nuclear hamiltonian. The tree-body interaction increases the binding of the system and produces an excellent agreement with the experimental values.

Method	Trial wave function	Energy (K)
VMC	McMillan	-1.08(2)
VMC	2B + 3B	-1.61(3)
VMC	2B + BF	-1.55(4)
VMC	2B + 3B + BF	-2.15(3)
GFMC	2B + 3B + BF	-2.44(4)
Exp.	-	-2.47

Table 4.3: Energies, expressed in K, of liquid He^3 calculated with VMC and GFMC by using different types of trial wave functions. Exp. inidicates the experimental value of the energy. Data taken from Ref. [Sch92].

The results of the GFMC calculations provide a quantitative, and positive, answer to the question about the validity of the assumptions done to tackle the many-body problem, those assumptions discussed in Chapter 1. The Schrödinger equation can describe well many-body systems in a non-relativistic regime. The essential point is that no approximation must be done. Even one simple approximation, such as that related to variational principle, can destroy this good description of the many-body system. Unfortunately, GFMC method has strong computational limitations, therefore it is necessary to develop approximated methods of solution of the many-body Schrödinger equation. Knowing, and controlling, these approximation is essential for the application of these theories.

4.4 Auxiliary Field Diffusion Monte Carlo (AFDMC)

The GFMC method is very powerful in describing nuclear systems up to ^{12}C. The main limitation of this method is the computational effort which increases exponentially with the particle numbers, because of the number of spin and isospin configurations. In the expression (4.41) of the wave function calculated at the time $\tau + \Delta\tau$, $\hat{V}(\boldsymbol{R})$ appears in the exponents. The potential contains terms which quadratically depends on the spin and on the isospin of the interacting particles. The quadratic form is because two particle are involved in the interaction, the terms of the tree-body force are even more complicated. These terms are the responsible of of the rapid increase of number of spin, and isospin, configurations.

This problem is tackled by using an approximated expression, called Hubbard-Stratonovich transformation. In this expression, the propagators containing quadratic operator terms can be written, approximatively, as propagators containing only linear terms of the operator

$$e^{-dt\frac{\hat{\mathcal{O}}^2}{2}} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2}} e^{-x\,\hat{\mathcal{O}}\sqrt{-dt}} \tag{4.45}$$

where the variables x are called auxiliary fields, and $\hat{\mathcal{O}}$ is a generic operator.

In order to use the expression (4.45) it is useful to rewrite the, local, interaction (4.17) separating the scalar part (SI), independent of the spin and of the isospin, from the spin and isospin dependent part (SD)

$$\hat{V}(i,j) = \hat{V}_{\rm SI}(i,j) + \hat{V}_{\rm SD}(i,j) \tag{4.46}$$

where the $V_{\rm SD}$ term contains the full operator dependence with $\hat{O}_{ij}^{p>1}$.

By using various transformation it is possible to rewrite the part of the interaction which depends on the operators, $V_{\rm SD}(i,j)$, such as the operator dependence can be expressed as

$$\hat{V}_{\rm SD}(i,j) \simeq \sum_n \lambda_n \hat{\mathcal{O}}_n^2 \tag{4.47}$$

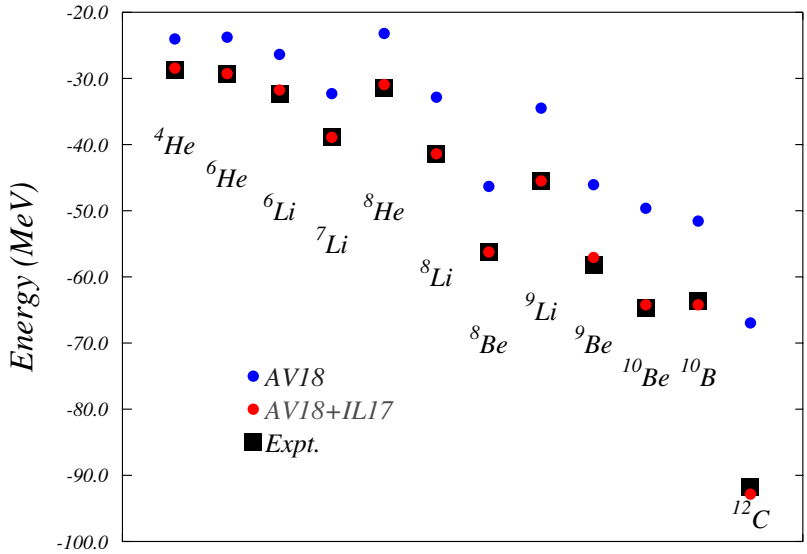

Figure 4.3: GFMC results for some nuclei [Car15]. The blu points show the energies obtained by considering only a two-body interaction (Argonne V18). The red points include the three-body interaction (IL-17). The black points show the experimental values.

where the λ_n coefficient are numbers.

Let's consider the operator dependent part of the two-body interaction

$$\begin{aligned}\hat{V}_{\rm SD}(i,j) &= \frac{1}{2}\sum_{i\alpha j\beta}\hat{\sigma}_\alpha(i)A^{(\sigma)}_{i\alpha j\beta}\hat{\sigma}_\beta(j) + \frac{1}{2}\sum_{i\alpha j\beta}\hat{\sigma}_\alpha(i)A^{(\sigma\tau)}_{i\alpha j\beta}\hat{\sigma}_\beta(j)\hat{\boldsymbol{\tau}}(i)\cdot\hat{\boldsymbol{\tau}}(j) \\ &+ \frac{1}{2}\sum_{ij}A^{(\tau)}_{ij}\hat{\boldsymbol{\tau}}(i)\cdot\hat{\boldsymbol{\tau}}(j) \qquad (4.48)\end{aligned}$$

where the labels i and j indicate the interacting fermions and α e β the cartesian coordinates. The $A^{(\sigma)}$ and $A^{(\sigma\tau)}$ matrices have $3A\times 3A$ components while the $A^{(\tau)}$ has $A\times A$ components. The elements of these matrices can be expressed in terms of the scalar functions of the definition (4.17) of the interaction:

$$A^{(\sigma)}_{i\alpha j\beta} = v_3(r_{ij})\delta_{\alpha\beta} + v_5(r_ij)(3\hat{r}^\alpha_{ij}\hat{r}^\beta_{ij} - \delta_{\alpha\beta}) \qquad (4.49)$$

$$A^{(\sigma\tau)}_{i\alpha j\beta} = v_4(r_{ij})\delta_{\alpha\beta} + v_6(r_ij)(3\hat{r}^\alpha_{ij}\hat{r}^\beta_{ij} - \delta_{\alpha\beta}) \qquad (4.50)$$

$$A^{(\tau)}_{ij} = v_2(r_{ij}) \qquad (4.51)$$

The A matrices are zero along the diagonal, for $i = j$, in order to avoid self-interaction. They are real and symmetric, and have real eigenvalues and eigenvectors which can be expressed as

$$\sum_{j\beta} A^{(\sigma)}_{i\alpha j\beta}\psi^{(\sigma)}_{n,j\beta} = \lambda^{(\sigma)}\psi^{(\sigma)}_{n,i\alpha} \quad (4.52)$$

$$\sum_{j\beta} A^{(\sigma\tau)}_{i\alpha j\beta}\psi^{(\sigma\tau)}_{n,j\beta} = \lambda^{(\sigma\tau)}\psi^{(\sigma\tau)}_{n,i\alpha} \quad (4.53)$$

$$\sum_{j\beta} A^{(\tau)}_{i\alpha j\beta}\psi^{(\tau)}_{n,j\beta} = \lambda^{(\tau)}\psi^{(\tau)}_{n,i\alpha} \quad (4.54)$$

It is possible to define new operators of the type

$$\hat{\mathcal{O}}^{(\sigma)}_{n} = \sum_{j\beta} \hat{\sigma}_\beta(j)\psi^{(\sigma)}_{n,j\beta} \quad (4.55)$$

$$\hat{\mathcal{O}}^{(\sigma\tau)}_{n\alpha} = \sum_{j\beta} \hat{\tau}(i)_\alpha\hat{\sigma}_\beta(j)\ \psi^{(\sigma\tau)}_{n,j\beta} \quad (4.56)$$

$$\hat{\mathcal{O}}^{(\tau)}_{n\alpha} = \sum_{j} \hat{\tau}(j)_\alpha\psi^{(\tau)}_{n,j} \quad (4.57)$$

The potential $\hat{V}_{\rm SD}$ can be rewritten as

$$\begin{aligned}\hat{V}_{\rm SD}(i,j) &= \frac{1}{2}\sum_{n=1}^{3A}(\hat{\mathcal{O}}^{(\sigma)}_n)^2\lambda^{(\sigma)}_n \\ &+ \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A}(\hat{\mathcal{O}}^{(\sigma\tau)}_{n\alpha})^2\lambda^{(\sigma\tau)}_n \\ &+ \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A}(\hat{\mathcal{O}}^{(\tau)}_{n\alpha})^2\lambda^{(\sigma\tau)}_n \end{aligned} \quad (4.58)$$

In this way it is possible to use the Hubbard-Stratonovich expression (4.45) and to rewrite Eq. (4.41) as

$$\begin{aligned}\Psi(\boldsymbol{R},\tau+\Delta\tau) \simeq & \int d\boldsymbol{R}'\left(\frac{\hbar}{m}\Delta\tau\right)^{-n/2}\exp\left[-\frac{m}{2\hbar\Delta\tau}(\boldsymbol{R}-\boldsymbol{R}')^2\right] \\ & \exp\left\{\left[-\frac{1}{2}\left(\hat{V}_{\rm SI}(\boldsymbol{R}')+\hat{V}_{\rm SI}(\boldsymbol{R})\right)-E_0\right]\frac{\Delta\tau}{\hbar}\right\} \\ & \times\prod_{n=1}^{15}\frac{1}{\sqrt{2\pi}}\int dx_n e^{-\frac{x_n^2}{2}}e^{-x\,\hat{\mathcal{O}}\sqrt{-\lambda_n\Delta t}}\ \Psi(\boldsymbol{R}',\tau)\end{aligned} \quad (4.59)$$

where the dependence on $\boldsymbol{R}'$ in the last term is inserted in the λ_n.

The key difference between the expressions (4.41) and (4.59) is the presence, in the latter expression, of an additional integral on the x_n variable, called auxiliary field. The effort in calculating this additional integral is compensated by the linear presence of the $\hat{\mathcal{O}}$ reducing enormously the number of spin and isospin configurations to be calculated.

The AFDMC allows calculations of nuclear systems with a number of particles larger than 12. There are difficulties in treating systems composed by particles of different type, in the nuclear case this is related to the presence of the isospin terms. For this reason systems containing only neutrons are favorite. Results obtained with a finite number of neutrons (66) have been compared with those obtained by other microscopic theories treating infinite neutron matter [Car15]. The comparison indicates a convergence of the results obtained with different theories for this specific system.

Part III

Theories inspired to Quantum Field Theories

Chapter 5

Occupation number representation

5.1 Slater determinants

The use of creation and destruction operators has been introduced in Quantum Field Theories where the number of particles is not constant, since it is possible to create particle-antiparticle pairs. Non relativistic Quantum Mechanics treats phenomena whose energetics are much smaller than the particles rest masses, therefore the creation of particle-antiparticle pairs is not possible. On the other hand, in the treatment of many-body systems, the formalism developed by using creation and destruction operators is very useful. As we discuss below, the physical meaning of the action of these operators is very different from that defined in field theory.

We consider only the case of fermions. The treatment of bosonic systems is not difficult, even though it is not a straightforward modification of the fermionic case. A system of A identical fermions can be described by the time-independent Schrödinger equation

$$\hat{H}\,\Psi(x_1, x_2 \ldots x_A) = E\,\Psi(x_1, x_2 \ldots x_A) \ , \tag{5.1}$$

where x indicates all the quantum numbers characterizing each particle: position ($\mathbf{r}$), spin (σ), isospin (τ) and eventually other quantum numbers such as flavour, color. Since we deal with fermions, the global wave function Ψ must be antisymmetric for the exchange of two particles:

$$\Psi(\ldots x_i, \ldots, x_j \ldots) = -\Psi(\ldots x_j, \ldots, x_i \ldots) \ . \tag{5.2}$$

Each eigenfunction of $\hat{H}$ can be written as linear combination of a complete system of orthonormal functions forming a basis. For example

$$\Psi = \sum_i C_i \Phi_i \ , \tag{5.3}$$

where Φ_i is a Slater determinant and the C_i coefficient is a number. The Slater determinant is built by products of single particle wave functions. As it has been discussed in Chapter 2, these single-particle wave functions, which form a basis, are obtained by solving a single-particle Schrödinger equation:

$$\hat{h}_\nu \phi_\nu(x) = \epsilon_\nu \phi_\nu(x) \ , \tag{5.4}$$

where ν is the set of quantum numbers characterising the single-particle state. These are the three components of the momentum $\mathbf{p}$, in the case of plane waves. For the wave functions in a potential with spherical symmetry they are the principal quantum number n, and those quantum numbers related to the orbital angular momentum l, total angular momentum, j, and its projection m on the quantisation axis quantum numbers

Once the single-particle wave functions ϕ_ν are known the Slater determinant for A particles is built as

$$\Phi(x_1, \dots x_A) = \frac{1}{\sqrt{A!}} \sum_P (-)^P P \phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2)\dots\phi_{\nu_N}(x_A) \ , \tag{5.5}$$

where P indicates the permutations between the indexes of the coordinates. The $\sqrt{A!}$ factor gives the normalisation

$$\langle \Phi \mid \Phi \rangle = 1 \ . \tag{5.6}$$

Eq. (5.5) can be written as

$$\Phi(x_1 \dots x_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{\nu_1}(x_1) & \dots & \phi_{\nu_A}(x_1) \\ \vdots & & \vdots \\ \phi_{\nu_1}(x_A) & \dots & \phi_{\nu_A}(x_A) \end{vmatrix} \ . \tag{5.7}$$

The Slater determinant is eigenstate of a many-body hamiltonian which is sum of single-particle hamiltonians:

$$\sum_\nu \hat{h}_\nu \Phi = \hat{H}_0 \Phi = \mathcal{E}_0 \Phi \ . \tag{5.8}$$

5.2 Creation and destruction operators

The Slater determinant contains redundant information. From the physics point of view, it is important to know whether the state ϕ_ν is occupied or not. The knowledge of what is the fermion occupying this state is not relevant since all the fermions composing the system are identical. The information contained in the Slater determinant can be summarised in a set of ordered numbers indicating which are the occupied single-particle states. It is possible to map this set of ordered numbers to the Slater determinant:

$$|\Phi\rangle \longrightarrow |\nu_A, \nu_{A-1} \dots \nu_1\rangle \ . \tag{5.9}$$

In a commonly used convention, the order of the indexes is that of decreasing values of energies. The ν_A state is that with with highest energy, and so on. This representation of a Slater determinant is usually called Occupation Number Representation (ONR).

It is useful to relate states with different particle numbers. For example, the single-particle state

$$|\phi_\nu\rangle \equiv |\nu\rangle, \tag{5.10}$$

can be imagined as obtained by adding a particle to the vacuum state $|0\rangle$. In symbols

$$|\nu\rangle = \hat{a}^+_\nu |0\rangle, \tag{5.11}$$

where $\hat{a}^+_\nu$ represents the operator which puts a particle on the single-particle state characterized by the ν quantum numbers.

In general one can write:

$$\hat{a}^+_\nu |\nu_A \dots \nu_1\rangle = |\nu\nu_A \dots \nu_1\rangle. \tag{5.12}$$

This state with $A+1$ particles is not necessarily ordered. The newly added particle, ν, must be correctly positioned. This is done by considering that any change of position produces a multiplicative negative phase, this is because we are dealing with a determinant describing a set of fermions. The possible ambiguities on the global sign of the state can be defined by choosing that the sign of the determinant does not change if the new particle remains in the first position, as we have assumed in writing Eq. (5.12).

For example:

$$\hat{a}^+_{\nu_1} |\nu_3\nu_2\rangle = |\nu_1\nu_3\nu_2\rangle = -|\nu_3\nu_1\nu_2\rangle = |\nu_3\nu_2\nu_1\rangle \ . \tag{5.13}$$

It follows from Eq. (5.11) and (5.12) that:

$$|\nu_A \dots \nu_1\rangle = \hat{a}^+_{\nu_A} \hat{a}^+_{\nu_A - 1} \dots \hat{a}^+_{\nu_1} |0\rangle \ . \tag{5.14}$$

For the properties of the Slater determinant we have that:

$$\hat{a}^+_\nu |\nu_A \dots \nu \dots \nu_1\rangle = 0 \ . \tag{5.15}$$

This operation inserts in a determinant a row, or a column, equal to a row, or a column already present. From the physics point of view Eq. (5.15) expresses the Pauli exclusion principle.

From what we have presented so far, it possible to deduce that the creation operators have the following anti-commutation properties

$$\hat{a}^+_{\nu_1} \hat{a}^+_{\nu_2} = -\hat{a}^+_{\nu_2} \hat{a}^+_{\nu_1} \ . \tag{5.16}$$

Let's demonstrate the validity of Eq. (5.16). We assume $\nu > \nu'$

$$\begin{aligned} \hat{a}^+_\nu \hat{a}^+_{\nu'} \Phi^A(A \dots \quad \dots 1) &= \theta^I_{\nu'} \hat{a}^+_\nu \Phi^{A+1}(A \dots \nu' \dots 1) = \theta^I_\nu \theta^I_{\nu'} \Phi^{A+2}(A \dots \nu \dots \nu' \dots 1) \ , \\ \hat{a}^+_{\nu'} \hat{a}^+_\nu \Phi^A(A \dots \quad \dots 1) &= \theta^{II}_\nu \hat{a}^+_{\nu'} \Phi^{A+1}(A \dots \nu \dots 1) = \theta^{II}_\nu \theta^{II}_{\nu'} \Phi^{A+2}(A \dots \nu \dots \nu' \dots 1) \ . \end{aligned} \tag{5.17}$$

We indicated with $\theta^I_\nu = (-)^p \equiv (-1)^p$ the phase acquired by carrying out the necessary permutations to put in the proper position the ν particle, and in analogy $\theta^I_{\nu'} = (-)^{p'}$. The phases obtained in the second case have been indicated as θ^{II}_ν and $\theta^{II}_{\nu'}$. Since $\nu > \nu'$, $\theta^I_\nu = \theta^{II}_\nu$ because the number of permutation to put in order ν is the same in both cases. On the other hand, $\theta^I_{\nu'} = -\theta^{II}_{\nu'}$ since in the second case, an additional permutation has to be done to arrange ν'. Therefore, we obtain

$$\hat{a}^+_\nu \hat{a}^+_{\nu'} \Phi = -\hat{a}^+_{\nu'} \hat{a}^+_\nu \Phi \ , \tag{5.18}$$

from where the relation (5.16) between operators is derived. Obviously Eq. (5.16) implies

$$\left(a^+_\nu\right)^2 = 0 \ , \tag{5.19}$$

which is another way to express Eq. (5.15), i.e. the Pauli exclusion principle.

It is possible to define the adjoint operator of $\hat{a}^+$ whose action can be understood by taking the adjoint of Eq. (5.11).

$$(\hat{a}^+_\nu)^+ = \hat{a}_\nu \ , \tag{5.20}$$

$$|\nu\rangle = \hat{a}^+_\nu |0\rangle \quad ; \quad \langle\nu| = \langle 0|\hat{a}_\nu \ , \tag{5.21}$$

$$\langle \nu_1 \nu_2 \dots \nu_N| = \langle 0|\hat{a}_{\nu_1} \dots \hat{a}_{\nu_{N-1}} \hat{a}_{\nu_N} \ , \tag{5.22}$$

since $\langle\nu|\nu\rangle = 1$ we obtain

$$\langle 0 \underbrace{|\hat{a}_\nu \hat{a}^+_\nu |0\rangle}_{|0\rangle} = 1 \ , \tag{5.23}$$

and therefore,

$$|0\rangle = \hat{a}_\nu \hat{a}^+_\nu |0\rangle = \hat{a}_\nu |\nu\rangle = |0\rangle \ . \tag{5.24}$$

The effect of applying $\hat{a}_\nu$ on the ket state is that of taking out a particle which occupied the $|\nu\rangle$ state. From this the name of destruction operator. Let's analyze the behaviour of $\hat{a}_{\nu_r}$.

$$\hat{a}_{\nu_r} |\nu_A \dots \nu_{r+1} \nu_r \nu_{r-1} \dots \nu_1\rangle = |\nu_A \dots \nu_{r+1} \nu_{r-1} \dots \nu_1\rangle (-)^{r-1} \ . \tag{5.25}$$

Since, by definition, in the vacuum all the single-particle states are empty, we can write

$$\hat{a}_\nu|0\rangle = 0 \ . \tag{5.26}$$

If the vector $|\nu_N \dots \nu_1\rangle$ does not contain the ν state, then

$$\hat{a}_\nu|\nu_A \dots \nu_1\rangle = 0 \ . \tag{5.27}$$

Also in the case of the destruction operators it is possible to show that

$$\hat{a}_{\nu_1}\hat{a}_{\nu_2} = -\hat{a}_{\nu_2}\hat{a}_{\nu_1} \qquad \text{and} \quad \text{therefore} \qquad (\hat{a}_\nu)^2 = 0 \ . \tag{5.28}$$

Analogously, it is possible to demonstrate that, for $\nu_1 \neq \nu_2$, the following relation holds:

$$\hat{a}_{\nu_1}\hat{a}^+_{\nu_2} = -\hat{a}^+_{\nu_2}\hat{a}_{\nu_1} \ . \tag{5.29}$$

By using the properties previously discussed we obtain:

$$\hat{a}_\nu\hat{a}^+_\nu|\nu_A \dots \nu_1\rangle = \begin{cases} 0 & \text{if} \quad \nu \in S \\ |\nu_A \dots \nu_1\rangle & \text{if} \quad \nu \notin S \end{cases} \qquad S = \{\nu_A \dots \nu_1\} \tag{5.30}$$

$$\hat{a}^+_\nu\hat{a}_\nu|\nu_A \dots \nu_1\rangle = \begin{cases} |\nu_A \dots \nu_1\rangle & \text{if} \quad \nu \in S \\ 0 & \text{if} \quad \nu \notin S \end{cases} \tag{5.31}$$

Eqs. (5.30) and (5.31) leads to the relation

$$\left(\hat{a}_\nu\hat{a}^+_\nu + \hat{a}^+_\nu\hat{a}_\nu\right)|\nu_A \dots \nu_1\rangle = |\nu_A \dots \nu_1\rangle \ . \tag{5.32}$$

This relation is valid for any vector $|\nu_A \dots \nu_1\rangle$ since one of the two terms gives a zero result, while the other one reproduces the starting vector.

Eq. (5.31) defines the occupation number operator

$$\hat{n}_\nu = \hat{a}^+_\nu\hat{a}_\nu \ , \tag{5.33}$$

whose eigenvalues are 1 or 0 whether the state to which is applied contains, or not, the single-particle state ν.

The relation between creation and destruction operators given by Eqs. (5.30) and (5.31) is:

$$\hat{a}_\nu\hat{a}^+_\nu + \hat{a}^+_\nu\hat{a}_\nu = 1 \ . \tag{5.34}$$

The relations (5.16), (5.28), (5.29), defining the properties of the creation and destruction operators, can be summarised as:

$$\left\{\hat{a}_\nu, \hat{a}^+_{\nu'}\right\} = \delta_{\nu\nu'} \qquad \{\hat{a}_\nu, \hat{a}_{\nu'}\} = 0 \qquad \left\{\hat{a}^+_\nu, \hat{a}^+_{\nu'}\right\} = 0 \ , \tag{5.35}$$

where the symbol $\{,\}$ indicates the anti-commutator operator.

When the many-body system has rotational symmetry is it convenient to work with operators which have the properties of the irreducible spherical tensors. For this reason, it is convenient the use of creation and destruction operators defined in a slightly different manner, as indicated in the Appendix B.

5.3 One- and two-body operators

We used the ONR to describe state vectors, Slater determinants to be precise, but the approach can continue to describe the operators.

We indicated with $|S\rangle$ and $|S'\rangle$ two vectors described in ONR, and with $|\Phi_S\rangle$ and $|\Phi_{S'}\rangle$ the two corresponding Slater determinants. Let's consider, in the configuration space, a generic many-body operator $\hat{O}_S(x_1 \dots x_A)$. Since the physical quantities which can be measured are related to the expectation value of operators between states, the two representations must provide the same value

$$\langle \Phi_{S'}|\hat{O}_S|\Phi_S\rangle = \langle S'|\hat{O}|S\rangle \ . \tag{5.36}$$

In the study of many-body systems, the most common operators are the one- and two-body operators. In the coordinate space, a one-body operator is given by the sum of operators acting on a single coordinate at the time:

$$\hat{O}^I_S(x_1 \dots x_A) = \sum_{i=1}^{A} \hat{o}^I(x_i) \ . \tag{5.37}$$

The kinetic energy is a typical one-body operator. For simplicity let's use a basis of single-particle wave functions where $\hat{O}^I$ is diagonal

$$\hat{o}^I(x)\phi_\nu(x) = \omega_\nu \phi_\nu(x). \tag{5.38}$$

By using the Slater determinant built on the ϕ_ν states we obtain:

$$\begin{aligned}
\hat{O}^I_S(x_1 \dots x_A)\Phi_S(x_1 \dots x_A) &= \\
&= \frac{1}{\sqrt{A!}} \sum_P (-)^P \sum_{i=1}^{A} \hat{o}^I(x_i)\hat{P}\phi_{\nu_1}(x_1)\dots\phi_{\nu_A}(x_A) = \\
&= \frac{1}{\sqrt{A!}} \sum_P (-)^P \sum_{i=1}^{A} \hat{P}\hat{o}^I(x_i)\phi_{\nu_1}(x_1)\dots\phi_{\nu_A}(x_A) \\
&= \frac{1}{\sqrt{A!}} \sum_P (-)^P \sum_{i=1}^{A} (\omega_{\nu_i}\hat{P}\phi_{\nu_1}(x_1)\dots\phi_{\nu_A}(x_A) \\
&= \sum_{i=1}^{A} \omega_{\nu_i}\Phi_S = \sum_{\nu\ occupied} \omega_\nu \Phi_S = \sum_\nu \omega_\nu n_\nu \Phi_S \ ,
\end{aligned} \tag{5.39}$$

where we have indicated with $\hat{P}$ the operator which makes all the possible P permutations. In the previous equations $n_\nu = 1$ for all the occupied levels and $n_\nu = 0$ for the empty ones. The evaluation of the matrix element is:

$$\begin{aligned}
\langle \Phi_{S'}|\hat{O}^I_S|\Phi_S\rangle &= \langle \Phi_{S'}| \sum_\nu \omega_\nu n_\nu |\Phi_S\rangle = & (5.40)\\
&= \sum_\nu \omega_\nu \langle S'|\hat{n}_\nu|S\rangle = \langle S'|O^I|S\rangle \ , & (5.41)
\end{aligned}$$

where we used the occupation number operator defined in Eq. (5.33). By substituting we obtain

$$\langle S'|O^I|S\rangle = \langle S'| \sum_\nu \omega_\nu \hat{a}^+_\nu \hat{a}_\nu |S\rangle \ , \tag{5.42}$$

and then:

$$\hat{O}^I = \sum_{\nu\nu} \omega_{\nu\nu} \hat{a}^+_\nu \hat{a}_\nu \ , \tag{5.43}$$

where

$$\omega_{\nu\nu} = \int d^3r \phi^*_\nu(\mathbf{r}) \hat{o}^I(\mathbf{r}) \phi_\nu(\mathbf{r}) \ . \tag{5.44}$$

The expression of the one-body operator for a generic single-particle basis is:

$$\hat{O}^I = \sum_{\nu\nu'} O^I_{\nu\nu'} \hat{a}^+_\nu \hat{a}_{\nu'} \tag{5.45}$$

$$O^I_{\nu\nu'} = \int dx \phi^*_\nu(x) \hat{o}^I(x) \phi_{\nu'}(x) \equiv \langle \nu | o^I | \nu' \rangle \tag{5.46}$$

where x is a generalized coordinate, containing space, spin and, eventually, also isospin. This expression shows that the one-body operator takes out a particle in ν' and puts a particle in the ν state. Obviously, ν' must be occupied and ν empty. This action is called creation of a particle-hole pair. In the case where $|S\rangle = |S'\rangle$ the only contributions different from zero are those where $\nu' = \nu$.

Analogous procedure can be used to obtain the ONR expression for the two-body operators, defined as sum of operators acting on two-coordinates at the time:

$$\hat{O}^{II}_S(x_1 \dots x_A) = \sum_{i<j} \hat{o}^{II}(x_i, x_j) = \frac{1}{2} \sum_{i \neq j} \hat{o}^{II}(x_i, x_j) \tag{5.47}$$

A typical example of two-body operator is the interaction potential $\hat{V} = \frac{1}{2} \sum_{i \neq j} V(x_i, x_j)$. In ONR, operators of this type are respresented as:

$$\hat{O}^{II} = \frac{1}{2} \sum_{\nu\nu'\mu\mu'} O^{II}_{\nu\mu\nu'\mu'} \hat{a}^+_\nu \hat{a}^+_\mu \hat{a}_{\mu'} \hat{a}_{\nu'} \ , \tag{5.48}$$

where $O^{II}_{\nu\mu\nu'\mu'}$, which is a number, is defined as:

$$O^{II}_{\nu\mu\nu'\mu'} = \langle \nu\mu | O^{II} | \nu'\mu' \rangle = \int dx dx' \phi^*_\nu(x) \phi^*_\mu(x') \hat{o}^{II}(x, x') \phi_{\nu'}(x) \phi_{\mu'}(x') \ . \tag{5.49}$$

It is worth to remark that the order of the two sub-indexes are inverted in the sequence of the creation and destruction operators with respect to that of the matrix element.

In this case the two-body operator takes out two particles from occupied states and puts them in two empty states.

5.4 Field operators

The creation and destruction operators $\hat{a}^+_\nu$ and $\hat{a}_\nu$ presented here follows the same algebra, defined by the anti-commutation relations (5.35), of the anaolgous operators introduced in the field theory. The physical interpretation of the action of these operators is different in the two theories. In field theory the operators describe the creation and the destruction of particles, as example in the formation of particle-antiparticle pairs. In many-body theory the idea is that the mean-field problem has already been solved, and its solution has provided a basis of single-particle states. The creation operator $\hat{a}^+_\nu$ puts a particle on the state characterised by the ν quantum numbers, and $\hat{a}_\nu$ takes out a particle occupying this state.

In field theory the field operator $\hat{\psi}^+(\mathbf{r})$ creates a particle in the point $\mathbf{r}$ and the operator $\hat{\psi}(\mathbf{r})$ destroys a particle positioned in $\mathbf{r}$. It is possible to define this kind of operators also in many-body theory. These

field operator are related to the creation and destruction operators through the single-particle wave functions $\phi_\nu(\mathbf{r})$ generated by the solution of the mean-field problem:

$$\hat{\psi}(\mathbf{r}) = \sum_\nu \hat{a}_\nu \phi_\nu(\mathbf{r}) \ , \tag{5.50}$$

$$\hat{\psi}^+(\mathbf{r}) = \sum_\nu \hat{a}^+_\nu \phi^*_\nu(\mathbf{r}) \ . \tag{5.51}$$

Because of the orthonormality of the ϕ, these two equations can be inverted to express the creation and destruction operators in terms of field operator:

$$\hat{a}_\nu = \int d^3r \phi^*_\nu(\mathbf{r})\hat{\psi}(\mathbf{r}) \qquad \text{and} \qquad \hat{a}^+_\nu = \int d^3r \phi_\nu(\mathbf{r})\hat{\psi}^+(\mathbf{r}) \ . \tag{5.52}$$

By using the anticommutation relations (5.35) in the above definitions, it is possible to obtain analogous relations for the field operators:

$$\left\{\hat{\psi}^+(\mathbf{r}), \hat{\psi}^+(\mathbf{r}')\right\} = 0 \qquad \left\{\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')\right\} = 0 \qquad \left\{\hat{\psi}^+(\mathbf{r}), \hat{\psi}(\mathbf{r}')\right\} = \delta(\mathbf{r}-\mathbf{r}') \ . \tag{5.53}$$

The one- and two-body operators can be expressed in terms of field operators as:

$$\hat{O}^I = \int d^3r \, \hat{\psi}^+(\mathbf{r})\hat{o}^I(\mathbf{r})\hat{\psi}(\mathbf{r}) \ , \tag{5.54}$$

$$\hat{O}^{II} = \frac{1}{2}\int d^3r d^3r' \, \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r}')\hat{o}^{II}(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) \ . \tag{5.55}$$

The hamiltonian operator can be written in terms of creation and destruction operators or in terms of field operators:

$$\hat{H} = = \sum_{\nu\nu'} \langle\nu|\hat{T}|\nu'\rangle \hat{a}^+_\nu \hat{a}_{\nu'} + \frac{1}{2}\sum_{\nu\nu'\mu\mu'} \langle\nu\mu|\hat{V}|\nu'\mu'\rangle \hat{a}^+_\nu \hat{a}^+_\mu \hat{a}_{\mu'}\hat{a}_{\nu'} \ , \tag{5.56}$$

$$= \int d^3r \hat{\psi}^+(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d^3r d^3r' \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) \ . \tag{5.57}$$

Chapter 6

Perturbation theory of many-body systems

6.1 Pictures

The values of the observable quantities, in Quantum Mechanics, are obtained by calculating expectation values of operators between states. These quantities are invariant if the same unitary transformation is applied to the states and to the operators. These unitary transformations can contain the time and, for example, they can transform states which depend on time in time-independent states. In this latter case, the dependence on the time is inserted in the operator expressions. These time-dependent unitary transformations are called **pictures** of the Quantum Mechanics.

Schrödinger picture

The most used picture is that of Schrödinger where the states describing the system depend on the time, while the operators are time-independent. In this picture, the time evolution of the system is described by the equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle = \hat{H}|\Psi_S(t)\rangle \ , \tag{6.1}$$

which is the well known time-dependent Schrödinger equation.

For those system where the energy is conserved, the hamilton operator $\hat{H}$ does not depend on the time. In this case, the formal solution of Eq. (6.1) is:

$$|\Psi_S(t)\rangle = e^{-i\frac{\hat{H}(t-t_0)}{\hbar}}|\Psi_S(t_0)\rangle \ . \tag{6.2}$$

In this equation the exponential function of an operator is present. The action of this function on the state $|\Psi_S(t_0)\rangle$ can be expressed in terms of a power expansion of the exponential. In addition, since $\hat{H}$ is an hermitian operator, $e^{\frac{i}{\hbar}\hat{H}t}$ is a unitary operator.

The Eq. (6.2) allows us to know the solution of the Schrödinger equation at any time t once the state of the system is known at a specific time value t_0.

Heisenberg picture

In this picture, the states are time-independent, while the operators have an explicit time dependence. The states in the Heisenberg picture are related to those of the Schrödinger picture by the relation

$$|\Psi_H(t)\rangle \equiv e^{i\frac{\hat{H}t}{\hbar}}|\Psi_S(t)\rangle \ . \tag{6.3}$$

The time evolution of these states in the Heisenberg picture is:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi_H(t)\rangle &= -\hat{H}e^{i\frac{\hat{H}t}{\hbar}}|\Psi_S(t)\rangle + e^{i\frac{\hat{H}t}{\hbar}}i\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle = \text{ for (6.1)} \\ &= -\hat{H}e^{i\frac{\hat{H}t}{\hbar}}|\Psi_S(t)\rangle + \hat{H}e^{i\frac{\hat{H}t}{\hbar}}|\Psi_S(t)\rangle = 0 \ . \end{aligned} \tag{6.4}$$

This clearly shows that $|\Psi_H\rangle$ does not depend on time.

The relation between the expressions of the operators in the two pictures is obtained by considering that the expectation values of the operators must be the same:

$$\langle\Psi_S(t)|\hat{O}_S|\Psi_S(t)\rangle = \langle\Psi_H|e^{i\frac{\hat{H}t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}t}{\hbar}}|\Psi_H\rangle \ , \tag{6.5}$$

obviously

$$\hat{O}_H \equiv e^{i\frac{\hat{H}t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}t}{\hbar}} \ . \tag{6.6}$$

The time evolution of the operator provides the equation of motion:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{O}_H(t) &= -\hat{H}e^{i\frac{\hat{H}t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}t}{\hbar}} + e^{i\frac{\hat{H}t}{\hbar}}\hat{O}_S\hat{H}e^{-i\frac{\hat{H}t}{\hbar}} = \\ &= -\hat{H}\hat{O}_H + \hat{O}_H\hat{H} = [\hat{O}_H, \hat{H}] \end{aligned} \tag{6.7}$$

where we exploited the fact that $\hat{H}$ and $e^{i\frac{\hat{H}t}{\hbar}}$ commute. In general, $\hat{O}_H$ and $\hat{H}$ do not commute. In case of commutation, Eq. (6.7) expresses the fact that $\hat{O}_H$ describes a constant of motion.

Interaction picture

This picture, intermediate between that of Heisenberg and that of Schrödinger, is that of main interest in the description of many-body systems.

Let's consider a time-independent hamiltonan in the Schrödinger picture, and let's separate it in two terms

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \ . \tag{6.8}$$

The state vector in the interaction picture is defined as:

$$|\Psi_I(t)\rangle \equiv e^{i\frac{\hat{H}_0 t}{\hbar}}|\Psi_S(t)\rangle \ . \tag{6.9}$$

The time evolution of the state $|\Psi_I(t)\rangle$ is given by:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle &= -\hat{H}_0 e^{i\frac{\hat{H}_0 t}{\hbar}}|\Psi_S(t)\rangle + e^{i\frac{\hat{H}_0 t}{\hbar}}i\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle \\ &= e^{i\frac{\hat{H}_0 t}{\hbar}}\left[-\hat{H}_0 + \hat{H}_0 + \hat{H}_1\right]e^{-i\frac{\hat{H}_0 t}{\hbar}}e^{i\frac{\hat{H}_0 t}{\hbar}}|\Psi_S(t)\rangle \\ &= e^{i\frac{\hat{H}_0 t}{\hbar}}\hat{H}_1 e^{-i\frac{\hat{H}_0 t}{\hbar}}|\Psi_I(t)\rangle = \hat{H}_{1,I}(t)|\Psi_I(t)\rangle \ , \end{aligned} \tag{6.10}$$

where in the second step we used Eq. (6.1). In general, $\hat{H}_1$ and $\hat{H}_0$ do not commute.

Also in this case, the expression of the operators in the interaction picture, in terms of the operator in Schrödinger picture, is obtained by considering that the expectation values must be the same in both pictures:

$$\langle\Psi_S(t)|\hat{O}_S|\Psi_S(t)\rangle = \langle\Psi_I|e^{+i\frac{\hat{H}_0 t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}_0 t}{\hbar}}|\Psi_I\rangle \ , \tag{6.11}$$

from where we obtain the definition:

$$\hat{O}_I(t) = e^{i\frac{\hat{H}_0 t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}_0 t}{\hbar}} \ . \tag{6.12}$$

From the above equations, it appears clear that, in the interaction picture, both states and operators depend on time. The equation of motion in the interaction picture is:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{O}_I(t) &= -\hat{H}_0 e^{i\frac{\hat{H}_0 t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}_0 t}{\hbar}} + e^{i\frac{\hat{H}_0 t}{\hbar}}\hat{O}_S\hat{H}_0 e^{-i\frac{\hat{H}_0 t}{\hbar}} \\ &= e^{i\frac{\hat{H}_0 t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}_0 t}{\hbar}}\hat{H}_0 - \hat{H}_0 e^{i\frac{\hat{H}_0 t}{\hbar}}\hat{O}_S e^{-i\frac{\hat{H}_0 t}{\hbar}} \\ &= \hat{O}_I\hat{H}_0 - \hat{H}_0\hat{O}_I = \left[\hat{O}_I(t), \hat{H}_0\right] \ . \end{aligned} \tag{6.13}$$

Since in the ONR all the operators can be expressed in terms of creation and destruction operators, it is convenient to obtain the expressions of these operators in the interaction picture. In order to simplify the calculation we consider a special situation where $\hat{H}_0$ is a one-body operator diagonal in the chosen single-particle basis:

$$\hat{H}_0 = \sum_k \hbar\omega_k \hat{a}_k^+ \hat{a}_k \ . \tag{6.14}$$

The equation of motion for an operator in the interaction picture is

$$\begin{aligned} i\hbar\frac{d}{dt}\hat{a}_{I,k}(t) &= e^{i\frac{\hat{H}_0 t}{\hbar}}\left[\hat{a}_{S,k}, \hat{H}_0\right] e^{-i\frac{\hat{H}_0 t}{\hbar}} = e^{i\frac{\hat{H}_0 t}{\hbar}}\left[\hat{a}_{S,k}, \sum_{k'}\hbar\omega_{k'}\hat{a}^+_{S,k'}\hat{a}_{S,k'}\right] e^{-i\frac{\hat{H}_0 t}{\hbar}} \\ &= e^{i\frac{\hat{H}_0 t}{\hbar}}\sum_{k'}\left[\hat{a}_{S,k}, \hat{a}^+_{S,k'}\hat{a}_{S,k'}\right] e^{-i\frac{\hat{H}_0 t}{\hbar}}\hbar\omega_{k'} \ , \end{aligned}$$

where I and S indicate the interaction and Schrödinger pictures respectively. The term in parentheses becomes:

$$[\hat{a}_{S,k}\hat{a}^+_{S,k'}\hat{a}_{S,k'} - \hat{a}^+_{S,k'}(-\hat{a}_{S,k}\hat{a}_{S,k'})] = [\hat{a}_{S,k}\hat{a}^+_{S,k'}\hat{a}_{S,k'} - (-\delta_{kk'}\hat{a}_{S,k'} + \hat{a}_{S,k}\hat{a}^+_{S,k'}\hat{a}_{S,k'})] = \hat{a}_{S,k} \ .$$

We have then:

$$i\hbar\frac{d}{dt}\hat{a}_{k,I}(t) = \hbar\omega_k\hat{a}_{k,I}(t) \ , \tag{6.15}$$

and, by assuming $\hat{a}_I(t=0) = \hat{a}_S$,

$$\hat{a}_{I,k}(t) = \hat{a}_{S,k}e^{-i\omega_k t} \ . \tag{6.16}$$

For the adjoint operator, we obtain:

$$\hat{a}^+_{I,k}(t) = \hat{a}^+_{S,k}e^{i\omega_k t} \ . \tag{6.17}$$

Since the time dependence is present only in the complex phase, the (anti-)commutation properties of the creation and destruction operators in the interaction picture are the same as those in the Schrödinger picture.

In order to obtain the expression of the whatever operator in the interaction picture, it is enogh to substitute the $\hat{a}_k$ with $\hat{a}_{I,k}(t)$ and analogously with the creation operators. Also the field operators can be expressed in terms of $\hat{a}_{S,k}$ and $\hat{a}^+_{S,k}$, therefore their expressions in the interaction picture can be obtained by using the same procedure.

6.2 Time-evolution operator

We define an operator $\hat{U}(t, t_0)$, the time evolution operator, which determines the state vector at the time t once the state vector is known at the t_0 time

$$|\Psi_I(t)\rangle = \hat{U}(t, t_0)|\Psi_I(t_0)\rangle \ . \tag{6.18}$$

From the definition of state in the interaction picture, and from Eq. (6.2) we can write:

$$\begin{aligned} |\Psi_I(t)\rangle &= e^{i\frac{\hat{H}_0 t}{\hbar}}|\Psi_S(t)\rangle = e^{i\frac{\hat{H}_0 t}{\hbar}}e^{-i\frac{\hat{H}}{\hbar}(t-t_0)}|\Psi_S(t_0)\rangle \\ &= e^{i\frac{\hat{H}_0 t}{\hbar}}e^{-i\frac{\hat{H}}{\hbar}(t-t_0)}e^{-i\frac{\hat{H}_0 t_0}{\hbar}}|\Psi_I(t_0)\rangle \ , \end{aligned}$$

and therefore

$$\hat{U}(t,t_0) \equiv e^{i\frac{\hat{H}_0 t}{\hbar}}e^{-i\frac{\hat{H}(t-t_0)}{\hbar}}e^{-i\frac{\hat{H}_0 t_0}{\hbar}} \ . \tag{6.19}$$

The properties of $\hat{U}(t,t_0)$ can be deduced by the above equation. For example:

$$\hat{U}(t_0,t_0) = 1 \ , \tag{6.20}$$

and

$$\hat{U}^+(t,t_0)\hat{U}(t,t_0) = \hat{U}(t,t_0)\hat{U}^+(t,t_0) = 1 \ , \tag{6.21}$$

which implies

$$\hat{U}^+(t,t_0) = \hat{U}^{-1}(t,t_0) \ , \tag{6.22}$$

and

$$\hat{U}(t_1,t_2)\hat{U}(t_2,t_3) = \hat{U}(t_1,t_3) \ , \tag{6.23}$$

and

$$\hat{U}(t,t_0)\hat{U}(t_0,t) = 1 \qquad \text{which implies} \quad \hat{U}(t_0,t) = \hat{U}^+(t,t_0) \ , \tag{6.24}$$

Eq. (6.19) is not very useful for the calculation of observables. From the computational point of view, the solution of Eq. (6.18) by using the expression (6.19) is equivalente to solve the Schrödinger equation. The usefulness of $\hat{U}(t,t_0)$ is related to the possibility of calculating it by doing a perturbation expansion. In order to acheive this goal it is convenient to use an integral expression of $\hat{U}(t,t_0)$.

Let's rewrite Eq.(6.10) as

$$i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \hat{H}_1(t)|\Psi_I(t)\rangle \tag{6.25}$$

where $\hat{H}_1(t)$ is the term of the hamiltonian in the interaction picture. To simplify the writing we did not write the sub-index I in hamiltonian term which will be understood henceforth. By using Eq. (6.18) we obtain:

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)|\Psi_I(t_0)\rangle = \hat{H}_1(t)\hat{U}(t,t_0)|\Psi_I(t_0)\rangle. \tag{6.26}$$

Since $|\Psi_I(t_0)\rangle$ is different from zero, we can divide by it the above equation and obtain a relation between operators:

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}_1(t)\hat{U}(t,t_0) \ . \tag{6.27}$$

By integrating from t_0 to t we obtain

$$\begin{aligned} \int_{t_0}^{t} i\hbar\frac{\partial}{\partial t'}\hat{U}(t',t_0)dt' &= \int_{t_0}^{t}\hat{H}_1(t')\hat{U}(t',t_0)dt' \\ = i\hbar\left[\hat{U}(t,t_0) - \hat{U}(t_0,t_0)\right] &= \int_{t_0}^{t} dt'\hat{H}_1(t')\hat{U}(t',t_0). \end{aligned}$$

By considering Eq. (6.20) we have:

$$\hat{U}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\hat{H}_1(t')\hat{U}(t',t_0) \tag{6.28}$$

We obtain a formal solution Eq. (6.28) by by inserting its expression of $\hat{U}(t',t_0)$ in the right hand side:

$$\begin{aligned}\hat{U}(t,t_0) &= 1-\frac{i}{\hbar}\int_{t_0}^{t}dt'\hat{H}_1(t')\left[1-\frac{i}{\hbar}\int_{t_0}^{t'}dt''\hat{H}_1(t'')[1-\ldots]\right]\\ \hat{U}(t,t_0) &= 1-\frac{i}{\hbar}\int_{t_0}^{t}dt'\hat{H}_1(t')+\left(\frac{-i}{\hbar}\right)^2\underbrace{\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{H}_1(t')\hat{H}_1(t'')}_{t>t'}+\ldots \end{aligned} \tag{6.29}$$

Let's consider the third term in the right hand side of the above equation:

$$\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{H}_1(t')\hat{H}_1(t'')=\frac{1}{2}\underbrace{\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{H}_1(t')\hat{H}_1(t'')}_{t'>t"}+\frac{1}{2}\underbrace{\int_{t_0}^{t}dt''\int_{t_0}^{t''}dt'\hat{H}_1(t'')\hat{H}_1(t')}_{t">t'} \quad . \tag{6.30}$$

In this expression the dummy indexes of the integration variables have been interchanged. In general, one has

$$\int_a^b dy\int_y^b dx f(x)f(y)=\int_a^b dx\int_a^x dy f(x)f(y) \quad , \tag{6.31}$$

therefore Eq. (6.30) can be written as:

$$\begin{aligned}&\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{H}_1(t')\hat{H}_1(t'')=\\ &\frac{1}{2}\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{H}_1(t')\hat{H}_1(t'')+\frac{1}{2}\int_{t_0}^{t}dt'\int_{t'}^{t}dt''\hat{H}_1(t'')\hat{H}_1(t')=\\ &\frac{1}{2}\int_{t_0}^{t}dt'\int_{t_0}^{t}dt''\left[\hat{H}_1(t')\hat{H}_1(t'')\theta(t'-t'')+\hat{H}_1(t'')\hat{H}_1(t')\theta(t''-t')\right]=\\ &\frac{1}{2}\int_{t_0}^{t}dt'\int_{t_0}^{t}dt''\hat{\mathbb{T}}\left[\hat{H}_1(t')\hat{H}_1(t'')\right] \quad , \end{aligned} \tag{6.32}$$

where I introduced a **time-ordering operator** $\hat{\mathbb{T}}$ whose action consists in ordering a product of operators in decreasing time from the left to the right.

Generalising the result (6.32) for each term, we obtain, for Eq. (6.29), the expression

$$\hat{U}(t,t_0)=\sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n\frac{1}{n!}\int_{t_0}^{t}dt_1\ldots\int_{t_0}^{t}dt_n\hat{\mathbb{T}}\left[\hat{H}_1(t_1)\ldots\hat{H}_1(t_n)\right]. \tag{6.33}$$

Demonstration of Eq. (6.31). Let's define

$$\frac{dF(x)}{dx}=f(x) \quad .$$

We consider the first term of Eq. (6.31).

$$\begin{aligned}&\int_a^b dy\int_y^b dx f(x)f(y)=\int_a^b dy f(y)\left[F(b)-F(y)\right]=F(b)\left[F(b)-F(a)\right]-\int_a^b dy f(y)F(y)\\ =\;& F(b)\left[F(b)-F(a)\right]-\int_a^b dy\frac{1}{2}\frac{d}{dy}\left[F(y)\right]^2=F^2(b)-F(b)F(a)-\frac{1}{2}\left[F^2(b)-F^2(a)\right]\\ =\;&\frac{1}{2}F^2(b)+\frac{1}{2}F^2(a)-F(b)F(a)=\frac{1}{2}\left[F(b)-F(a)\right]^2 \quad .\end{aligned}$$

The second term of Eq. (6.31) is

$$\int_a^b dx \int_a^x dy f(x)f(y) = \int_a^b dx f(x)\left[F(x) - F(a)\right] = \int_a^b dx f(x)F(x) - F(a)\left[F(b) - F(a)\right]$$
$$= \int_a^b dx \frac{1}{2}\frac{d}{dx}\left[F(x)\right]^2 - F(a)F(b) + F^2(a) = \frac{1}{2}\left[F^2(b) - F^2(a)\right] - F(a)F(b) + F^2(a)$$
$$= \frac{1}{2}F^2(b) + \frac{1}{2}F^2(a) - F(b)F(a) = \frac{1}{2}\left[F(b) - F(a)\right]^2 \quad .$$

6.3 Wick's theorem

Before considering the use of the time-evolution operator in the perturbation expansion we shall present a theorem which is very useful in the calculations of the expectation values of operators expressed in ONR.

Time-ordering operator $\hat{\mathbb{T}}$

I have already introduced in Eq. (6.32) the time-ordering operator

$$\hat{\mathbb{T}}[\hat{A}\hat{B}\hat{C}\ldots], \tag{6.34}$$

which orders a sequence of time-dependent operators, such as those expressed in the interaction picture, with the latest times to the left. Since these operators can be expressed in terms of creation and destruction operators, it is necessary to take care of the anticommutation relations in doing this ordering. This means one has to add a -1 sign for each interchange of fermion operators.

For example, assuming $t_{n+1} < t_n$, we have that:

$$\hat{\mathbb{T}}\left[\hat{a}(t_3)\hat{a}^+(t_1)\hat{a}^+(t_2)\right] = \quad \hat{a}^+(t_1)\hat{a}^+(t_2)\hat{a}(t_3). \tag{6.35}$$

Another example:

$$\hat{\mathbb{T}}\left[\hat{a}(t_2)\hat{a}^+(t_1)\hat{a}^+(t_3)\right] = \quad -\hat{a}^+(t_1)\hat{a}(t_2)\hat{a}^+(t_3) \ . \tag{6.36}$$

Normal order product

By definition, the expectation value of a normally ordered set of creation and destruction operators with respect to the ground state of the system is zero. This enforces the construction of an operator $\hat{\mathbb{N}}$ which arranges the sequence of creation and destruction operators to obtain a zero value. The action of $\hat{\mathbb{N}}$ depends on the definition of the system ground state.

In field theory, the ground state of the system is the physical vacuum, i.e. a state without particles, $|0\rangle$. In this case, the action of $\hat{\mathbb{N}}$ consists in putting on the right hand side the destruction operators, and to the left hand side the creation operators. This because $\hat{a}|0\rangle = 0$, and $\langle 0|\hat{a}^+ = 0$. For example:

$$\hat{\mathbb{N}}[\hat{a}_1\hat{a}_2^+\hat{a}_3\hat{a}_4^+] = \quad -\hat{a}_2^+\hat{a}_4^+\hat{a}_1\hat{a}_3 \ , \quad \text{field theory}. \tag{6.37}$$

In the case of many-body systems, it is much more convenient to consider a ground state given by the solution of the mean-field problem $|\Phi_0\rangle$, where all the levels below the Fermi surface are occupied (hole states) and those above the Fermi surface are empty (particle states). The action of $\hat{\mathbb{N}}$ on the creation and destruction operators is more involved than in the previous case. Following the traditional nomenclature we indicate with the latin letters $(ijkl)$ the hole states, and with $(mnpq)$ the particle states. We shall

use the greek letters to indicate a generic state which can be hole or particle. The action of the creation and destruction operators on the mean-field ground state is:

$$\begin{aligned} \hat{a}_j|\Phi_0\rangle \neq 0 \quad &; \quad \hat{a}_m|\Phi_0\rangle = 0 \ ; \\ \hat{a}_j^+|\Phi_0\rangle = 0 \quad &; \quad \hat{a}_m^+|\Phi_0\rangle \neq 0 \ . \end{aligned} \tag{6.38}$$

In this case, the action of $\hat{\mathbb{N}}$ consists in moving to the right hand side the $\hat{a}_m$ and the $\hat{a}_j^+$ operators, and to the left hand side the operators $\hat{a}_j$ and $\hat{a}_m^+$. Also in this case, every change in the position of the operators inserts a minus sign. The following example contains two minus signs:

$$\hat{\mathbb{N}}[\hat{a}_m\hat{a}_j^+\hat{a}_j\hat{a}_m^+] = (-\hat{a}_j\hat{a}_m^+)(-\hat{a}_m\hat{a}_j^+) = \quad \hat{a}_j\hat{a}_m^+\hat{a}_m\hat{a}_j^+ \ . \tag{6.39}$$

Contraction

The contraction is defined as the difference between two time-ordered and normal-ordered operators.

$$\overbrace{\hat{A}\hat{B}} \equiv \hat{\mathbb{T}}[\hat{A}\hat{B}] - \hat{\mathbb{N}}[\hat{A}\hat{B}] \ . \tag{6.40}$$

We identify the two operators to contract by a line joining them.

If the operators are time-independent, or if they are defined at the same time:

$$\hat{\mathbb{T}}[\hat{A}\hat{B}] = \hat{A}\hat{B} \ . \tag{6.41}$$

For example, the contraction of a particle creation operator with a hole destruction operator is:

$$\overbrace{\hat{a}_m^+\hat{a}_i} = \hat{\mathbb{T}}[\hat{a}_m^+\hat{a}_i] - \hat{\mathbb{N}}[\hat{a}_m^+\hat{a}_i] = \hat{a}_m^+\hat{a}_i - \hat{a}_m^+\hat{a}_i = 0 \ . \tag{6.42}$$

The result of the contraction is not an operator, or an operator sequence, but it is a number. This is a consequence of the anti-commutation rules of the creation and destruction operators. The contraction is related to the anti-commutator of these operators.

The contraction is the expectation value of the two operators on the ground state:

$$\langle\Phi_0|\hat{A}\hat{B}|\Phi_0\rangle = \langle\Phi_0|\overbrace{\hat{A}\hat{B}}|\Phi_0\rangle + \langle\Phi_0|\hat{\mathbb{N}}[\hat{A}\hat{B}]|\Phi_0\rangle = \overbrace{\hat{A}\hat{B}}\langle\Phi_0|\Phi_0\rangle \ , \tag{6.43}$$

where we used the fact that $\langle\Phi_0|\hat{\mathbb{N}}[\hat{A}\hat{B}]|\Phi_0\rangle = 0.$ by definition.

In a set of various operators, eventually with more than one contraction, the pair of operators which has to be contracted must be arranged such as the operators to be contracted are close to each other. This procedure includes a -1 for each operator exchange. The global sign must take care of For example:

$$\overbrace{\hat{A}\hat{B}\hat{C}\hat{D}\hat{E}\hat{F}} = -\overbrace{\hat{A}\hat{C}}\overbrace{\hat{B}\hat{F}}\hat{D}\hat{E} \ . \tag{6.44}$$

Formulation of the Wick's theorem

The Wick's theorem states that a time-ordered product of operators can be written as sum of normal-ordered products where all the possible contractions are executed:

$$\begin{aligned} \hat{\mathbb{T}}[\hat{A}\hat{B}\hat{C}\ldots\hat{Z}] = \hat{\mathbb{N}}[\hat{A}\hat{B}\hat{C}\ldots\hat{Z}] \quad &+ \quad \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}}\ldots\hat{Z}] + \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}\hat{C}}\ldots\hat{Z}] \\ &+ \quad \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}}\overbrace{\hat{C}\hat{D}}\ldots\hat{Z}] + \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}\overbrace{\hat{C}\hat{D}}}\ldots\hat{Z}] \\ &+ \quad \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}\overbrace{\hat{C}\hat{D}}}\ldots\hat{Z}] + \ldots \ . \end{aligned}$$

Since the result of a contraction is a number, all the contracted operators are not involved by the action of $\hat{\mathbb{N}}$. For example, the Wick's theorem applied to the product of four operators gives:

$$\begin{aligned}
\hat{A}\hat{B}\hat{C}\hat{D} = \hat{\mathbb{N}}[\hat{A}\hat{B}\hat{C}\hat{D}] &+ \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}}\hat{C}\hat{D}] + \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}\hat{C}}\hat{D}] + \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}\hat{C}\hat{D}}] \\
&+ \hat{\mathbb{N}}[\hat{A}\overbrace{\hat{B}\hat{C}}\hat{D}] + \hat{\mathbb{N}}[\hat{A}\overbrace{\hat{B}\hat{C}\hat{D}}] + \hat{\mathbb{N}}[\hat{A}\hat{B}\overbrace{\hat{C}\hat{D}}] \\
&+ \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}}\overbrace{\hat{C}\hat{D}}] + \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}\hat{C}}\hat{D}] + \hat{\mathbb{N}}[\overbrace{\hat{A}\hat{B}}\overbrace{\hat{C}\hat{D}}] \\
= \hat{\mathbb{N}}[\hat{A}\hat{B}\hat{C}\hat{D}] &+ \overbrace{\hat{A}\hat{B}}\,\hat{\mathbb{N}}[\hat{C}\hat{D}] - \overbrace{\hat{A}\hat{C}}\,\hat{\mathbb{N}}[\hat{B}\hat{D}] + \overbrace{\hat{A}\hat{D}}\,\hat{\mathbb{N}}[\hat{B}\hat{C}] \\
&+ \overbrace{\hat{B}\hat{C}}\,\hat{\mathbb{N}}[\hat{A}\hat{D}] - \overbrace{\hat{B}\hat{D}}\,\hat{\mathbb{N}}[\hat{A}\hat{C}] + \overbrace{\hat{C}\hat{D}}\,\hat{\mathbb{N}}[\hat{A}\hat{B}] \\
&+ \overbrace{\hat{A}\hat{B}\hat{C}}\hat{D} - \overbrace{\hat{A}\hat{B}\hat{C}}\hat{D} + \overbrace{\hat{A}\hat{B}\hat{C}}\hat{D} \ . \qquad (6.45)
\end{aligned}$$

From this expression it appears clear that the calculation of the expectation value of these operators with respect to the ground state is reduced to the evaluation of the contractions since all the terms containing $\hat{\mathbb{N}}$ are zero, by definition.

6.4 Adiabatic switching on of the interaction

We use here the adiabatic switching on of the interaction as a mathematical expedient to write the eigenstates of a system of interacting particles in terms of states of non-interacting particles, i.e. MF states. This is very useful since the MF problem is easily solved.

Let's consider a hamiltonian of the form

$$\hat{H} = \hat{H}_0 + e^{-\epsilon|t|}\hat{H}_1 \ , \qquad (6.46)$$

where ϵ is a real, and positive, number. Obviously:

$$\lim_{t\to\pm\infty} \hat{H} = \hat{H}_0 \ , \qquad (6.47)$$

and at the time $t = 0$ the hamiltonian (6.46) is the full hamiltonian:

$$\lim_{t\to 0} \hat{H} = \hat{H}_0 + \hat{H}_1 \ . \qquad (6.48)$$

The ϵ parameter can be chosen in order to switch on and off, slowly at pleasure, the perturbation. The final results must be independent of the value of ϵ.

The eigenstates of the hamiltonian (6.46) in interaction picture can be expressed as:

$$|\Psi_I(t)\rangle = \hat{U}_\epsilon(t, t_0)|\Psi_I(t_0)\rangle \ . \qquad (6.49)$$

The sub-index ϵ has been added to the time evolution operator $\hat{U}$ since in its definition, Eq. (6.19), instead of $\hat{H}_1(t)$ we use $e^{-\epsilon|t|}\hat{H}_1(t)$.

Eq. (6.33), expressing the time-evolution operator in perturbative terms, becomes:

$$\begin{aligned}
\hat{U}_\epsilon(t, t_0) &= \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \ldots \int_{t_0}^{t} dt_n \\
&\quad e^{-\epsilon|[t_1|+|t_2|+\ldots]}\hat{\mathbb{T}}[\hat{H}_1(t_1)\ldots\hat{H}_1(t_n)] \ , \qquad (6.50)
\end{aligned}$$

where the exponential terms have been exctracted from $\hat{\mathbb{T}}$ since they commute with $\hat{H}_1$. The equation of motion (6.10) for a system described by the hamiltonian (6.46) can be expressed as:

$$i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = e^{-\epsilon|t|}\hat{H}_1(t)|\Psi_I(t)\rangle \to_{t\to\pm\infty} 0 \ , \tag{6.51}$$

therefore, in the limit $t \to \pm\infty$ one has that $|\Psi_I(\pm\infty)\rangle$ is time independent. For $t \to \pm\infty$ the hamiltonian reduces to $\hat{H}_0$, therefore we have

$$|\Psi_I(t)\rangle = \hat{U}_\epsilon(t,-\infty)|\Phi_0\rangle \ , \tag{6.52}$$

where $|\Phi_0\rangle$ is eigenstate of $\hat{H}_0$.

If the interaction term $\hat{H}_1$ would not be present, $|\Psi_I\rangle$ would be always equal to $|\Phi_0\rangle$. When the time increases the interaction is switched on up to $t = 0$ when it is fully active. After that the interaction it is slowly switch off up to become zero for $t = +\infty$.

The definitions of the state in the Heisenberg, Schrödinger and interaction pictures determine the states at $t = 0$:

$$|\Psi_H(t)\rangle_{t\to 0} = \lim_{t\to 0} e^{i\frac{\hat{H}t}{\hbar}}|\Psi_S(t)\rangle \quad = \quad |\Psi_S(0)\rangle \tag{6.53}$$

$$|\Psi_I(t)\rangle_{t\to 0} = \lim_{t\to 0} e^{i\frac{\hat{H}_0 t}{\hbar}}|\Psi_S(t)\rangle \quad = \quad |\Psi_S(0)\rangle \tag{6.54}$$

$$|\Psi_H(0)\rangle = |\Psi_I(0)\rangle \quad = \quad |\Psi_S(0)\rangle \ , \tag{6.55}$$

and then:

$$|\Psi_S(0)\rangle = |\Psi_H(0)\rangle = |\Psi_I(0)\rangle = \hat{U}_\epsilon(0,-\infty)|\Phi_0\rangle \ . \tag{6.56}$$

Eq. (6.56) expresses the eigenstate of an interacting hamiltonian $\hat{H}$ in terms of an eigenstates of a non-interacting, mean-field, hamiltonian $\hat{H}_0$. The result obtained is physically meaningful if all the quantities calculated in the $\lim \epsilon \to 0$ are finite.

The *Gell-Mann and Low theorem* answer to this question. Let's consider a perturbation expansion of the following mathematical entity

$$\frac{\hat{U}_\epsilon(0,-\infty)|\Phi_0\rangle}{\langle\Phi_0|\hat{U}_\epsilon(0,-\infty)|\Phi_0\rangle} \equiv \frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = \sum_{n=0}^{\infty}|\xi_\epsilon^{(n)}\rangle\, g^n \ , \tag{6.57}$$

where g^n is a generic expansion parameter. If, for each n the $\lim_{\epsilon\to 0}|\xi_\epsilon^{(n)}\rangle$ exists, i.e. it is finite, then, the full quantity defined in Eq. (6.57) is eigenstate of the hamiltonian $\hat{H}$:

$$\hat{H}\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = E_0\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} \ . \tag{6.58}$$

Multiplying on the left both terms of the above equation by $\langle\Phi_0|$ we obtain:

$$\begin{aligned}\frac{\langle\Phi_0|\hat{H}|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = E_0 \quad &= \quad \frac{\langle\Phi_0|\hat{H}_0|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} + \frac{\langle\Phi_0|\hat{H}_1|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} \\ &= \quad \mathcal{E}_0 + \frac{\langle\Phi_0|\hat{H}_1|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} \ ,\end{aligned}$$

teherefore:

$$E_0 - \mathcal{E}_0 = \frac{\langle \Phi_0 | \hat{H}_1 | \Psi_0 \rangle}{\langle \Phi_0 | \Psi_0 \rangle} = \frac{\langle \Phi_0 | H_1 \, \hat{U}(0, -\infty) | \Phi_0 \rangle}{\langle \Phi_0 | \hat{U}(0, -\infty) | \Phi_0 \rangle} \quad . \tag{6.59}$$

Detailed proofs of the Gell-Mann and Low theorem can be found in various textbooks, for example [Fet71, Gro91]. We would like here to emphasize the essential point of the theorem, by pointing out that in the $\lim_{\epsilon \to 0}$ numerator and denominator of Eq. (6.57) do not separately exists, but the limit of they ratio is finite. The numerator has divergencies of ϵ^{-1} order which are canceled by analogous divergencies present in the denominator.

The result (6.59) is important since it expresses the difference between the energy of a system of interacting particles with that of non-interacting particles described by a mean-field model. All the ingredients necessary to calculate this quantity are known. The basic assumption of our approach is that the mean-field problem is solved, which implies that $|\Phi_0\rangle$ is known. The time-evolution operator $\hat{U}$ is calculated by using the perturbation expansion given by the expression (6.33) where the Wick's theorem allows the evaluation of the time-ordering operator $\hat{\mathbb{T}}$ applied to the various $\hat{H}_1$ acting at different times.

Chapter 7

Goldstone theorem

7.1 Goldstone diagrams

The analysis of the various terms of the perturbative expansion is simplified by the use of graphic techniques. These techniques consist in associating a graphic symbol to every element of the equation which is perturbatively expanded. Every expansion term is identified by a diagram.

In relativistic field theory, these diagrams are called *Feynman diagrams*. There is a set of rule which allows the exact reconstruction of the mathematical expression of the perturbative term graphically described.

It is not our interest here to use the graphic techniques in this manner. We use these diagrams to identify the terms of the perturbative expansion having similar characteristics.

Since the Feynman diagrams are used in relativistic field theory, we call *Goldstone diagrams* those used in non-relativistic Quantum Mechanics.

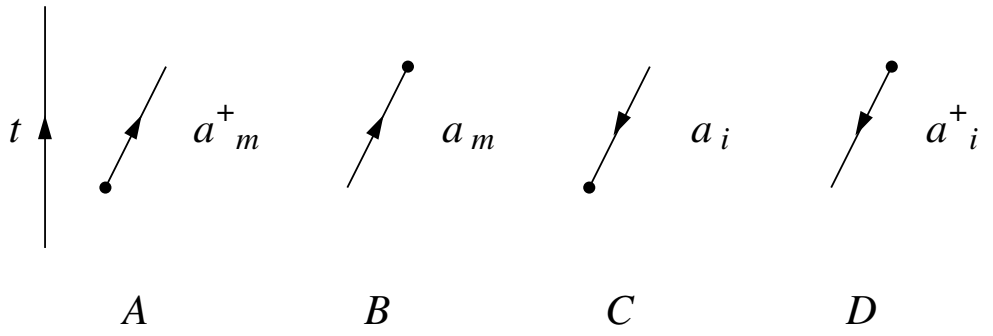

Figure 7.1:

In Fig. 7.1 the various elements composing the diagram are presented. In this representation let's imagine an ideal time arrow oriented from the lower to the upper sides of the diagram. This line has been drawn in Fig. 7.1 but it will be understood in all the other figures.

An oriented line coming out from a point and moving in the direction of positive times (A in the figure) represents the creation of a particle. This diagram is related to the creation operator $\hat{a}^+_m$. We remember the convention adopted to indicate with the m, n, p, q, r, the states above the Fermi surface,

and with the i, j, k, l letters the states below it. In case of coordinate representation, this symbol is related to the field operator $\hat{\psi}^{+}(\mathbf{r})$, which indicates the creation of a particle in the point $\mathbf{r}$. An oriented line moving in the positive time direction and disappearing in a point (B in the Figure) represents the destruction of a particle, and the operators associated to it are $\hat{a}_m$ or $\hat{\psi}(\mathbf{r})$.

In relativistic field theory, the lines oriented in opposite direction with respect to the time arrow (negative times) represent antiparticles. In our case, Goldstone diagrams, they, instead, represent hole states, i.e. single particle states below the Fermi surface. A disappearing line (case D of the Figure) indicates the creation of a hole state, and the associated operators are $\hat{a}_i^{+}$ or $\hat{\psi}(\mathbf{r})$. Obviously, the oriented line moving back in the time and disappearing in a point (case C of the Figure) indicates the destruction of a hole state. In this case, the related operators are $\hat{a}_i$ o $\hat{\psi}^{+}(\mathbf{r})$.

The last graphic element required to compose the diagrams is that related to the interaction $\hat{V}(\mathbf{r}_1, \mathbf{r}_2)$. We have chosen a dashed line joining two points, which describe the action of a two-body interactions. Since the framework is non relativistic, the action of the interaction is instantaneous, therefore in the Goldstone diagrams the dashed lines are always horizontal. This is not the case in the Feynmann where the interaction propagates at finite velocity.

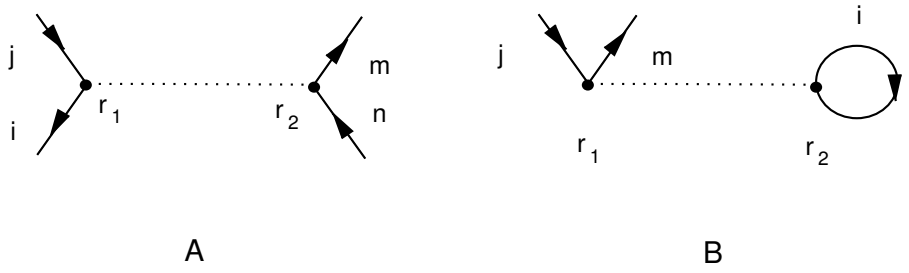

Figure 7.2:

As example, we present in Fig. 7.2 two diagrams of which we calculate the explicit expressions. The diagrams represent the expectation values of the type:

$$\langle \Phi_a | \hat{V} | \Phi_b \rangle \ , \tag{7.1}$$

where $|\Phi_a\rangle$ indicates the initial state and $|\Phi_b\rangle$ the final one.

Let's consider the A diagram of Fig. 7.2. The initial state is formed by a particle state n and by a hole state i:

$$\langle \Phi_a | = \langle \Phi_0 | \hat{a}_i^{+} \hat{a}_n \ , \ |\Phi_a\rangle = \hat{a}_n^{+} \hat{a}_i | \Phi_0 \rangle \tag{7.2}$$

In this diagram also the final state is composed by hole and particle states which are different with respect to those of the initial state:

$$|\Phi_b\rangle = \hat{a}_m^{+} \hat{a}_j | \Phi_0 \rangle. \tag{7.3}$$

The expression of the A diagram of the Fig. 7.2 is:

$$\langle \Phi_0 | \hat{a}_i^{+} \hat{a}_n \hat{V} \hat{a}_m^{+} \hat{a}_j | \Phi_0 \rangle. \tag{7.4}$$

At this point one has to insert the expression of $\hat{V}$ in ONR:

$$\hat{V} = \frac{1}{2} \sum_{\nu\nu'\mu\mu'} V_{\nu\mu\nu'\mu'} \hat{a}^+_\nu \hat{a}^+_\mu \hat{a}_{\mu'} \hat{a}_{\nu'}, \tag{7.5}$$

and then to use the Wick's theorem to evaluate the expectation value.

The evaluation of the B diagram of Fig. 7.2 proceeds in analogous manner. The difference with the previous case that the hole states of the initial and final states are the same. The expression of the diagram is:

$$\langle \Phi_0 | \hat{a}^+_i \hat{a}_j \hat{V} \hat{a}_i \hat{a}^+_m | \Phi_0 \rangle. \tag{7.6}$$

7.2 Goldstone theorem

The Goldstone theorem states that the difference between the energy of system of interacting particles and that of a system of non-interacting particles can be expressed as:

$$E_0 - \mathcal{E}_0 = \langle \Phi_0 | \hat{H}_1 \sum_{n=0}^{\infty} \left(\frac{1}{\mathcal{E}_0 - \hat{H}_0} \hat{H}_1 \right)^n |\Phi_0\rangle_c \ , \tag{7.7}$$

where $\hat{H}_0$ and $\hat{H}_1$ are time-independent operators in the Schrödinger picture, and $|\Phi_0\rangle$ is the eigenstate of $\hat{H}_0$, the MF hamiltonian. The meaning of the important sub-index c will be clarified below.

Let's write explicitly the first terms of Eq. (7.7):

$$\begin{aligned} E_0 - \mathcal{E}_0 &= \langle \Phi_0 | \hat{H}_1 | \Phi_0 \rangle \\ &+ \langle \Phi_0 | \hat{H}_1 \frac{1}{\mathcal{E}_0 - \hat{H}_0} \hat{H}_1 | \Phi_0 \rangle_c \\ &+ \langle \Phi_0 | \hat{H}_1 \frac{1}{\mathcal{E}_0 - \hat{H}_0} \hat{H}_1 \frac{1}{\mathcal{E}_0 - \hat{H}_0} \hat{H}_1 | \Phi_0 \rangle_c \\ &+ \ \ldots \ . \end{aligned} \tag{7.8}$$

Some of the diagrams related to the expansion terms are shown in Fig. 7.3. The diagram A is contained in the first term of Eq. (7.8). A single dashed line indicates the presence of only one interaction $\hat{H}_1$. There are not open lines of particle or holes since the expectation value is evaluated on the mean-field ground state. The other diagram present in the first expansion term is that called exchange term. In this diagram the particle and hole lines are interchanged between the various points. This is the diagram B of Fig. 7.4).

The diagram B of Fig. 7.3 is one of the diagrams of the second term of Eq. (7.8) since it contains to interaction lines $\hat{H}_1$. Also in this case it is necessary to add the exchange term. This diagram show that $\hat{H}_1$ creates an intermediate state characterised by 2 particle states and 2 hole states ($2p-2h$). This happens since $\hat{H}_1$ is a two-body operator. This intermediate state propagates (the term $(\mathcal{E}_0 - \hat{H}_0)^{-1}$ is the Fourier transform of the time propagation operator) and it is de-excited by the action of another $\hat{H}_1$ term.

The traditional expression of the perturbative expansion can be obtained by inserting a completeness of $\hat{H}_0$ eigenstates $\hat{\mathbb{I}} = \sum_{n\neq 0} |\Phi_n\rangle\langle\Phi_n|$, (where $\hat{\mathbb{I}}$ is the identity operator):

$$E_0 - \mathcal{E}_0 = \langle \Phi_0 | \hat{H}_1 | \Phi_0 \rangle + \sum_{n\neq 0} \frac{\langle \Phi_0 | \hat{H}_1 | \Phi_n \rangle \langle \Phi_n | \hat{H}_1 | \Phi_0 \rangle}{\mathcal{E}_0 - \mathcal{E}_n} + \ldots \tag{7.9}$$

The absence of the $n = 0$ terms is a subtle point which we clarify here below where we show how to obtain Eq. (7.7) starting from the expression of the Gell-Mann and Low theorem.

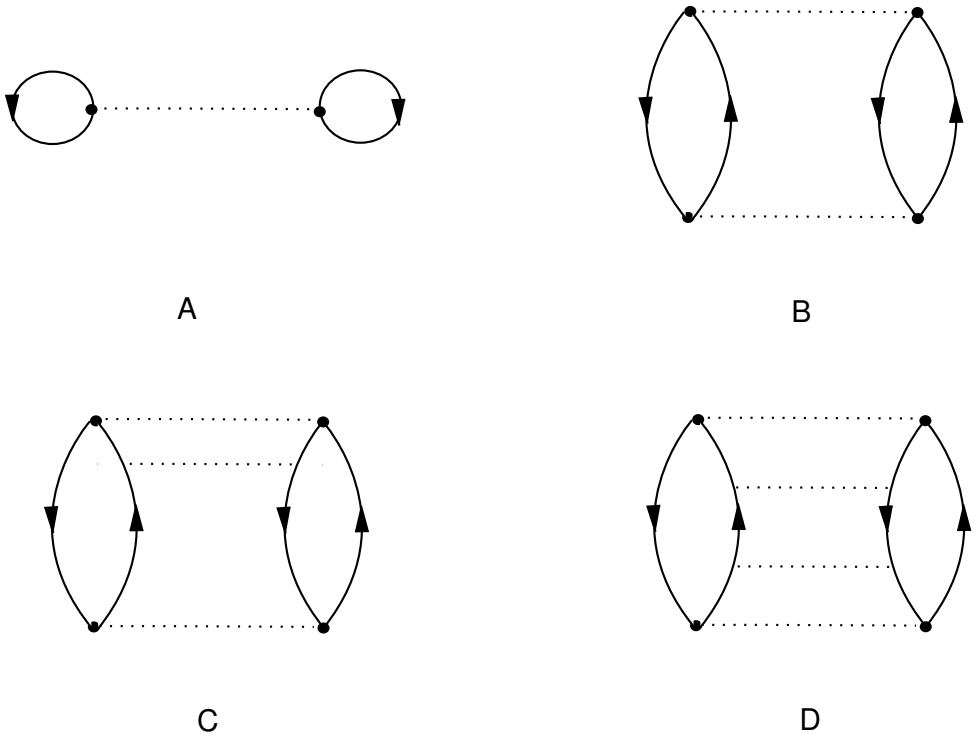

Figure 7.3:

Eq. (6.59) can be rewritten as:

$$E_0 - \mathcal{E}_0 = \frac{\langle\Phi_0|\hat{H}_1|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = \frac{\langle\Phi_0|\hat{H}_1\hat{U}(0,-\infty)|\Phi_0\rangle}{\langle\Phi_0|\hat{U}(0,-\infty)|\Phi_0\rangle} \ . \tag{7.10}$$

By using the expression (6.33) of the time evolution operator, we obtain, for the numerator:

$$\begin{aligned}\langle\Phi_0|\hat{H}_1\hat{U}(0,-\infty)|\Phi_0\rangle &= \sum_{\nu=0}\left(\frac{-i}{\hbar}\right)^{\nu}\frac{1}{\nu!}\int_{-\infty}^{0}dt_1\ldots\int_{-\infty}^{0}dt_\nu \\ &\quad \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1,\hat{H}_1(t_1)\ldots,\hat{H}_1(t_\nu)]|\Phi_0\rangle \ ,\end{aligned} \tag{7.11}$$

where we used the $\lim\varepsilon\to 0$ of Eq. (6.50). The H_1 operator which in (7.10) is out of the action of $\hat{\mathbb{T}}$ here it has been included in the first position between the operators which have to be ordered by $\hat{\mathbb{T}}$. This operation does not modify the results since this $\hat{H}_1$ is defined at $t=0$ which is the latest time involved.

The various terms of the perturbative expansion can be calculated by using the Wick theorem. The investigation of the diagrams which are here generated indicates the possibility of classify them in two categories: *linked* and *unlinked*. The linked diagrams are those where there are contractions between the creation and destruction operators defining $\hat{H}_1(0)$ and other operators defined at earlier times.

Let's consider, for example, the term with $\nu=1$:

$$\begin{aligned}&\langle\Phi_0|\hat{H}_1(0)\hat{H}_1(t_1)|\Phi_0\rangle \sim \\ &\langle\Phi_0|\hat{V}_{\mu\nu\mu'\nu'}\hat{a}^+_\mu(0)\hat{a}^+_\nu(0)\hat{a}_{\nu'}(0)\hat{a}_{\mu'}(0)\hat{V}_{\eta\xi\eta'\xi'}\hat{a}^+_\eta(t_1)\hat{a}^+_\xi(t_1)\hat{a}_{\xi'}(t_1)\hat{a}_{\eta'}(t_1)|\Phi_0\rangle \ ,\end{aligned} \tag{7.12}$$

where we have explicitly written $\hat{H}_1$ in terms of creation and destruction operators in interaction picture. For simplicity in writing we understand the sum on the repeated greek indexes.

In absence of contraction between operators defined at the time t_1 and those defined at $t=0$, the two terms can be separated by inserting an identity operator $|\Phi_0\rangle\langle\Phi_0| = \hat{\mathbb{I}}$:

$$\langle\Phi_0|V_{\mu\nu\mu'\nu'}a^+_\mu a^+_\nu a_{\nu'}a_{\mu'}|\Phi_0\rangle_{t=0}\langle\Phi_0|V_{\eta\xi\eta'\xi'}a^+_\eta a^+_\xi a_{\xi'}a_{\eta'}|\Phi_0\rangle_{t=t_1} \ . \tag{7.13}$$

The contractions different from zero in these two terms are:

$$\hat{a}^+_\mu(t)\hat{a}^+_\nu(t)\hat{a}_{\nu'}(t)\hat{a}_{\mu'}(t) \ , \tag{7.14}$$

and

$$\hat{a}^+_\mu(t)\hat{a}^+_\nu(t)\hat{a}_{\nu'}(t)\hat{a}_{\mu'}(t) \ . \tag{7.15}$$

The first of these terms is presented in the diagram A of Fig. 7.4 and the second term by the diagram B of the same figure. By using this result we observe that the term of Eq. (7.13) produces four diagrams, each of them obtained by coupling two of the diagrams of Fig. 7.4: one at the time $t=0$ and the other one at the time $t=t_1$. Clearly these diagrams are unlinked.

On the other hand, if we apply the Wick theorem by using contractions relating operators defined at $t=0$ with those defined at $t=t_1$, we obtain linked diagrams. For example:

$$\langle\Phi_0|V_{\mu\nu\mu'\nu'}\hat{a}^+_\mu(0)\hat{a}^+_\nu(0)\hat{a}_{\nu'}(0)\hat{a}_{\mu'}(0)V_{\eta\xi\eta'\xi'}\hat{a}^+_\eta(t)\hat{a}^+_\xi(t)\hat{a}_{\xi'}(t)\hat{a}_{\eta'}(t)|\Phi_0\rangle \ . \tag{7.16}$$

The diagram representing this term is shown in Fig. 7.5.

The term with $\nu=1$ in Eq. (7.12) produces both unlinked diagrams, as the diagram A of Fig. 7.6, and linked diagrams, as the diagram B of the same figure.

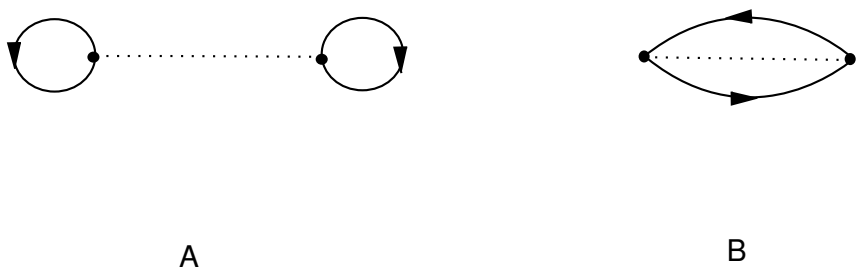

Figure 7.4:

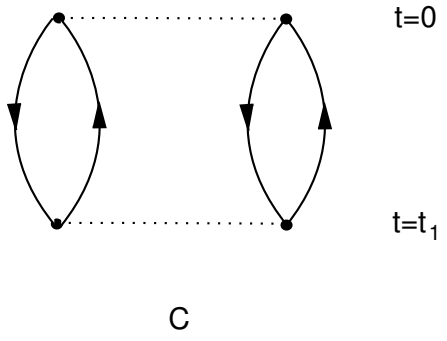

Figure 7.5:

After this discussion on the structure of the various terms of the expansion we present a derivation of Eq. (7.7). Let's consider a term of Eq. (7.11) and assume it is composed by two unlinked parts, as, for example, the diagram shown in Fig. 7.7. The contribution of a diagram of this type is:

$$\begin{aligned}\langle\Phi_0|\hat{H}_1\hat{U}(0,-\infty)|\Phi_0\rangle_\nu \quad &= \\ \left(\frac{-i}{\hbar}\right)^\nu \frac{1}{\nu!}\int_{-\infty}^{0} dt_1 \quad \dots \quad &\int_{-\infty}^{0} dt_n \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1(0)\dots\hat{H}_1(t_n)]|\Phi_0\rangle_c \\ \int_{-\infty}^{0} dt_{n+1} \quad \dots \quad &\int_{-\infty}^{0} dt_{n+m} \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1(t_{n+1})\dots\hat{H}_1(t_{n+m})]|\Phi_0\rangle_c \ . \end{aligned} \tag{7.17}$$

We factorized the two linked parts, the first one containing n interaction terms $\hat{H}_1$ and the second one with m interactions.

In general, the total contribution of a diagrams of ν order which can divided in two parts, of n and m ($\nu = m + n$) order. Diagrams of this type can be obtained by exchanging the position of the $\hat{H}_1$ under the action of $\hat{\mathbb{T}}$. By exchanging two $\hat{H}_1$ operators defined at different times there is an exchange of 4 creation and destruction operators, therefore the total phase generated by this exchange is always positive. The number of possibile permutations is $\nu!$. On the other hand, two $\hat{H}_1$ operators belonging to

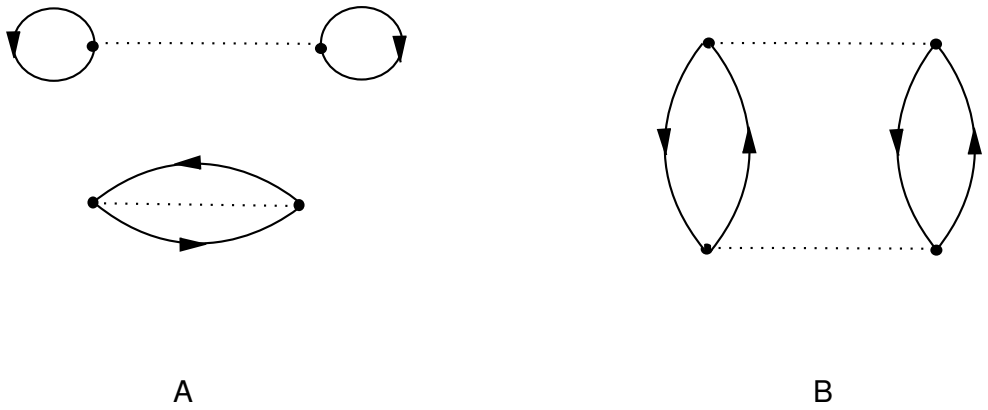

Figure 7.6:

the same partition do not produce a new diagram, since the time ordering operator re-order the various terms. The number of permutations which do not produce any new diagram is $n!\ m!$.

The total contribution to Eq. (7.11) of diagrams such as that of Fig. 7.7 is:

$$\sum_n \sum_m \left(\frac{-i}{\hbar}\right)^{n+m} \frac{\nu!}{n!m!}\frac{1}{\nu!}\int_{-\infty}^{0} dt_1 \quad \dots \quad \int_{-\infty}^{0} dt_n \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1, \hat{H}_1(t_1)\dots\hat{H}_n(t_n)]|\Phi_0\rangle_c$$
$$\int_{-\infty}^{0} dt_{n+1} \quad \dots \quad \int_{-\infty}^{0} dt_{n+m} \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1(t_{n+1})\dots\hat{H}_1(t_{n+m})]|\Phi_0\rangle_c \quad (7.18)$$

The second term of this expression is present in the denominator of Eq. (7.10). In this second term, under the action of the time-ordering operator $\hat{\mathbb{T}}$ is not present $\hat{H}_1(0)$ which is the only extraneous term with respect to those present in the denominator of Eq. (7.10). Eq. (7.10) can be rewritten as:

$$\begin{aligned} E_0 - \mathcal{E}_0 &= \left[\sum_{\nu=0}^{\infty}\left(\frac{-i}{\hbar}\right)^{\nu}\frac{1}{\nu!}\int_{-\infty}^{0} dt_1 \dots \int_{-\infty}^{0} dt_\nu \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1(0), \hat{H}_1(t_1)\dots, \hat{H}_1(t_\nu)]|\Phi_0\rangle\right]_c \\ &\left[\sum_{\mu=0}^{\infty}\left(\frac{-i}{\hbar}\right)^{\mu}\frac{1}{\mu!}\int_{-\infty}^{0} dt_1 \dots \int_{-\infty}^{0} dt_\mu \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1(t_1)\dots, \hat{H}_1(t_\mu)]|\Phi_0\rangle\right] / \langle\Phi_0|\hat{U}(0,-\infty)|\Phi_0\rangle \\ &= \left[\sum_{\nu=0}^{\infty}\left(\frac{-i}{\hbar}\right)^{\nu}\frac{1}{\nu!}\int_{-\infty}^{0} dt_1 \dots \int_{-\infty}^{0} dt_\nu \langle\Phi_0|\hat{\mathbb{T}}[\hat{H}_1, \hat{H}_1(t_1)\dots, \hat{H}_1(t_\nu)]|\Phi_0\rangle\right]_c , \end{aligned}$$

where we used the fact that ν, μ and the times t are dummy indexes since they are summed or integrated. All the diagrams not linked to $\hat{H}_1(0)$ are eliminated by the denominator.

After having clarified why in the expression of the Goldstone theorem only linked diagrams appear, we calculate the time integrals. Let's consider the order n of the expansion and use the explicit expression of the $\hat{H}_1$ operator in interaction picture:

$$\hat{H}_1(t) = e^{i\frac{\hat{H}_0 t}{\hbar}}\hat{H}_1 e^{-i\frac{\hat{H}_0 t}{\hbar}}. \quad (7.19)$$

The term of order n can be written as:

$$[E_0 - \mathcal{E}_0]_n = \left(\frac{-i}{\hbar}\right)^n \int_{-\infty}^{0} dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n e^{\epsilon(t_1+\dots t_n)}$$

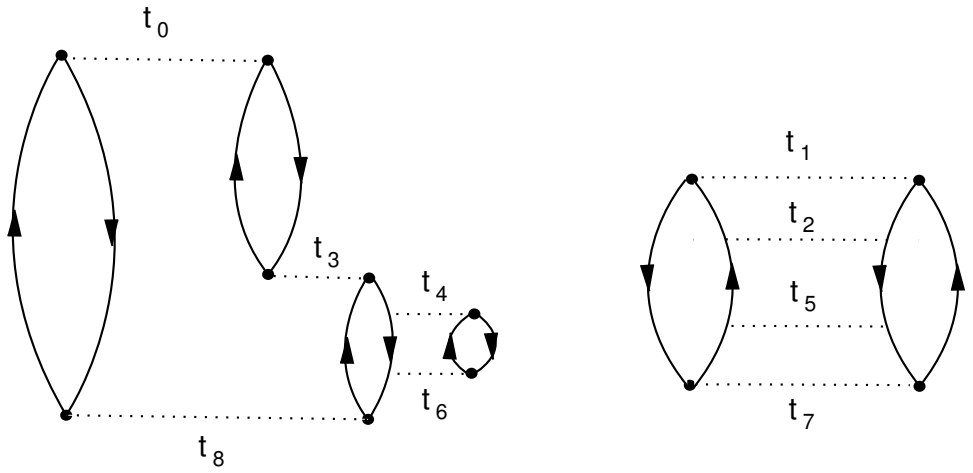

Figure 7.7:

$$\langle\Phi_0|\hat{H}_1 e^{i\frac{\hat{H}_0 t_1}{\hbar}}\hat{H}_1 e^{-i\frac{\hat{H}_0 t_1}{\hbar}} e^{i\frac{\hat{H}_0 t_2}{\hbar}}\hat{H}_1 \dots e^{-i\frac{\hat{H}_0}{\hbar}t_{n-1}} e^{i\frac{\hat{H}_0}{\hbar}t_n}\hat{H}_1 e^{-i\frac{\hat{H}_0}{\hbar}t_n}|\Phi_0\rangle_c$$

where $\hat{\mathbb{T}}$ has been eliminated since we have explicitly written the integration limits and we inserted the factor $e^{\epsilon t}$. We make a change of the integration variables:

$$\begin{aligned} &x_1 = t_1 \quad , \quad x_2 = t_2 - t_1 \quad , \quad x_3 = t_3 - t_2 \quad , \quad \dots \quad , \quad x_n = t_n - t_{n-1} \\ &t_1 = x_1 \quad , \quad t_2 = x_2 + x_1 \quad , \quad t_3 = x_3 + x_2 + x_1 \quad , \quad \dots \quad , \quad t_n = \sum_n x_n \end{aligned}$$

and, by using $\hat{H}_0|\Phi_0\rangle = \mathcal{E}_0|\Phi_0\rangle$ we obtain:

$$\begin{aligned} &[E_0 - \mathcal{E}_0]_n = \left(\frac{-i}{\hbar}\right)^n \langle\Phi_0| \int_{-\infty}^0 dx_1 \int_{-\infty}^0 dx_2 \dots \int_{-\infty}^0 dx_n \\ &e^{\epsilon(x_1+(x_2+x_1)+(x_3+x_2+x_1)+\dots(x_n+x_{n-1}\dots+x_2+x_1)} \\ &\hat{H}_1 e^{i\frac{\hat{H}_0 x_1}{\hbar}}\hat{H}_1 e^{i\frac{\hat{H}_0 x_2}{\hbar}}\hat{H}_1 \dots e^{i\frac{\hat{H}_0 x_n}{\hbar}}\hat{H}_1 e^{-i\frac{\hat{H}_0 t_n}{\hbar}}|\Phi_0\rangle_c \end{aligned}$$

Let's consider the term on the right hand side of the above equation,

$$e^{-i\frac{\hat{H}_0 t_n}{\hbar}}|\Phi_0\rangle = e^{-i\frac{\mathcal{E}_0}{\hbar}t_n}|\Phi_0\rangle = e^{-i\frac{\mathcal{E}_0}{\hbar}(x_1+\dots x_n)}|\Phi_0\rangle \tag{7.20}$$

and insert it in the integral:

$$\begin{aligned} &[E_0 - \mathcal{E}_0]_n = \left(\frac{-i}{\hbar}\right)^n \langle\Phi_0|\hat{H}_1 \int_{-\infty}^0 dx_1\, e^{n\epsilon x_1} e^{i\frac{(\hat{H}_0-\mathcal{E}_0)}{\hbar}x_1}\cdot\hat{H}_1 \\ &\int_{-\infty}^0 dx_2\, e^{(n-1)\epsilon x_2} e^{i\frac{(\hat{H}_0-\mathcal{E}_0)}{\hbar}x_2}\cdot\hat{H}_1 \dots \int_{-\infty}^0 dx_N\, e^{\epsilon x_n} e^{i\frac{(\hat{H}_0-\mathcal{E}_0)}{\hbar}x_n}\hat{H}_1|\Phi_0\rangle_c \end{aligned}$$

The nth term is expressed as product of integrals of the type:

$$\int_{-\infty}^0 dx_1 e^{\frac{i}{\hbar}(\hat{H}_0 - \mathcal{E}_0 - in\epsilon\hbar)x_1} = \frac{\hbar}{-i}\frac{1}{[\mathcal{E}_0 - \hat{H}_0 + in\varepsilon\hbar]} \tag{7.21}$$

Since there are n equal terms, there is a factor $\left(\frac{\hbar}{-i}\right)^n$ which can be factorized, therefore:

$$[E-\mathcal{E}_0]_n = \langle\Phi_0|\hat{H}_1\frac{1}{\mathcal{E}_0-\hat{H}_0+i\epsilon n\hbar}\hat{H}_1\frac{1}{\mathcal{E}_0-\hat{H}_0+i\epsilon(n-1)\hbar}\ldots\hat{H}_1\frac{1}{\mathcal{E}_0-\hat{H}_0+i\epsilon\hbar}\hat{H}_1|\Phi_0\rangle_c \tag{7.22}$$

By executing the $\lim\epsilon\to 0$ we obtain the expression of the Goldstone theorem.

Since Eq. (7.7) is valid only for linked diagram, as the sub-index c indicates, it is prohibited to insert $|\Phi_0\rangle\langle\Phi_0|$ terms, therefore there are not divergencies since the contribution of the denominator $\mathcal{E}_0-\hat{H}_0$ is always different from zero.

Chapter 8

Brueckner theory

8.1 Introduzione

The evaluation of the ground state energy of a system of interacting particles is based on the Goldstone equation which we rewrite

$$E_0 - \mathcal{E}_0 = \langle \Phi_0 | \hat{H}_1 \sum_{n=0}^{\infty} \left(\frac{1}{\mathcal{E}_0 - \hat{H}_0} \hat{H}_1 \right)^n |\Phi_0\rangle_c \ , \tag{8.1}$$

where E_0 is the energy of the system of interacting particles, $\mathcal{E}_0$ is the smallest eigenvalue of H_0, i.e. the ground state energy of the MF solution of the many-body problem, and the sub-index c indicates that only the linked diagrams must be considered in the expansion formula. This last point avoids the divergencies produced by zeros of the denominator.

The computational scheme is, in principle, well defined. After obtaining $\hat{V}$, included in $\hat{H}_1$, from the study of the two-fermions systems as indicated in Chapter 3 one has to insert it in the Goldstone expansion (8.1) to obtain the value of the ground state energy. The problem is in the behaviour of the two-fermion potential at short distances. The microscopic interaction becomes extremely large, it can even diverge, for small values of the relative distance between the two fermions. This empirical evidence has been found for most different two-fermions systems, from nucleons to molecules. The same problem is present also in the electron gas where the Coulomb interaction has a divergence for zero relative distances.

This problem, related to the divergence, or a strong repulsion, for small distances is sketched in Fig. 8.1 where we indicated with ψ the wave function describing the relative motion of the two fermions which interact by means of the potential $\hat{V}(r)$. Since ψ is eigenstate of the full hamiltonian, the product $\hat{V}(r)\ \psi(r)$ is always finite for every value of r. At short distances where the potential becomes very large, the $\psi(r)$ wave function is very small. In the limit of a potential going to infinity, the wave function goes to zero more rapidly than the divergence of the potential such as the product $\hat{V}(r)\ \psi(r)$ remains always finite. This is not the case if one multiplies the potential for the relative wave functions ϕ of two free, therefore non-interacting, particles. The ϕ is eigenstate of the $\hat{H}_0$ hamiltonian.

In the Goldstone equation (8.1) one has to calculate matrix elements of the interaction between eigenstates $|\Phi_0\rangle$ of $\hat{H}_0$. The problem arising in this procedure appears clear if one assumes that the potential $\hat{V}(r)$ goes to infinity at short distances. Each expansion term goes to infinity and the solution of the Goldstone equation would consists in obtaining a finite value by summing and subtracting infinities. Even by assuming finite, but large, values of the potential at short distances, the problem remains. The value of each expansion term would be much larger than the expected energy value. This is exactly the opposite of the basic assumption of the perturbation expansions. Evidently, *the microscopic potentials are not pertubative*, and, therefore, they should not be directly used in Goldstone expansions.

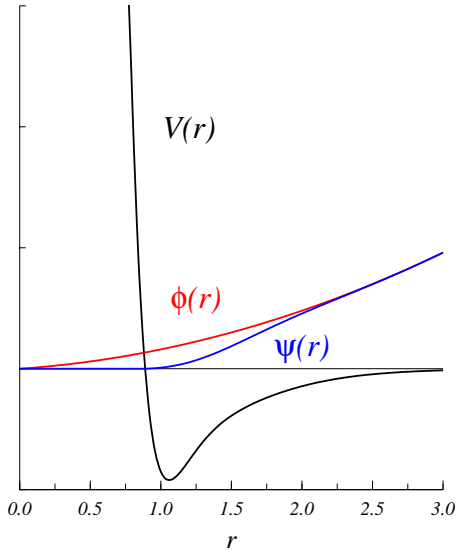

Figure 8.1: Microscopic potential between two fermions and relative wave functions. With ψ we indicate the wave function describing the relative motion of the two interacting particles, while with ϕ that of two non-interacting particles. The figure is sketching the behaviour of potential and wave functions, therefore the units are indicative.

The idea of the Brueckner theory is that of using in the Goldstone expansion (8.1) an effective interaction which behaves well at short distances in order to be perturbative. This implies the definition of a new interaction $\hat{\mathcal{G}}$ such as

$$\hat{\mathcal{G}}|\Phi_0\rangle = \hat{V}|\Psi_0\rangle \ , \tag{8.2}$$

where

$$\hat{H}_0|\Phi_0\rangle = \mathcal{E}_0|\Phi_0\rangle \ , \tag{8.3}$$

and

$$\hat{H}|\Psi_0\rangle = (\hat{H}_0 + \hat{H}_1)|\Psi_0\rangle = (\hat{H}_0 + \hat{V})|\Psi_0\rangle = E_0|\Psi_0\rangle \ . \tag{8.4}$$

8.2 The Bethe-Goldstone equation

The equation which satisfies the definition (8.2) of effective interaction $\hat{\mathcal{G}}$ is called *Bethe-Goldstone equation*. We derived it by starting from the definition (8.2) and by using the relations

$$\hat{H}_0|\Phi_n\rangle = \mathcal{E}_n|\Phi_n\rangle \tag{8.5}$$

$$\hat{H}|\Psi_n\rangle = (\hat{H}_0 + \hat{H}_1)|\Psi_n\rangle = E_n|\Psi_n\rangle \ . \tag{8.6}$$

Since the eigenstates of Eq. (8.5) form a complete basis, it is possible to expand $|\Psi_0\rangle$ on this basis. Neglecting the role of a global constant used for the proper normalization of the state, we obtain

$$|\Psi_0\rangle \simeq |\Phi_0\rangle + \sum_{n\neq 0} a_n|\Phi_n\rangle \ . \tag{8.7}$$

where a_n are complex numbers. We use Eq. (8.6) to express the ground state

$$(\hat{H}_0+\hat{H}_1)\left(|\Phi_0\rangle+\sum_{n\neq 0}a_n|\Phi_n\rangle\right) = E_0\left(|\Phi_0\rangle+\sum_{n\neq 0}a_n|\Phi_n\rangle\right) \ , \tag{8.8}$$

$$(\hat{H}_0-E_0)\left(|\Phi_0\rangle+\sum_{n\neq 0}a_n|\Phi_n\rangle\right) + \hat{H}_1|\Psi_0\rangle = 0 \ . \tag{8.9}$$

Multiplying on the left hand side by $\langle\Phi_0|$, and considering the orthogonality of the $|\Phi_n\rangle$ states, we obtain:

$$\langle\Phi_0|(\hat{H}_0-E_0)\Big(|\Phi_0\rangle+\sum_{n\neq 0}a_n|\Phi_n\rangle\Big)+\langle\Phi_0|\hat{H}_1|\Psi_0\rangle = 0 \ ,$$

$$\mathcal{E}_0 - E_0 + \langle\Phi_0|\hat{H}_1|\Psi_0\rangle = 0 \ . \tag{8.10}$$

Repeating an analogous operation on the (8.9), but by using $\langle\Phi_n|$ with $n>0$, we have

$$\langle\Phi_n|(\hat{H}_0-E_0)\Big(|\Phi_0\rangle+\sum_{n'\neq 0}a_{n'}|\Phi_{n'}\rangle\Big)+\langle\Phi_n|\hat{H}_1|\Psi_0\rangle = 0 \ , \tag{8.11}$$

and, since $\langle\Phi_n|\Phi_{n'}\rangle=\delta_{n,n'}$,

$$(\mathcal{E}_n-E_0)a_n+\langle\Phi_n|\hat{H}_1|\Psi_0\rangle = 0 \ . \tag{8.12}$$

By using the expression of a_n taken from the above equation, and inserting it in (8.7) we obtain

$$\begin{aligned} |\Psi_0\rangle &\simeq |\Phi_0\rangle+\sum_{n\neq 0}\frac{1}{E_0-\mathcal{E}_n}|\Phi_n\rangle\langle\Phi_n|\hat{H}_1|\Psi_0\rangle \\ &= |\Phi_0\rangle+\hat{Q}\frac{1}{E_0-\hat{H}_0}\hat{H}_1|\Psi_0\rangle \ , \end{aligned} \tag{8.13}$$

where we defined the operator $\hat{Q}$ as

$$\hat{Q}=\sum_{n\neq 0}|\Phi_n\rangle\langle\Phi_n| \ . \tag{8.14}$$

Multiplying on the left hand side by $\hat{H}_1$ we get the expression

$$\hat{H}_1|\Psi_0\rangle=\hat{H}_1|\Phi_0\rangle+\hat{H}_1\frac{\hat{Q}}{E_0-\hat{H}_0}\hat{H}_1|\Psi_0\rangle \ , \tag{8.15}$$

and considering the definition (8.2) of the operator $\hat{\mathcal{G}}$, and the fact that in the present derivation $\hat{H}_1=\hat{V}$, we obtain the Bethe-Goldstone equation

$$\hat{\mathcal{G}}|\Phi_0\rangle=\hat{H}_1|\Phi_0\rangle+\hat{H}_1\frac{\hat{Q}}{E_0-\hat{H}_0}\hat{\mathcal{G}}|\Phi_0\rangle=\left(\hat{H}_1+\hat{H}_1\frac{\hat{Q}}{E_0-\hat{H}_0}\hat{\mathcal{G}}\right)|\Phi_0\rangle \ . \tag{8.16}$$

8.3 The sum of the ladder diagrams

In this section, we show how the Bethe-Goldstone equation can be obtained by considering the diagrams techniques presented in Chapter 7. This different derivation of the Bethe-Goldstone equation provides insight which allows a better understanding of the physical content of this equation.

We consider a hamiltonian containing only two-body interaction,

$$\hat{H} = \sum_i \hat{t}_i + \sum_{i<j} \hat{v}_{ij} = \sum_i (\hat{t}_i + \hat{u}_i) + \sum_{i<j} \hat{v}_{ij} - \sum_i \hat{u}_i \ , \tag{8.17}$$

where the mean-field potential $\hat{u}_i$ has been summed and subtracted. We define

$$\hat{H}_0|\Phi_0\rangle = (\hat{T} + \hat{U})|\Phi_0\rangle = \sum_i (\hat{t}_i + \hat{u}_i)|\Phi_0\rangle = \sum_i \hat{h}_i|\Phi_0\rangle \ , \tag{8.18}$$

where Φ_0 is the Slater determinant

$$\Phi_0(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_A) = \frac{1}{\sqrt{A!}} \det |\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\cdots\phi_A(\mathbf{r}_A)| \ , \tag{8.19}$$

and the single-particle wave functions are defined as:

$$\hat{h}_i|\phi_i\rangle = \epsilon_i|\phi_i\rangle \ , \tag{8.20}$$

and

$$\mathcal{E}_0 = \sum_i \epsilon_i \ . \tag{8.21}$$

In ONR the two terms of the hamiltonian under consideration can be expressed as:

$$\hat{H}_0 = \sum_\nu \big(\langle\nu|\hat{t}|\nu\rangle + \langle\nu|\hat{u}|\nu\rangle\big)\hat{a}^+_\nu \hat{a}_\nu \ , \tag{8.22}$$

and

$$\hat{H}_1 = \frac{1}{2}\sum_{\nu\nu'\mu\mu'} \langle\nu\mu|\hat{v}|\nu'\mu'\rangle \hat{a}^+_\nu \hat{a}^+_\mu \hat{a}_{\mu'}\hat{a}_{\nu'} - \sum_\nu \langle\nu|\hat{u}|\nu\rangle \hat{a}^+_\nu \hat{a}_\nu \ . \tag{8.23}$$

By definition we have that

$$\mathcal{E}_0 = \langle\Phi_0|\hat{H}_0|\Phi_0\rangle = \langle\Phi_0|\hat{T}|\Phi_0\rangle + \langle\Phi_0|\hat{U}|\Phi_0\rangle \ . \tag{8.24}$$

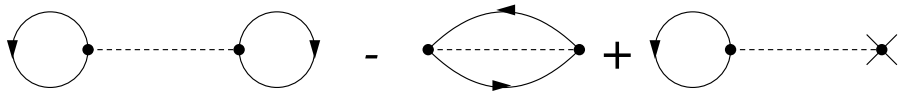

Figure 8.2: Diagrams corresponding to the (8.25) term.

The first term of the expansion (8.1) is that with $n = 0$

$$\begin{aligned}
(E_0 - \mathcal{E}_0)_{(n=0)} &= \langle\Phi_0|\hat{H}_1|\Phi_0\rangle = \langle\Phi_0|\hat{V} - \hat{U}|\Phi_0\rangle \\
&= \frac{1}{2}\sum_{\nu\nu'\mu\mu'} \langle\nu\mu|\hat{v}|\nu'\mu'\rangle\langle\Phi_0|\hat{a}^+_\nu \hat{a}^+_\mu \hat{a}_{\mu'}\hat{a}_{\nu'}|\Phi_0\rangle - \sum_\nu \langle\nu|\hat{u}|\nu'\rangle\langle\Phi_0|\hat{a}^+_\nu \hat{a}_{\nu'}|\Phi_0\rangle \\
&= \frac{1}{2}\sum_{ij} \big(\langle ij|\hat{v}|ij\rangle - \langle ij|\hat{v}|ji\rangle\big) - \sum_i \langle i|\hat{u}|i\rangle \ .
\end{aligned} \tag{8.25}$$

The diagrams corresponding to the three terms of the above equation are shown in Fig. 8.2. We use the usual convention of indicating with the i, j, k, l letters single-particle states of hole type and the m, n, p, q, r the particle states.

Let's consider now the term $n = 1$.

$$\begin{aligned}(E_0 - \mathcal{E}_0)_{(n=1)} &= \langle\Phi_0|\hat{H}_1(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{H}_1|\Phi_0\rangle_c \\ &= \langle\Phi_0|\hat{V}(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{V}|\Phi_0\rangle_c - \langle\Phi_0|\hat{U}(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{V}|\Phi_0\rangle_c \\ &- \langle\Phi_0|\hat{V}(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{U}|\Phi_0\rangle_c + \langle\Phi_0|\hat{U}(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{U}|\Phi_0\rangle_c \ . \end{aligned} \tag{8.26}$$

The first term of the above expression can be written as

$$\begin{aligned}&\langle\Phi_0|\hat{V}(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{V}|\Phi_0\rangle_c \\ = \ &\frac{1}{4}\langle\Phi_0|\sum_{\nu\nu'\mu\mu'}\langle\nu\mu|\hat{v}|\nu'\mu'\rangle\hat{a}^+_\nu\hat{a}^+_\mu\hat{a}_{\mu'}\hat{a}_{\nu'}(\mathcal{E}_0 - \hat{H}_0)^{-1}\sum_{\alpha\beta\alpha'\beta'}\langle\alpha\beta|\hat{v}|\alpha'\beta'\rangle\hat{a}^+_\alpha\hat{a}^+_\beta\hat{a}_{\beta'}\hat{a}_{\alpha'}|\Phi_0\rangle_c \ . \end{aligned} \tag{8.27}$$

We insert in the left and right hand side of the denominator $(E_0 - \hat{H}_0)^{-1}$ a projection operator $|\Phi_n\rangle\langle\Phi_n| = \hat{\mathbb{I}}$ taking care that $n \neq 0$ otherwise unliked diagrams would be produced against the requirement imposed by the sub-index c. These Slater determinants $|\Phi_n\rangle$ represents excited states of the system of non interacting particles formed by 2-particles 2-hole $(2p-2h)$ excitations, whose energy is given by

$$|\Phi_n\rangle = \hat{a}^+_m\hat{a}^+_n\hat{a}_j\hat{a}_i|\Phi_0\rangle \ ; \ \mathcal{E}_0 + \epsilon_m + \epsilon_n - \epsilon_i - \epsilon_j \ , \tag{8.28}$$

where the ϵ indicate the energy of the single-particle state.

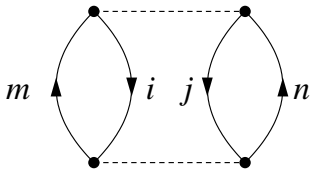

Figure 8.3: Diagram corresponding the the (8.29) term.

Since $|\Phi_n\rangle$ is eigenstate of $\hat{H}_0$, the denominator of (8.29) is diagonal with respect to these states, therefore the non zero contributions are those with the same state on the left and right hand side of the denominator. For this reason the particle and hole lines created by the interaction on the left hand side are linked to those destroyed by the interaction on the right hand side. The direct diagram corrresponding to this term is presented in Fig. 8.3. The contribution to this diagram is:

$$\begin{aligned}\langle\Phi_0|\hat{V}(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{V}|\Phi_0\rangle_c &= \frac{1}{4}\sum_{ijmn}\left(\langle ij|\hat{v}|mn\rangle(\mathcal{E}_0 - (\mathcal{E}_0 + \epsilon_m + \epsilon_n - \epsilon_i - \epsilon_j))^{-1}\langle mn|\hat{v}|ij\rangle\right) \\ &= \frac{1}{4}\sum_{ijmn}\left(\langle ij|\hat{v}|mn\rangle(\epsilon_i + \epsilon_j - \epsilon_m - \epsilon_n)^{-1}\langle mn|\hat{v}|ij\rangle\right) \ . \end{aligned} \tag{8.29}$$

The other terms of Eq. (8.29) can be calculated in analogous manner. For example:

$$\langle\Phi_0|\hat{V}(\mathcal{E}_0 - \hat{H}_0)^{-1}\hat{U}|\Phi_0\rangle_c = \frac{1}{2}\sum_{ijm}\left(\langle ij|\hat{v}|mj\rangle(\epsilon_i - \epsilon_m)^{-1}\langle m|\hat{u}|i\rangle\right) \ . \tag{8.30}$$

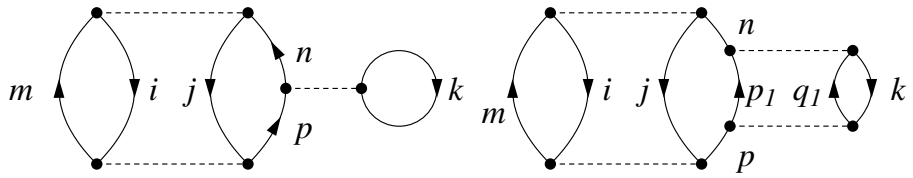

Figure 8.4: Insertion of interactions on a particle lines.

We consider now a generic diagram and we focus our attention to an interaction acting between the particle lines. The choice of operating only on particle lines is related to the fact that the interaction changes the state $|\phi_\alpha\rangle$, and working on particle lines avoid problems related to the blocking due to the Pauli exclusion principle.

Let's consider the diagram of Fig. 8.4 and insert the interaction lines in the part of the p e n line. The diagram with a single interaction between p and n is given by

$$\begin{aligned} & \langle\Phi_0|\hat{V}(\mathcal{E}_0-\hat{H}_0)^{-1}\hat{V}(\mathcal{E}_0-\hat{H}_0)^{-1}\hat{V}|\Phi_0\rangle_c \\ = & \frac{1}{8}\sum_{ijmp}\langle ij|\hat{v}|mp\rangle(\epsilon_i+\epsilon_j-\epsilon_m-\epsilon_p)^{-1}\sum_{kn}\langle pk|\hat{v}|nk\rangle(\epsilon_i+\epsilon_j-\epsilon_m-\epsilon_n)^{-1}\langle mn|\hat{v}|ij\rangle \ . \end{aligned} \tag{8.31}$$

The diagram with two interaction lines between p and n is given by

$$\begin{aligned} & \langle\Phi_0|\hat{V}(\mathcal{E}_0-\hat{H}_0)^{-1}\hat{V}(\mathcal{E}_0-\hat{H}_0)^{-1}\hat{V}(\mathcal{E}_0-\hat{H}_0)^{-1}\hat{V}|\Phi_0\rangle_c \\ = & \frac{1}{16}\sum_{ijmp}\langle ij|\hat{v}|mp\rangle(\epsilon_i+\epsilon_j-\epsilon_m-\epsilon_p)^{-1} \\ & \sum_{kn}\left[\sum_{p_1q_1}\langle pk|\hat{v}|p_1q_1\rangle(\epsilon_i+\epsilon_j+\epsilon_k-\epsilon_m-\epsilon_{p_1}-\epsilon_{q_1})^{-1}\langle p_1q_1|\hat{v}|nk\rangle\right] \\ & (\epsilon_i+\epsilon_j-\epsilon_m-\epsilon_n)^{-1}\langle mn|\hat{v}|ij\rangle \ . \end{aligned} \tag{8.32}$$

In the above equation it is possible to identify terms present also in Eq. (8.31) and not modified. These are the first and the last terms of the equation. The part which is modified is in square brackets. Also in this latter term there is a part, in the denominator, identical to that in Eq. (8.31) representing the energy differences between the parts of the diagram which did not changed after the inclusion of a new interaction line. I define

$$W=\epsilon_i+\epsilon_j+\epsilon_k-\epsilon_m \ . \tag{8.33}$$

The terms of the diagram which are modified by inserting the interaction lines are:

$$\text{1 line} \qquad \frac{1}{2}\langle pk|\hat{v}|nk\rangle\equiv\langle pk|\hat{V}|nk\rangle \tag{8.34}$$

$$\begin{aligned} \text{2 lines} \qquad & \frac{1}{4}\sum_{p'q'}\langle pk|\hat{v}|p_1q_1\rangle(W-\epsilon_{p_1}-\epsilon_{q_1})^{-1}\langle p_1q_1|\hat{v}|nk\rangle \\ \equiv \ & \langle pk|\hat{V}|p_1q_1\rangle(W-\epsilon_{p_1}-\epsilon_{q_1})^{-1}\langle p_1q_1|\hat{V}|nk\rangle \end{aligned} \tag{8.35}$$

$$\text{3 lines} \qquad \frac{1}{8}\sum_{p_1q_1p_2q_2}\langle pk|\hat{v}|p_1q_1\rangle(W-\epsilon_{p_1}-\epsilon_{q_1})^{-1}\langle p_1q_1|\hat{v}|p_2q_2\rangle(W-\epsilon_{p_2}-\epsilon_{q_2})^{-1}\langle p_2q_2|\hat{v}|nk\rangle$$

$$\equiv \sum_{p_1 q_1 p_2 q_2} \langle pk|\hat{V}|p_1 q_1\rangle (W - \epsilon_{p_1} - \epsilon_{q_1})^{-1} \langle p_1 q_1|\hat{V}|p_2 q_2\rangle (W - \epsilon_{p_2} - \epsilon_{q_2})^{-1} \langle p_2 q_2|\hat{V}|nk\rangle \quad (8.36)$$

n lines $\cdots$

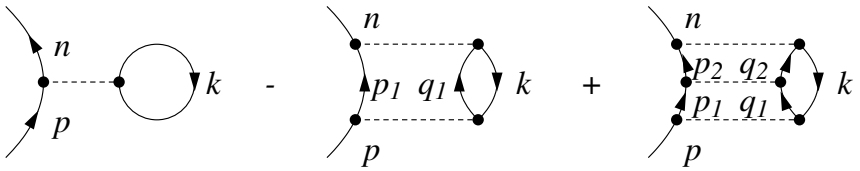

Figure 8.5: Insertion of interactions in a particle line.

We can build an operator $\hat{\mathcal{G}}$ whose action is the insertion of interaction lines between the states $\langle pk|$ and $|nk\rangle$. For this purpose we define an operator $\hat{Q}$ such as:

$$\hat{Q}|\alpha\beta\rangle = |\alpha\beta\rangle \text{ , if } \epsilon_\alpha, \epsilon_\beta > \epsilon_{\rm F} \quad (8.37)$$

$$\hat{Q}|\alpha\beta\rangle = 0 \text{ , (if } \epsilon_\alpha, \epsilon_\beta < \epsilon_{\rm F}) \ . \quad (8.38)$$

This operator selects only particle lines in the diagram. It is useful to consider also the operator $\hat{\mathcal{W}}$ whose action is

$$\hat{\mathcal{W}}|pq\rangle = (W - \epsilon_p - \epsilon_q)|pq\rangle \ , \quad (8.39)$$

where W is defined in Eq. (8.33). In the example we are discussing, the expectation value of $\hat{\mathcal{G}}$ is

$$\begin{aligned}\langle pk|\hat{\mathcal{G}}|nk\rangle &= \langle pk|\hat{V}|nk\rangle \\ &+ \sum_{p_1 q_1} \langle pk|\hat{V}|p_1 q_1\rangle (W - \epsilon_{p_1} - \epsilon_{q_1})^{-1} \langle p_1 q_1|\hat{V}|nk\rangle \\ &+ \sum_{p_1 q_1 p_2 q_2} \langle pk|\hat{V}|p_2 q_2\rangle (W - \epsilon_{p_2} - \epsilon_{q_2})^{-1} \langle p_2 q_2|\hat{V}|p_1 q_1\rangle (W - \epsilon_{p_1} - \epsilon_{q_1})^{-1} \langle p_1 q_1|\hat{V}|nk\rangle\end{aligned}$$

$$
\begin{aligned}
+ & \quad \cdots \\
= & \quad \langle pk|\hat{V} + \hat{V}\frac{\hat{Q}}{\hat{W}}\hat{V} + \hat{V}\frac{\hat{Q}}{\hat{W}}\hat{V}\frac{\hat{Q}}{\hat{W}}\hat{V} + \cdots |nk\rangle \\
= & \quad \langle pk|\hat{V} + \hat{V}\frac{\hat{Q}}{\hat{W}}\hat{\mathcal{G}}|nk\rangle \ . \qquad (8.40)
\end{aligned}
$$

From the operators point of view, we obtain the Bethe-Goldstone equation (8.16)

$$\hat{\mathcal{G}} = \hat{V} + \hat{V}\frac{\hat{Q}}{\hat{W}}\hat{\mathcal{G}} \ . \qquad (8.41)$$

This equation, gives a prescription how to construct an effective interaction whose behaviour at short distances does not produces the divergences. The idea is to use $\hat{\mathcal{G}}$ instead of $\hat{V}$ in the Goldstone expansion (8.1). Since the effective interaction $\hat{\mathcal{G}}$ has been obtained by considering an infinite set of ladder diagrams, it is necessary to care about the possibility that, in this procedure, some of the diagrams of the Goldstone expansion are already included in the definition of $\hat{\mathcal{G}}$. In order to avoid this problem of double counting, the selection of the Goldstone diagrams to calculate has to be accurate. For example, in the diagram of Fig. 8.6 the two upper lines represents a double counting.

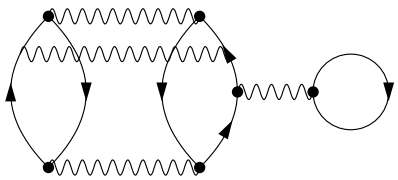

Figure 8.6: Diagram showing a double counting.

8.4 Comparison with the Lippmann-Schwinger equation

The Bethe-Goldstone equation (8.41) has strong analogies with an integral equation, the Lippmann-Schwinger equation, used to make a formal description of the scattering of two particles. In this section we recall the main physics assumptions leading to the Lippmann-Schwinger equation useful to clarify the differences between these two very similar equations. More detailed discussions and derivations of the Lippmann-Schwinger equation can be found in the basic Quantum Mechanics textbooks, such as [Mes61].

Let's consider the scattering of two particles in vacuum which interacts with a central potential. The asymptotic behaviour of the wave function describing the relative motion of the two particles can be expressed as:

$$\lim_{r\to\infty} \psi_{k_a}(\mathbf{r}) = e^{i\mathbf{k}_a\cdot\mathbf{r}} + f_{k_a}(\Omega)\frac{e^{ik_a r}}{r} \quad . \tag{8.42}$$

The cross section is related to the transition amplitude by the relation

$$\frac{d\sigma}{d\Omega} = |f_{k_a}(\Omega)|^2 \quad . \tag{8.43}$$

For a hamiltonian $\hat{H} = \hat{T} + \hat{V}$ the scattering amplitude is defined by the relation [Mes61]

$$\langle\phi_b|\hat{V}|\psi_a\rangle = -\frac{2\pi\hbar^2}{m} f_a(\Omega) \ , \tag{8.44}$$

where the writing has been simplified by indicating $a \equiv k_a$ and analogously for b. Strictly speaking, Eq. (8.44) does not describe a matrix element since the two state of the expectation value are not eigenstates of the same hamiltonian. We indicated with ϕ the eigenfunction of $\hat{H}_0 = \hat{T}$, and with ψ that of he full hamiltonian $\hat{H}$.

We define here the Green's function as a resolvent of the free and interacting hamiltonian. For the free Green's function we have the expression

$$\frac{\hbar^2}{2m}\left[\nabla^2 + k^2\right] G^0(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \ , \tag{8.45}$$

implying

$$G^0(\mathbf{r},\mathbf{r}') = -\frac{m}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \ , \tag{8.46}$$

where the energy of the free particle is

$$E = \frac{\hbar^2 k^2}{2m} \ . \tag{8.47}$$

The validity of the expression (8.46) can be verified by substitution and remembering that

$$\nabla^2 \frac{1}{|\mathbf{r}-\mathbf{r}'|} = -4\pi\delta(\mathbf{r}-\mathbf{r}') \ .$$

The solution of the Schrödinger equation for the two-interacting particles is

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int d^3r'\, G^0(\mathbf{r},\mathbf{r}')\hat{V}(\mathbf{r}')\psi(\mathbf{r}') \ , \tag{8.48}$$

in fact, by inserting the above expression in the equation

$$\frac{\hbar^2}{2m}\left[\nabla^2 + k^2\right]\psi(\mathbf{r}) = \hat{V}(\mathbf{r})\psi(\mathbf{r}) \ , \tag{8.49}$$

we obtain

$$\begin{aligned} & \frac{\hbar^2}{2m}\left[\nabla^2+k^2\right]e^{i\mathbf{k}\cdot\mathbf{r}}+\int d^3r'\,\frac{\hbar^2}{2m}\left[\nabla^2+k^2\right]G^0(\mathbf{r},\mathbf{r}')\hat{V}(\mathbf{r}')\psi(\mathbf{r}') \\ = & \frac{\hbar^2}{2m}\left[-k^2+k^2\right]e^{i\mathbf{k}\cdot\mathbf{r}}+\int d^3r'\,\delta(\mathbf{r}-\mathbf{r}')\hat{V}(\mathbf{r}')\psi(\mathbf{r}') \\ = & 0+\hat{V}(\mathbf{r})\psi(\mathbf{r})\ . \end{aligned}$$

Let's define an operator $\hat{\mathcal{T}}$ such as

$$\langle\phi_b|\hat{\mathcal{T}}|\phi_a\rangle=\langle\phi_b|\hat{V}|\psi_a\rangle\ . \tag{8.50}$$

which is the analogous of the definition (8.2) of $\hat{Q}$ but for two particles in vacuum.

We can consider Eq. (8.45) as an equality between operators

$$(E-\hat{H}_0)G^0=\hat{\mathbb{I}}\ ;\ G^0=\frac{\hat{\mathbb{I}}}{(E-\hat{H}_0)}\ , \tag{8.51}$$

and Eq. (8.48) can be written as

$$|\psi_a\rangle=|\phi_a\rangle+G^0\hat{V}|\psi_a\rangle=|\phi_a\rangle+\frac{1}{E-\hat{H}_0+i\eta}\hat{V}|\psi_a\rangle\ , \tag{8.52}$$

where the $i\eta$ term has been inserted to avoid divergences. Multiplying on the left hand side for $\hat{V}$ and considering the definition (8.50) of $\hat{\mathcal{T}}$ we obtain

$$\hat{V}|\psi_a\rangle=\hat{V}|\phi_a\rangle+\hat{V}\frac{\hat{\mathbb{I}}}{E-\hat{H}_0+i\eta}\hat{V}|\psi_a\rangle \tag{8.53}$$

or equivalently

$$\hat{\mathcal{T}}|\phi_a\rangle=\left(\hat{V}+\hat{V}\frac{\hat{\mathbb{I}}}{E-\hat{H}_0+i\eta}\hat{\mathcal{T}}\right)|\phi_a\rangle\ , \tag{8.54}$$

which is the Lippmann-Schwinger equation.

The analogy with the Bethe-Goldstone equation (8.16) is evident. Rhe Bethe-Goldstone equation describes the interaction between two particles which scatter in the medium. The most remarkable difference is related to the presence of the operator $\hat{Q}$ which takes into account the Pauli exclusion principle. In the medium, only the reactions populating states above the Fermi surface are allowed. In the vacuum there are not limitations to the final states.

Another difference is related to the energy denominator. In the Lippmann-Schwinger equation, the denominator contains only the kinetic energies of the colliding particles, and the presence of the imaginary term is necessary since there is the possibility that the denominator can be zero. In the Bethe-Goldstone equation, the denominator is never equal to zero since there are not unlinked diagrams. Furthermore, the single particle energies are not the kinetic energies of the particles, but they contain also the mean-field energy term. Finally, there is also the W term, defined by Eq. (8.33) inserting in the denominator the dependence on the single particle energies of the diagrams terms which are not directly involved by the interaction of the two particles.

8.5 Application to nuclear matter

The most remarkable application of the Brueckner theory to physical system has been done on nuclear matter. This is a fictitious system of a infinite number nucleons which has translational symmetry. These properties simplify the mean-field problems since the potential is constant and the single-particle wave functions are plane waves. The Coulomb interaction is switched off, and, here, we shall consider the case of equal number of protons and neutrons. The single-particle wave functions are characterized by the wave number $\mathbf{k} = \mathbf{p}/\hbar c$, where $\mathbf{p}$ is the momentum of the particle (see section 2.3).

The empirical evidences coming from the elastic electron scattering off nuclei indicate that the charge distributions at the nuclear center have similar values for the different nuclei on the nuclide chart [Kra88]. By simplifying the situation let's consider the nucleus as a rigid sphere of constant density with a radius R. We then obtain the density value by dividing the number of nucleons by the volume of the sphere:

$$\rho = \frac{A}{\frac{4}{3}\pi R^3} = \frac{A}{\frac{4}{3}\pi r_0^3 A} = \frac{3}{4\pi r_0^3} = 0.17 \pm 0.02 \ \text{fm}^{-3} \ , \tag{8.55}$$

where the empirical relation $R = r_0 A^{\frac{1}{3}}$ with r_0=1.12 fm has been used.

In order to estimate the binding energy of this system, we consider the following expression of the semi-empirical mass formula [Kra88]

$$B(A,Z) = a_v A + a_s A^{\frac{2}{3}} + a_c \frac{Z^2}{A^{\frac{1}{3}}} + a_i \frac{(N-Z)^2}{A} + \delta(A) \ , \tag{8.56}$$

and we study its behaviour under the assumptions mentioned above. Since we assume that the number of protons and neutrons is the same, the asymmetry term, the fourth term in the right hand side, is zero. This approximation is done here to simplify the treatment, but it not necessary for the system stablilty. There are studies on asymmetric nuclear matter, and especially on neutron matter. Neutron stars, associated to the pulsars, are, at the moment, the physical systems most similar to nuclear matter.

Much more relevant the other assumption: the Coulomb interaction is switched off. This assumption is necessary for the stability of the infinite system. Because the Coulomb interaction has infinite range, all the protons interact among them. In the limit for an infinite number of protons there will be an infinite repulsion.

With these assumptions the expression of the binding energy per nucleon of nuclear matter is:

$$\frac{B(A,Z)}{A} = a_v + a_s A^{-\frac{1}{3}} + \frac{\delta(A)}{A} \ , \tag{8.57}$$

and neglecting the last term, the pairing term, in the limit for A going to infinity only the volume term survives: $a_v = 16.0$ MeV.

A proper description of nuclear matter should predict an equation of state relating the binding energy per nucleon with the density of the system. The minimum of this function should appear in the empirical region where for $\rho = 0.17 \pm 0.02$, fm^{-3} one has $B(A,Z)/A = 16.0 \pm 1.0$ MeV.

The mean-field treatment of a system with translational invariance has been presented in Section 2.3. Eq. (2.54) expresses the density of the system as a function of the Fermi momentum

$$\rho(\mathbf{r}) = \frac{2}{3\pi^2} {k_\text{F}}^3 \ . \tag{8.58}$$

By using the empirical value of the density we find that the numerical value of the Fermi momentum is $k_\text{F} = 1.36$ fm^{-1} = 250 MeV/c. Eq. (2.57) gives he kinetic energy per particle of the system

$$\frac{T}{A} = \frac{3}{5}\epsilon_\text{F} \ , \tag{8.59}$$

where the Fermi energy is given by

$$\epsilon_{\rm F} = \frac{\hbar^2}{2m} {k_{\rm F}}^2 \ . \tag{8.60}$$

We present here below how the Brueckner theory is applied to this system. We define the relative coordinates of the two interacting particles p and q

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_p + \mathbf{r}_q) \quad ; \quad \mathbf{r} = \mathbf{r}_p - \mathbf{r}_q \tag{8.61}$$

$$\mathbf{K}_{pq} = \mathbf{k}_p + \mathbf{k}_q \quad ; \quad \mathbf{k}_{pq} = \mathbf{k}_p - \mathbf{k}_q \ . \tag{8.62}$$

The unperturbed wave function describing the motion of the two particles is

$$\Phi_{pq}(\mathbf{r}_p, \mathbf{r}_q) = \frac{1}{\mathcal{V}} e^{i\mathbf{k}_p\cdot\mathbf{r}_p} e^{i\mathbf{k}_q\cdot\mathbf{r}_q} = \frac{1}{\mathcal{V}} e^{i\mathbf{K}_{pq}\cdot\mathbf{R}} e^{i\mathbf{k}_{pq}\cdot\mathbf{r}} = \frac{1}{\mathcal{V}} e^{i\mathbf{K}_{pq}\cdot\mathbf{R}} \phi_{pq}(\mathbf{r}) \ , \tag{8.63}$$

where we indicated with $\mathcal{V}$ the volume, which will go to infinity at the end of the calculation, and we neglected the spin and isospin terms.

The operators $\hat{Q}$ and $\hat{\mathcal{W}}$ previously defined act on this wave function. The action of $\hat{Q}$ on the wave function

$$\hat{Q}|\Phi_{pq}\rangle = |\Phi_{pq}\rangle \ , \tag{8.64}$$

is different from zero only when both $|\mathbf{k}_p|$ and $|\mathbf{k}_q|$ are larger than $\mathbf{k}_{\rm F}$, and the action of $\hat{\mathcal{W}}$ is

$$\hat{\mathcal{W}}|\Phi_{pq}\rangle = \left[W - \epsilon(\mathbf{k}_p) - \epsilon(\mathbf{k}_q)\right]|\Phi_{pq}\rangle = e(\mathbf{k}_p, \mathbf{k}_q)|\Phi_{pq}\rangle \ . \tag{8.65}$$

The wave function of the two interacting particles can be written by factorizing the free motion of the center of mass with respect to the relative motion

$$\Psi_{pq}(\mathbf{r}_p, \mathbf{r}_q) = \frac{1}{\mathcal{V}} e^{i\mathbf{K}_{pq}\cdot\mathbf{R}} \psi_{pq}(\mathbf{r}) \ . \tag{8.66}$$

Because of he definition (8.2) we can write

$$\begin{aligned} \langle\Phi_{pq}|\hat{\mathcal{G}}|\Phi_{rs}\rangle &= \int d^3r_p\, d^3r_q\, \Phi_{pq}(\mathbf{r}_p, \mathbf{r}_q)\hat{V}(\mathbf{r})\Psi_{rs}(\mathbf{r}_p, \mathbf{r}_q) \\ &= \frac{1}{(2\pi)^3}\delta(\mathbf{K}_{pq} - \mathbf{K}_{sr}) \int d^3r e^{i\mathbf{k}_{pq}\cdot\mathbf{r}} \hat{V}(\mathbf{r})\psi_{rs}(\mathbf{r}) \equiv \langle\phi_{pq}|\hat{\mathcal{G}}|\phi_{rs}\rangle \ . \end{aligned} \tag{8.67}$$

The part related to the center of mass coordinate can be factorized, therefore, by considering Eq. (8.66), we obtain

$$\psi_{pq}(\mathbf{r}) = \phi_{pq}(\mathbf{r}) + \int d^3r'\, \mathcal{K}_{pq}(\mathbf{r}, \mathbf{r}')\hat{V}(r')\psi_{pq}(\mathbf{r}') \ , \tag{8.68}$$

with

$$\mathcal{K}_{pq}(\mathbf{r}, \mathbf{r}') = \frac{1}{(2\pi)^3} \int d^3k \frac{\hat{Q}(\mathbf{K}_{pq}, \mathbf{k})}{e(\mathbf{K}_{pq}, \mathbf{k})} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \ . \tag{8.69}$$

In the solution of the Goldstone equation (8.1) it is necessary to select the type of diagram to calculate. In this diagram there is certainly a matrix element of the (8.67) type. The procedure adopted to solve the set of equations giving the value of this matrix element is composed by the following steps.

1. Choice of $\hat{U}$ to select the single particle energies of the denominator.
2. Numerical solution of Eq. (8.69).
3. Insertion of the kernel (8.69) in Eq. (8.68).
4. Insertion of Eq. (8.68) in the matrix element (8.67).

8.6 Final considerations

1. In the scattering in vacuum, the denominator of the Lippmann-Schwinger equation (8.54) has an imaginary part. This implies that asymptotically there is a phase shift between scattering and free wave functions. In the Bethe-Goldstone equation (8.16) the imaginary term is not present, therefore there is no phase shift between the relative wave functions of the interacting particles ψ_{pq} and those of the non interacting particles ϕ_{pq}. The difference between these two wave functions is present only at short distances where the, finite range, potential plays an important role, essentially in the region of the strongly repulsive core.

2. The key parameter of the Goldstone expansion is not the number of interacting lines but the number of hole lines. Diagrams differing by one interaction line generate contribution of the same order of magnitude. On the other hand diagrams with an additional hole lines produce contributions one order of magnitude smaller with respect to the diagrams with a hole line less [Day67]. The hole line expansion is an expansion in density powers. In many-body physics one has to consider the relative density, i.e. the number of pointlike particles present in the volume defined by the strongly repulsive core of the interaction (see Section 3.4).

3. In principle, the interaction $\hat{\mathcal{G}}$ should be independent of the choice of the mean-field potential $\hat{U}$. In reality this does not happens since the Goldstone expansion (8.1) is truncated. The convergence of the expansion by using $\hat{\mathcal{G}}$, calculated with $\hat{H}_1 = \hat{V}$ is very slow. The insertion in the perturbative term of the hamiltonian of a one-body term, $\hat{H}_1 = \hat{V} - \hat{U}$ contributes to speed up the convergence. The self-consistent choice of $\hat{U}$ is
$$\hat{U} = \sum_{\alpha} \langle \phi_\alpha | \hat{\mathcal{G}}(W) | \phi_\alpha \rangle \tag{8.70}$$
The so-called *normal* choice consists in considering in the above sum only the states below the Fermi surface. In this choice there is a discontinuity in the single particle energies. Those below the Fermi energy contain also the potential term, while those above the Fermi energy are only kinetic energies. This, relatively simple, choice does not guarantee stability of the results which are strongly dependent on the choice of $\hat{U}$. When it has been possible, thanks to the improvement of the computational capacities, the *continous* choice, consisting in considering the full space in the sum of Eq. (8.70), showed a remarkable independence of the results on the choice of $\hat{U}$.

Chapter 9

Mean-field applications of the variational principle

9.1 Introduction

The variational principle is one of the most used methods to solve the Schrödinger equation in approximated manner. The basic idea is that the wave function which minimizes the energy, considered a functional of the many-body wave function, is the correct eigenfunction of the hamiltonian. This is correct if the search for the minimum is carried out by considering the full Hilbert space. In reality the problem is simplified by assuming a specific expression of the wave function and the search for the minimum is done in the subspace spanned by all the wave functions which have the chosen expression. In this manner the energy value obtained is an upper bound of the correct energy eigenvalue of the hamiltonian. The formal properties of the variational principle are discussed in the Quantum Mechanics textbooks, for example [Mes61]. A summary of the properties of our interest is given in the Appendix A.

We have already shown an application of the variational principle in Sect. 4.2. In that case the multi-dimensional integrals required by the calculation of the energy were carried out with Monte Carlo techniques. In that calculation the expression of the trial wave functions was given by Eq. (4.12) which represented the product of a Slater determinant by a correlation function. Another application of the variational principle with this type of trial wave function will be presented in Chapter 13.

In this chapter, we shall concentrate our attention on the application of the variational principle to much simpler trial wave functions whose expression is that of a singular Slater determinant. This choice of the trial wave function leads to theories which, in the language of the many-body physics, are classified as MF theories: Hartree-Fock (HF) and Density Functional Theory (DFT).

The microscopic theories describing many-body systems consider the MF problem has been solved and make use of the single-particle basis generated by this solution. We have presented in Chapter 2 how the MF model is solved for different kinds of many-body systems. Those approaches were of phenomenological type. The average potentials contained parameters whose choice was guided by the requirement of reproducing some, selected, experimental data. In this chapter, we present an approach which provides a solid theoretical ground of the phenomenological models of Chapter 2.

9.2 Hartree-Fock

9.2.1 The Hartee-Fock hamiltonian

In this section we obtain an expression of the hamiltonian very convenient for its use in HF calculations. No new physics is presented, it is only a rewriting of the expression of the hamiltonian. In this new expression it will become evident the approximation made by the HF theory.

Let's consider the expression of the hamiltonian in ONR Eq. (5.56):

$$\begin{aligned}\hat{H} &= \sum_{\nu\nu'} T_{\nu\nu'}\hat{a}^+_\nu\hat{a}_{\nu'} + \frac{1}{2}\sum_{\nu\mu\nu'\mu'} V_{\nu\mu\nu'\mu'}\hat{a}^+_\nu\hat{a}^+_\mu\hat{a}_{\mu'}\hat{a}_{\nu'} \\ &= \sum_{\nu\nu'} T_{\nu\nu'}\hat{a}^+_\nu\hat{a}_{\nu'} + \frac{1}{4}\sum_{\nu\nu'\mu\mu'} \overline{V}_{\nu\mu\nu'\mu'}\hat{a}^+_\nu\hat{a}^+_\mu\hat{a}_{\mu'}\hat{a}_{\nu'} \ . \end{aligned} \tag{9.1}$$

where only two-body interactions have been considered. The antisymmetrized matrix element is defined as:

$$\overline{V}_{\nu\mu\nu'\mu'} \equiv \langle\nu\mu|V|\nu'\mu'\rangle - \langle\nu\mu|V|\mu'\nu'\rangle \ . \tag{9.2}$$

From the definition of contraction (see Sect. 6.3), for ν and $\nu' < \epsilon_{\rm F}$ we have that

$$\hat{a}^+_\nu\,\hat{a}_{\nu'} = \delta_{\nu\nu'}\delta_{\nu' i} \ \ ; \ \ \hat{a}_\nu\,\hat{a}^+_{\nu'} = 0 \ \ ; \ \ \hat{a}_\nu\,\hat{a}_{\nu'} = 0 \ \ ; \ \ \hat{a}^+_\nu\,\hat{a}^+_{\nu'} = 0 \ . \tag{9.3}$$

By considering the definition of normal ordered product $\hat{\mathbb{N}}$ we obtain

$$\hat{a}^+_\nu\,\hat{a}_{\nu'} = \hat{\mathbb{N}}[\hat{a}^+_\nu\,\hat{a}_{\nu'}] + \hat{a}^+_\nu\,\hat{a}_{\nu'} \ , \tag{9.4}$$

and, for the Wick's theorem,

$$\begin{aligned}\hat{a}^+_\nu\hat{a}^+_\mu\,\hat{a}_{\mu'}\,\hat{a}_{\nu'} &= \hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}^+_\mu\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}] \\ &+ \hat{\mathbb{N}}[\hat{a}^+_\mu\hat{a}_{\mu'}]\hat{a}^+_\nu\,\hat{a}_{\nu'} + \hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}_{\nu'}]\hat{a}^+_\mu\,\hat{a}_{\mu'} \\ &- \hat{\mathbb{N}}[\hat{a}^+_\mu\hat{a}_{\nu'}]\hat{a}^+_\nu\,\hat{a}_{\mu'} - \hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}_{\mu'}]\hat{a}^+_\mu\,\hat{a}_{\nu'} \\ &+ \hat{a}^+_\mu\hat{a}_{\mu'}\hat{a}^+_\nu\,\hat{a}_{\nu'} - \hat{a}^+_\nu\hat{a}_{\mu'}\hat{a}^+_\mu\,\hat{a}_{\nu'} \ . \end{aligned} \tag{9.5}$$

Let's insert the above expression in Eq. (9.1)

$$\begin{aligned}\hat{H} &= \sum_{\nu\nu'} T_{\nu\nu'}\hat{a}^+_\nu\hat{a}_{\nu'} + \frac{1}{4}\sum_{\mu\mu'\nu\nu'} \overline{V}_{\nu\mu\nu'\mu'}\Big\{\hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}^+_\mu\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}] \\ &+ \hat{\mathbb{N}}[\hat{a}^+_\mu\hat{a}_{\mu'}]\delta_{\nu\nu'}\delta_{\nu i} + \hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}_{\nu'}]\delta_{\mu\mu'}\delta_{\mu i} - \hat{\mathbb{N}}[\hat{a}^+_\mu\hat{a}_{\nu'}]\delta_{\nu\mu'}\delta_{\nu i} - \hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}_{\mu'}]\delta_{\mu\nu'}\delta_{\mu i} \\ &+ \delta_{\nu\nu'}\delta_{\nu i}\delta_{\mu\mu'}\delta_{\mu j} - \delta_{\nu\mu'}\delta_{\nu i}\delta_{\mu\nu'}\delta_{\mu j}\Big\} \end{aligned} \tag{9.6}$$

where we have already considered the fact that a contraction is different from zero only if the single-particle state is of hole type, i.e. if its energy is below the Fermi surface. We used the common convention of indicating with i, j, k, l the hole states and with m, n, p, q, r the particle states.

By considering the restrictions imposed by the indexes of the Kronecker δ, we obtain

$$\hat{H} = \sum_{\nu\nu'} T_{\nu\nu'}\hat{a}^+_\nu\hat{a}_{\nu'} + \frac{1}{4}\sum_{\mu\mu'\nu\nu'} \overline{V}_{\nu\mu\nu'\mu'}\hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}^+_\mu\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}]$$

$$
\begin{aligned}
&+ \quad \frac{1}{4}\sum_{\mu\mu' i}\overline{V}_{\mu i\mu' i}\hat{\mathbb{N}}[\hat{a}^+_\mu\hat{a}_{\mu'}] + \frac{1}{4}\sum_{\nu\nu' i}\overline{V}_{i\nu i\nu'}\hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}_{\nu'}] \\
&- \quad \frac{1}{4}\sum_{\mu\nu' i}\overline{V}_{i\mu\nu' i}\hat{\mathbb{N}}[\hat{a}^+_\mu\hat{a}_{\nu'}] - \frac{1}{4}\sum_{\nu\mu' i}\overline{V}_{\nu i i\mu'}\hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}_{\mu'}] \\
&+ \quad \frac{1}{4}\sum_{ij}\overline{V}_{iji j} - \frac{1}{4}\sum_{ij}\overline{V}_{ijji} \ . \qquad (9.7)
\end{aligned}
$$

The definition (9.2) of the antisymmetric matrix element implies the following relations:

$$
\overline{V}_{\nu\mu\nu'\mu'} = -\overline{V}_{\mu\nu\nu'\mu'} = \overline{V}_{\mu\nu\mu'\nu'} = -\overline{V}_{\nu\mu\mu'\nu'} \ , \qquad (9.8)
$$

therefore

$$
\begin{aligned}
\hat{H} \quad &= \quad \sum_{\nu\nu'} T_{\nu\nu'}\hat{a}^+_\nu\hat{a}_{\nu'} + \frac{1}{4}\sum_{\mu\mu'\nu\nu'}\overline{V}_{\nu\mu\nu'\mu'}\hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}^+_\mu\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}] \\
&+ \quad \sum_{\nu\nu' i}\overline{V}_{\nu i\nu' i}\hat{\mathbb{N}}[\hat{a}^+_\nu\,\hat{a}_{\nu'}] + \frac{1}{2}\sum_{ij}\overline{V}_{iji j} \ . \qquad (9.9)
\end{aligned}
$$

Let's consider the normal ordered product of two operators and write it following the definition of contraction

$$
\hat{\mathbb{N}}[\hat{a}^+_\nu\,\hat{a}_{\nu'}] = \hat{a}^+_\nu\,\hat{a}_{\nu'} - \hat{a}^+_\nu\,\hat{a}_{\nu'} \ . \qquad (9.10)
$$

The last but one term of Eq. (9.9) becomes

$$
\sum_{\nu\nu' i}\overline{V}_{\nu i\nu' i}\hat{\mathbb{N}}[\hat{a}^+_\nu\,\hat{a}_{\nu'}] = \sum_{\nu\nu' i}\overline{V}_{\nu i\nu' i}\hat{a}^+_\nu\,\hat{a}_{\nu'} - \sum_{ij}\overline{V}_{iji j} \ , \qquad (9.11)
$$

therefore, the hamiltonian can be expressed as

$$
\begin{aligned}
\hat{H} \quad &= \quad \sum_{\nu\nu'}\left(T_{\nu\nu'} + \sum_i \overline{V}_{\nu i\nu' i}\right)\hat{a}^+_\nu\hat{a}_{\nu'} \\
&+ \quad \frac{1}{4}\sum_{\mu\mu'\nu\nu'}\overline{V}_{\nu\mu\nu'\mu'}\hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}^+_\mu\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}] - \frac{1}{2}\sum_{ij}\overline{V}_{iji j} \ . \qquad (9.12)
\end{aligned}
$$

This expression makes evident the presence in the hamiltonian of a one-body operator, the term multiplying $\hat{a}^+_\nu\hat{a}_{\nu'}$. It is interesting to notice that part of the interaction $\overline{V}$ contributes to the one-body term. So far, we did not make any assumption on the structure of the basis of single-particle wave functions composing the Slater determinant on which the creation and destruction operators are acting. For this reason we can choose the single-particle basis which diagonalizes the one-body term of Eq. (9.12), that is

$$
h_{\nu\nu'} = T_{\nu\nu'} + \sum_i \overline{V}_{\nu i\nu' i} \ , \qquad (9.13)
$$

therefore

$$
\langle\nu|h|\nu\rangle = \epsilon_\nu \ . \qquad (9.14)
$$

The expression of the hamiltonian in this basis is

$$
\hat{H} = \sum_\nu \epsilon_\nu\hat{a}^+_\nu\hat{a}_\nu - \frac{1}{2}\sum_{ij}\overline{V}_{iji j} + \frac{1}{4}\sum_{\mu\mu'\nu\nu'}\overline{V}_{\nu\mu\nu'\mu'}\hat{\mathbb{N}}[\hat{a}^+_\nu\hat{a}^+_\mu\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}] = \hat{H}_0 + \hat{V}_{\rm res} \ . \qquad (9.15)
$$

In the above expression $\hat{H}_0$ has been defined as the one-body term plus the constant term and $\hat{V}_{\rm res}$, called residual interaction, is the last operator term containing the normal ordered product of four creation and destruction operators.

The expectation value of the hamiltonian (9.15) on the Slater determinant built with the eigenstates of $\hat{h}$ and describing the ground state of the system is

$$\begin{aligned} & \langle\Phi_0|\hat{H}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_0|\Phi_0\rangle + \langle\Phi_0|\hat{V}_{\rm res}|\Phi_0\rangle \\ = & \sum_\nu \epsilon_\nu \langle\Phi_0|\hat{a}^+_\nu \hat{a}_\nu|\Phi_0\rangle - \frac{1}{2}\sum_{ij}\overline{V}_{ijij}\langle\Phi_0|\Phi_0\rangle \\ + & \frac{1}{4}\sum_{\mu\mu'\nu\nu'}\overline{V}_{\nu\mu\nu'\mu'}\langle\Phi_0|\hat{\mathbb{N}}[\hat{a}^+_\nu \hat{a}^+_\mu\, \hat{a}_{\mu'}\, \hat{a}_{\nu'}]|\Phi_0\rangle \\ = & \sum_i \epsilon_i - \frac{1}{2}\sum_{ij}\overline{V}_{ijij} = \mathcal{E}_0 \ . \end{aligned} \tag{9.16}$$

Let's summarize here below the remarkable results of this section.

- The expression (9.15) of the hamiltonian is only a different way of writing Eq. (9.1), but in the former expression the normal ordered product is highlighted. There is not difference in the physics contents of the two expressions.
- The expectation value of the hamiltonian calculated for the ground state Slater determinant neglects one term of the hamiltonian. In the description of a many-body system in terms of a single Slater determinant, or in other words in terms of MF model, the contribution of the term related to the normal ordered product is zero, by definition. This is the great approximation implicit in any MF description of a many-body system. The term of the hamiltonian which is not considered in this description is called *residual interaction*. The one-body part, $\hat{H}_0$, of the hamiltonian is responsible of the IPM, or MF model. Phenomena beyond this description are due the presence of the residual interaction $\hat{V}_{\rm res}$, ad they are generically called *long-range correlations* to distinguish them from other effects related to the strongly repulsive core of the interaction which are, instead, called *short-range correlations*.
- The total energy of the many-body system in the framework of a mean-field model can be calculated by knowing only the two-body interaction $\hat{V}$. The expression (9.16) indicates that the total energy is not simply the sum of the single-particle energies but it explicitly contains an interaction term.

It is evident from the discussion done in Chapter 8 that the interaction used in the HF calculations is not one of the microscopic interactions presented in Chapter 3. The strongly repulsive core of these interactions is not properly handled in these calculations which require the use of the effective interactions such as that presented in Chapter 8.

9.2.2 Hartree-Fock equations

The variational calculation of the energy of the system is carried out by using Eq. (9.16). In the HF theory the search is for that Slater determinant which minimizes this value. It is therefore matter of searching for the minimum of E_0, considered a functional of the many-body wave function, in the subspace of the Hilbert space spanned by all the possible Slater determinants which can be built. The variational principle is applied by selecting the set of single particle states forming the Slater determinant. Clearly, these single-particle wave functions must be orthonormalized to form a basis. This is an external condition which has to be imposed. Therefore, the problem to be solved is in the search of a constrained minimum which is tackled by using the Lagrange multipliers technique.

The variational principle with the orthonormalization conditions can be expressed as

$$\delta \left[E(\Phi) - \sum_{ij} \lambda_{ij} \langle i|j\rangle \right] = 0 \ , \tag{9.17}$$

and, by using the hamiltonian operator $\hat{H}$

$$\delta\langle\Phi|\hat{H}|\Phi\rangle - \sum_{ij} \lambda_{ij}\delta\langle i|j\rangle = 0 \ , \tag{9.18}$$

where $|\Phi\rangle$ is the Slater determinant formed by the functions $|i\rangle$, and λ_{ij} is the Lagrange multiplier.

By using the expression (9.12) of the hamiltonian operator we obtain

$$\sum_i \delta\langle i|\hat{T}|i\rangle + \frac{1}{2}\sum_{ij}\left[\delta\langle ij|\hat{V}|ij\rangle - \delta\langle ij|\hat{V}|ji\rangle\right] - \sum_{ij}\lambda_{ij}\delta\langle i|j\rangle = 0 \ . \tag{9.19}$$

Since i and j are dummy indexes indicating hole states, we have that

$$\sum_{ij}\delta\langle ij| = \sum_{ij}[\langle(\delta i)j| + \langle i(\delta j)|] = 2\sum_{ij}\langle(\delta i)j| \ , \tag{9.20}$$

and therefore,

$$\sum_i \langle\delta i|\hat{T}|i\rangle + \sum_{ij}\left[\langle(\delta i)j|\hat{V}|ij\rangle - \langle(\delta i)j|\hat{V}|ji\rangle\right] - \sum_{ij}\lambda_{ij}\langle(\delta i)|j\rangle = 0 \ . \tag{9.21}$$

Since the variations $\langle\delta i|$ are independent of each other, each term of the above sum on i must be zero. This implies that for a generic term with $i = k$ we have

$$\langle\delta k|\hat{T}|k\rangle + \sum_j\left[\langle\delta k|\langle j|\hat{V}|j\rangle|k\rangle - \langle\delta k|\langle j|\hat{V}|k\rangle|j\rangle\right] = \sum_j \lambda_{kj}\langle\delta k|j\rangle \ . \tag{9.22}$$

Since $|\delta k\rangle$ is different from zero, I can simplify the above expression by writing

$$\hat{T}|k\rangle + \sum_j\left[\langle j|\hat{V}|j\rangle|k\rangle - \langle j|\hat{V}|k\rangle|j\rangle\right] = \sum_j \lambda_{kj}|j\rangle \ . \tag{9.23}$$

The Lagrange multiplier λ_{ij} is a real number, therefore it can be considered as the expectation value of a single-particle hamiltonian $\hat{h}$

$$\lambda_{kj} = \langle k|\hat{h}|j\rangle \ . \tag{9.24}$$

By using a unitary transformation, it is possible to find a single-particle basis where $\hat{h}$ is diagonal:

$$\langle\tilde{k}|\hat{h}|\tilde{j}\rangle = \epsilon_k\delta_{kj} \ . \tag{9.25}$$

The operator $\hat{\mathcal{U}}$ which makes the unitary transformation from a single-particle basis to another one is given by

$$|\tilde{k}\rangle = \sum_{k'}\hat{\mathcal{U}}_{kk'}|k'\rangle \quad \text{with} \quad \sum_{kk'}\hat{\mathcal{U}}^\dagger_{kk'}\hat{\mathcal{U}}_{k'k} = \hat{\mathbb{I}} \ . \tag{9.26}$$

The Slater determinant in the new basis is

$$|\tilde{\Phi}\rangle = \det(\hat{\mathcal{U}})|\Phi\rangle \ , \tag{9.27}$$

The $\hat{\mathcal{U}}$ is unitary operator which means that it satisfies the relation $|\det(\mathcal{U})| = 1$. This implies that the value of the determinant in the two bases is the same, apart from a phase factor, therefore the value of the functional $E(\Phi)$ is invariant under a unitary transformation of the basis, and, clearly, also its variation is invariant.

In the new basis (and here we substituted k to $\tilde{k}$ to simplify the writing), we obtain the expression

$$\hat{h}|k\rangle = \hat{T}|k\rangle + \sum_j \Big[\langle j|\hat{V}|j\rangle|k\rangle - \langle j|\hat{V}|k\rangle|j\rangle\Big] = \epsilon_k|k\rangle \ . \tag{9.28}$$

We define the average potential as

$$\hat{U}(\mathbf{r}) = \sum_j \langle j|\hat{V}|j\rangle = \sum_j \int d^3r' \phi_j^*(\mathbf{r}')\hat{V}(\mathbf{r},\mathbf{r}')\phi_j(\mathbf{r}') \ , \tag{9.29}$$

which is also called Hartree term. The sum is carried on all the states below the Fermi surface. This term describes the interaction of the k particle with all the other ones.

The second term containing the interaction is non-local, and is called Fock - Dirac term

$$\hat{W}(\mathbf{r},\mathbf{r}') = \sum_j \phi_j^*(\mathbf{r}')\hat{V}(\mathbf{r},\mathbf{r}')\phi_j(\mathbf{r}) \ . \tag{9.30}$$

In configuration space, the expression of Eq. (9.29) is

$$\hat{h}\phi_k(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m}\phi_k(\mathbf{r}) + \underbrace{\hat{U}(\mathbf{r})\phi_k(\mathbf{r})}_{\text{Hartree}} - \underbrace{\int d^3r' \hat{W}(\mathbf{r},\mathbf{r}')\phi_k(\mathbf{r}')}_{\text{Fock-Dirac}} = \epsilon_k\phi_k(\mathbf{r}) \ . \tag{9.31}$$

By neglecting the Fock-Dirac term we obtain a differential equation of mean-field type. The Fock-Dirac term, also called exchange term, changes the bare mean-field equation by inserting the effect of the Pauli exclusion principle.

It is worth to remark that the sums on the equations (9.29) and (9.30) do not have any limitations. If separately considered in the Eq. (9.28) they contain self-interaction terms when $j = k$. In the HF case, the two terms are identical but with opposite sign, therefore in the expression (9.28) there are not self-interactions.

The differential equations (9.31) are numerically solved by using an iterative procedure. One starts with a set of trial wave functions $|k\rangle_{(1)}$ built with mean-field methods, using for example harmonic oscillator or Woods-Saxon potentials. With these trial wave functions the Hartree (9.29) and Fock-Dirac (9.30) terms are calculated and included in Eq. (9.31). The solution of the Equations (9.31), solved with standard numerical methods, generates a new set of wave functions $|k\rangle_{(2)}$ which can be used to calculate new $\hat{U}$ and $\hat{W}$ potentials. The process continues up to convergence. Normally, the converge criterium is chosen by considering the differences between the total energies of the system (9.16) calculated in the i and $i+1$ iteration.

Koopmans' theorem

The physical meaning of the Lagrange multiplier ϵ_k is clarified by what is called *Koopmans' theorem* indicating that this quantity corresponds to the energy required to add a particle to the system of A particles.

We call $|\Phi_A\rangle$ the HF state describing the A nucleon system, and with $\mathcal{E}_A$ the energy of this system calculated with the HF theory. In the framework of the HF theory, we define the state of the system with an additional particle as

$$|\Phi_{A+1}\rangle = \hat{a}_k^+ |\Phi_A\rangle \quad . \tag{9.32}$$

The difference between the energies of the two systems is given by:

$$\begin{aligned}
\Delta\mathcal{E}_k^{\rm HF} &\equiv \langle\Phi_{A+1}|\hat{H}_0 + \hat{V}_{\rm res}|\Phi_{A+1}\rangle - \langle\Phi_A|\hat{H}_0|\Phi_A\rangle \\
&= \langle\Phi_A|\hat{a}_k\hat{H}_0\hat{a}_k^+|\Phi_A\rangle + \langle\Phi_A|\hat{a}_k\hat{V}_{\rm res}\hat{a}_k^+|\Phi_A\rangle - \langle\Phi_A|\hat{H}_0|\Phi_A\rangle \\
&= \langle\Phi_A|\hat{a}_k\hat{H}_0\hat{a}_k^+|\Phi_A\rangle + \langle\Phi_A|\hat{a}_k\hat{V}_{\rm res}\hat{a}_k^+|\Phi_A\rangle - \mathcal{E}_A^{\rm HF} \equiv \mathcal{E}_{A+1}^{\rm HF} - \mathcal{E}_A^{\rm HF} \quad ,
\end{aligned} \tag{9.33}$$

where we used the fact that the property

$$\langle\Phi_A|\hat{\mathbb{N}}[\cdots]|\Phi_A\rangle = 0 \quad , \tag{9.34}$$

is defined for the ground state of the A fermion system, but, in general, one has that

$$\langle\Phi_{A+1}|\hat{\mathbb{N}}[\cdots]|\Phi_{A+1}\rangle \neq 0 \quad . \tag{9.35}$$

Let's calculate the first term of Eq. (9.33)

$$\begin{aligned}
\langle\Phi_A|\hat{a}_k\hat{H}_0\hat{a}_k^+|\Phi_A\rangle &= \sum_{\nu=1}^{A+1}\epsilon_\nu - \frac{1}{2}\sum_{i,j=1}^{A+1}\overline{V}_{ijij} \\
&= \sum_{\nu=1}^{A}\epsilon_\nu + \epsilon_k - \frac{1}{2}\sum_{i,j=1}^{A}\overline{V}_{ijij} - \sum_{i=1}^{A}\left(\frac{1}{2}\overline{V}_{ikik} + \frac{1}{2}\overline{V}_{kiki}\right) - \frac{1}{2}\overline{V}_{kkkk} \qquad (9.36) \\
&= \mathcal{E}_A^{\rm HF} + \epsilon_k - \sum_{i=1}^{A}\overline{V}_{ikik} \quad , \qquad (9.37)
\end{aligned}$$

since for the definition of $\overline{V}$ we have that

$$\overline{V}_{ikik} = \overline{V}_{kiki} \quad \text{and} \quad \overline{V}_{kkkk} = 0 \quad . \tag{9.38}$$

Here ϵ_k is the Lagrange multiplier associated to the k single-particle state. The term of Eq. (9.33) related to he residual interaction is

$$\langle\Phi_A|\hat{a}_k\hat{V}_{\rm res}\hat{a}_k^+|\Phi_A\rangle = \frac{1}{4}\sum_{\mu\mu'\nu\nu'}\overline{V}_{\nu\mu\nu'\mu'}\langle\Phi_A|\hat{a}_k\hat{\mathbb{N}}[\hat{a}_\nu^+\hat{a}_\mu^+\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}]\hat{a}_k^+|\Phi_A\rangle \quad . \tag{9.39}$$

The expectation value of the term containing the creation and destruction operators is

$$\begin{aligned}
&\langle\Phi_A|\hat{a}_k\hat{\mathbb{N}}[\hat{a}_\nu^+\hat{a}_\mu^+\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}]\hat{a}_k^+|\Phi_A\rangle = \\
&\langle\Phi_A|\hat{a}_k\hat{a}_\nu^+\hat{a}_\mu^+\hat{a}_{\mu'}\hat{a}_{\nu'}\hat{a}_k^+|\Phi_A\rangle + \langle\Phi_A|\hat{a}_k\hat{a}_\nu^+\hat{a}_\mu^+\hat{a}_{\mu'}\hat{a}_{\nu'}\hat{a}_k^+|\Phi_A\rangle \\
+ \quad &\langle\Phi_A|\hat{a}_k\hat{a}_\nu^+\hat{a}_\mu^+\hat{a}_{\mu'}\hat{a}_{\nu'}\hat{a}_k^+|\Phi_A\rangle + \langle\Phi_A|\hat{a}_k\hat{a}_\nu^+\hat{a}_\mu^+\hat{a}_{\mu'}\hat{a}_{\nu'}\hat{a}_k^+|\Phi_A\rangle \\
= \quad &\delta_{k\nu}\delta_{k\nu'}\delta_{\mu\mu'}\delta_{\mu,i} - \delta_{k\nu}\delta_{k\mu'}\delta_{\mu\nu'}\delta_{\mu,i} - \delta_{k\mu}\delta_{k\nu'}\delta_{\nu\mu'}\delta_{\mu',i} + \delta_{k\mu}\delta_{k\mu'}\delta_{\nu\nu'}\delta_{\nu,i} \quad .
\end{aligned} \tag{9.40}$$

by exploiting the properties of $\overline{V}$ we can write

$$\langle\Phi_A|a_k\hat{V}_{\rm res}a_k^+|\Phi_A\rangle = \sum_i \overline{V}_{kiki} \tag{9.41}$$

Therefore

$$\Delta\mathcal{E}_k^{\rm HF} = \mathcal{E}_A^{\rm HF} + \epsilon_k - \sum_{i=1}^{A}\overline{V}_{ikik} + \sum_{i=1}^{A}\overline{V}_{kiki} - \mathcal{E}_A^{\rm HF} = \epsilon_k \quad , \tag{9.42}$$

which is Koopmans' theorem. The Lagrange multipliers ϵ_k of the constrained minimisation problem correspond to the energy differences between the MF energies of the $A+1$ and A fermions.

9.2.3 Hartree-Fock in Fermi gas

A simple application of the HF theory is the description of an infinite and homogeneous system of fermions. This is the system that in Sect. 2.3 we called *Fermi gas*.

We rewrite the HF equations in the coordinate space

$$\begin{aligned} -\frac{\hbar^2}{2m}\nabla^2\phi_k(\mathbf{r}) \quad &+ \quad \sum_{k'\le k_{\rm F}} \int d^3r' \, |\phi_{k'}(\mathbf{r}')|^2 \hat{V}(\mathbf{r},\mathbf{r}') \\ &- \quad \sum_{k'\le k_{\rm F}} \int d^3r' \phi^*_{k'}(\mathbf{r}') \hat{V}(\mathbf{r},\mathbf{r}') \phi_k(\mathbf{r}') \phi_{k'}(\mathbf{r}) = \epsilon_k \phi_k(\mathbf{r}) \ , \end{aligned} \tag{9.43}$$

where the sums on the occupied states are indicated as sums on the wave number k whose values are smaller than the Fermi value, k_F. The translational invariance implies that $\hat{V}(\mathbf{r},\mathbf{r}') = \hat{V}(\mathbf{r}-\mathbf{r}')$. The single-particle wave functions are eigenstates of the momentum $\mathbf{p} = \hbar\mathbf{k}$, that is the plane waves defined in Eq. (2.40), and satisfy the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi_k(\mathbf{r}) = \epsilon^{(0)}_k \phi_k(\mathbf{r}) \ . \tag{9.44}$$

The term $\hat{V}(\mathbf{r}-\mathbf{r}')$ represents the interaction between two of the fermions of the system. In Fermi gas case, there is not interaction among the particles composing the system. Each particle moves independently of the presence of the other particles in a uniform, and constant, potential which can also be eliminated by defining the zero of the energy in appropriated way.

The HF theory proposes a different approximated solution of the many-body problem. The total wave function is again a Slater determinant, but the interaction between fermions is switched on.

We define the Fourier transform of the interaction between two fermions as

$$\tilde{V}(\mathbf{k}) = \int d^3x \, \hat{V}(\mathbf{x}) \, e^{i\mathbf{k}\cdot\mathbf{x}} \ . \tag{9.45}$$

Let's consider the third term of Eq. (9.43), the Fock–Dirac term, by including the normalization factor (2.48)

$$\begin{aligned} & \frac{\mathcal{V}}{(2\pi)^3} \int d^3k' \Theta(k_{\rm F}-k) \int d^3\mathbf{r}' \frac{e^{-i\mathbf{k}'\cdot\mathbf{r}'}}{\mathcal{V}^{1/2}} \left[e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \hat{V}(\mathbf{r}-\mathbf{r}') \frac{e^{i\mathbf{k}\cdot\mathbf{r}'}}{\mathcal{V}^{1/2}} \frac{e^{-i\mathbf{k}'\cdot\mathbf{r}}}{\mathcal{V}^{1/2}} \\ = \quad & \frac{1}{(2\pi)^3} \int d^3k' \Theta(k_{\rm F}-k) \int d^3(r'-r) e^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}'-\mathbf{r})} \hat{V}(\mathbf{r}-\mathbf{r}') \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\mathcal{V}^{1/2}} \\ = \quad & \frac{1}{(2\pi)^3} \int d^3k' \Theta(k_{\rm F}-k) \tilde{V}(\mathbf{k}-\mathbf{k}') \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\mathcal{V}^{1/2}} \ . \end{aligned} \tag{9.46}$$

Since the density of the system is defined as (2.51),

$$\rho(r) = \sum_{k\le k_{\rm F}} |\phi_a(\mathbf{r})|^2 \ , \tag{9.47}$$

by using (9.44) we can write the HF equation (9.43) as

$$\left[\epsilon^{(0)}_k + \rho \, \tilde{V}(0) - \frac{1}{(2\pi)^3} \int d^3k' \Theta(k_{\rm F}-k) \tilde{V}(\mathbf{k}-\mathbf{k}') \right] \phi_k(\mathbf{r}) = \epsilon_k \phi_k(\mathbf{r}) \ . \tag{9.48}$$

where

$$\tilde{V}(0) = \int d^3x \, \hat{V}(\mathbf{x}) \tag{9.49}$$

is called volume integral of the interaction.

The presence of the interaction modifies the energy of the particle

$$\epsilon_k = \epsilon_k^{(0)} + \mathcal{U}_{\rm HF}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} + \mathcal{U}_{\rm HF}(\mathbf{k}) \ , \tag{9.50}$$

where

$$\mathcal{U}_{\rm HF}(\mathbf{k}) = \rho\,\tilde{V}(0) - \frac{1}{(2\pi)^3}\int d^3k'\Theta(k_{\rm F}-k')\tilde{V}(\mathbf{k}-\mathbf{k}') \ . \tag{9.51}$$

9.3 Density Functional Theory

The HF model is widely used in nuclear and atomic physics. There are two problems related to its use. A first one is related to the formal development of the theory and it shows up mainly in the nuclear physics framework. Since HF is a MF theory it is necessary to use effective interactions, i.e. interactions without the strongly repulsive core at short distances between the two interacting particles. The commonly used interactions adopted in nuclear physics have a phenomenological input and they contain also terms explicitly dependent on the density of the system. Without these terms the HF calculations are unable to reproduce binding energies and densities of nuclei. The addition of these terms allows the construction of interactions able to produce high quality results in all the nuclide table. What are the parts of the bare nucleon-nucleon interaction, or the many-body effects which renormalize it, simulated by the density dependence of the effective interaction are still matter of study. The formal fact is that the variational principle above defined is not valid if the interaction $\hat{V}$ depends explicitly on the density.

The second problem consists in the difficulty of evaluating the Fock-Dirac term in Eq. (9.31). Nuclei and atoms, even those showing a deformation, are systems which develop around a central point which can be conveniently used as a center of the coordinate system. The evaluation of the Fock-Dirac term is not easy but feasible in these system. The situation becomes prohibitive in the case of complex molecules which do not have a precise reference central point or translational invariance.

The Density Functional Theroy (DFT), solves both problems. The theory is based on a theorem formulated in the second half of the 60's of the last century. On this theoretical basis a set of equations has been obtained. These equations are very similar to the HF equations but they contain an effective local term which takes into account the Pauli principle, and also correlations beyond mean-field approach, and substitute the Fock-Dirac term.

9.3.1 Theorem of Hoenberg-Kohn

The starting point of the DFT is the theorem of Hohenberg-Kohn stating that the ground state of a many-particle system can be completely characterized bt the density of the particles and by correlated quantities. Let's consider the hamiltonian of a system of A fermions of mass m, and spin 1/2. we write it as

$$\hat{H} = \hat{T} + \hat{U}_{ext} + \hat{V} \ , \tag{9.52}$$

where

$$\hat{T} = \sum_{i=1} -\hbar^2\frac{\bigtriangledown_i^2}{2m} \quad , \quad \hat{U}_{ext} = \sum_{i=1}\hat{u}_{ext}(i) \quad , \quad \hat{V} = \frac{1}{2}\sum_{ij}\hat{v}(i,j) \ , \tag{9.53}$$

where all the sums run on all the A fermions. The kinetic energy term, $\hat{T}$, and the external potential $\hat{U}_{ext}$, are one-body operators, while the interaction term $\hat{V}$ is a two-body potential. Other many-body interactions are not considered. The kinetic energy term plus $\hat{V}$ are characteristic of the many-fermion system, while $\hat{U}_{ext}$ depends on external situations, and therefore, in principle, can be modified. For example, in an atomic system $\hat{U}_{ext}$ is given by the interaction of the electrons with the nucleus and it

can be modified if the neutron number changes, modifying in this manner the charge distribution of the nucleus, even though the global electric charge of the nucleus remains the same. This is the origin of the so-called isotope shift effects on the atomic spectra. In an electon gas of a crystal the external field can be modified by changing the position of the ions in the crystal, or by considering the system of positive charges as uniform, and homogeneous, distribution with a defined charge density. In the case of the nucleus, the external field can be the mean-field where the nucleons are immersed and it can be described by potentials of harmonic oscillator or Woods-Saxon type.

Let's consider the set of all the hamiltonians of type (9.53) having non degenerate ground states, i.e. the set of external potentials $\hat{U}_{ext}$ generating a specific ground state $|\Psi_0\rangle$. This set of hamiltonians contain not only the physically reasonable potentials, but also an infinite number of potentials which have only a mathematical relevance. In addition, for each $\hat{U}_{ext}$ there is an infinite number of copies obtained by adding a constant. These copies generate the same ground state, therefore, from the physics point of view they are equivalent. The presence of degenerate states can be removed by inserting a small perturbation which removes the symmetry of the system.

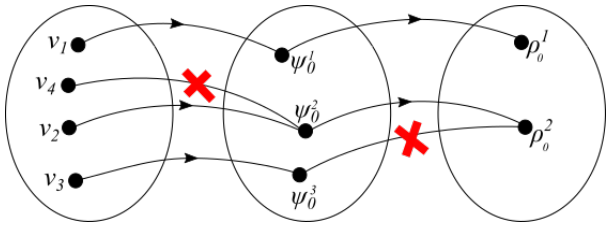

Figure 9.1:

The theorem states that there is a *bijective correspondence between the external potential* $\hat{U}_{ext}$*, the ground state* $|\Psi_0\rangle$ *and the number density*

$$\rho_0(\mathbf{r}) = \langle\Psi_0|\sum_{i=1}^{N}\delta(\mathbf{r}-\mathbf{r}_i)|\Psi_0\rangle \quad , \tag{9.54}$$

of the system. This means that it is not possible that the same potential generates more than one ground state, and that a ground state is generated by more than one external potential. In addition, every ground state produces only one density ρ_0, and each density is not generated by more than one Ψ_0 state. This is sketched in Fig. 9.1 where we indicated that $\Psi_0^{(2)}$ is generated only by v_2, and $\rho_0^{(2)}$ is generated only by $\Psi_0^{(2)}$. The important feature of the theorem is that the two maps are injective, and therefore unique.

The proof of the theorem requires two steps:
(i) for each $\hat{U}_{ext}$ only one Ψ_0 exists,
(ii) there is not Ψ_0 which is simultaneously the ground state of two potentials $\hat{U}_{ext}$ and $\hat{U}'_{ext}$ which can differ by more than a constant value.

(i) Since we consider a non degenerate system, by definition for each hamiltonian there is only one Ψ_0.
(ii) The proof of the second point is done by absurd. Let's assume that the same state $|\Psi_0\rangle$ is eigenstate of two hamiltonians differing by more than a constant term.

$$\begin{aligned}\hat{H}|\Psi_0\rangle &= [\hat{T}+\hat{V}+U_{ext}]|\Psi_0\rangle = E_0|\Psi_0\rangle \\ \hat{H}'|\Psi_0\rangle &= [\hat{T}+\hat{V}+U'_{ext}]|\Psi_0\rangle = E'_0|\Psi_0\rangle \ .\end{aligned}$$

By subtracting the two terms of these equations we obtain

$$[\hat{U}_{ext} - \hat{U}'_{ext}]|\Psi_0\rangle = (E_0 - E'_0)|\Psi_0\rangle \ ,$$

and dividing by $|\Psi_0\rangle$

$$\sum_i [\hat{U}_{ext}(\mathbf{r}_i) - \hat{U}'_{ext}(\mathbf{r}_i)] = E_0 - E'_0 \ .$$

The previous equation implies that $\hat{U}_{ext}(\mathbf{r}_i) - \hat{U}'_{ext}(\mathbf{r}_i)$ is constant for each value of $\mathbf{r}_i$ and for each i. This means that the two potentials differ by a constant value. If we exclude this situation, the above equation leads to a contradiction. The left hand side changes if $\mathbf{r}_i$ changes, while the right hand side remains constant. Therefore every $\hat{U}_{ext}$, apart from a constant value, defines a hamiltonian with only one eigenstate describing the ground state of the system.

Also the second part of the statement, each density ρ_0 is generated by a single state $|\Psi_0\rangle$, is demonstrated by absurd. Let's assume that the same density is produced both by the $|\Psi_0\rangle$ and the $|\Psi'_0\rangle$ eigenstates of the hamiltonians H and H' above defined. For the variational principle we obtain the inequality

$$E_0 = \langle\Psi_0|\hat{H}|\Psi_0\rangle < \langle\Psi'_0|\hat{H}|\Psi'_0\rangle \ , \tag{9.55}$$

where $\hat{H}$ is the hamiltonian of which $|\Psi_0\rangle$ is eigenstate, and the inequality comes from the fact that the system is not degenerate. I can rewrite the right hand side by adding and subtracting $\hat{U}'_{ext}$

$$\begin{aligned} E_0 &< \langle\Psi'_0|[(\hat{T} + \hat{V} + \hat{U}_{ext}) + \hat{U}'_{ext} - \hat{U}'_{ext}]|\Psi'_0\rangle = \langle\Psi'_0|[(\hat{T} + \hat{V} + \hat{U}'_{ext}) + \hat{U}_{ext} - \hat{U}'_{ext}]|\Psi'_0\rangle \\ &= E'_0 + \langle\Psi'_0|\hat{U}_{ext} - \hat{U}'_{ext}|\Psi'_0\rangle \ , \end{aligned}$$

The contribution of the one-body external potential can be written as:

$$\langle\Psi'_0|\sum_i \hat{U}_{ext}(\mathbf{r}_i)|\Psi'_0\rangle = \int d^3r\, \hat{U}_{ext}(\mathbf{r})\langle\Psi'_0|\sum_i \delta(\mathbf{r} - \mathbf{r}_i)|\Psi'_0\rangle = \int d^3r\, \hat{U}_{ext}(\mathbf{r})\, \rho_0(\mathbf{r}) \ ,$$

where we assumed that

$$\langle\Psi'_0|\sum_i \delta(\mathbf{r} - \mathbf{r}_i)|\Psi'_0\rangle = \rho_0(\mathbf{r}) = \langle\Psi_0|\sum_i \delta(\mathbf{r} - \mathbf{r}_i)|\Psi_0\rangle$$

which is what we want to prove wrong. We can write the inequality as

$$E_0 < E'_0 + \int d^3r\, [U_{ext}(\mathbf{r}) - U'_{ext}(\mathbf{r})]\, \rho_0(\mathbf{r})$$

All the discussion has been done by assuming Eq. (9.55) and it could be repeated by inverting the role of the two hamiltonians. Therefore we would obtain

$$E'_0 < E_0 + \int d^3r\, [\hat{U}'_{ext}(\mathbf{r}) - \hat{U}_{ext}(\mathbf{r})]\, \rho_0(\mathbf{r}) \ ,$$

from where, by summing the two equations member to member

$$E_0 + E'_0 < E_0 + E'_0 \ ,$$

which is absurd. Therefore there is unique mapping between $|\Psi_0\rangle$ and ρ_0.

The Hoenberg-Kohn theorem has the following implications.

(a) There is a bijective mapping between external potential $\hat{U}_{ext}$ and the, not degenerate, ground state $|\Psi_0\rangle$ obtained by the solution of the Schrödinger equation, and the ground state density ρ_0

$$\hat{U}_{ext} \Longleftrightarrow |\Psi_0\rangle \Longleftrightarrow \rho_0 \ . \tag{9.56}$$

Since the three quantities are related by bijective mappings, I can consider the states as functionals of the density $|\Psi_0[\rho]\rangle$.

(b) Because of (a), $|\Psi_0[\rho]\rangle$ is a functional of ρ, every observable is also a functional od ρ: $O[\rho]$. Specifically, this is true for the energy of the system

$$E[\rho] = \langle \Psi[\rho]|\hat{H}|\Psi[\rho]\rangle = F[\rho] + \int d^3r\, \hat{U}_{ext}(\mathbf{r})\, \rho_0(\mathbf{r}) \quad , \tag{9.57}$$

where the universal part, the part independent of the external potential, is defined as

$$F[\rho] \equiv \langle \Psi[\rho]|\hat{T} + \hat{V}|\Psi[\rho]\rangle \quad . \tag{9.58}$$

(c) There is a principle related to the minimum of E. If ρ_0 is the ground state density corresponding to a specific value of $\hat{U}_{ext}$, then, for each $\rho \neq \rho_0$ the following relation holds:

$$E_0 \equiv E[\rho_0] < E[\rho] \tag{9.59}$$

This is a consequence of the unicity of the relation between density, eigenstate and external potential, and of the variational principle.

9.3.2 Khon and Sham equations

The application of the Hoenberg-Khon theorem is based on the idea of building the ground state density ρ_0 of a system of interacting fermions by using a fictitious system of non-interacting fermions by changing the hamiltonian. The idea is graphically described in Fig. 9.2. The green line represents the density, and

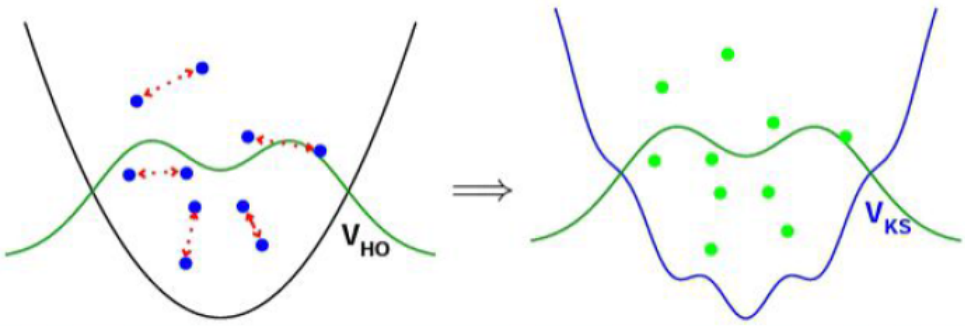

Figure 9.2:

it is the same in the system described in the left part of the figure, a system of interacting fermions, and in that represented in the right part. In the system of the left part the external potential $\hat{U}_{HO}$ is very different from that $\hat{U}_{KS}$ of the right part. The first potential is included in a hamiltonian containing $\hat{V}$, while the second one is included in a hamiltonian which does not contain $\hat{V}$.

The idea of describing a system of interacting fermions by using an effective system of non interacting fermions is analogous to that used by Landau to describe the Fermi liquids (see Chapter 17). In this latter case the properties of the fermions are modified, they acquire effective masses and charges. In the Khon e Sham approach is the hamiltonian to be modified by changing the potentials external to the system.

The starting point consists in writing the density (9.54) as a sum of orthonormalized single-particle wave functions

$$\rho_0(\mathbf{r}) = \rho_0^{\mathrm{KS}}(\mathbf{r}) = \sum_{i<\epsilon_{\mathrm{F}}} |\phi_i^{\mathrm{KS}}(\mathbf{r})|^2 \quad , \tag{9.60}$$

where KS indicates Kohn-Sham. The density (9.60) is generated by a one-body hamiltonian whose eigenstate is a Slater determinant $|\Phi^{\rm KS}\rangle$.

The energy functional built in this system is usually expressed as:

$$E[\rho_0] = T^{\rm KS}[\rho_0] + E^{\rm KS}_{\rm H}[\rho_0] + E^{\rm KS}_{\rm ext}[\rho_0] + E^{\rm KS}_{\rm xc}[\rho_0] \ , \tag{9.61}$$

where there is a kinetic energy term,

$$T^{\rm KS}[\rho_0] = \langle \Phi^{\rm KS}|\hat{T}|\Phi^{\rm KS}\rangle = \int d^3r \sum_i \phi^{*\rm KS}_i(\mathbf{r}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \phi^{\rm KS}_i(\mathbf{r}) \ , \tag{9.62}$$

a Hartree term,

$$E^{\rm KS}_{\rm H}[\rho_0] = \int d^3r_i \int d^3r_j \rho_0(\mathbf{r}_i)\hat{V}(\mathbf{r}_i,\mathbf{r}_j)\rho_0(\mathbf{r}_j) \ , \tag{9.63}$$

and an external mean-field term

$$E^{\rm KS}_{\rm ext}[\rho_0] = \int d^3r \rho_0(\mathbf{r}_i)\hat{U}^{\rm KS}_{\rm ext}(\mathbf{r}_i) \ . \tag{9.64}$$

The additional term is called of exchange and correlation $E^{\rm KS}_{\rm xc}$.

The application of the variational principle follows the path outlined in the case of HF. The final result is again a set of equations which allows the evaluation of the KS single-particle wave functions

$$\left\{-\frac{\hbar^2\nabla^2}{2m} + \int d^3r_j \hat{V}(\mathbf{r},\mathbf{r}_j)\rho_0(\mathbf{r}_j) + \hat{U}^{\rm KS}_{\rm ext}(\mathbf{r}) + \hat{U}^{\rm KS}_{\rm xc}(\mathbf{r})\right\} \phi^{\rm KS}_i(\mathbf{r}) = \epsilon_i \phi^{\rm KS}_i(\mathbf{r}) \ . \tag{9.65}$$

This integro-differential equation is numerically solved by using iterative techniques analogous to those used in the HF case.

- In Eq. (9.65) only local terms appear, contrary to the HF equation containing the non-local Fock-Dirac term. This makes the numerical solution of the KS equations much simpler than that of the HF equations.
- The expression of the operators of kinetic energy and in the Hartree term of the KS functional are the same as in the interacting system. This does not mean that from the quantitative point of view the values of the kinetic energy and of the Hartree term are equal in the two systems. In effect, the expectation values are evaluated between the Slater determinant for the KS functional, and between $|\Psi_0\rangle$ for the interacting systems.
- In the KS energy functional (9.61) the part which sums the contributions of kinetic energy, Hartree term and external potential are much larger than the contribution of the exchange and correlation term.
- The KS equations (9.61) are equivalent to the minimization of the ground state energy, in the same spirit of the HF equations. This because the bijection between density and energy functional.
- The Slater determinant $|\Phi^{\rm KS}\rangle$ is not the exact eigenvalue $|\Psi_0\rangle$ of the many-body hamiltonian. The DFT is based on the equality between densities (9.60), called one-body densities. The one-body densities contain poorer information than the states. I shall discuss this point in more detail in the next section.
- The single-particle wave functions $\phi^{\rm KS}_i(\mathbf{r})$ do not have a precise physical meaning, but they must be considered a mathematical instrument to obtain the density, which in the DFT is the only physically meaningful tool to obtain values of observables. Also the eigenvalues ϵ_i have to be considered only as Lagrange multipliers and not single-particle energies as indicated by the Koopmans' theorem in the HF case.

- There are not theoretical prescriptions or bounds to regulate the choice of the exchange and correlation term. The selection of this term is done on pragmatical basis. Great part of the theoretical work in the DFT framework is related to the construction of this term.
- The DFT is an independent particle model.

9.4 Density and single-particle wave functions

In this section we discuss about the definitions of the particle densities in view of their relevance in the framework of HF and DFT. We use a formalism considering a definition of the density in most general aspect, i.e. independent of the modelization of the many-body wave function. We define the density matrix of a many-body system as

$$\rho(\mathbf{r}_1,\mathbf{r}'_1) = \frac{A}{\langle\Psi|\Psi\rangle}\int d^3r_2\, d^3r_3\cdots d^3r_A \Psi^*(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_A)\Psi(\mathbf{r}'_1,\mathbf{r}_2,\cdots,\mathbf{r}_A)\ , \tag{9.66}$$

where Ψ is the wave function describing the system.

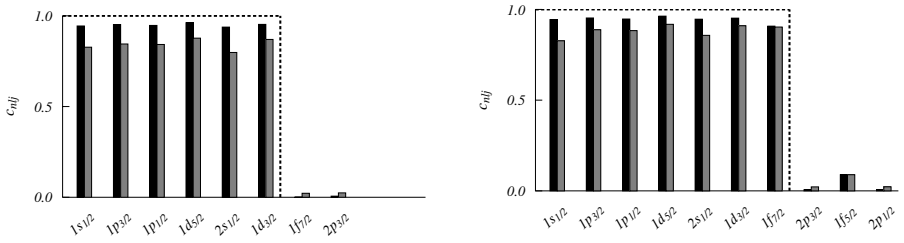

Figure 9.3: Comparison between the occupation numbers of an IPM, dashed lines and those of natural orbits indicated by the histograms. These latter numbers are calculated by using two different correlation functions. The system under investigation is the ^{48}Ca nucleus. The figure on the left hand side indicates the results for the protons, the figure on the right hand side that for the neutrons.

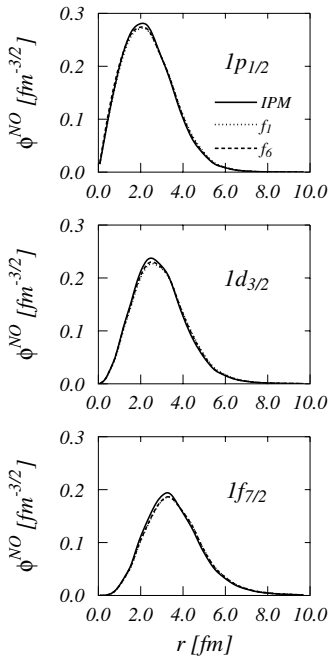

Figure 9.4: Independent particle model

For sake of precision, this is the definition of one-body density matrix, since in the equation (9.66) all the coordinates but one are integrated. The density matrix (9.66) is normalized to the particle number A, as it can be obtained by integrating on the $\mathbf{r}_1$ e $\mathbf{r}'_1$ coordinates and by inserting a $\delta(\mathbf{r}_1-\mathbf{r}'_1)$ factor. The density used in the DFT is the diagonal part of the one-body density matrix. It is evident that by integrating on $A-1$ coordinates a lot of the information contained in Ψ is lost. This limitation becomes evident when the observables studied are of two body-type or they are sensitive to the off-diagonal part of the density matrix.

In the IPM, the state $|\Psi\rangle$ is a Slater determinant $|\Phi\rangle$ composed by a set of orthonormal single-particle states $|\phi_i\rangle$. By inserting in Eq. (9.66) the Slater determinant we obtain a density matrix given by

$$\rho^{\rm IPM}(\mathbf{r}_1,\mathbf{r}'_1) = \sum_{i\le\epsilon_{\rm F}} \phi^*_i(\mathbf{r}_1)\phi_i(\mathbf{r}'_1) \tag{9.67}$$

The **mean-field single particles** are those generated in a independent particle model and produce densities of the type (9.67).

The **natural orbits** are defined as those single particle wave functions which diagonalize the density matrix (9.66) which can be described as

$$\rho(\mathbf{r}_1, \mathbf{r}'_1) = \sum_\alpha c_\alpha \phi^{*\mathrm{NO}}_\alpha(\mathbf{r}_1)\phi^{\mathrm{NO}}_\alpha(\mathbf{r}'_1) \tag{9.68}$$

The difference between the expressions (9.67) and (9.68) consists in the fact that, in the second expression, the sum is extended up to infinity and the, real, coefficients c_α are the diagonal terms of the density matrix, and indicate the occupation of the natural orbit. The two densities are normalized such as

$$\begin{aligned} A &= \int d^3 r_1 \rho^{\mathrm{IPM}}(\mathbf{r}_1, \mathbf{r}'_1)\delta(\mathbf{r}_1 - \mathbf{r}'_1) \\ &= \int d^3 r_1 \rho^{\mathrm{NO}}(\mathbf{r}_1, \mathbf{r}'_1)\delta(\mathbf{r}_1 - \mathbf{r}'_1) = \sum_\alpha c_\alpha \ . \end{aligned} \tag{9.69}$$

This allows the interpretation of the expression (9.67) in analogy to (9.68) where the occupation numbers are 1 for the states below the Fermi surface, and 0 for those above it.

In Fig. 9.3 we compare the occupation numbers of an IPM with those obtained by a microscopic calculations (FHNC see Chapter 13) carried out with two different correlation functions. The many-body system under investigation is the ^{48}Ca. The left panel shows the result for protons, the right panel that for neutrons.

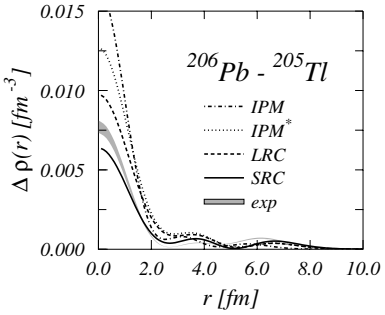

Figure 9.5: Difference between the charge distributions of ^{206}Pb and ^{205}Tl. IPM indicates the results with mean-field wave functions. The other lines have been obtained by considering different types of correlations, at short- and long-range, SRC and LRC respectively.

The IPM predicts full occupation for the states below the Fermi surface, while above it the occupation is zero. The calculations which include correlations show that the natural orbits are only partially occupied below the Fermi surface, even though the occupation numbers are very close to 1. Above the Fermi surface, the occupation numbers are very small but not zero.

In Fig. 9.4 we compare some wave functions of the IPM with the neutron natural orbits in ^{48}Ca. There is a great similarity between single-particle wave functions and natural orbits. The effects of correlations are mainly related to the changes of the occupation numbers rather than on the shape of the wave functions.

Another type of wave function referred to the individual fermion is that of the **quasi-particle wave functions** defined as the superposition of the wave functions describing systems with A and $A-1$ particles

$$\psi_\alpha(\mathbf{r}) = \frac{\sqrt{A}\langle\Psi(A-1)|\delta(\mathbf{r}-\mathbf{r}_A)|\Psi(A)\rangle}{\langle\Psi(A-1)|\Psi(A-1)\rangle^{1/2}\langle\Psi(A)|\Psi(A)\rangle^{1/2}} \ . \tag{9.70}$$

In Fig. 9.5 we show the difference between the charge distributions of the ^{206}Pb and ^{205}Tl nuclei. The shell structure of these nuclei indicates that the difference between these two charge distributions is due to the absence of a proton in the $3s_{1/2}$ state.

The line indicated as IPM shows the square modulus of this single-particle wave function in the IPM. The form of the wave function is similar to that indicated by the experiment. On the other hand, the IPM results is much above the experimental curve. In order to have a proper description of this charge distribution is necessary the inclusion of various effects which take care that in ^{206}Pb the neutrons do not completely fill all the levels, IPM*, of the collective surface vibrations of the nuclei LRC, and, finally, of the fact that the interaction between two nucleons has strongly repulsive core, SRC. All these phenomena are not considered in the IPM and they are included in the generic category of *correlations*.

If one adopts for the many-body system an IPM, than single-particle wave function, natural orbits and quasi-particle wave functions coincide. In calculations beyond IPM the subtle differences between these three types of wave functions become evident only in very special cases. This is what makes very useful mean-field calculations such as HF and DFT. In the framework of the latter theory, formulated in terms of the functional of the density, the correlation effects are visible only on observables which are sensitive to the off-diagonal part of the one-body density matrix (9.66).

One observable of this type is the momentum distribution, traditionally indicated as $n(\mathbf{k})$, and defined as:

$$n(\mathbf{k}) = \frac{1}{(2\pi)^3}\frac{1}{\langle\Psi|\Psi\rangle}\int d^3(r-r')\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\rho(\mathbf{r},\mathbf{r}') \ . \qquad (9.71)$$

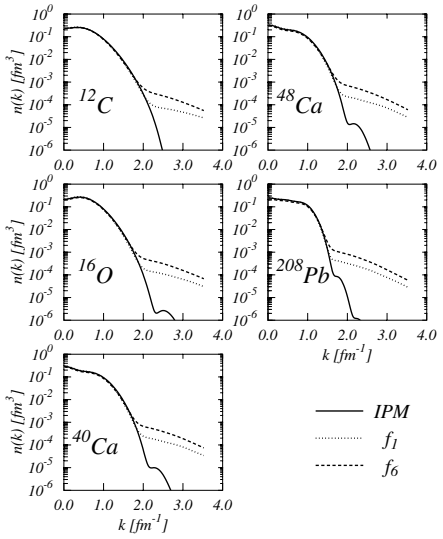

Figure 9.6: Momentum distributions for five spherical and doubly-magic nuclei obtained in IPM and with a theory which consider the correlations between the particles.

The momentum distribution is, in momentum space, analogous to the number density. It answer to the question of what is the probability of finding in the many-body system a particle with momentum, wave number, with value between $\mathbf{k}$ and $\mathbf{k} + d\mathbf{k}$.

In Fig. 9.6 we show the momentum distributions for five spherical and doubly magic nuclei. The full lines have been obtained by considering an IPM, or, in other words, a diagonal density matrix. The other lines have been obtained by solving the many-body problem in the framework of the Correlated Basis Function theory (see Chapter 13). The difference between the IPM results and the correlated ones is remarkable at large values of k, which indicate that the off-diagonal parts of the density matrix generates high-momentum components.

Chapter 10

Excited states

In the previous chapters we focused our attention to the description of the ground state of systems composed by many-fermions. In this Chapter we present the Random Phase Approximation (RPA) a theory aiming to describe the excitation spectrum of these system. The RPA is an approach which goes beyond the IPM since it considers also effects generated by the residual interaction, defined in Eq. (9.16).

The RPA theory has been proposed in the middle of the 50's of the last century to describe plasma excitations [Boh53]. The name has an historical motivation since the authors of Ref. [Boh53] made the assumption of neglecting the coupling of plasma oscillations with different momenta. This assumption concerned the system under investigation and not the theory which does not contain any random phase.

The RPA theory will be proposed again in Sect. 12.5, by using the two-body Green's functions. The formulation used in this chapter, the so-called Equation of Motion Method, is less general, but it has the advantage of a simpler interpretation. The is a third method to get the RPA equations, a method based on time-dependent HF theory. Obviously all the formulations lead to the same set of equations to be numerically solved, and each of them emphasizes aspects that are hidden in other formulations. Usually, in the treatment of infinite systems with translational invariance the Green's function formulation is preferred, while for systems with rotational invariance, the Equation of Motion method is usually chosen.

10.1 The equations of motion method

This method is inspired to the Heisenberg picture of the Quantum Mechanics. Also in this case, the commutation properties of a hamiltonian with an operator are exploited.

Let's consider the Schrödinger equation

$$\hat{H}\left|\Psi_\nu\right\rangle = E_\nu \left|\Psi_\nu\right\rangle \quad , \tag{10.1}$$

where $|\Psi_\nu\rangle$ describe an excited state of the system. We define the $\hat{Q}^+_\nu$ operator whose action on the system ground state defines the excited states:

$$\hat{Q}^+_\nu \left|\Psi_0\right\rangle = \left|\Psi_\nu\right\rangle \;\; ; \;\; \hat{Q}_\nu \left|\Psi_0\right\rangle = 0 \;\; . \tag{10.2}$$

The choice of $\hat{Q}^+_\nu$ defines completely the problem to be solved, and also the ground state of the system. Let's calculate the commutator of the $\hat{Q}^+_\nu$ operator with the hamiltonian

$$\begin{aligned} \left[\hat{H}, \hat{Q}^+_\nu\right] \left|\Psi_0\right\rangle &= \left(\hat{H}\hat{Q}^+_\nu - \hat{Q}^+_\nu \hat{H}\right) \left|\Psi_0\right\rangle = \hat{H}\left|\Psi_\nu\right\rangle - \hat{Q}^+_\nu E_0 \left|\Psi_0\right\rangle \\ &= E_\nu \left|\Psi_\nu\right\rangle - \hat{Q}^+_\nu E_0 \left|\Psi_0\right\rangle = \left(E_\nu - E_0\right) \hat{Q}^+_\nu \left|\Psi_0\right\rangle \quad , \end{aligned} \tag{10.3}$$

and for the operator $\hat{Q}_\nu$ we obtain

$$\left[\hat{H},\hat{Q}_\nu\right]|\Psi_0\rangle = \left(\hat{H}\hat{Q}_\nu - \hat{Q}_\nu\hat{H}\right)|\Psi_0\rangle = \hat{H}\hat{Q}_\nu|\Psi_0\rangle - E_0\hat{Q}_\nu|\Psi_0\rangle = 0 \ . \tag{10.4}$$

We multiply Eq. (10.3) by a generic operator $\hat{\mathcal{O}}$ and by $\langle\Psi_0|$, and we subctract the complex conjugate

$$\begin{aligned}
\langle\Psi_0|\left[\hat{\mathcal{O}},[\hat{H},\hat{Q}_\nu^+]\right]|\Psi_0\rangle &= \langle\Psi_0|\hat{\mathcal{O}}[\hat{H},\hat{Q}_\nu^+]|\Psi_0\rangle - \langle\Psi_0|[\hat{H},\hat{Q}_\nu^+]\hat{\mathcal{O}}|\Psi_0\rangle \\
&= \langle\Psi_0|\left(\hat{\mathcal{O}}[\hat{H},\hat{Q}_\nu^+] - [\hat{H},\hat{Q}_\nu^+]\hat{\mathcal{O}}\right)|\Psi_0\rangle \ \text{for Eqs. (10.3) and (10.4)} \\
&= (E_\nu - E_0)\langle\Psi_0|\hat{\mathcal{O}}\hat{Q}_\nu^+|\Psi_0\rangle - \langle\Psi_0|\hat{H}\hat{Q}_\nu^+\hat{\mathcal{O}}|\Psi_0\rangle + \langle\Psi_0|\hat{Q}_\nu^+\hat{H}\hat{\mathcal{O}}|\Psi_0\rangle \\
&= (E_\nu - E_0)\langle\Psi_0|\hat{\mathcal{O}}\hat{Q}_\nu^+|\Psi_0\rangle - E_0\langle\Psi_0|\hat{Q}_\nu^+\hat{\mathcal{O}}|\Psi_0\rangle + \langle\Psi_0|\hat{Q}_\nu^+\hat{H}\hat{\mathcal{O}}|\Psi_0\rangle \ .
\end{aligned}$$

Since $\langle\Psi_0|\,\hat{Q}_\nu^+ = 0$, we can write

$$\langle\Psi_0|\left[\hat{\mathcal{O}},[\hat{H},\hat{Q}_\nu^+]\right]|\Psi_0\rangle = (E_\nu - E_0)\langle\Psi_0|\hat{\mathcal{O}}\hat{Q}_\nu^+|\Psi_0\rangle = (E_\nu - E_0)\langle\Psi_0|\left[\hat{\mathcal{O}},\hat{Q}_\nu^+\right]|\Psi_0\rangle \ . \tag{10.5}$$

This result is independent on the expression of the operator $\hat{\mathcal{O}}$. In the construction of the various theories describing the system excited states, the $\hat{\mathcal{O}}$ operator is substituted by the $\delta\hat{Q}_\nu$ operator representing an infinitesimal variation of the excitation operator defined by the Eqs. (10.2).

10.2 Tamm-Dankoff approximation (TDA)

A first choice of the $\hat{Q}_\nu^+$ consists in considering the excited state as linear combination of particle-hole excitations. Clearly, this implies that the mean-field problem has already been solved, and a set of orthonormal single-particle wave functions, with the relative single-particle energies, is available. The ground state is characterized by fully occupied hole states, those below the Fermi energy, and totally empty particle states, those above the Fermi energy. The set of single-particle wave functions can be obtained by using the MF techniques presented in Chapter 2 or by solving the HF or the KS equations as indicated in Chapter 9.

The definition of $\hat{Q}_\nu^+$ in terms of creation and destruction operators is

$$\hat{Q}_\nu^+ = \sum_{p\,h} X_{ph}^\nu \hat{a}_p^+\hat{a}_h \tag{10.6}$$

and then

$$\delta\hat{Q}_\nu = \sum_{p\,h} \hat{a}_h^+\hat{a}_p\delta X_{ph}^{*\nu} \ . \tag{10.7}$$

In the above equation X_{ph}^ν is a number and the usual convention of indicating the hole states with the letters h,i,j,k,l and the particle states with m,n,p,q,r has been adopted. The ground state $|\Psi_0\rangle$ satisfying the Eqs. (10.3) and (10.4) is the MF ground state $|\Phi_0\rangle$, in effect

$$\hat{Q}_\nu|\Phi_0\rangle = \sum_{p\,h} X_{ph}^\nu \hat{a}_h^+\hat{a}_p|\Phi_0\rangle = 0 \ , \tag{10.8}$$

since it is not possible to remove particles above the Fermi surface or to put particles below it (see Chapter 5).

By substituting Eq. (10.7) in Eq. (10.5) we obtain

$$\begin{aligned} & \langle\Phi_0|\Big[\sum_{p\,h}\hat{a}_h^+\hat{a}_p\delta X_{ph}^{*\nu},\big[\hat{H},\sum_{p'\,h'}X_{p'h'}^{\nu}\hat{a}_{p'}^+\hat{a}_{h'}\big]\Big]|\Phi_0\rangle \\ = \quad & (E_\nu - E_0)\,\langle\Phi_0|\Big[\sum_{m\,i}\hat{a}_i^+\hat{a}_m\delta X_{mi}^{*\nu},\sum_{n\,j}X_{nj}^{\nu}\hat{a}_n^+\hat{a}_j\Big]|\Phi_0\rangle \quad . \end{aligned} \tag{10.9}$$

Every variation $\delta X_{ph}^{*\nu}$ is independent on the other ones. For this reason, the above equation is a sum of terms independent of each other. The equation is satisfied if all the terms related to the same variation of X_{ph}^{ν} satisfy the relation. Let's consider a single term of the sum, and, since $\delta X_{ph}^{*\nu} \neq 0$, we can divide it by this factor and obtain a system of connected equations which can be expressed as

$$\langle\Phi_0|\Big[\hat{a}_i^+\hat{a}_m,\big[\hat{H},\sum_{n\,j}X_{nj}^{\nu}\hat{a}_n^+\hat{a}_j\big]\Big]|\Phi_0\rangle = (E_\nu - E_0)\sum_{qk}X_{qk}^{\nu}\,\langle\Phi_0|\left[a_i^+a_m,a_q^+a_k\right]|\Phi_0\rangle \quad . \tag{10.10}$$

Let's calculate the right hand side of Eq. (10.10):

$$\langle\Phi_0|\left[\hat{a}_i^+\hat{a}_m,\hat{a}_q^+\hat{a}_k\right]|\Phi_0\rangle = \langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_q^+\hat{a}_k|\Phi_0\rangle - \langle\Phi_0|\hat{a}_q^+\hat{a}_k,\hat{a}_i^+\hat{a}_m|\Phi_0\rangle \quad .$$

We apply the Wick theorem to the first term

$$\langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_q^+\hat{a}_k|\Phi_0\rangle = \delta_{mq}\delta_{ik} \quad .$$

The second term is zero since

$$\hat{a}_m\,|\Phi_0\rangle = 0 \quad .$$

By using this result in Eq. 10.10) we obtain

$$\langle\Phi_0|\Big[\hat{a}_i^+\hat{a}_m,\big[\hat{H},\sum_{n\,j}X_{nj}^{\nu}\hat{a}_n^+\hat{a}_j\big]\Big]|\Phi_0\rangle = (E_\nu - E_0)\,X_{mi}^{\nu} \quad . \tag{10.11}$$

For the calculation of the left hand side of Eq. (10.11) we use the expression of the hamiltonian given in Eq. (9.15)

$$\hat{H} = \sum_{\alpha\beta}h_{\alpha\beta}\hat{a}_\alpha^+\hat{a}_\beta - \frac{1}{2}\sum_{ij}\overline{V}_{ijij} + \frac{1}{4}\sum_{\mu\mu'\nu\nu'}\overline{V}_{\nu\mu\nu'\mu'}\hat{\mathbb{N}}[\hat{a}_\nu^+\hat{a}_\mu^+\,\hat{a}_{\mu'}\,\hat{a}_{\nu'}] \quad , \tag{10.12}$$

where the greek indexes can assume values above or below the Fermi surface, while for the latin indexes we used the common convention. The calculation of the double commutator is carried out here below.

We calculate the double commutators of Eq. (10.11) by considering a term at the time. For the first commutator of the first term of Eq. (10.12) we obtain, by considering the anti-commutation rules of the creation and destruction operators,

$$[\hat{a}_\alpha^+\hat{a}_\beta,\hat{a}_n^+\hat{a}_j] = \delta_{n\beta}\hat{a}_\alpha^+\hat{a}_j - \delta_{j\alpha}\hat{a}_n^+\hat{a}_\beta \quad ,$$

therefore, the commutator of the hamiltonian can be written as

$$\begin{aligned} [\hat{H},\hat{a}_n^+\hat{a}_j] \quad = \quad & \sum_{\alpha\beta}h_{\alpha\beta}\left(\delta_{n\beta}\hat{a}_\alpha^+\hat{a}_j - \delta_{j\alpha}\hat{a}_n^+\hat{a}_\beta\right) \\ + \quad & \frac{1}{4}\sum_{\alpha\alpha'\beta\beta'}\overline{V}_{\alpha\beta\alpha'\beta'}\Big[\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}],\hat{a}_n^+\hat{a}_j\Big] \quad . \end{aligned}$$

We did not considered the second term of the hamiltonian (10.12) since it is a number, therefore commuting with every operator. We consider the expectation value of the double commutator

$$\langle\Phi_0|\left[\hat{a}_i^+\hat{a}_m,[\hat{H},\hat{a}_n^+\hat{a}_j]\right]|\Phi_0\rangle$$

The contribution of the first term of the hamiltonian can be rewritten as

$$\begin{aligned}
& h_{\alpha\beta}\,\langle\Phi_0|\left[\hat{a}_i^+\hat{a}_m,\left(\delta_{n\beta}\hat{a}_\alpha^+\hat{a}_j-\delta_{j\alpha}\hat{a}_n^+\hat{a}_\beta\right)\right]|\Phi_0\rangle \\
= \;& h_{\alpha\beta}\,\langle\Phi_0|\left(\hat{a}_i^+\hat{a}_m\delta_{n\beta}\hat{a}_\alpha^+\hat{a}_j-\hat{a}_i^+\hat{a}_m\delta_{j\alpha}\hat{a}_n^+\hat{a}_\beta\right)|\Phi_0\rangle \\
= \;& h_{\alpha\beta}\,\langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_\alpha^+\hat{a}_j|\Phi_0\rangle\,\delta_{n\beta}-h_{\alpha\beta}\,\langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_n^+\hat{a}_\beta|\Phi_0\rangle\,\delta_{j\alpha} \\
= \;& h_{\alpha\beta}\delta_{ij}\delta_{m\alpha}\delta_{n\beta}-h_{\alpha\beta}\delta_{i\beta}\delta_{mn}\delta_{j\alpha} \\
= \;& (\epsilon_m-\epsilon_i)\delta_{ij}\delta_{mn}\quad , \qquad (10.13)
\end{aligned}$$

where in the last step we considered the diagonal expression of $h_{\alpha,\beta}$. For the calculation of the second term of the hamiltonian we consider that

$$\left[\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}],\hat{a}_n^+\hat{a}_j\right]=\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]\hat{a}_n^+\hat{a}_j-\hat{a}_n^+\hat{a}_j\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]\quad ,$$

therefore

$$\begin{aligned}
& \langle\Phi_0|\left[\hat{a}_i^+\hat{a}_m,\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]\hat{a}_n^+\hat{a}_j-\hat{a}_n^+\hat{a}_j\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]\right]|\Phi_0\rangle \\
= \;& \langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]\hat{a}_n^+\hat{a}_j|\Phi_0\rangle \qquad (10.14) \\
- \;& \langle\Phi_0|\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]\hat{a}_n^+\hat{a}_j\hat{a}_i^+\hat{a}_m|\Phi_0\rangle \qquad (10.15) \\
- \;& \langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_n^+\hat{a}_j\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]|\Phi_0\rangle \qquad (10.16) \\
+ \;& \langle\Phi_0|\hat{a}_n^+\hat{a}_j\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\,\hat{a}_{\beta'}\,\hat{a}_{\alpha'}]\hat{a}_i^+\hat{a}_m|\Phi_0\rangle\quad . \qquad (10.17)
\end{aligned}$$

The terms (10.15) and (10.17) are zero since $a_m\,|\Phi_0\rangle=0$. The situation for the term (10.16) is more involved. In the application of the Wick's theorem one can see that in all the possible set of contractions there are always terms where $\hat{a}_n^+$ is contracted with $\hat{a}_{\alpha'}$ or $\hat{a}_{\beta'}$, and these contractions are zero. Only the term (10.14) is different from zero, and, by applying the Wick's theorem we have to consider all the possible contractions and we obtain

$$\begin{aligned}
\langle\Phi_0|a_i^+a_mN[a_\alpha^+a_\beta^+\,a_{\beta'}\,a_{\alpha'}]a_n^+a_j|\Phi_0\rangle \;=\;& \delta_{i\alpha'}\delta_{m\alpha}\delta_{\beta'n}\delta_{\beta j}-\delta_{i\alpha'}\delta_{m\beta}\delta_{\beta'n}\delta_{\alpha j} \\
-\;& \delta_{i\beta'}\delta_{m\alpha}\delta_{\alpha'n}\delta_{\beta j}+\delta_{i\beta'}\delta_{m\beta}\delta_{\alpha'n}\delta_{\alpha j} \qquad (10.18)
\end{aligned}$$

By inserting the above result in Eq. (10.11) and by considering the symmetry properties of $\overline{V}_{\alpha,\beta,\alpha',\beta'}$ we obtain the TDA equations

$$\boxed{\sum_{nj}X_{nj}^\nu\left[(\epsilon_n-\epsilon_j)\delta_{mn}\delta_{ij}+\overline{V}_{mjin}\right]=(E_\nu-E_0)X_{mi}^\nu\quad ,} \qquad (10.19)$$

where

$$\overline{V}_{mjin}\equiv\langle mj|V|in\rangle-\langle mj|V|ni\rangle\quad . \qquad (10.20)$$

The expression (10.19) represents a homogenous system of linear equations whose unknown are the X^{ν}_{mi}. The number of unknowns, and therefore of the solutions, is given by the number of the particle-hole pairs which truncates the sum.

The normalization condition of the excited state induces a relation between the X^{ν}_{mi} amplitudes:

$$\begin{aligned} 1 &= \langle\Psi_\nu|\Psi_\nu\rangle = \langle\Phi_0|\hat{Q}_\nu\hat{Q}^+_\nu|\Phi_0\rangle = \langle\Phi_0|\sum_{p\,h}\hat{a}^+_h\hat{a}_p X^{*\nu}_{ph}\sum_{p'\,h'}X^{\nu}_{p'h'}\hat{a}^+_{p'}\hat{a}_{h'}|\Phi_0\rangle \\ &= \sum_{p\,h}\sum_{p'\,h'}X^{*\nu}_{ph}X^{\nu}_{p'h'}\,\langle\Phi_0|\overbrace{\hat{a}^+_h\hat{a}_p\hat{a}^+_{p'}}\hat{a}_{h'}|\Phi_0\rangle = \sum_{p\,h}|X^{\nu}_{ph}|^2 \quad , \end{aligned} \tag{10.21}$$

which defines without ambiguity the values of the X^{ν}_{ph} and proposes a probabilistic interpretation. Here below we present an example of TDA equations applied to the case of only two particle-hole pairs.

Let's consider the case where there are only two possible particle-hole excitation pairs. The TDA equations are

$$\begin{pmatrix} \epsilon_{p_1}-\epsilon_{h_1}-\omega+\overline{V}_{p_1h_1h_1p_1} & \overline{V}_{p_2h_2h_1p_1} \\ \overline{V}_{p_1h_1h_2p_2} & \epsilon_{p_2}-\epsilon_{h_2}-\omega+\overline{V}_{p_2h_2h_2p_2} \end{pmatrix}\begin{pmatrix} X_{p_1h_1} \\ X_{p_2h_2} \end{pmatrix} = 0 \quad , \tag{10.22}$$

with $\omega = E - E_0$.

The system has solutions different from the trivial one only if the determinant of the known terms matrix is zero, therefore

$$(\epsilon_{p_1}-\epsilon_{h_1}-\omega+\overline{V}_{p_1h_1h_1p_1})(\epsilon_{p_2}-\epsilon_{h_2}-\omega+\overline{V}_{p_2h_2h_2p_2}) - \overline{V}_{p_2h_2h_1p_1}\overline{V}_{p_2h_2h_2p_2} = 0 \quad . \tag{10.23}$$

The equation is quadratic in ω, therefore it is satisfied by two values.

In case $\overline{V} = 0$ the two values are $\omega = \epsilon_{p_1} - \epsilon_{h_1}$ and $\omega = \epsilon_{p_2} - \epsilon_{h_2}$, which are the energy of the possible excitations in a pure MF model. The presence of the residual interaction mixes the components of the two particle-hole pairs in each excited state, and also the energy eigenvalues are modified with respect to the MF solution. The stronger is the effect of $\hat{V}$ the larger is the mixing of the particle-hole pairs. These type of states with large mixing of particle-hole pairs are called collective states.

The TDA theory describes not only the energy spectrum of the system, but, for each excited state it provides the many-body wave function written in terms of single particle states. This allows the calculation of the transition probability from the ground state to an excited state.

Let's assume that the action of the external field which excites the system is described by a one-body operator

$$\hat{F} = \sum_{\mu\mu'}\langle\mu|\hat{f}|\mu'\rangle\,\hat{a}^+_\mu\hat{a}_{\mu'} \equiv \sum_{\mu\mu'}f_{\mu\mu'}\hat{a}^+_\mu\hat{a}_{\mu'} \quad . \tag{10.24}$$

The transition probability from the ground state to an excited state is

$$\begin{aligned} \langle\Phi_\nu|\hat{F}|\Phi_0\rangle &= \langle\Phi_0|\hat{Q}_\nu\hat{F}|\Phi_0\rangle \\ &= \langle\Phi_0|\sum_{mi}X^{*\nu}_{mi}\hat{a}^+_i\hat{a}_m\sum_{\mu\mu'}f_{\mu\mu'}\hat{a}^+_\mu\hat{a}_{\mu'}|\Phi_0\rangle \\ &= \sum_{mi}X^{*\nu}_{mi}\sum_{\mu\mu'}f_{\mu\mu'}\,\langle\Phi_0|\hat{a}^+_i\hat{a}_m\hat{a}^+_\mu\hat{a}_{\mu'}|\Phi_0\rangle \\ &= \sum_{mi}X^{*\nu}_{mi}\sum_{\mu\mu'}f_{\mu\mu'}\delta_{i\mu'}\delta_{m\mu} = \sum_{mi}X^{*\nu}_{mi}\,\langle m|\hat{f}|i\rangle \quad . \end{aligned} \tag{10.25}$$

The many-body transition probabilities are described in terms of single-particle transition probabilities.

10.3 Random Phase Approximation (RPA)

10.3.1 Limits of the TDA

The comparison between the TDA results and the experimental data is not satisfying, especially for the nuclear physics case, therefore from the second half of the 60's of the last century the assumptions related to the TDA theory have been carefully analyazed. These assumptions are those of the choice of the expression (10.7) of the $\hat{Q}_\nu$ operator. From these studies it appeared clear that this choice is inconsistent with the the equations of motion (10.5). The inconsistency can be pointed out in the following manner. The equation of motions (10.5) have been obtained without making any assumption on the operator $\hat{\mathcal{O}}$. For an operator of the type $\hat{a}_m^+\hat{a}_i$, the equation of motion are:

$$\langle\Psi_0|\left[\hat{a}_m^+\hat{a}_i,[\hat{H},\hat{Q}_\nu^+]\right]|\Psi_0\rangle = (E_\nu - E_0)\,\langle\Psi_0|\hat{a}_m^+\hat{a}_i\hat{Q}_\nu^+|\Psi_0\rangle = (E_\nu - E_0)\,\langle\Psi_0|\left[\hat{a}_m^+\hat{a}_i,\hat{Q}_\nu^+\right]|\Psi_0\rangle \quad . \tag{10.26}$$

By inserting the expression of the TDA operator (10.7) for the right hand side of the above equation we obtain

$$\sum_{nj} X_{nj}^\nu\,\langle\Phi_0|\left[\hat{a}_m^+\hat{a}_i,\hat{a}_n^+\hat{a}_j\right]|\Phi_0\rangle = \sum_{nj} X_{nj}^\nu\left\{\langle\Phi_0|\hat{a}_m^+\hat{a}_i\hat{a}_n^+\hat{a}_j|\Phi_0\rangle - \langle\Phi_0|\hat{a}_n^+\hat{a}_j\hat{a}_m^+\hat{a}_i|\Phi_0\rangle\right\} = 0 \quad . \tag{10.27}$$

This result requires that also the left hand side of the equation (10.26) must be zero. In effects, the one-body term of the hamiltonian has a double commutator equal to zero

$$\sum_{\alpha\beta} h_{\alpha,\beta}\,\langle\Phi_0|\hat{a}_m^+\hat{a}_i,(\hat{a}_\alpha^+\hat{a}_j\delta_{n\beta} - \hat{a}_n^+\hat{a}_\beta\delta_{j\alpha})|\Phi_0\rangle = 0 \quad ,$$

but the double commutator of the interaction term, in general is not equal to zero,

$$\sum_{\alpha,\beta,\alpha',\beta'} \overline{V}_{\alpha,\beta,\alpha',\beta'}\,\langle\Phi_0|\left[\hat{a}_m^+\hat{a}_i,\left[\hat{\mathbb{N}}[\hat{a}_\alpha^+\hat{a}_\beta^+\hat{a}_{\beta'}\hat{a}_{\alpha'}],\hat{a}_n^+\hat{a}_j\right]\right]|\Phi_0\rangle \neq 0 \quad .$$

In the evaluation of this double commutator there are terms of the type

$$\sum_{\alpha,\beta,\alpha',\beta'} \overline{V}_{\alpha,\beta,\alpha',\beta'}\,\langle\Phi_0|\hat{a}_m^+\hat{a}_i\hat{a}_\alpha^+\hat{a}_\beta^+\hat{a}_{\beta'}\hat{a}_{\alpha'}\hat{a}_n^+\hat{a}_j|\Phi_0\rangle \quad ,$$

evidently different from zero.

10.3.2 The RPA equations

Instead than the choice (10.7) the RPA excitation operator is defined as

$$\hat{Q}_\nu^+ \equiv \sum_{p\,h} X_{ph}^\nu\hat{a}_p^+\hat{a}_h - \sum_{p\,h} Y_{ph}^\nu\hat{a}_h^+\hat{a}_p \quad , \tag{10.28}$$

where both X_{ph}^ν and Y_{ph}^ν are numbers, called *RPA amplitudes*.

The RPA ground state is defined by the equation $\hat{Q}_\nu\,|\nu_0\rangle = 0$. Evidently $|\nu_0\rangle$ is not a MF ground state. In this last case we would have

$$\hat{Q}_\nu\,|\Phi_0\rangle = \sum_{p\,h} X_{ph}^{*\nu}\hat{a}_h^+\hat{a}_p\,|\Phi_0\rangle - \sum_{p\,h} Y_{ph}^{*\nu}\hat{a}_p^+\hat{a}_k\,|\Phi_0\rangle \quad ,$$

The first term is certainly zero, while the second one is not zero. The RPA ground state $|\nu_0\rangle$ is more complex than the mean-field ground state and it contains effects beyond it. These effects, *correlations*, here are described in terms of hole-particle excitations as we shall discuss in Sect. 10.3.6.

By using the definition (10.28) of the RPA amplitudes the equations of motion (10.5) becomes

$$\langle\nu_0|\Big[\delta\hat{Q}_\nu,\big[\hat{H},\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle = (E_\nu - E_0)\,\langle\nu_0|\Big[\delta\hat{Q}_\nu,\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle \quad ,$$

therefore

$$\begin{aligned}
&\langle\nu_0|\Big[\left(\sum_{mi}\hat{a}^+_i\hat{a}_m\delta X^\nu_{mi} - \sum_{mi}\hat{a}^+_m\hat{a}_i\delta Y^\nu_{mi}\right),\big[\hat{H},\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle \\
= \quad & (E_\nu - E_0)\,\langle\nu_0|\Big[\left(\sum_{mi}\hat{a}^+_i\hat{a}_m\delta X^\nu_{mi} - \sum_{mi}\hat{a}^+_m\hat{a}_i\delta Y^\nu_{mi}\right),\hat{Q}^+_\nu\Big]|\nu_0\rangle \quad ,
\end{aligned}$$

and making explicit the the variations on the RPA amplitudes we obtain

$$\begin{aligned}
&\sum_{mi}\delta X^\nu_{mi}\,\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\big[\hat{H},\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle - \sum_{mi}\delta Y^\nu_{mi}\,\langle\nu_0|\Big[\hat{a}^+_m\hat{a}_i,\big[\hat{H},\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle \\
= \quad & (E_\nu - E_0)\left\{\sum_{mi}\delta X^\nu_{mi}\,\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\hat{Q}^+_\nu\Big]|\nu_0\rangle - \sum_{mi}\delta Y^\nu_{mi}\,\langle\nu_0|\Big[\hat{a}^+_m\hat{a}_i,\hat{Q}^+_\nu\Big]|\nu_0\rangle\right\} \quad .
\end{aligned}$$

As in the TDA case, the above equation represent a sum of independent terms since each variation is independent of the other ones. By equating the terms related to the same variation we obtain the following relations

$$\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\big[\hat{H},\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle = (E_\nu - E_0)\,\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\hat{Q}^+_\nu\Big]|\nu_0\rangle \tag{10.29}$$

$$\langle\nu_0|\Big[\hat{a}^+_m\hat{a}_i,\big[\hat{H},\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle = (E_\nu - E_0)\,\langle\nu_0|\Big[\hat{a}^+_m\hat{a}_i,\hat{Q}^+_\nu\Big]|\nu_0\rangle \quad . \tag{10.30}$$

Let's consider the left hand side of Eq. (10.29)

$$\begin{aligned}
&\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\big[\hat{H},\hat{Q}^+_\nu\big]\Big]|\nu_0\rangle \\
= \quad & \sum_{nj}X^\nu_{nj}\,\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\big[\hat{H},\hat{a}^+_n\hat{a}_j\big]\Big]|\nu_0\rangle - \sum_{nj}Y^\nu_{nj}\,\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\big[\hat{H},\hat{a}^+_j\hat{a}_n\big]\Big]|\nu_0\rangle \\
\equiv \quad & \sum_{nj}X^\nu_{nj}A_{minj} + \sum_{nj}Y^\nu_{nj}B_{minj} \quad .
\end{aligned} \tag{10.31}$$

These equations define the elements of the A and B matrices. The sign of the element of B has to be pointed out.

To calculate the left hand side of Eq. (10.29) we use an approximation know in the literature as *Quasi-Boson-Approximation* (QBA) consisting in considering that the expectation value of commutator between RPA states has the same value of the commutator between MF states $|\Phi_0\rangle$. In the specific case under study we have that

$$\langle\nu_0|\Big[\hat{a}^+_i\hat{a}_m,\hat{Q}^+_\nu\Big]|\nu_0\rangle \simeq \langle\Phi_0|\Big[\hat{a}^+_i\hat{a}_m,\hat{Q}^+_\nu\Big]|\Phi_0\rangle \quad . \tag{10.32}$$

It is worth to remark that the QBA can be applied only if the matrix element is expressed in terms of commutators. The idea is that the pairs of creation and destruction operators behave as

$$[\hat{a}^+_i\hat{a}_m,\hat{a}^+_n\hat{a}_j] = \delta_{mn}\delta_{ij} \quad ,$$

this means that the operators $\hat{\mathcal{O}}_{im} \equiv \hat{a}_i^+ \hat{a}_m$ and $\hat{\mathcal{O}}_{jn}^+ \equiv a_n^+ a_j$ would be boson operators.

By using the QBA we can write

$$\begin{aligned}
& \langle \nu_0 | \left[\hat{a}_i^+ \hat{a}_m, \hat{Q}_\nu^+ \right] | \nu_0 \rangle \\
\simeq & \sum_{nj} X_{nj}^\nu \langle \Phi_0 | [\hat{a}_i^+ \hat{a}_m, \hat{a}_n^+ \hat{a}_j] | \Phi_0 \rangle - \sum_{nj} Y_{nj}^\nu \langle \Phi_0 | [\hat{a}_i^+ \hat{a}_m, \hat{a}_j^+ \hat{a}_n] | \Phi_0 \rangle \\
= & \sum_{nj} X_{nj}^\nu \left\{ \langle \Phi_0 | \hat{a}_i^+ \hat{a}_m, \hat{a}_n^+ \hat{a}_j | \Phi_0 \rangle - \langle \Phi_0 | \hat{a}_n^+ \hat{a}_j \hat{a}_i^+ \hat{a}_m | \Phi_0 \rangle \right\} \\
- & \sum_{nj} Y_{nj}^\nu \left\{ \langle \Phi_0 | \hat{a}_i^+ \hat{a}_m \hat{a}_j^+ \hat{a}_n | \Phi_0 \rangle - \langle \Phi_0 | \hat{a}_j^+ \hat{a}_n \hat{a}_i^+ \hat{a}_m | \Phi_0 \rangle \right\} \\
= & \sum_{nj} X_{nj}^\nu \langle \Phi_0 | \hat{a}_i^+ \hat{a}_m, \hat{a}_n^+ \hat{a}_j | \Phi_0 \rangle = X_{mi}^\nu \delta_{mn} \delta_{ij} \ , \qquad (10.33)
\end{aligned}$$

where we have taken into account that the terms multiplying Y_{nj}^ν do not conserve the particle number and, furthermore, that $a_m |\Phi_0\rangle = 0$. Eq. (10.29) becomes

$$\sum_{nj} X_{nj}^\nu A_{minj} + \sum_{nj} Y_{nj}^\nu B_{minj} = (E_\nu - E_0) X_{mi}^\nu \ . \qquad (10.34)$$

For the calculation of the left hand side of equation (10.30) we consider that:

$$[\hat{H}, \hat{a}_n^+ \hat{a}_j]^+ = (\hat{H} \hat{a}_n^+ \hat{a}_j - \hat{a}_n^+ \hat{a}_j \hat{H})^+ = \hat{a}_j^+ \hat{a}_n \hat{H} - \hat{H} \hat{a}_j^+ \hat{a}_n = -[\hat{H}, \hat{a}_j^+ \hat{a}_n] \ , \qquad (10.35)$$

since $\hat{H} = \hat{H}^+$, and then

$$\left[\hat{a}_i^+ \hat{a}_m, [\hat{H}, \hat{a}_j^+ \hat{a}_n] \right]^+ = -\left[\hat{a}_m^+ \hat{a}_i, -[\hat{H}, \hat{a}_n^+ \hat{a}_j] \right] = \left[\hat{a}_m^+ \hat{a}_i, [\hat{H}, \hat{a}_n^+ \hat{a}_j] \right] \ . \qquad (10.36)$$

The double commutator becomes

$$\begin{aligned}
& \langle \nu_0 | \left[a_m^+ a_i, \left[H, Q_\nu^+ \right] \right] | \nu_0 \rangle \\
= & \sum X_{nj}^\nu \langle \nu_0 | \left[a_m^+ a_i, \left[H, a_n^+ a_j \right] \right] | \nu_0 \rangle - \sum Y_{nj}^\nu \langle \nu_0 | \left[a_m^+ a_i, \left[H, a_j^+ a_n \right] \right] | \nu_0 \rangle \\
= & \sum X_{nj}^\nu \langle \nu_0 | \left[a_i^+ a_m, \left[H, a_j^+ a_n \right]^+ \right] | \nu_0 \rangle - \sum Y_{nj}^\nu \langle \nu_0 | \left[a_i^+ a_m, \left[H, a_n^+ a_j \right]^+ \right] | \nu_0 \rangle \\
= & \sum_{nj} X_{nj}^\nu (-B_{minj}^*) + \sum_{nj} Y_{nj}^\nu (-A_{minj}^*) \ , \qquad (10.37)
\end{aligned}$$

where we considered the definitions of the matrix elements A e B in Eq. (10.31).

For the calculation of the right hand side of Eq. (10.30) by using the QBA we have

$$\langle \nu_0 | \left[\hat{a}_m^+ \hat{a}_i, Q_\nu^+ \right] | \nu_0 \rangle \rightarrow \text{ (QBA)} \rightarrow - \sum_{nj} Y_{nj}^\nu \langle \Phi_0 | \left[\hat{a}_m^+ \hat{a}_i, \hat{a}_j^+ \hat{a}_n \right] | \Phi_0 \rangle = Y_{mi}^\nu \delta_{ij} \delta_{mn} \ , \qquad (10.38)$$

therefore Eq. (10.30) becomes

$$\sum_{nj} X_{nj}^\nu (-B_{minj}^*) + \sum_{nj} Y_{nj}^\nu (-A_{minj}^*) = (E_\nu - E_0) Y_{mi}^\nu \ . \qquad (10.39)$$

The equations (10.34) and (10.39) represent a homogenous system of linear equations whose unknown are the RPA amplitudes X_{ph}^ν and Y_{ph}^ν. Usually, this system is presented as

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = (E_\nu - E_0) \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = (E_\nu - E_0) \begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix} \ , \qquad (10.40)$$

where A and B are square matrices whose dimensions are those of the number of the particle-hole pairs describing the excitation, and X e Y are vectors of the same dimensions.

The expressions of the matrix elements of A and B in terms of effective interaction between two interacting particles are

$$A_{minj} \rightarrow (\text{QBA}) \rightarrow \langle\Phi_0|\Big[\hat{a}_i^+\hat{a}_m,\big[\hat{H},\hat{a}_n^+\hat{a}_j\big]\Big]|\Phi_0\rangle = (\epsilon_m-\epsilon_i)\delta_{mn}\delta_{ij}+\overline{V}_{mjin} \ , \tag{10.41}$$

$$B_{minj} \rightarrow (\text{QBA}) \rightarrow -\langle\Phi_0|\Big[\hat{a}_i^+\hat{a}_m,\big[\hat{H},\hat{a}_j^+\hat{a}_n\big]\Big]|\Phi_0\rangle = \overline{V}_{mnij} \ . \tag{10.42}$$

The element A_{minj} is the same as that of the TDA, Eq. (10.19).
For the term B_{minj} we consider, again, the expression (10.12) of the hamiltonian. Also in this case, as in the case of the TDA, the scalar term $\overline{V}_{ijij}$ does not contribute to the double commutator. Also the contribution of the one-body term is zero. By considering the anti-commutation properties of the creation and destruction operators we obtain

$$[\hat{a}_\alpha^+\hat{a}_\beta,\hat{a}_j^+\hat{a}_n] = \delta_{\beta j}\hat{a}_\alpha^+\hat{a}_n - \delta_{n\alpha}\hat{a}_j^+\hat{a}_\beta \ ,$$

therefore

$$\begin{aligned}
& \langle\Phi_0|\Big[\hat{a}_i^+\hat{a}_m,\Big[\hat{a}_\alpha^+\hat{a}_\beta,\hat{a}_j^+a_n\Big]\Big]|\Phi_0\rangle \\
= \ & \langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_\alpha^+\hat{a}_n|\Phi_0\rangle \rightarrow 0 \\
- \ & \langle\Phi_0|\hat{a}_\alpha^+\hat{a}_n\hat{a}_i^+\hat{a}_m|\Phi_0\rangle \rightarrow 0 \\
- \ & \langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_j^+\hat{a}_\beta|\Phi_0\rangle = \delta_{j\beta}\delta_{im} \rightarrow 0 \\
+ \ & \langle\Phi_0|\hat{a}_j^+\hat{a}_\beta\hat{a}_i^+\hat{a}_m|\Phi_0\rangle \rightarrow 0 \ .
\end{aligned}$$

For the two-body term we have to evaluate

$$\langle\Phi_0|\Big[a_i^+a_m,\Big[N[a_\alpha^+a_\beta^+a_{\beta'}a_{\alpha'},a_j^+a_n\Big]\Big]|\Phi_0\rangle \ .$$

Three terms of the double commutators are zero since the contain $a_m\,|\Phi_0\rangle = 0$. Only the term

$$-\langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_j^+\hat{a}_n\hat{a}_\alpha^+\hat{a}_\beta^+\hat{a}_{\beta'}\hat{a}_{\alpha'}|\Phi_0\rangle \ ,$$

is different from zero, therefore

$$B_{minj} = \frac{1}{4}\sum_{\alpha\beta\alpha'\beta'}\overline{V}_{\alpha\beta\alpha'\beta'}\,\langle\Phi_0|\hat{a}_i^+\hat{a}_m\hat{a}_j^+\hat{a}_n\hat{a}_\alpha^+\hat{a}_\beta^+\hat{a}_{\beta'}\hat{a}_{\alpha'}|\Phi_0\rangle \ .$$

By considering the symmetry properties of $\overline{V}$ and all the possible contractions one obtains Eq. (10.42).

10.3.3 Properties of the RPA equations

We consider the RPA equations in the form

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix} \ ,$$

where $\omega = E_\nu - E_0$ is the excitation energy.

- If $B = 0$ we obtain the TDA equations.
- The two RPA equations can be written as the system

$$\begin{aligned} A\,X^\nu + B\,Y^\nu &= \omega_\nu\,X^\nu \\ -B^*\,X^\nu - A^*\,Y^\nu &= \omega_\nu\,Y^\nu \quad . \end{aligned}$$

We take the complex conjugate of the above equations

$$\begin{aligned} A^*\,X^{*\nu} + B^*\,Y*^\nu &= \omega_\nu\,X^{*\nu} \\ B\,X^{*\nu} + A\,Y^{*\nu} &= -\omega_\nu\,Y^\nu \quad , \end{aligned}$$

which can be written as

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Y^{*\nu} \\ X^{*\nu} \end{pmatrix} = -\omega_\nu \begin{pmatrix} Y^{*\nu} \\ -X^{*\nu} \end{pmatrix} \quad .$$

Therefore the RPA equations allow positive and negative eigenvalues with the same absolute value.

- The RPA matrix is not hermitian. A is hermitian but B is symmetric but not hermitian $B_{minj} = B_{njmi}$. It possible to show that the eigenvalues are real numbers.

  Normally real interactions are used, therefore the matrix element of the A and B matrices are real. Also the X and Y amplitudes are real.

- Eigenvectors corresponding to different eigenvalues are orthogonal.

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix} \quad ; \quad \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\mu \\ Y^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} X^\mu \\ -Y^\mu \end{pmatrix} \quad .$$

Let's calculate the hermitian conjugate of the second equation

$$(X^{\mu+}, Y^{\mu+}) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} = (X^{\mu+}, -Y^\mu)\omega_\mu \quad .$$

We multiply the first equation by $(X^{\mu+}, Y^{\mu+})$ on the left hand side, and the second equation on the right hand side by

$$\begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix}$$

and we obtain

$$\begin{aligned} (X^{\mu+}, Y^{\mu+}) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} &= \omega_\nu (X^{\mu+}, Y^{\mu+}) \begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix} \\ (X^{\mu+}, Y^{\mu+}) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} &= \omega_\mu (X^{\mu+}, -Y^\mu) \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} \end{aligned}$$

By subtracting the two equations we have

$$0 = (\omega_\nu - \omega_\mu)(X^{\mu+}X^\nu - Y^{\mu+}Y^\nu) \quad .$$

Since we have assumed $\omega_\nu \neq \omega_\mu$ we obtain

$$(X^{\mu+}X^{\nu} - Y^{\mu+}Y^{\nu}) = 0 \ .$$

- The normalization between two excited states requires

$$\begin{aligned}\delta_{\nu\nu'} &= \langle\nu|\nu'\rangle = \langle\nu_0|\hat{Q}_\nu\hat{Q}^+_{\nu'}|\nu_0\rangle = \langle\nu_0|[\hat{Q}_\nu,\hat{Q}^+_{\nu'}]|\nu_0\rangle \rightarrow \text{ (QBA)} \rightarrow \langle\Phi_0|[\hat{Q}_\nu,\hat{Q}^+_{\nu'}]|\Phi_0\rangle \\ &= \sum_{mi}\left(X^\nu_{mi}X^{\nu'}_{mi} - Y^\nu_{mi}Y^{\nu'}_{mi}\right) \ ,\end{aligned}$$

where we used the fact that $\hat{Q}_\nu\,|\nu_0\rangle = 0$.

10.3.4 Transition probabilities in RPA

In analogy to the TDA case, we assume that the action of the external field exciting the system is described by a one-body operator expressed as in Eq. (10.24). The transition probability between the RPA ground state and excited state is described by

$$\langle\nu|\hat{F}|\nu_0\rangle = \langle\nu_0|\hat{Q}_\nu\hat{F}|\nu_0\rangle = \langle\nu_0|[\hat{Q}_\nu,\hat{F}]|\nu_0\rangle \ , \tag{10.43}$$

where we used the fact that $\hat{Q}_\nu\,|\nu_0\rangle = 0$. Since the equation is expressed in terms of commutator we can use the QBA

$$\begin{aligned}&\langle\nu|\hat{F}|\nu_0\rangle \rightarrow \text{ (QBA)} \rightarrow \langle\Phi_0|[\hat{Q}_\nu,\hat{F}]|\Phi_0\rangle \\ &= \sum_{\mu\mu'} f_{\mu\mu'}\Big\{\sum_{mi} X^\nu_{mi}\,\langle\Phi_0|[\hat{a}^+_i\hat{a}_m,\hat{a}^+_\mu\hat{a}_{\mu'}]|\Phi_0\rangle - \sum_{mi} Y^\nu_{mi}\,\langle\Phi_0|[\hat{a}^+_m\hat{a}_i,\hat{a}^+_\mu\hat{a}_{\mu'}]|\Phi_0\rangle\Big\} \ .\end{aligned} \tag{10.44}$$

The two matrix elements are

$$\begin{aligned}\langle\Phi_0|[\hat{a}^+_i\hat{a}_m,\hat{a}^+_\mu\hat{a}_{\mu'}]|\Phi_0\rangle &= \langle\Phi_0|\hat{a}^+_i\hat{a}_m\hat{a}^+_\mu\hat{a}_{\mu'}|\Phi_0\rangle - \langle\Phi_0|\hat{a}^+_\mu\hat{a}_{\mu'}\hat{a}^+_i\hat{a}_m|\Phi_0\rangle = \delta_{m\mu}\delta_{i\mu'} - 0 \ , \\ \langle\Phi_0|[a^+_m a_i,a^+_\mu a_{\mu'}]|\Phi_0\rangle &= \langle\Phi_0|a^+_m a_i a^+_\mu a_{\mu'}|\Phi_0\rangle - \langle\Phi_0|a^+_\mu a_{\mu'} a^+_m a_i|\Phi_0\rangle = 0 - \delta_{m\mu'}\delta_{i\mu} \ ,\end{aligned}$$

Therefore

$$\langle\nu|\hat{F}|\nu_0\rangle \simeq \sum_{\mu\mu'} f_{\mu\mu'}\left(\sum_{mi} X^\nu_{mi}\delta_{m\mu}\delta_{i\mu'} + \sum_{mi} Y^\nu_{mi}\delta_{m\mu'}\delta_{i\mu}\right) = \sum_{mi}\left(X^\nu_{mi}\,\langle m|f|i\rangle + Y^\nu_{mi}\,\langle i|f|m\rangle\right) \ . \tag{10.45}$$

Also in this case the transition amplitude of a many-body system is expressed as linear combination of single particle transitions.

10.3.5 Sum rules

In general, by indicating with $|\Psi_\nu\rangle$ the eigenstates of the hamiltonian $\hat{H}$

$$\hat{H}\,|\Psi_\nu\rangle = E_\nu\,|\Psi_\nu\rangle \ ,$$

for an external operator $\hat{F}$ inducing a transition of the system from the ground state to the excited state one has that:

$$2\sum_\nu (E_\nu - E_0)\left|\langle\Psi_\nu|\hat{F}|\Psi_0\rangle\right|^2 = \langle\Psi_0|\Big[\hat{F},\big[\hat{H},\hat{F}\big]\Big]|\Psi_0\rangle \ . \tag{10.46}$$

We derive here the above expression

$$\begin{aligned}\langle\Psi_0|\Big[\hat{F},(\hat{H}\hat{F}-\hat{F}\hat{H})\Big]|\Psi_0\rangle &= \langle\Psi_0|\Big[\hat{F}\hat{H}\hat{F}-\hat{F}\hat{F}\hat{H}-\hat{H}\hat{F}\hat{F}+\hat{F}\hat{H}\hat{F})\Big]|\Psi_0\rangle \\ &= \Big[2\langle\Psi_0|\hat{F}\hat{H}\hat{F}|\Psi_0\rangle-\langle\Psi_0|\hat{F}\hat{F}|\Psi_0\rangle E_0-E_0\langle\Psi_0|\hat{F}\hat{F}|\Psi_0\rangle\Big] \\ &= 2\langle\Psi_0|\hat{F}(\hat{H}-E_0)|\Psi_0\rangle \quad .\end{aligned}$$

We insert the completness

$$\begin{aligned}& 2\langle\Psi_0|\hat{F}\sum_\nu|\Psi_\nu\rangle\langle\Psi_\nu|(\hat{H}-E_0)\hat{F}|\Psi_0\rangle \\ = \;& 2\langle\Psi_0|\hat{F}\sum_\nu|\Psi_\nu\rangle\langle\Psi_\nu|(E_\nu-E_0)\hat{F}|\Psi_0\rangle = 2(E_\nu-E_0)\sum_\nu\langle\Psi_0|\hat{F}|\Psi_\nu\rangle\langle\Psi_\nu|\hat{F}|\Psi_0\rangle \quad .\end{aligned}$$

This expression puts a quantitative limit on the total value of the excitation strength of a many-body system to an external probe. This value is determined by the ground state properties only, and the knowledge of the excited states structure is not required. The validity of Eq. (10.46) is related to the fact that the $|\Psi_\nu\rangle$ are eigenstates of $\hat{H}$. In actual calculations, states based on models or approximated solutions of the Schrödinger equations are used.

For example, for the RPA theory it is possible to derive the following relation

$$2\sum_\nu(E_\nu-E_0)\left|\langle\nu|\hat{F}|\nu_0\rangle\right|^2=\langle\Phi_0|\Big[\hat{F},\big[\hat{H},\hat{F}\big]\Big]|\Phi_0\rangle \quad , \tag{10.47}$$

which, formally, is not a true sum rule since in the left hand side there are RPA states, both ground and excited states, while in the right hand side there is a mean-field ground state. The demonstration of Eq. (10.47) is presented in detail in Ref. [Tho61].

When the residual interaction is neglected, one obtains mean-field excited states $|\Phi_{ph}\rangle$, i.e. single Slater determinants with particle-hole excitations. In this case, Eq. (10.46) is verified since all these mean-field states are eigenstate of the unperturbed hamiltonian $\hat{H}_0$

$$2\sum_{ph}(\epsilon_p-\epsilon_h)\left|\langle\Phi_{ph}|\hat{F}|\Phi_0\rangle\right|^2=\langle\Phi_0|\Big[\hat{F},\big[\hat{H}_0,\hat{F}\big]\Big]|\Phi_0\rangle\,, \tag{10.48}$$

where the excitation energies of the full system are given by the difference between the single-particle energies of the particle-hole excitation.

Since in the RPA the full hamiltonian $\hat{H}=\hat{H}_0+\hat{V}_{\rm res}$ is considered, by inserting this expression in Eq. (10.47) we obtain

$$2\sum_\nu(E_\nu-E_0)\left|\langle\nu|\hat{F}|\nu_0\rangle\right|^2=\langle\Phi_0|\Big[\hat{F},\big[\hat{H}_0,\hat{F}\big]\Big]|\Phi_0\rangle+\langle\Phi_0|\Big[\hat{F},\big[\hat{V}_{\rm res},\hat{F}\big]\Big]|\Phi_0\rangle \quad . \tag{10.49}$$

For operators $\hat{F}$ which commute with $\hat{V}_{\rm res}$ the IPM and RPA sum rules coincide.

10.3.6 The RPA ground state

We have already indicated that the RPA ground state is not a mean-field state but it contains effects beyond it, correlations, expressed in terms of hole-particle excitations. A more precise representation

of the RPA ground state comes from a theorem demonstrated by D. J. Thouless [Tho61] leading to an expression of the RPA ground state of the type [Rin80]:

$$|\nu_0\rangle = \mathcal{N} e^{\hat{S}} |\Phi_0\rangle \quad , \tag{10.50}$$

where $\mathcal{N}$ is a normalization constant and the operator $\hat{S}$ is defined as

$$\hat{S} \equiv \frac{1}{2} \sum_{\nu,minj} s_{\nu,minj} \hat{a}_m^+ \hat{a}_i \hat{a}_j^+ \hat{a}_n \quad . \tag{10.51}$$

The sum considers all the particle-hole $\hat{a}_m^+ \hat{a}_i$ and hole-particle $\hat{a}_j^+ \hat{a}_n$ pairs, and the index ν runs on all the possible angular momentum and parity combinations allowed by the particle-hole, and hole-particle, quantum numbers. We indicated with $s_{\nu,minj}$ an amplitude weighting the contribution of each pair.

Starting from the above expression it is possible to calculate the $s_{\nu,minj}$ from the knowledge of the RPA X_{ph}^{ν} e Y_{ph}^{ν} amplitudes [Suh07]. What is relevant is that by using these expressions the expectation value of a one-body operator with respect to the RPA ground state can be expressed as

$$\begin{aligned} \langle \nu_0 | \hat{F} | \nu_0 \rangle &= \langle \nu_0 | \sum_{\mu\mu'} \langle \mu | f | \mu' \rangle \, \hat{a}_\mu^+ \hat{a}_{\mu'} | \nu_0 \rangle \\ &= \sum_h \langle h | f | h \rangle \left[1 - \frac{1}{2} \sum_\nu \sum_p |Y_{ph}^\nu|^2 \right] + \sum_p \langle p | f | p \rangle \left[\frac{1}{2} \sum_\nu \sum_h |Y_{ph}^\nu|^2 \right] \quad . \end{aligned} \tag{10.52}$$

This clearly shows that the Y_{ph}^{ν} amplitudes modify the value with respect to the MF result.

10.3.7 Application of the RPA

The RPA formulation implies, in the definition of the excitation operator (10.28), a sum running on all the particle-hole pairs. The hole states are well defined: all the states below the Fermi surface. On the other hand, the number of particle states is infinite, since they are all the states above the Fermi surface. From the operative point of view a truncation of the sum is required, which implies the use of a limited set of particle states. This defines the so-called *configuration space*.

The selection of the configuration space is usually done by defining a maximal energy of the single particle states. The mean-field problem is solved by obtaining single particle wave functions and energies up to a selected maximum value. After the configuration space has been chosen, all the particle-hole pairs compatible with the values of the angular momentum and parity of the excited states under study are selected. At this point it is possible to calculate the A and B matrix elements defined in Eq. (10.31), and, finally, to carry out the diagonalization of the RPA matrix.

The result, as already pointed out in the TDA case, is a number of eigenstates and eigenvalues identical to the number of particle-hole pairs identified. In absence of residual interaction, the eigenvalues correspond to the difference between the energies of the particle and hole states $\omega_\nu = \epsilon_p - \epsilon_h$. The residual interaction modifies these values of the energy. In some situation the effect of the residual interaction is relevant and the values of the RPA eigenstates are very different from those of the mean-field model. In this cases, the eigenstates are described by a remarkable mixing of the particle-hole excitations. This fact is indicated by values of the X_{ph}^{ν} which are similar for various particle-hole pairs. These are collective excitation of the system.

On the opposite side there are excited states which essentially single particle excitations characterized by a single $X_{ph}^{\nu} \simeq 1$, while the other amplitudes are negligible. In this case the RPA eiegenvalue is rather close to the particle-hole energy difference of the dominant pair.

Examples of this type of RPA results are given in Tables 10.1 and 10.2 where we present a selection of the results obtained for the $J^\pi = 3^-$ and $J^\pi = 14^-$ states of the ^{208}Pb. In both tables we show only

^{208}Pb	3^-	$\omega = 3.689$ MeV		
		protons		
p	h	$\epsilon_p - \epsilon_h$ MeV	X	Y
$2f_{7/2}$	$3s_{1/2}$	5.8168	0.364778	-0.076573
$1h_{9/2}$	$2d_{3/2}$	5.8038	0.425067	-0.096266
$1i_{13/2}$	$1h_{11/2}$	8.8699	0.252087	-0.097650
		neutrons		
p	h	$\epsilon_p - \epsilon_h$ MeV	X	Y
$1i_{11/2}$	$2f_{5/2}$	7.2150	0.326432	-0.101974
$2g_{9/2}$	$3p_{3/2}$	6.0838	0.410392	-0.096913
$1j_{15/2}$	$1i_{13/2}$	8.8621	0.277879	-0.110192

Table 10.1: Exctracted from the results of a RPA calculation for the $J^\pi = 3^-$ state of the ^{208}Pb nucleus. The RPA eigenvalue is 3.689 MeV, a number quite distant from the energies of the single particle excitations $\epsilon_p - \epsilon_h$. The calculation considered 1284 particle-hole pairs, and here only those with amplitude greater than 0.1 are shown.

^{208}Pb	14^-	$\omega = 9.098$ MeV		
		neutrons		
p	h	$\epsilon_p - \epsilon_h$ MeV	X	Y
$1j_{15/2}$	$1i_{13/2}$	8.8699	-0.999661	0.012288

Table 10.2: The same as Table 10.1 for the state $J^\pi = 14^-$ of the ^{208}Pb nucleus. The RPA energy eigenvalue is 9.098 MeV rather close to the energy of the dominant particle-hole pair.

the particle-hole transitions whose X^ν_{ph} amplitude is greater than 0.1. In the tables the single-particle states are identified in the usual nuclear shell-model scheme [Rin80].

In the calculation of the 3^- state, the chosen configuration space predicted 1284 particle-hole pairs, which is also the number of the obtained solutions. The results we show in Tab. 10.1 is that with the smallest energy eigenvalue, $\omega = 3.69$ MeV. It is worth to remark that the minimal value of the particle-hole energy is 5.80 MeV. This indicates that the residual interaction acts by strongly modifying the energy values. There are 6 particle-hole pairs with $X^\nu_{ph} > 0.1$. This indicates a high degree of collectivity.

The situation shown in Tab. 10.2 regarding the state 14^-, is completely different. Also in this case we show the results for the lowest energy eigenvalue. The chosen configuration space selected 306 particle-hole pairs in this case, and only one $X^\nu_{ph} > 0.1$, and its contribution is about the 99 % of the RPA eigenstate. The RPA energy eigenvalue is 9.10 MeV to be compared with the 8.87 MeV of the dominant particle-hole configuration. This is the typical single-particle excited state. In this case the contribution of the residual interaction is very small. The RPA is able to describe within the same theoretical framework both collective and single-particle excitations of the many-body system.

We presented results of RPA calculations where all the configuration space is described by discrete single-particle states, even when the single-particle energy is grater than zero. The choice of these configuration spaces is done to make stable the solution for the first, discrete, excited sates. It is a good approximation for the discrete states, but it has many failures when one wants to describe excitations in the continuum. This implies that the system is fragmented because it looses one of its elements. It is possible to formulate the RPA to consider the fact for $\epsilon_p > 0$ the particle is in the continuum, and therefore the excited states describe a system which is loosing a particle, in the atomic case an electron which is in the ionisation condition.

In Fig. 10.1 we show the results of a RPA calculation which consider particle-hole excitations in the

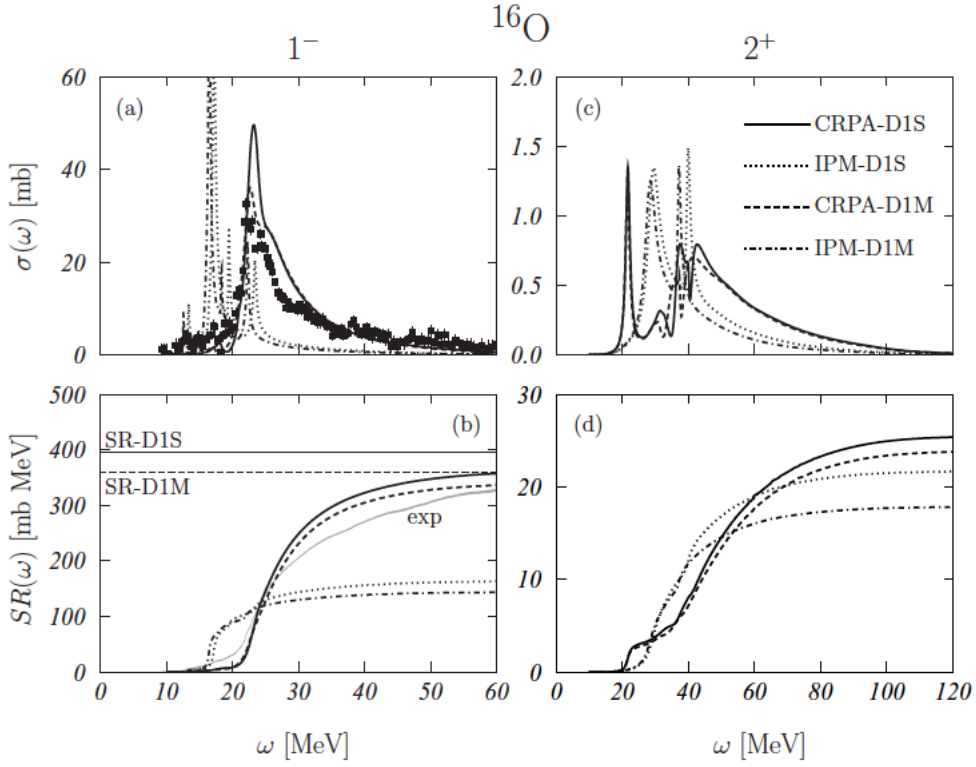

Figure 10.1: Results of RPA calculations which consider the excitations in the continuum (CRPA) compared to the IPM results. The acronyms D1S and D1M indicate two different effective interactions. In the panels (a) and (b) the cross sections of photo-absorption for electric dipole (a) and quadrupole (b) are shown. In the panel (a) also the experimental data are shown [Ahr75]. In the lower panels the value of the integrals of the above cross sections are shown as a function of the upper limit of the energy integration. The horizontal lines are estimates of the sum rule values done in nuclear matter for the two interactions considered [Don11].

continuum. [Don11]. In the upper panels we show the total photoabsorption cross sections for the ^{16}O nucleus. In the left panel (a), there is the electric dipole excitation $J^\pi = 1^-$, in the right panel the electric quadrupole transition $J^\pi = 2^+$. The calculations have been carried out by using two different residual interactions, identified with the names D1S and D1M. Together with the RPA results, also the IPM results are presented.

In the panel (a) also the experimental data are presented. It is evident an increase of the cross section around 23 MeV. This effect is known to be present in all nuclei with more than 10 nucleons since 30's of the last century. This excitation has been called *giant resonance*. The first descriptions of this resonance were based on hydrodynamical model which described the nucleus as liquid drop. This specific case was treated as a two drops, one for protons and one for neutrons, oscillating out of phase. A description in terms of IPM is unable to describe the presence of the resonance, as it is evident in the panel (a). The RPA which takes care of the residual interaction effect, predicts the collective motion of the giant resonance. The contribution of the 2^+ to the total cross section is negligible, as it can be seen by observing the differences in the scales of the (a) and (b) panels.

The lower panels show the value of the integral

$$SR(\omega) = \int_0^\omega d\omega' \sigma(\omega') \ .$$

The behaviour of the curves related to the RPA results is rather similar to those of the experimental data, and for $\omega = 60$ MeV the values are rather close. This means that the total strength of the transition is well described by the RPA. These results indicate that the RPA is able to reproduce the position of the giant resonance. As it is shown in the panel (a) the maximum values of the RPA cross sections coincide with those of the experimental data. Also the total RPA strengths coincide with the experimental one. The distribution of the width of the resonance is not properly described. The comparison with the sum rules calculated with the IPM shows that in Eq. (10.28) the contribution of the term which does not commute with the hamiltonian is very important.

Probably the reason of the failure of the RPA in reproducing the experimental width is related to the fact that in the assumptions on the $\hat{Q}^+_\nu$ operators (10.28) only one-particle one-hole, and one-hole one-particle, pairs are considered. The inclusion of two-particle two-hole pairs would produce an increase of the width which would lower the peak value since the total strength would remain the same.

Chapter 11

Green's function

Up to now we avoided the use of that theoretical entity introduced in Quantum Field Theory and in Many-Body Theories and know as Green's function. In reality, we mentioned the Green's function in Sect. 8.4 as the resolvent of a differential equation. The mathematical expressions of the Green's function we introduce in this chapter and that of Sect. 8.4 are identical, but their interpretation is completely different.

The Green's function is extremely useful in the description of the many-body systems for the calculation of observable quantities, included the energy of the system. The Green's function contains general aspects of the many-body system independently of the specific observable under investigation.

The Green's function is not uniquely defined since its definition depends on the number of field operators which are considered. In this chapter we first present the one-body Green's function, we give the physical interpretation, we show how to use it to calculate observables and we related it to the Green's function of Sect. 8.4. After that, we define the two-body Green's function At the end of the chapter we present a set of linked equations which give a relation between Green's functions defined for any number of particles. The difficulties in solving this set of coupled equations pushes to the formulation of an alternative technique of calculating Green's functions, a technique based on perturbative theory. This will be the subject of Chapter 12.

11.1 One-body Green's functions

The fermionic field operator in Heisenberg representation is defined as

$$\hat{\psi}_{\mathrm{H},\alpha}(\mathbf{x},t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{\psi}_{\alpha}(\mathbf{x})e^{-\frac{i}{\hbar}\hat{H}t} \tag{11.1}$$

where the sub-index H indicates Heisenberg while $\hat{H}$ is the system hamiltonian. With α we indicated all the quantum numbers different from space and time which characterize the particle, for example spin and isospin.

The **one-body Green's function** for a fermion system is defined as

$$i\,G_{\alpha\beta}(\mathbf{x},t,\mathbf{x}',t') = \frac{\langle\Psi_0|\hat{\mathbb{T}}\left[\hat{\psi}_{\mathrm{H},\alpha}(\mathbf{x},t)\hat{\psi}^{+}_{\mathrm{H},\beta}(\mathbf{x}',t')\right]|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \tag{11.2}$$

In the above expression $|\Psi_0\rangle$ indicates the ground state of the system in Heisenberg representation

$$\hat{H}|\Psi_0\rangle = E|\Psi_0\rangle \tag{11.3}$$

and $\hat{\mathbb{T}}$ indicates the time-ordering operator

$$\hat{\mathbb{T}}\left[\hat{\psi}_{\mathrm{H},\alpha}(\mathbf{x},t)\hat{\psi}^{+}_{\mathrm{H},\beta}(\mathbf{x}',t')\right] = \begin{cases} & \hat{\psi}_{\mathrm{H},\alpha}(\mathbf{x},t)\hat{\psi}^{+}_{\mathrm{H},\beta}(\mathbf{x}',t') \quad t>t' \\ - & \hat{\psi}^{+}_{\mathrm{H},\beta}(\mathbf{x}',t')\hat{\psi}_{\mathrm{H},\alpha}(\mathbf{x},t) \quad t<t' \end{cases} \tag{11.4}$$

The one-body Green's functions can be related to the following observable quantities:

- expectation value od a one-body operator with respect to the system ground state,
- energy of the ground state,
- excitation spectrum of the system for single particle excitations.

Henceforth, to simplify the writing, we shall not explicitly write the quantum numbers α e β, understanding their sum each time that we indicate an integration on the coordinates.

Assuming that the hamiltonian $\hat{H}$ is time independent we can write the Green's function (11.2) as

$$i\,G(\mathbf{x},t,\mathbf{x}',t') = \begin{cases} & e^{\frac{i}{\hbar}E(t-t')}\dfrac{\langle\Psi_0|\hat{\psi}(\mathbf{x})e^{-\frac{i}{\hbar}\hat{H}(t-t')}\hat{\psi}^{+}(\mathbf{x}')|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \quad t>t' \\ & \\ - & e^{-\frac{i}{\hbar}E(t-t')}\dfrac{\langle\Psi_0|\hat{\psi}^{+}(\mathbf{x}')e^{\frac{i}{\hbar}\hat{H}(t-t')}\hat{\psi}(\mathbf{x})|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \quad t<t' \end{cases} . \tag{11.5}$$

For the calculation of the expectation value of a one-body operator on the ground state of the system, we use the expression of one-body operator in terms of field operators

$$\hat{\mathcal{O}}^{I} = \int d^3x\,\hat{\psi}^{+}(\mathbf{x})\hat{\mathcal{O}}(\mathbf{x})\hat{\psi}(\mathbf{x}) \ . \tag{11.6}$$

We can write its expectation value with respect to the ground state as

$$\langle\hat{\mathcal{O}}^{I}\rangle = \int d^3x\,\frac{\langle\Psi_0|\hat{\psi}^{+}(\mathbf{x})\hat{\mathcal{O}}(\mathbf{x})\hat{\psi}(\mathbf{x})|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \int d^3x\,\lim_{\mathbf{x}'\to\mathbf{x}}\hat{\mathcal{O}}(\mathbf{x})\frac{\langle\Psi_0|\hat{\psi}^{+}(\mathbf{x}')\hat{\psi}(\mathbf{x})|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \ . \tag{11.7}$$

where the limit $\mathbf{x}'\to\mathbf{x}$ has been inserted to allow the commutation of $\hat{\mathcal{O}}(\mathbf{x})$ with $\hat{\psi}^{+}(\mathbf{x}')$. By using the second equation (11.5), and indicating with t^{+} a time greater than t, we obtain

$$\langle\hat{\mathcal{O}}^{I}\rangle = -i\lim_{t'\to t^{+}\to t}\int d^3x\,\lim_{\mathbf{x}\to\mathbf{x}'}\hat{\mathcal{O}}(\mathbf{x})G(\mathbf{x},t,\mathbf{x}',t') \ . \tag{11.8}$$

Let's make an example of this kind of calculation by considering the number density operator. The operator related the number of particles of the system can be expressed as a function of the density operator

$$\hat{\rho}(\mathbf{x}) = \int d^3x'\delta(\mathbf{x}-\mathbf{x}') \tag{11.9}$$

as

$$\hat{n} \equiv \int d^3x\,\hat{\psi}^{+}(\mathbf{x})\hat{\rho}(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{x}) = \int d^3x\,\int d^3x'\delta(\mathbf{x}-\mathbf{x}')\,\hat{\psi}^{+}(\mathbf{x})\,\hat{\psi}(\mathbf{x}) = \int d^3x\,\hat{\psi}^{+}(\mathbf{x})\,\hat{\psi}(\mathbf{x}) \ . \tag{11.10}$$

The expectation value of this operator with respect to the ground state of the system is:

$$\begin{aligned} \langle\hat{n}\rangle &= -i\lim_{t'\to t^{+}}\int d^3x\,\lim_{\mathbf{x}\to\mathbf{x}'}\hat{\rho}(\mathbf{x})G(\mathbf{x},t,\mathbf{x}',t') \\ &= -i\lim_{t'\to t^{+}}\int d^3x\,\lim_{\mathbf{x}\to\mathbf{x}'}G(\mathbf{x},t,\mathbf{x}',t') \\ &= -i\int d^3x\,G(\mathbf{x},t,\mathbf{x},t) = \int d^3x\,\frac{\langle\Psi_0|\hat{\psi}^{+}(\mathbf{x})\hat{\psi}(\mathbf{x})|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \end{aligned} \tag{11.11}$$

In the case of non-interacting fermions we have $|\Psi_0\rangle = |\Phi_0\rangle$ and we obtain

$$\langle \hat{n} \rangle = \int d^3x \frac{\langle \Phi_0 | \hat{\psi}^+(\mathbf{x}) \hat{\psi}(\mathbf{x}) | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} \tag{11.12}$$

By using the representation of the field operators in terms of creation and destruction operators, Eqs. (5.50) and (5.51), we have

$$\begin{aligned} \langle \hat{n} \rangle &= \int d^3x \sum_{\alpha,\alpha'} \phi^*_\alpha(\mathbf{x}) \phi_{\alpha'}(\mathbf{x}) \langle \Phi_0 | \hat{a}^+_\alpha \hat{a}_{\alpha'} | \Phi_0 \rangle \\ &= \int d^3x \sum_{\alpha,\alpha'=1}^{\epsilon_F} \phi^*_\alpha(\mathbf{x}) \phi_{\alpha'}(\mathbf{x}) \delta_{\alpha,\alpha'} = \int d^3\, x \sum_{\alpha=1}^{\epsilon_F} |\phi_\alpha(x)|^2 \ , \end{aligned} \tag{11.13}$$

where we have assumed the orthonormality of the single particle wave functions ϕ_α and that the many-body state $|\Phi_0\rangle$ is normalized to 1. We indicated with ϵ_F the Fermi energy. The final expression under the integration symbol is the traditional expression of the density for a system of non interacting particles.

The ground state energy of the system is related to the one-body Green's function by the expression

$$\begin{aligned} E_0 &= \frac{\langle \Psi_0 | \hat{T} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} + \frac{\langle \Psi_0 | \hat{V} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \\ &= -\frac{i}{2} \int d^3r \lim_{\mathbf{r}' \to \mathbf{r}} \lim_{t' \to t} \left[i\hbar \frac{\partial}{\partial t} + \left(-\hbar^2 \frac{\nabla^2_{\mathbf{r}}}{2m} \right) \right] G(\mathbf{r}, t, \mathbf{r}', t') \ . \end{aligned} \tag{11.14}$$

We show here below how to obtain the above expression.

WE shall use the following expressions of the commutators of 3 operators:

$$[\hat{A}, \hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{A}\hat{C} \tag{11.15}$$

$$\left[\hat{A}, \hat{B}\hat{C}\right] = \{\hat{A}, \hat{B}\}\hat{C} - \hat{B}\{\hat{A}, \hat{C}\} \tag{11.16}$$

$$\left[\hat{A}, \hat{B}\hat{C}\right] = [\hat{A}, \hat{B}]\hat{C} - \hat{B}[\hat{C}, \hat{A}] \ , \tag{11.17}$$

and also

$$\{\hat{A}, \hat{B}\hat{C}\} = \{\hat{A}, \hat{B}\}\hat{C} - \hat{B}[\hat{A}, \hat{C}] \ . \tag{11.18}$$

We consider the commutator of the hamiltonian

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{V} = \int d^3x\, \hat{\psi}^+(\mathbf{x}) \left(-\hbar^2 \frac{\nabla^2_{\mathbf{x}}}{2m} \right) \hat{\psi}(\mathbf{x}) \\ &+ \frac{1}{2} \int d^3x\, d^3y\, \hat{\psi}^+(\mathbf{x}) \hat{\psi}^+(\mathbf{y}) \hat{V}(\mathbf{x}, \mathbf{y}) \hat{\psi}(\mathbf{y}) \hat{\psi}(\mathbf{x}) \ , \end{aligned} \tag{11.19}$$

with the operator $\hat{\psi}(\mathbf{r})$. I first evaluate the commutator with the kinetic energy term

$$[\psi(\mathbf{r}), \hat{T}] = \left[\underbrace{\hat{\psi}(\mathbf{r})}_{\hat{A}}, \int d^3x\, \underbrace{\hat{\psi}^+(\mathbf{x})}_{\hat{B}} \underbrace{\left(-\hbar^2 \frac{\nabla^2_{\mathbf{x}}}{2m} \right) \hat{\psi}(\mathbf{x})}_{\hat{C}} \right] \ . \tag{11.20}$$

We apply Eq. (11.16)

$$\begin{aligned}[\hat{\psi}(\mathbf{r}),\hat{T}] &= \int d^3x\, \underbrace{\{\hat{\psi}(\mathbf{r}),\hat{\psi}^+(\mathbf{x})\}}_{\delta(\mathbf{x}-\mathbf{r})}\left(-\hbar^2\frac{\nabla^2_{\mathbf{x}}}{2m}\hat{\psi}(\mathbf{x})\right) - \int d^3x\,\hat{\psi}^+(\mathbf{x})\left(-\hbar^2\frac{\nabla^2_{\mathbf{x}}}{2m}\right)\underbrace{\{\hat{\psi}(\mathbf{r}),\hat{\psi}(\mathbf{x})\}}_{0} \\ &= \int d^3x\,\delta(\mathbf{x}-\mathbf{r})\left(-\hbar^2\frac{\nabla^2_{\mathbf{x}}}{2m}\hat{\psi}(\mathbf{x})\right) = -\frac{\hbar^2\nabla^2_{\mathbf{r}}}{2m}\hat{\psi}(\mathbf{r})\ . \end{aligned} \tag{11.21}$$

For the interaction term we consider

$$[\hat{\psi}(\mathbf{r}),\hat{V}] = \frac{1}{2}\int d^3x\,d^3y\,\left[\underbrace{\hat{\psi}(\mathbf{r})}_{\hat{A}},\underbrace{\hat{\psi}^+(\mathbf{x})}_{\hat{B}}\underbrace{\hat{\psi}^+(\mathbf{y})\hat{V}(\mathbf{x},\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})}_{\hat{C}}\right]\ . \tag{11.22}$$

By applying Eq. (11.16) we obtain

$$\begin{aligned}[\hat{\psi}(\mathbf{r}),\hat{V}] &= \frac{1}{2}\int d^3x\,d^3y\,\left[\underbrace{\{\psi(\mathbf{r}),\psi^+(\mathbf{x})\}}_{\delta(\mathbf{r}-\mathbf{x})}\hat{C} - \hat{\psi}^+(\mathbf{x})\left\{\underbrace{\hat{\psi}(\mathbf{r})}_{\hat{A}'},\underbrace{\hat{\psi}^+(\mathbf{y})}_{\hat{B}'}\underbrace{\hat{V}(\mathbf{x},\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})}_{\hat{C}'}\right\}\right] \\ &= \frac{1}{2}\int d^3y\,\hat{\psi}^+(\mathbf{y})\hat{V}(\mathbf{r},\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{r}) \\ &+ \frac{1}{2}\int d^3x\,d^3y\,\left(-\hat{\psi}^+(\mathbf{x})\right)\underbrace{\left\{\hat{\psi}(\mathbf{r}),\hat{\psi}^+(\mathbf{y})\right\}}_{\delta(\mathbf{r}-\mathbf{y})}\hat{V}(\mathbf{x},\mathbf{y})\underbrace{\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})}_{-\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{y})} \\ &- \frac{1}{2}\int d^3x\,d^3y\,\left(-\hat{\psi}^+(\mathbf{x})\right)\hat{\psi}^+(\mathbf{y})\hat{V}(\mathbf{x},\mathbf{y})\underbrace{[\hat{\psi}(\mathbf{r}),\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})]}_{0} \\ &= \frac{1}{2}\int d^3y\,\hat{\psi}^+(\mathbf{y})\hat{V}(\mathbf{r},\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d^3x\,\hat{\psi}^+(\mathbf{x})\hat{V}(\mathbf{x},\mathbf{r})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{r})\ . \end{aligned} \tag{11.23}$$

where we used Eq. (11.18) and the anti-commutation rules of the field operators. For the symmetry of the potential $\hat{V}(\mathbf{x},\mathbf{y}) = \hat{V}(\mathbf{y},\mathbf{x})$, the two terms of the last expression are equal, therefore

$$[\hat{\psi}(\mathbf{r}),\hat{V}] = \int d^3x\,\hat{\psi}^+(\mathbf{x})\hat{V}(\mathbf{r},\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{r})\ . \tag{11.24}$$

Putting together Eqs. (11.21) and (11.24) we obtain

$$[\hat{\psi}(\mathbf{r}),\hat{H}] = -\hbar^2\frac{\nabla^2_{\mathbf{r}}}{2m}\hat{\psi}(\mathbf{r}) + \int d^3x\,\hat{\psi}^+(\mathbf{x})\hat{V}(\mathbf{r},\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{r})\ . \tag{11.25}$$

We use this expression in the equation of motion for the field operator in Heisenberg representation

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{\psi}_{\rm H}(\mathbf{r},t) &= \left[\hat{\psi}_{\rm H}(\mathbf{r},t),\hat{H}\right] = e^{\frac{i}{\hbar}\hat{H}t}\left[\hat{\psi}(\mathbf{r}),\hat{H}\right]e^{-\frac{i}{\hbar}\hat{H}t} \\ &= -\hbar^2\frac{\nabla^2_{\mathbf{r}}}{2m}\hat{\psi}_{\rm H}(\mathbf{r},t) + \int d^3x\,\hat{\psi}^+_{\rm H}(\mathbf{x},t)\hat{V}(\mathbf{r},\mathbf{x})\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}_{\rm H}(\mathbf{r},t)\ . \end{aligned} \tag{11.26}$$

We multiply on the left by the operator $\hat{\psi}^+_{\rm H}(\mathbf{r}',t')$, then we evaluate the expectation value on the ground state $|\Psi_0\rangle$ and divide it by its norm

$$\begin{aligned} &\left[i\hbar\frac{\partial}{\partial t} - \left(-\hbar^2\frac{\nabla^2_{\mathbf{r}}}{2m}\right)\right]\frac{\langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{r}',t')\hat{\psi}_{\rm H}(\mathbf{r},t)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \\ &= \frac{1}{\langle\Psi_0|\Psi_0\rangle}\int d^3x\,\langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{r}',t')\hat{\psi}^+_{\rm H}(\mathbf{x},t)\hat{V}(\mathbf{r},\mathbf{x})\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}_{\rm H}(\mathbf{r},t)|\Psi_0\rangle\ . \end{aligned} \tag{11.27}$$

We take the limit for $\mathbf{r}' \to \mathbf{r}$ e $t' \to t$ and after we integrate on d^3r,

$$\int d^3r \lim_{\mathbf{r}'\to\mathbf{r}} \lim_{t'\to t} \left[i\hbar\frac{\partial}{\partial t} - \left(-\hbar^2\frac{\nabla^2_{\mathbf{r}}}{2m}\right)\right] \left[-iG(\mathbf{r},t,\mathbf{r}',t')\right] = 2\frac{\langle\Psi_0|\hat{V}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \ , \tag{11.28}$$

where the factor 2 is due to the definition of $\hat{V}$ given by Eq. (11.19).
We use Eq. (11.7) to calculate the expectation value of the kinetic energy operator

$$\frac{\langle\Psi_0|\hat{T}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = -i\int d^3r \lim_{\mathbf{r}'\to\mathbf{r}} \lim_{t'\to t} \left(-\hbar^2\frac{\nabla^2_{\mathbf{r}}}{2m}\right) G(\mathbf{r},t,\mathbf{r}',t') \ . \tag{11.29}$$

Combining these two equations, by adding $2\hat{T}$ on the left and right hand sides, we can eliminate the potential term from the energy expectation value and than we obtain Eq. (11.14).

11.1.1 System of non-interacting fermions

In this section, we obtain an expression of the one-body Green's function for an infinite system of non-interacting fermions. This result is the starting point of the perturbative calculation of the Green's function describing a system of interacting particles.

The system of non-interacting particle is defined by the fact that it is described by a MF hamiltonian

$$\hat{H} \equiv \hat{H}_0 = \sum_\alpha \hat{h}_\alpha \tag{11.30}$$

where $\hat{h}_\alpha$ are single particle hamiltonians of which $|\phi_\alpha\rangle$ are the eigenstates. In this case, all the operators in the Heisenberg picture correspond to those expressed in the interaction picture

$$\hat{\mathcal{O}}_{\rm H} \equiv e^{\frac{i}{\hbar}\hat{H}t}\hat{\mathcal{O}}e^{-\frac{i}{\hbar}\hat{H}t} = e^{\frac{i}{\hbar}\hat{H}_0t}\hat{\mathcal{O}}e^{-\frac{i}{\hbar}\hat{H}_0t} \equiv \hat{\mathcal{O}}_{\rm I} \ . \tag{11.31}$$

To simplify the writing we assume normalized to 1 the many-body states $|\Phi_0\rangle$. By definition, the one-body Green's function can be expressed as

$$\begin{aligned} i\,G^0(\mathbf{x},t,\mathbf{x}',t') &= \langle\Phi_0|\hat{\mathbb{T}}\left[\hat{\psi}_{\rm I}(\mathbf{x},t)\hat{\psi}^+_{\rm I}(\mathbf{x}',t')\right]|\Phi_0\rangle \\ &= \langle\Phi_0|\hat{\psi}_{\rm I}(\mathbf{x},t)\hat{\psi}^+_{\rm I}(\mathbf{x}',t')|\Phi_0\rangle\Theta(t-t') - \langle\Phi_0|\hat{\psi}^+_{\rm I}(\mathbf{x}',t')\hat{\psi}_{\rm I}(\mathbf{x},t)|\Phi_0\rangle\Theta(t'-t) \ , \end{aligned} \tag{11.32}$$

where $\Theta(x)$ is the step function.

Let's consider the field operators in the interaction picture and express them in terms of creation and destruction operators

$$\hat{\psi}_{\rm I}(\mathbf{x},t) = \sum_k \hat{a}_{I,k}(t)\phi_k(\mathbf{x}) \ \text{ and } \ \hat{\psi}^+_{\rm I}(\mathbf{x},t) = \sum_k \hat{a}^+_{I,k}(t)\phi^*_k(\mathbf{x}) \ , \tag{11.33}$$

therefore

$$\begin{aligned} i\,G^0(\mathbf{x},t,\mathbf{x}',t') &= \langle\Phi_0|\sum_k \phi_k(\mathbf{x})\hat{a}_k e^{-i\omega_k t}\sum_{k'}\phi^*_{k'}(\mathbf{x}')\hat{a}^+_{k'}e^{i\omega_{k'}t'}|\Phi_0\rangle\Theta(t-t') \\ &- \langle\Phi_0|\sum_{k'}\phi^*_{k'}(\mathbf{x}')\hat{a}^+_{k'}e^{i\omega_{k'}t'}\sum_k \phi_k(\mathbf{x})\hat{a}_k e^{-i\omega_k t}|\Phi_0\rangle\Theta(t'-t) \\ &= \sum_{k\,k'}\phi_k(\mathbf{x})\phi^*_{k'}(\mathbf{x}')e^{-i\omega_k t}e^{i\omega_{k'}t'} \\ &\quad \left[\langle\Phi_0|\hat{a}_k\hat{a}^+_{k'}|\Phi_0\rangle\Theta(t-t') - \langle\Phi_0|\hat{a}^+_{k'}\hat{a}_k|\Phi_0\rangle\Theta(t'-t)\right] \ , \end{aligned} \tag{11.34}$$

where we defined $\omega_k = E_k/\hbar$.

By definition of $|\Phi_0\rangle$ the following relations hold

$$\langle\Phi_0|\hat{a}_k\hat{a}^+_{k'}|\Phi_0\rangle = \delta_{k\,k'}\Theta(k'-k_F), \text{ and } \langle\Phi_0|\hat{a}^+_{k'}\hat{a}_k|\Phi_0\rangle = \delta_{k\,k'}\Theta(k_F-k) \ . \tag{11.35}$$

In an infinite, and homogeneos, system the expression of the single-particle wave function is

$$\phi_k(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}}e^{-i\mathbf{k}\cdot\mathbf{x}} \ , \tag{11.36}$$

where spin and isospin dependent terms have been neglected. The unperturbed Green's function (11.34) assumes the expression

$$i\,G^0(\mathbf{x},t,\mathbf{x}',t') = \frac{1}{\mathcal{V}}\sum_k e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}e^{-i\omega_k(t-t')}\left[\Theta(k-k_F)\Theta(t-t') - \Theta(k_F-k)\Theta(t'-t)\right] \ . \tag{11.37}$$

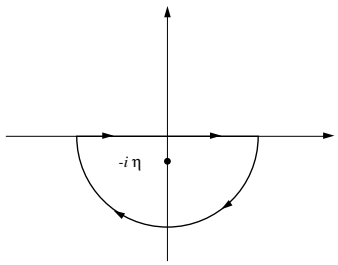

Figure 11.1: Integration contour for the integral (11.41).

We remember that, for an infinite system, we have to substitute the sums in integrals following the prescription

$$\sum_k \to \frac{\mathcal{V}}{(2\pi)^3}\int d^3\,k \ . \tag{11.38}$$

By using the integral representation of the step function

$$\Theta(x) = -\lim_{\eta\to 0}\int_{-\infty}^{\infty} dk\left(\frac{1}{2\pi\,i}\right)\frac{e^{-ikx}}{k+i\eta} \ , \tag{11.39}$$

we can write

$$\begin{aligned} i\,G^0(\mathbf{x},t,\mathbf{x}',t') &= \frac{1}{(2\pi)^3}\int d^3k\,e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}e^{-i\omega_k(t-t')} \\ &\left[-\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi\,i}\frac{e^{-i\omega'(t-t')}}{\omega'+i\eta}\Theta(k-k_F) - \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi\,i}\frac{e^{-i\omega'(t-t')}}{\omega'-i\eta}\Theta(k_F-k)\right] \ . \end{aligned} \tag{11.40}$$

Let's show the validity of Eq. (11.39) by exploiting the residue theorem.

$$\int_{-\infty}^{\infty} dk \frac{1}{2\pi\, i} \frac{e^{-ikx}}{k+i\eta} = -\lim_{k\to -i\eta} 2\pi\, i \frac{1}{2\pi\, i}(k+i\eta)\frac{e^{-ikx}}{k+i\eta} = -e^{-\eta x} \ , \tag{11.41}$$

where the overall minus sign is due to the direction of the integration contour for $x > 0$. In the case $x < 0$ the integration contour will be closed without considering the pole, therefore the integral will be zero. At this point one has that

$$\lim_{\eta\to 0} -e^{-\eta x} = -1 \ . \tag{11.42}$$

from which Eq. (11.39) .

Putting everything together and multiplying by $-i$, we obtain

$$\begin{aligned} G^0(\mathbf{x},t,\mathbf{x}',t') &= \frac{1}{(2\pi)^4}\int d^3k\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\int_{-\infty}^{\infty} d\omega' e^{-i\omega'(t-t')}e^{-i\omega_k(t-t')} \\ &\quad \left[\frac{\Theta(k-k_F)}{\omega'+i\eta}+\frac{\Theta(k_F-k)}{\omega'-i\eta}\right] \ . \end{aligned} \tag{11.43}$$

We define a new variable $\omega = \omega' + \omega_k$ and rewrite the above equation as

$$G^0(\mathbf{x},t,\mathbf{x}',t') = \frac{1}{(2\pi)^4}\int d^3k\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega(t-t')}\left[\frac{\Theta(k-k_F)}{\omega-\omega_k+i\eta}+\frac{\Theta(k_F-k)}{\omega-\omega_k-i\eta}\right] \ , \tag{11.44}$$

From the above expression we extract the definition of the unperturbed one-body Green's function depending on the energy and on the momentum

$$\tilde{G}^0(\mathbf{k},\omega) \equiv \left[\frac{\Theta(k-k_F)}{\omega-\omega_k+i\eta}+\frac{\Theta(k_F-k)}{\omega-\omega_k-i\eta}\right] \ . \tag{11.45}$$

11.1.2 Lehmann representation

Let's consider the full Green's function, i. e. that of the system of interacting particles, and, to simplify the writing, let's assume that the ground state is normalized to unity $\langle\Psi_0|\Psi_0\rangle = 1$. We rewrite the expression of the Green's function by inserting a complete set of eigenstates of the hamiltonian $\hat{H}$

$$\begin{aligned} i\,G(\mathbf{x},t,\mathbf{x}',t') &= \langle\Psi_0|\hat{\mathbb{T}}\left[\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\right]|\Psi_0\rangle \\ &= \sum_n \langle\Psi_0|\hat{\psi}_{\rm H}(\mathbf{x},t)|\Psi_n\rangle\langle\Psi_n|\hat{\psi}^+_{\rm H}(\mathbf{x}',t')|\Psi_0\rangle\Theta(t-t') \\ &- \sum_{n'} \langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{x}',t')|\Psi_{n'}\rangle\langle\Psi_{n'}|\hat{\psi}_{\rm H}(\mathbf{x},t)|\Psi_0\rangle\Theta(t'-t) \end{aligned} \tag{11.46}$$

The eigenstates $|\Psi_n\rangle$ and $|\Psi_{n'}\rangle$ of $\hat{H}$ contain different number of particles. Specifically, the $|\Psi_n\rangle$ multiplying $\Theta(t-t')$ have $A+1$ particles, while $|\Psi_{n'}\rangle$ multiplying $\Theta(t'-t)$ have $A-1$ particles.

Let's indicate with A the number of particles, eigenvalue of the particle number operator

$$\hat{n} = \int d^3x\, \hat{\psi}^+(\mathbf{x})\hat{\psi}(\mathbf{x}) \ . \tag{11.47}$$

We calculate the commutator

$$[\hat{n},\hat{\psi}(\mathbf{z})] = \int d^3x[\hat{\psi}^+(\mathbf{x})\hat{\psi}(\mathbf{x}),\hat{\psi}(\mathbf{z})] = \int d^3x\,[\hat{\psi}^+(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{z}) - \hat{\psi}(\mathbf{z})\hat{\psi}^+(\mathbf{x})\hat{\psi}(\mathbf{x})]$$
$$= \int d^3x\,[\hat{\psi}^+(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{z}) - \hat{\psi}^+(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{z}) - \hat{\psi}(\mathbf{z})\delta(\mathbf{x}-\mathbf{z})] = -\hat{\psi}(\mathbf{z}) \ .$$

From the operator point of view we can write

$$[\hat{n},\hat{\psi}] = -\hat{\psi} \ , \ \hat{n}\hat{\psi} - \hat{\psi}\hat{n} = -\hat{\psi} \ , \ \hat{n}\hat{\psi} = \hat{\psi}(\hat{n}-1) \tag{11.48}$$

therefore

$$\hat{n}\hat{\psi}|\Psi_0\rangle = \hat{\psi}(\hat{n}-1)|\Psi_0\rangle = \hat{\psi}(A-1)|\Psi_0\rangle = (A-1)\hat{\psi}|\Psi_0\rangle \ , \tag{11.49}$$

which indicates that the states of the second term of Eq. (11.46) have a particle less than the states $|\Psi_0\rangle$.

We use in Eq. (11.46) the field operators in the Schrödinger picture.

$$\hat{\mathcal{O}}_H = e^{\frac{i}{\hbar}\hat{H}t}\hat{\mathcal{O}}_S e^{-\frac{i}{\hbar}\hat{H}t} \ , \tag{11.50}$$

$$\begin{aligned} i\,G(\mathbf{x},t,\mathbf{x}',t') &= \sum_n \Theta(t-t')e^{-\frac{i}{\hbar}(E_n-E_0)(t-t')}\langle\Psi_0|\hat{\psi}(\mathbf{x})|\Psi_n\rangle\langle\Psi_n|\hat{\psi}^+(\mathbf{x}')|\Psi_0\rangle \\ &- \sum_{n'} \Theta(t-t')e^{\frac{i}{\hbar}(E_{n'}-E_0)(t-t')}\langle\Psi_0|\hat{\psi}^+(\mathbf{x}')|\Psi_{n'}\rangle\langle\Psi_{n'}|\hat{\psi}(\mathbf{x})|\Psi_0\rangle \ . \end{aligned} \tag{11.51}$$

By substituting the expressions of the field operators

$$\hat{\psi}(\mathbf{x}) = \sum_k \hat{a}_k\phi_k(\mathbf{x}) \ \text{ and } \ \hat{\psi}^+(\mathbf{x}) = \sum_k \hat{a}_k^+\phi_k^*(\mathbf{x}) \tag{11.52}$$

we obtain

$$\begin{aligned} i\,G(\mathbf{x},t,\mathbf{x}',t') &= \sum_n \Theta(t-t')e^{-\frac{i}{\hbar}(E_n-E_0)(t-t')}\sum_{k,k'}\phi_k(\mathbf{x})\phi_{k'}^*(\mathbf{x}')\langle\Psi_0|\hat{a}_k|\Psi_n\rangle\langle\Psi_n|\hat{a}_{k'}^+|\Psi_0\rangle \\ &- \sum_{n'} \Theta(t'-t)e^{\frac{i}{\hbar}(E_{n'}-E_0)(t-t')}\sum_{k,k'}\phi_k(\mathbf{x})\phi_{k'}^*(\mathbf{x}')\langle\Psi_0|\hat{a}_{k'}^+|\Psi_{n'}\rangle\langle\Psi_{n'}|\hat{a}_k|\Psi_0\rangle \ . \end{aligned} \tag{11.53}$$

By considering that, for an infinite system, Eqs. (11.36) and (11.38) hold, we can write

$$\begin{aligned} &i\,G(\mathbf{x},t,\mathbf{x}',t') = \\ &\sum_n \Theta(t-t')e^{-\frac{i}{\hbar}(E_n-E_0)(t-t')}\frac{1}{(2\pi)^3}\int d^3k\,e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\langle\Psi_0|\hat{a}_k|\Psi_n\rangle\langle\Psi_n|\hat{a}_k^+|\Psi_0\rangle \\ &- \sum_{n'} \Theta(t'-t)e^{\frac{i}{\hbar}(E_{n'}-E_0)(t-t')}\frac{1}{(2\pi)^3}\int d^3k\,e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\langle\Psi_0|\hat{a}_k^+|\Psi_{n'}\rangle\langle\Psi_{n'}|\hat{a}_k|\Psi_0\rangle \ . \end{aligned} \tag{11.54}$$

In the above equations we considered that $|\Psi_n\rangle$ is characterized by the momentum k, therefore

$$\mathbb{I} = \sum_n |\Psi_n\rangle\langle\Psi_n| \equiv \frac{1}{(2\pi)^3}\int d^3k\,|k\rangle\langle k'| = \delta_{k,k'} \ .$$

By using the integral expression of the step function (11.39) we obtain

$$G(\mathbf{x},t,\mathbf{x}',t') = \frac{1}{(2\pi)^4}\int d^3k\, e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\int d\omega e^{-i\omega(t-t')} \left[\sum_n \frac{\langle\Psi_0|\hat{a}_k|\Psi_n\rangle\langle\Psi_n|\hat{a}_k^+|\Psi_0\rangle}{\omega-(E_n-E_0)/\hbar+i\eta} + \sum_{n'}\frac{\langle\Psi_0|\hat{a}_k^+|\Psi_{n'}\rangle\langle\Psi_{n'}|\hat{a}_k|\Psi_0\rangle}{\omega+(E_{n'}-E_0)/\hbar-i\eta}\right] . \tag{11.55}$$

We define the Fourier transform

$$\begin{aligned}\tilde{G}(\mathbf{k},\omega) &= \int d^3(x-x')\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\int d(t-t')e^{i\omega(t-t')}G(\mathbf{x},t,\mathbf{x}',t') \\ &= \sum_n \frac{\langle\Psi_0|\hat{a}_k|\Psi_n\rangle\langle\Psi_n|\hat{a}_k^+|\Psi_0\rangle}{\omega-(E_n-E_0)/\hbar+i\eta} + \sum_{n'}\frac{\langle\Psi_0|\hat{a}_k^+|\Psi_{n'}\rangle\langle\Psi_{n'}|\hat{a}_k|\Psi_0\rangle}{\omega+(E_{n'}-E_0)/\hbar-i\eta} .\end{aligned} \tag{11.56}$$

Let's consider the denominator of the first term. The energy E_0 is eigenvalue of $|\Psi_0\rangle$ describing the system with A particles, while E_n is eiegenvalue of $|\Psi_n\rangle$ which has $A+1$ particles. We rewrite the denominator indicating in round brackets the number of particles of the system which the energy refers to.

$$\begin{aligned}&\hbar\omega - E_n(A+1) + E_0(A) = \hbar\omega - E_n(A+1) + E_0(A+1) - E_0(A+1) + E_0(A) \\ =\ &\hbar\omega - [E_n(A+1) - E_0(A+1)] - [E_0(A+1) - E_0(A)] = \hbar\omega - \hbar\omega_n(A+1) - \mu\ .\end{aligned}$$

In the above equations we call $\omega_n(A+1)$ the excitation energy of the system with $A+1$ particles and with μ the **chemical potential** defined as

$$\mu = \left(\frac{\partial E}{\partial \mathrm{A}}\right)_V \equiv \left[\frac{E_0(A+1)-E_0(A)}{\Delta 1}\right] . \tag{11.57}$$

where we indicated with $\Delta 1$ the variation of one unit of the number of fermions.

The Green's function in Lehmann representation is

$$\tilde{G}(\mathbf{k},\omega) = \sum_n \frac{\langle\Psi_0|\hat{a}_k|\Psi_n\rangle\langle\Psi_n|\hat{a}_k^+|\Psi_0\rangle}{\omega-\omega_n-\mu/\hbar+i\eta} + \sum_{n'}\frac{\langle\Psi_0|\hat{a}_k^+|\Psi_{n'}\rangle\langle\Psi_{n'}|\hat{a}_k|\Psi_0\rangle}{\omega+\omega_{n'}-\mu/\hbar-i\eta} . \tag{11.58}$$

The sign of the chemical potential in the second denominator is due to the definition (11.57) where the derivative has positive sign when a particle is added to the system. It worth to remark that ω_n in the first term is refers to the system with $A+1$ particles, while $\omega_{n'}$ in the second term to a system with $A-1$ particles.

11.1.3 Physical interpretation

Let's consider a state in the interaction picture and add a particle in the point $\mathbf{x}'$, at the time t'

$$\hat{\psi}_{\mathrm{I}}^+(\mathbf{x}',t')|\Psi_{\mathrm{I}}(t')\rangle\ . \tag{11.59}$$

This states propagates at the time t as

$$\hat{U}(t,t')\hat{\psi}_{\mathrm{I}}^+(\mathbf{x}',t')|\Psi_{\mathrm{I}}(t')\rangle\ . \tag{11.60}$$

We shall calculate the overlap with $\hat{\psi}_{\mathrm{I}}^+(\mathbf{x},t)|\Psi_{\mathrm{I}}(t)\rangle$ for $t > t'$.

Let's recall here below some property of the time propagation operator $\hat{U}(t,t')$

$$\begin{aligned}
&\hat{U}(t,t')\hat{U}(t',t) = \hat{U}(t,t) = 1 \\
&|\Psi_{\rm H}\rangle = |\Psi_{\rm I}(0)\rangle = \hat{U}(0,-\infty)|\Phi_0\rangle = |\Psi_0\rangle \\
&\hat{U}(t,t_0) = e^{\frac{i}{\hbar}\hat{H}_0 t}e^{-\frac{i}{\hbar}(\hat{H}_0+\hat{H}_1)(t-t_0)}e^{-\frac{i}{\hbar}\hat{H}_0 t_0} \\
&\hat{U}(t,0) = e^{-\frac{i}{\hbar}\hat{H}_1 t} \;\; ; \;\; \hat{U}(0,t) = e^{\frac{i}{\hbar}\hat{H}_1 t} \\
&\hat{\mathcal{O}}_{\rm I}(t) = e^{-\frac{i}{\hbar}\hat{H}_1 t}\hat{\mathcal{O}}_{\rm H}(t)e^{\frac{i}{\hbar}\hat{H}_1 t} = \hat{U}(t,0)\hat{\mathcal{O}}_{\rm H}\hat{U}(0,t) \\
&\hat{\mathcal{O}}_{\rm H}(t) = e^{\frac{i}{\hbar}\hat{H} t}\hat{\mathcal{O}}_{\rm S}e^{-\frac{i}{\hbar}\hat{H} t} \;\; ; \;\; \hat{\mathcal{O}}_{\rm I}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{\mathcal{O}}_{\rm S}e^{-\frac{i}{\hbar}\hat{H}_0 t} \\
&|\Psi_{\rm I}(t')\rangle = \hat{U}(t',-\infty)|\Phi(0)\rangle \;\; .
\end{aligned}$$

At the time t' in the point $\mathbf{x}'$, a particle is added to the system, the state propagates and, later on, at the time t, in the position $\mathbf{x}$ the particle is eliminated. This process can be described as

$$\begin{aligned}
&\langle\Psi(t)|\hat{\psi}_{\rm I}(\mathbf{x},t)\hat{U}(t,t')\hat{\psi}^+_{\rm I}(\mathbf{x}',t')|\Psi(t')\rangle = \\
&\langle\Phi_0|\hat{U}(\infty,t)\left[\hat{U}(t,0)\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{U}(0,t)\right]\hat{U}(t,t')\left[\hat{U}(t',0)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\hat{U}(0,t')\right]\hat{U}(t',-\infty)|\Phi_0\rangle = \\
&\left\{\langle\Phi_0|\hat{U}(\infty,t)\hat{U}(t,0)\right\}\hat{\psi}_{\rm H}(\mathbf{x},t)\left[\hat{U}(0,t)\hat{U}(t,t')\hat{U}(t',0)\right]\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\left\{\hat{U}(0,t')\hat{U}(t',-\infty)|\Phi_0\rangle\right\} = \\
&\langle\Psi_0|\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')|\Psi_0\rangle
\end{aligned}$$

The last expression is that of the one-body Green's function for $t > t'$. The Green's function is the probability amplitude that a particle created in the point $\mathbf{x}'$ at the time t' is destroyed in the point $\mathbf{x}$ at the time t.

11.2 Two-body Green's function

Also in this section, to simplify the writing, we assume $\langle\Psi_0|\Psi_0\rangle = 1$. The two-body Green's function is defined as

$$(-i)^2 G(\mathbf{x}_1,t_1,\mathbf{x}_2,t_2,\mathbf{x}_3,t_3,\mathbf{x}_4,t_4) \equiv \langle\Psi_0|\hat{\mathbb{T}}[\hat{\psi}_{\rm H}(\mathbf{x}_1,t_1)\hat{\psi}_{\rm H}(\mathbf{x}_2,t_2)\hat{\psi}^+_{\rm H}(\mathbf{x}_3,t_3)\hat{\psi}^+_{\rm H}(\mathbf{x}_4,t_4)]|\Psi_0\rangle \;\; , \qquad (11.61)$$

For the one-body Green's function it has been necessary to consider two cases, $t > t'$ and viceversa. For the two-body Green's function there are $4! = 24$ cases. In reality for the symmetry properties

$$G(1234) = -G(2134) = -G(1243) = G(2143) \;\; , \qquad (11.62)$$

there are only 6 independent cases. Out of these 6 cases only 3 have physically interesting properties.

1. $t_1, t_2 > t_3, t_4$. This case implies

$$(-i)^2 G(\mathbf{x}_1,t_1,\mathbf{x}_2,t_2,\mathbf{x}_3,t_3,\mathbf{x}_4,t_4) \equiv \langle\Psi_0|\hat{\psi}_{\rm H}(\mathbf{x}_1,t_1)\hat{\psi}_{\rm H}(\mathbf{x}_2,t_2)\hat{\psi}^+_{\rm H}(\mathbf{x}_3,t_3)\hat{\psi}^+_{\rm H}(\mathbf{x}_4,t_4)|\Psi_0\rangle \;\; , \qquad (11.63)$$

   and describes the evolution of a state to which, at the times t_3 and t_4, two particles have been added.

2. $t_1, t_2 < t_3, t_4$. This case implies

$$(-i)^2 G(\mathbf{x}_1,t_1,\mathbf{x}_2,t_2,\mathbf{x}_3,t_3,\mathbf{x}_4,t_4) \equiv \langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{x}_3,t_3)\hat{\psi}^+_{\rm H}(\mathbf{x}_4,t_4)\hat{\psi}_{\rm H}(\mathbf{x}_1,t_1)\hat{\psi}_{\rm H}(\mathbf{x}_2,t_2)|\Psi_0\rangle \;\; , \qquad (11.64)$$

   and describes the evolution of a state to which, at the times t_1 and t_2, two holes have been created.

3. $t_1, t_3 > t_2, t_4$. This case implies

$$(-i)^2 G(\mathbf{x}_1, t_1, \mathbf{x}_2, t_2, \mathbf{x}_3, t_3, \mathbf{x}_4, t_4) = -\langle \Psi_0 | \hat{\psi}_{\rm H}(\mathbf{x}_1, t_1) \hat{\psi}^+_{\rm H}(\mathbf{x}_3, t_3) \hat{\psi}_{\rm H}(\mathbf{x}_2, t_2) \hat{\psi}^+_{\rm H}(\mathbf{x}_4, t_4) | \Psi_0 \rangle \ , \quad (11.65)$$

and describes the time evolution of a particle-hole pair.

This latter case is that of major interest to us and it is the only case treated in this section.

Since we work in non-relativistic framework the creation, and also the destruction, of a particle-hole pair is instantaneous, we have that

$$t_1 = t_3 = t' \ \text{ e } \ t_2 = t_4 = t \ . \quad (11.66)$$

For this case, we express the two-body Green's function in terms of creation and destruction operators

$$\begin{aligned} & G(\mathbf{x}_1, t', \mathbf{x}_2, t, \mathbf{x}_3, t', \mathbf{x}_4, t) = \\ & \sum_{\nu_1 \nu_2 \nu_3 \nu_4} \phi_{\nu_1}(\mathbf{x}_1) \phi^*_{\nu_3}(\mathbf{x}_3) \phi_{\nu_2}(\mathbf{x}_2) \phi^*_{\nu_4}(\mathbf{x}_4) \langle \Psi_0 | \hat{\mathbb{T}}[\hat{a}_{\nu_1}(t') \hat{a}^+_{\nu_3}(t') \hat{a}_{\nu_2}(t) \hat{a}^+_{\nu_4}(t)] | \Psi_0 \rangle \\ = & \sum_{\nu_1 \nu_2 \nu_3 \nu_4} \phi_{\nu_1}(\mathbf{x}_1) \phi_{\nu_2}(\mathbf{x}_2) \phi^*_{\nu_3}(\mathbf{x}_3) \phi^*_{\nu_4}(\mathbf{x}_4) G(\nu_1, t', \nu_2, t, \nu_3, t', \nu_4, t) \ . \end{aligned} \quad (11.67)$$

where it is understood that all the creation and destruction operators are expressed in the Heisenberg picture. The previous equation defines a two-body Green's function depending on the quantum numbers ν characterizing the single-particle states.

We define the *retarded* part of the Green's function by considering the $t' > t$ case

$$\begin{aligned} & G^R(\nu_1, t', \nu_2, t, \nu_3, t', \nu_4, t) = \langle \Psi_0 | \hat{a}_{\nu_1}(t') \hat{a}^+_{\nu_3}(t') \hat{a}_{\nu_2}(t) \hat{a}^+_{\nu_4}(t) | \Psi_0 \rangle \\ = & \langle \Psi_0 | e^{\frac{i}{\hbar}\hat{H}t'} \hat{a}_{\nu_1} e^{-\frac{i}{\hbar}\hat{H}t'} e^{\frac{i}{\hbar}\hat{H}t'} \hat{a}^+_{\nu_3} e^{-\frac{i}{\hbar}\hat{H}t'} e^{\frac{i}{\hbar}\hat{H}t} \hat{a}_{\nu_2} e^{-\frac{i}{\hbar}\hat{H}t} e^{\frac{i}{\hbar}\hat{H}t} \hat{a}^+_{\nu_4} e^{-\frac{i}{\hbar}\hat{H}t} | \Psi_0 \rangle \\ = & \langle \Psi_0 | \hat{a}_{\nu_1} \hat{a}^+_{\nu_3} e^{-\frac{i}{\hbar}(\hat{H} - E_0)(t'-t)} \hat{a}_{\nu_2} \hat{a}^+_{\nu_4} | \Psi_0 \rangle \ , \end{aligned} \quad (11.68)$$

where we made explicit the expression of the creation and destruction operators in the Heisenberg picture, and we used $\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle$. In analogous manner we define the *advanced* part of the Green's function for the $t' < t$ case,

$$G^A(\nu_1, t', \nu_2, t, \nu_3, t', \nu_4, t) = \langle \Psi_0 | \hat{a}_{\nu_2} \hat{a}^+_{\nu_4} e^{+\frac{i}{\hbar}(\hat{H} - E_0)(t'-t)} \hat{a}_{\nu_1} \hat{a}^+_{\nu_3} | \Psi_0 \rangle \quad (11.69)$$

We can express the two-body Green's function as

$$G(\nu_1, \nu_2, \nu_3, \nu_4, \tau) = \begin{cases} G^A(\nu_1, t', \nu_2, t, \nu_3, t', \nu_4, t) & \text{per } \tau = t' - t < 0 \\ G^R(\nu_1, t', \nu_2, t, \nu_3, t', \nu_4, t) & \text{per } \tau = t' - t > 0 \end{cases} \ . \quad (11.70)$$

11.2.1 Lehmann representation

We define the energy dependent two-body Green's function as

$$\tilde{G}(\nu_1, \nu_2, \nu_3, \nu_4, E) = \int_{-\infty}^{\infty} d\tau \, G(\nu_1, \nu_2, \nu_3, \nu_4, \tau) \, e^{\frac{i}{\hbar} E \tau} \ , \quad (11.71)$$

where $\tau = t' - t$. We consider the retarded part

$$\tilde{G}^R(\nu_1, \nu_2, \nu_3, \nu_4, E) = \langle \Psi_0 | \hat{a}_{\nu_1} \hat{a}^+_{\nu_3} \int_0^{\infty} d\tau \, e^{-\frac{i}{\hbar}(\hat{H} - E_0 - E)\tau} \hat{a}_{\nu_2} \hat{a}^+_{\nu_4} | \Psi_0 \rangle \ . \quad (11.72)$$

We can express the value of the time integral as

$$\lim_{\eta\to 0}\int_0^\infty d\tau\, e^{\frac{i}{\hbar}(-\hat{H}+E_0+E+i\eta)\tau} = \lim_{\eta\to 0}\frac{e^{\frac{i}{\hbar}(E-\hat{H}+E_0)\tau}e^{-\eta\tau}}{\frac{i}{\hbar}(E-\hat{H}+E_0+i\eta)}\Big|_0^\infty = \lim_{\eta\to 0}\frac{i\hbar}{E-\hat{H}+E_0+i\eta}\ , \tag{11.73}$$

therefore

$$\tilde{G}^R(\nu_1,\nu_2,\nu_3,\nu_4,E) = \hbar\langle\Psi_0|\hat{a}_{\nu_1}\hat{a}^+_{\nu_3}\frac{i}{E-\hat{H}+E_0+i\eta}\hat{a}_{\nu_2}\hat{a}^+_{\nu_4}|\Psi_0\rangle\ . \tag{11.74}$$

With an analogous calculation we obtain for the advanced part

$$\tilde{G}^A(\nu_1,\nu_2,\nu_3,\nu_4,E) = \langle\Psi_0|\hat{a}_{\nu_2}\hat{a}^+_{\nu_4}\int_{-\infty}^0 d\tau\, e^{\frac{i}{\hbar}(\hat{H}-E_0+E)\tau}\hat{a}_{\nu_1}\hat{a}^+_{\nu_3}|\Psi_0\rangle\ , \tag{11.75}$$

$$\lim_{\eta\to 0}\int_{-\infty}^0 d\tau\, e^{\frac{i}{\hbar}(\hat{H}-E_0+E-i\eta)\tau} = \lim_{\eta\to 0}\frac{e^{\frac{i}{\hbar}(E+\hat{H}-E_0)\tau}e^{\eta\tau}}{\frac{i}{\hbar}(E+\hat{H}-E_0-i\eta)}|_{-\infty}^0 = \lim_{\eta\to 0}\frac{-i\hbar}{E+\hat{H}-E_0-i\eta}\ , \tag{11.76}$$

$$\tilde{G}^A(\nu_1,\nu_2,\nu_3,\nu_4,E) = (-1)\hbar\langle\Psi_0|\hat{a}_{\nu_2}\hat{a}^+_{\nu_4}\frac{i}{E+\hat{H}-E_0-i\eta}\hat{a}_{\nu_1}\hat{a}^+_{\nu_3}|\Psi_0\rangle\ , \tag{11.77}$$

therefore

$$\begin{aligned}-\frac{i}{\hbar}\tilde{G}(\nu_1,\nu_2,\nu_3,\nu_4,E) = -\frac{i}{\hbar}(\tilde{G}^R+\tilde{G}^A) &= \langle\Psi_0|\hat{a}_{\nu_1}\hat{a}^+_{\nu_3}\frac{1}{E-\hat{H}+E_0+i\eta}\hat{a}_{\nu_2}\hat{a}^+_{\nu_4}|\Psi_0\rangle \\ &- \langle\Psi_0|\hat{a}_{\nu_2}\hat{a}^+_{\nu_4}\frac{1}{E+\hat{H}-E_0-i\eta}\hat{a}_{\nu_1}\hat{a}^+_{\nu_3}|\Psi_0\rangle\ .\end{aligned} \tag{11.78}$$

By inserting the completeness of the eigenfunctions of $\hat{H}$, $\sum_n|\Psi_n\rangle\langle\Psi_n| = 1$, and considering $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$ we obtain the expression

$$\begin{aligned}&-\frac{i}{\hbar}\tilde{G}(\nu_1,\nu_2,\nu_3,\nu_4,E) \\ &= \sum_n\left[\frac{\langle\Psi_0|\hat{a}_{\nu_1}\hat{a}^+_{\nu_3}|\Psi_n\rangle\langle\Psi_n|\,\hat{a}_{\nu_2}\hat{a}^+_{\nu_4}|\Psi_0\rangle}{E-(E_n-E_0)+i\eta} - \frac{\langle\Psi_0|\hat{a}_{\nu_2}\hat{a}^+_{\nu_4}|\Psi_n\rangle\langle\Psi_n|\hat{a}_{\nu_1}\hat{a}^+_{\nu_3}|\Psi_0\rangle}{E+(E_n-E_0)-i\eta}\right]\ .\end{aligned} \tag{11.79}$$

In this expression, the states $|\Psi_n\rangle$ have the same particle number of the ground state. The energy values related to the poles, $E = E_n - E_0$, represent the excitation energies of the A particle system.

11.3 Linear response

Let's consider the situation where the many-body system is subject to an external perturbation. We express the total hamiltonian describing the perturbed system as sum of the hamiltonian $\hat{H}$ describing the system in absence of the perturbation, and we indicate its eigenstates as $|\Psi\rangle$. The external perturbation is described by the term $\hat{H}^{\rm ext}(t)$

$$\hat{H}^{\rm tot} = \hat{H} + \hat{H}^{\rm ext}(t) = \hat{H} + \hat{B}F(t)\ , \tag{11.80}$$

where $\hat{B}$ is the operator describing the action of the external perturbation on the system. For example the perturbation can be generated by photons, electrons, hadrons, etc.. The function $F(t)$ describes how the perturbation acts on the time, and it is defined such as $\hat{F}(t) = 0$ for $t < t_0 = 0$. This means that the perturbation is switched on after a specific time, t_0 which we define as zero time.

We assume that, under the action of the external perturbation, the many-body system reacts with time much faster than the time needed to the perturbation to switch on and off. Then, when the perturbation is totally switched on the hamiltonian is $\hat{H}^{\rm tot} = \hat{H} + \hat{B}$. In this case we can treat $\hat{B}$ as a perturbative term of the total time-dependent hamiltonian. For this reason, we can consider the equation of motion in the interaction picture (see Chapter 6)

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\rm I}(t)\rangle = \hat{B}_{\rm I}(t)|\Psi_{\rm I}(t)\rangle \ , \tag{11.81}$$

where

$$\hat{B}_{\rm I}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}t} \quad \text{e} \quad |\Psi_{\rm I}(t)\rangle = e^{\frac{i}{\hbar}\hat{H}t}|\Psi(t)\rangle \ . \tag{11.82}$$

In this section we use the convention that states and operators without sub-indexes are expressed in the Schrödinger picture. We integrate Eq. (11.81)

$$\begin{aligned} i\hbar\int_{-\infty}^{t} dt' \, \frac{\partial}{\partial t'}|\Psi_{\rm I}(t')\rangle &= \int_{-\infty}^{t} dt' \, \hat{B}_{\rm I}(t')|\Psi_{\rm I}(t')\rangle \\ i\hbar\Big[|\Psi_{\rm I}(t)\rangle - |\Psi_{\rm I}(-\infty)\rangle\Big] &= \int_{-\infty}^{t} dt' \, \hat{B}_{\rm I}(t')|\Psi_{\rm I}(t')\rangle \\ |\Psi_{\rm I}(t)\rangle &= |\Psi_{\rm I}(-\infty)\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \hat{B}_{\rm I}(t')|\Psi_{\rm I}(t')\rangle \ . \end{aligned} \tag{11.83}$$

Since the perturbation is off when $t = -\infty$ we have that $|\Psi_{\rm I}(-\infty)\rangle = |\Psi_0\rangle$. We can express the above equation in perturbative terms by iterating the presence of $|\Psi_{\rm I}(-\infty)\rangle$

$$|\Psi_{\rm I}(t)\rangle = |\Psi_0\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \hat{B}_{\rm I}(t')|\Psi_0\rangle \quad + \quad \cdots \tag{11.84}$$

We call $\hat{D}$ the operator which describe how the system reacts to the external perturbation induced by the operator $\hat{B}$. The expectation value of this operator is given by

$$\begin{aligned} & \langle\Psi_{\rm I}(t)|\hat{D}_{\rm I}(t)|\Psi_{\rm I}(t)\rangle \\ = & \left\{\langle\Psi_0| + \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \hat{B}_{\rm I}(t')\langle\Psi_0| \quad + \quad \cdots\right\}\hat{D}_{\rm I}(t)\left\{|\Psi_0\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \hat{B}_{\rm I}(t')|\Psi_0\rangle \quad + \quad \cdots\right\} \\ = & \langle\Psi_0|\hat{D}_{\rm I}(t)|\Psi_0\rangle + \frac{i}{\hbar}\int_{-\infty}^{t} dt'\langle\Psi_0|[\hat{B}_{\rm I}(t'), \hat{D}_{\rm I}(t)]|\Psi_0\rangle \quad + \cdots \end{aligned} \tag{11.85}$$

We define the response function as

$$R(t'-t) = \begin{cases} 0 & \text{per } \ t' < t \\ \dfrac{i}{\hbar}\langle\Psi_0|[\hat{B}_{\rm I}(t'), \hat{D}_{\rm I}(t)]|\Psi_0\rangle & \text{per } \ t' > t \end{cases} \ . \tag{11.86}$$

This definition implies causality. The system cannot respond before that the perturbation is switched on.

By making explicit the time dependence of $\hat{B}_{\rm I}(t')$ and $\hat{D}_{\rm I}(t)$,

$$\hat{B}_{\rm I}(t') = e^{\frac{i}{\hbar}\hat{H}t'}\hat{B}e^{-\frac{i}{\hbar}\hat{H}t'} \quad ; \quad \hat{D}_{\rm I}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{D}e^{-\frac{i}{\hbar}\hat{H}t} \ , \tag{11.87}$$

we can express the response as

$$R(t'-t) = \frac{i}{\hbar}\langle\Psi_0|\hat{B}e^{\frac{i}{\hbar}(\hat{H}-E_0)(t-t')}\hat{D}|\Psi_0\rangle - \frac{i}{\hbar}\langle\Psi_0|\hat{D}e^{-\frac{i}{\hbar}(\hat{H}-E_0)(t-t')}\hat{B}|\Psi_0\rangle \ , \tag{11.88}$$

and, since it depends only on the time difference $\tau = t - t'$, by using the definition of Fourier transform, we obtain

$$\begin{aligned} R(E) &= \int_{-\infty}^{\infty} d\tau\, R(\tau)\, e^{\frac{i}{\hbar}E\tau} \\ &= \frac{i}{\hbar}\langle\Psi_0|\hat{B}\int_{-\infty}^{\infty} d\tau e^{\frac{i}{\hbar}(\hat{H}-E_0+E)\tau}\hat{D}|\Psi_0\rangle - \frac{i}{\hbar}\langle\Psi_0|\hat{D}\int_{-\infty}^{\infty} d\tau e^{-\frac{i}{\hbar}(\hat{H}-E_0-E)\tau}\hat{B}|\Psi_0\rangle \\ &= -\langle\Psi_0|\hat{B}(\hat{H}-E_0+E+i\eta)^{-1}\hat{D}|\Psi_0\rangle - \langle\Psi_0|\hat{D}(\hat{H}-E_0-E-i\eta)^{-1}\hat{B}|\Psi_0\rangle \ . \end{aligned} \tag{11.89}$$

We insert the completeness $\sum_n |\Psi_n\rangle\langle\Psi_n| = 1$ and obtain

$$R(E) = \sum_n \left[\frac{\langle\Psi_0|\hat{D}|\Psi_n\rangle\langle\Psi_n|\hat{B}|\Psi_0\rangle}{E-(E_n-E_0)+i\eta} - \frac{\langle\Psi_0|\hat{B}|\Psi_n\rangle\langle\Psi_n|\hat{D}|\Psi_0\rangle}{E+(E_n-E_0)+i\eta} \right] \ . \tag{11.90}$$

The poles of $R(E)$ correspond to the excitation energies of the system. For each positive pole there is a negative pole, equal in absolute value to the positive one.

We consider the Dirac expression

$$\frac{1}{x'-x\pm i\eta} = \mathscr{P}\frac{1}{x'-x} \mp i\pi\delta(x-x') \ , \tag{11.91}$$

where $\mathscr{P}$ indicates the principal part, therefore

$$\delta(x-x') = -\frac{1}{\pi}\Im\left(\frac{1}{x'-x\pm i\eta}\right) \ , \tag{11.92}$$

with the symbol $\Im$ indicating the imaginary part.

We assume $\hat{D} = \hat{B}$, as it usually happens, and consider only positive energies. The transition probability from the ground state to an excited state is given by

$$S(E) = -\frac{1}{\pi}\Im\big(R(E)\big) = \sum_n |\langle\Psi_0|\hat{B}|\Psi_n\rangle|^2\delta\big(E-(E_n-E_0)\big) \ . \tag{11.93}$$

This is the traditional expression obtained by applying the time-dependent perturbation theory [Mes61]. Assuming that $\hat{B}$ is a one-body operator

$$\hat{B} = \sum_{\nu_1\nu_2} B_{\nu_1\nu_2}\hat{a}_{\nu_1}\hat{a}^+_{\nu_2} \ \text{ and } \ B_{\nu_1\nu_2} = \int d^3r\, \phi^*_{\nu_1}(\mathbf{r})\, \hat{B}(\mathbf{r})\, \phi_{\nu_2}(\mathbf{r}) \ , \tag{11.94}$$

we obtain

$$\begin{aligned} R(E) = \sum_{\nu_1\nu_2}\sum_{\nu_3\nu_4}\sum_n \quad & \Big[B_{\nu_1\nu_2}B^*_{\nu_3\nu_4}\frac{\langle\Psi_0|\hat{a}_{\nu_1}\hat{a}^+_{\nu_2}|\Psi_n\rangle\langle\Psi_n|\hat{a}_{\nu_3}\hat{a}^+_{\nu_4}|\Psi_0\rangle}{E-(E_n-E_0)+i\eta} \\ - \quad & B_{\nu_3\nu_4}B^*_{\nu_1\nu_2}\frac{\langle\Psi_0|\hat{a}_{\nu_3}\hat{a}^+_{\nu_4}|\Psi_n\rangle\langle\Psi_n|\hat{a}_{\nu_1}\hat{a}^+_{\nu_2}|\Psi_0\rangle}{E+(E_n-E_0)+i\eta}\Big] \ , \end{aligned} \tag{11.95}$$

Since $\hat{B}$ is hermitian, $B_{\nu_1\nu_2} = B^*_{\nu_2\nu_1}$ and the indexes ν are dummy, we can write

$$\begin{aligned} R(E) &= \sum_{\nu_1\nu_2}\sum_{\nu_3\nu_4} B_{\nu_1\nu_2}B^*_{\nu_3\nu_4} \\ &\quad \sum_n \Big[\frac{\langle\Psi_0|\hat{a}_{\nu_1}\hat{a}^+_{\nu_2}|\Psi_n\rangle\langle\Psi_n|\hat{a}_{\nu_3}\hat{a}^+_{\nu_4}|\Psi_0\rangle}{E-(E_n-E_0)+i\eta} - \frac{\langle\Psi_0|\hat{a}_{\nu_3}\hat{a}^+_{\nu_4}|\Psi_n\rangle\langle\Psi_n|\hat{a}_{\nu_1}\hat{a}^+_{\nu_2}|\Psi_0\rangle}{E+(E_n-E_0)+i\eta}\Big] \\ &= \sum_{\nu_1\nu_2}\sum_{\nu_3\nu_4} B_{\nu_1\nu_2}B^*_{\nu_3\nu_4}(-i)\tilde{G}(\nu_1,\nu_3,\nu_2,\nu_4,E) \ , \end{aligned} \tag{11.96}$$

where, in the last step, we considered the expression (11.79) of the two-body Green's function in Lehmann representation. The transition probability is given by

$$S(E) = -\frac{1}{\pi}\Im\big(R(E)\big) = \sum_{\nu_1\nu_2}\sum_{\nu_3\nu_4} B_{\nu_1\nu_2}B^*_{\nu_3\nu_4}\frac{\Im}{\pi}\left(i\hbar\tilde{G}(\nu_1,\nu_3,\nu_2,\nu_4,E)\right) \ . \tag{11.97}$$

11.4 Equation of motion

In this section we shall obtain a set of equation describing the time evolution of the Green's functions. Let's consider the total hamiltonian as sum of one-body term $\hat{H}_0$ and a two-body term $\hat{H}_1$.

$$\begin{aligned}\hat{H} &= \hat{H}_0 + \hat{H}_1 = \int d^3x\, \hat{\psi}^+(\mathbf{x})\hat{h}(\mathbf{x})\hat{\psi}(\mathbf{x}) \\ &+ \frac{1}{2}\int d^3x\, d^3y\, \hat{\psi}^+(\mathbf{x})\hat{\psi}^+(\mathbf{y})\hat{V}(\mathbf{x},\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \ ,\end{aligned} \tag{11.98}$$

where $\hat{h}(\mathbf{x})$, in addition to the kinetic energy term, can also contain a MF, one-body, potential term. By using the techniques adopted to obtain (11.21) and (11.24), we have

$$[\hat{\psi}(\mathbf{r}),\hat{H}_0] = \hat{h}(\mathbf{r})\hat{\psi}(\mathbf{r}) \tag{11.99}$$

$$\left[\hat{\psi}(\mathbf{r}),\hat{H}_1\right] = \int d^3x\, \hat{\psi}^+(\mathbf{x})\hat{V}(\mathbf{r},\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{r}) \tag{11.100}$$

$$\left[\hat{\psi}^+(\mathbf{r}),\hat{H}_0\right] = -\hat{\psi}^+(\mathbf{r})\hat{h}(\mathbf{r}) \tag{11.101}$$

$$\left[\hat{\psi}^+(\mathbf{r}),\hat{H}_1\right] = -\int d^3x\, \hat{\psi}^+(\mathbf{r})\hat{\psi}^+(\mathbf{x})\hat{V}(\mathbf{r},\mathbf{x})\hat{\psi}(\mathbf{x}) \tag{11.102}$$

From the definition of one-body Green's function we obtain

$$\begin{aligned}i\frac{\partial}{\partial t}G(\mathbf{x},t,\mathbf{x}',t') &= \langle\Psi_0|\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')|\Psi_0\rangle\frac{\partial\,\theta(t-t')}{\partial t} \\ &- \langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\hat{\psi}_{\rm H}(\mathbf{x},t)|\Psi_0\rangle\frac{\partial\,\theta(t'-t)}{\partial t} \\ &+ \langle\Psi_0|\frac{\partial\hat{\psi}_{\rm H}(\mathbf{x},t)}{\partial t}\hat{\psi}^+_{\rm H}(\mathbf{x}',t')|\Psi_0\rangle\theta(t-t') \\ &- \langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\frac{\partial\hat{\psi}_{\rm H}(\mathbf{x},t)}{\partial t}|\Psi_0\rangle\theta(t'-t) \ .\end{aligned}$$

By considering the equations of motion in the Heisenberg picture

$$i\hbar\frac{\partial}{\partial t}\hat{\psi} = [\hat{\psi},\hat{H}] \ , \tag{11.103}$$

we can write

$$\begin{aligned}i\frac{\partial}{\partial t}G(\mathbf{x},t,\mathbf{x}',t') &= \langle\Psi_0|\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')|\Psi_0\rangle\delta(t-t') \\ &- \langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\hat{\psi}_{\rm H}(\mathbf{x},t)|\Psi_0\rangle\,(-\delta(t-t')) \\ &+ (-i)\langle\Psi_0|[\hat{\psi}_{\rm H}(\mathbf{x},t),\hat{H}]\hat{\psi}^+_{\rm H}(\mathbf{x}',t')|\Psi_0\rangle\theta(t-t')\hbar^{-1} \\ &- (-i)\langle\Psi_0|\hat{\psi}^+_{\rm H}(\mathbf{x}',t')[\hat{\psi}_{\rm H}(\mathbf{x},t),\hat{H}]|\Psi_0\rangle\theta(t'-t)\hbar^{-1} \ .\end{aligned}$$

The first two terms can be written as anti-commutator between $\hat{\psi}$ and $\hat{\psi}^+$

$$\langle\Psi_0|\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t') + \hat{\psi}^+_{\rm H}(\mathbf{x}',t')\hat{\psi}_{\rm H}(\mathbf{x},t)|\Psi_0\rangle = \langle\Psi_0|\left\{\hat{\psi}_{\rm H}(\mathbf{x},t),\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\right\}|\Psi_0\rangle = \delta(\mathbf{x}-\mathbf{x}')\,. \quad (11.104)$$

By considering the commutators between hamiltonian and field operators written above we have

$$\begin{aligned} i\frac{\partial}{\partial t}\,G(\mathbf{x},t,\mathbf{x}',t') &= \delta(\mathbf{x}-\mathbf{x}')\delta(t-t') + \hat{h}(\mathbf{x})\langle\Psi_0|\hat{\mathbb{T}}[\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')]|\Psi_0\rangle(-i)\hbar^{-1} \\ &+ \langle\Psi_0|\hat{\mathbb{T}}\left[[\hat{\psi}_{\rm H}(\mathbf{x},t),H_1]\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\right]|\Psi_0\rangle(-i)\hbar^{-1}\ , \end{aligned} \quad (11.105)$$

where, as usual, $\hat{\mathbb{T}}$ indicates the time-ordering operator.

The factor at the second term is the definition of one-body Green's function, therefore

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{h}(\mathbf{x})\right]G(\mathbf{x},t,\mathbf{x}',t') = \hbar\delta(\mathbf{x}-\mathbf{x}')\delta(t-t') - i\langle\Psi_0|\hat{\mathbb{T}}\left[[\hat{\psi}_{\rm H}(\mathbf{x},t),\hat{H}_1]\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\right]|\Psi_0\rangle\ . \quad (11.106)$$

By considering Eq. (11.100) the last term can be written as

$$\begin{aligned} &\langle\Psi_0|\hat{\mathbb{T}}\left[\int d^3y\,\hat{\psi}^+_{\rm H}(\mathbf{y},t)\hat{V}(\mathbf{x},\mathbf{y})\hat{\psi}_{\rm H}(\mathbf{y},t)\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\right]|\Psi_0\rangle \\ = &\int d^3y\,\hat{V}(\mathbf{x},\mathbf{y})\langle\Psi_0|\hat{\mathbb{T}}\left[\hat{\psi}_{\rm H}(\mathbf{y},t)\hat{\psi}_{\rm H}(\mathbf{x},t)\hat{\psi}^+_{\rm H}(\mathbf{y},t)\hat{\psi}^+_{\rm H}(\mathbf{x}',t')\right]|\Psi_0\rangle \\ = &\int d^3y\,\hat{V}(\mathbf{x},\mathbf{y})(i)^2G(\mathbf{y},t,\mathbf{x},t,\mathbf{y},t,\mathbf{x}',t')\ , \end{aligned} \quad (11.107)$$

where the definition of the two-body Green's function has been used. The ambiguity in the choice of the time to be associated to $\mathbf{y}$ and $\mathbf{x}$ is clarified by considering that the three field operators, depending on these variables, are part of a single block defined at the time t. The equation of motion can be written as

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{h}(\mathbf{x})\right]G(\mathbf{x},t,\mathbf{x}',t') = \hbar\delta(\mathbf{x}-\mathbf{x}')\delta(t-t') + i\int d^3y\,\hat{V}(\mathbf{x},\mathbf{y})G(\mathbf{y},t,\mathbf{x},t,\mathbf{y},t,\mathbf{x}',t')\ . \quad (11.108)$$

For a system of non-interacting particles $\hat{V}(\mathbf{x},\mathbf{y}) = 0$ therefore we can write

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{h}(\mathbf{x})\right]G^0(\mathbf{x},t,\mathbf{x}',t') = \hbar\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')\ . \quad (11.109)$$

This expression shows that, for a system of non interacting particles, the Green's function defined in this chapter coincide with the resolvent of the Schrödinger equation [Mes61], as it has been defined in Chapter 6.

The integral expression of the equation of motion (11.108) is

$$G(\mathbf{x},t,\mathbf{x}',t') = G^0(\mathbf{x},t,\mathbf{x}',t') + \frac{i}{\hbar}\int d^3y\,d^3z\,G^0(\mathbf{x},t,\mathbf{y},t)\,\hat{V}(\mathbf{y},\mathbf{z})\,G(\mathbf{z},t,\mathbf{y},t,\mathbf{z},t,\mathbf{x}',t')\ . \quad (11.110)$$

A test of the validity of this expression can be done by inserting it in Eq. (11.108) and, by using Eq. (11.109).

The equation of motion of the one-body Green's function contains the two-body Green's function in both its differential (11.108) or integral (11.110) expressions. In general, it is possible to define a n-body Green's function as

$$\begin{aligned} &(i)^nG_n(\mathbf{x}_1,t1,\cdots,\mathbf{x}_n,t_n;\mathbf{x}'_1,t'_1,\cdots,\mathbf{x}'_n,t'_n) \\ \equiv &\frac{\langle\Psi_0|\hat{\mathbb{T}}\left[\hat{\psi}_{\rm H}(\mathbf{x}_1,t_1)\cdots\hat{\psi}_{\rm H}(\mathbf{x}_n,t_n)\hat{\psi}^+_{\rm H}(\mathbf{x}'_1,t'_1)\cdots\hat{\psi}^+_{\rm H}(\mathbf{x}'_n,t'_n)\right]|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}\ . \end{aligned} \quad (11.111)$$

The equation of motion for a n body Green's function requires the information on the $n+1$ body Green's function.

$$\begin{aligned}
&\left[i\hbar\frac{\partial}{\partial t_1} - h(\mathbf{x}_1)\right] G_n(\mathbf{x}_1, t_1, \cdots, \mathbf{x}_n, t_n; \mathbf{x}'_1, t'_1, \cdots, \mathbf{x}'_n, t'_n) \\
= \;& \hbar\sum_{i=1}^{n} \delta(\mathbf{x}_1 - \mathbf{x}_i)\delta(t_1 - t_i)(-1)^{n-i} G_{n-1}(\mathbf{x}_1, t_1, \cdots, \mathbf{x}_{n-1}, t_{n-1}; \mathbf{x}'_1, t'_1, \cdots, \mathbf{x}'_{n-1}, t'_{n-1}) \\
+ \;& i\int d^3y\, \hat{V}(\mathbf{x}, \mathbf{y}) G_{n+1}(\mathbf{x}_1, t_1, \cdots, \mathbf{x}_{n+1}, t_{n+1}; \mathbf{x}'_1, t'_1, \cdots, \mathbf{x}'_{n+1}, t'_{n+1}) \ . \qquad (11.112)
\end{aligned}$$

This is a system of coupled equations connecting Green's functions with different numbers of particles.

This problem is very difficult to solve since it is necessary to have the information on a Green's function of a number of particles larger than that one is interested. The problem is formulated with a set of equations which become always more complicated. If it would be possible to break the hierarchy by making an assumption on the n-body Green's function, then one could calculate the Green's functions with a smaller number of particles. From the operative point of view is in any case a very complicated procedure, and normally it is preferred to use a pertubative procedure such as that described in Chapter 12.

Chapter 12

Perturbative description of the Green's function

The perturbation theory developed in Chapter 6 can be used for the calculation of the Green's functions. We first consider the case of the one-body Green's function and then, at the end of the chapter, the two-body Green's function.

We recall some relations presented in Sect. 11.1.3.

$$\begin{aligned}
\hat{U}(t,0) &= e^{-\frac{i}{\hbar}\hat{H}_1 t} \;;\; \hat{U}(0,t) = e^{\frac{i}{\hbar}\hat{H}_1 t} && (12.1)\\
\hat{\mathcal{O}}_{\rm H}(t) &= e^{\frac{i}{\hbar}\hat{H}_1 t}\hat{\mathcal{O}}_{\rm I}(t)e^{-\frac{i}{\hbar}\hat{H}_1 t} = \hat{U}(0,t)\hat{\mathcal{O}}_{\rm I}\hat{U}(t,0) && (12.2)\\
|\Psi_{\rm H}\rangle &= |\Psi_{\rm I}(0)\rangle = |\Psi_{\rm S}(0)\rangle = \hat{U}_\epsilon(0,-\infty)|\Phi_0\rangle = |\Psi_0\rangle \;. && (12.3)
\end{aligned}$$

where $\hat{\mathcal{O}}$ is a generic operator, and the meanings of the other symbols is the same as those used in Chapter 6.

We express the expectation value of an operator $\hat{\mathcal{O}}$ in the Heisenberg picture by exploiting the technique of the adiabatic switch on of the interaction

$$\begin{aligned}
\frac{\langle\Psi_0|\hat{\mathcal{O}}_{\rm H}(t)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} &= \lim_{\epsilon\to 0}\frac{\langle\Phi_0|\hat{U}_\epsilon(+\infty,0)\left[\hat{U}_\epsilon(0,t)\hat{\mathcal{O}}_{\rm I}(t)\hat{U}_\epsilon(t,0)\right]\hat{U}_\epsilon(0,-\infty)|\Phi_0\rangle}{\langle\Phi_0|\hat{U}_\epsilon(\infty,-\infty)|\Phi_0\rangle}\\
&= \lim_{\epsilon\to 0}\frac{\langle\Phi_0|\hat{U}_\epsilon(+\infty,t)\hat{\mathcal{O}}_{\rm I}(t)\hat{U}_\epsilon(t,-\infty)|\Phi_0\rangle}{\langle\Phi_0|\hat{U}_\epsilon(+\infty,-\infty)|\Phi_0\rangle} \;.
\end{aligned}$$

Since

$$\begin{aligned}
&\hat{U}_\epsilon(+\infty,t)\,\hat{\mathcal{O}}_{\rm I}(t)\,\hat{U}_\epsilon(t,-\infty) =\\
&\sum_{n=0}^{\infty}(-i)^n\frac{1}{n!}\int_t^\infty dt_1\cdots\int_t^\infty dt_n\, e^{-\epsilon(|t_1|+\cdots|t_n|)}\,\hat{\mathbb{T}}\left[\hat{H}_{{\rm I},1}(t_1)\cdots\hat{H}_{{\rm I},1}(t_n)\right]\hat{\mathcal{O}}_{\rm I}(t)\\
&\sum_{m=0}^{\infty}(-i)^m\frac{1}{m!}\int_{-\infty}^t dt'_1\cdots\int_{-\infty}^t dt_m\, e^{-\epsilon(|t'_1|+\cdots|t'_m|)}\,\hat{\mathbb{T}}\left[\hat{H}_{{\rm I},1}(t'_1)\cdots\hat{H}_{{\rm I},1}(t'_m)\right] \;, \qquad (12.4)
\end{aligned}$$

we can rewrite the one-body Green's function as

$$iG(x,y) = \sum_{\mu=0}^{\infty}(-i)^\mu\frac{1}{\mu!}\int_{-\infty}^\infty dt_1\cdots\int_{-\infty}^\infty dt_\mu\,\frac{\langle\Phi_0|\hat{\mathbb{T}}\left[\hat{H}_{{\rm I},1}(t_1)\cdots\hat{H}_{{\rm I},1}(t_\mu)\hat{\psi}_I(x)\hat{\psi}^+_{\rm I}(y)\right]|\Phi_0\rangle}{\langle\Phi_0|\hat{U}(\infty,-\infty)|\Phi_0\rangle} \;, \qquad (12.5)$$

where we used the symbol $x \equiv (\mathbf{x}, t_x)$, and analogously for y. In the above expression we have already carried out the limit for $\epsilon \to 0$. Furthermore, we have considered that $\hat{H}_1$ is hermitian, therefore the expression (12.4) is valid for both $\hat{\mathcal{O}}_{\rm I}(t)$ and for $\hat{\mathcal{O}}^+_{\rm I}(t)$.

We consider an instantaneous interaction

$$\hat{\mathcal{U}}(x,x') \equiv \hat{V}(\mathbf{x},\mathbf{x}')\delta(t-t') \ , \tag{12.6}$$

therefore we can express the perturbative term of the hamiltonian as

$$\hat{H}_{\rm I,1}(t,t') = \frac{1}{2}\int d^3x \int d^3x' \hat{\psi}^+_{\rm I}(x)\hat{\psi}^+_{\rm I}(x')\hat{V}(\mathbf{x},\mathbf{x}')\delta(t-t')\hat{\psi}_{\rm I}(x')\hat{\psi}_{\rm I}(x) \ . \tag{12.7}$$

The numerator of Eq. (12.5) can be expressed as

$$\begin{aligned} iG^{\rm num}(x,y) &= \langle\Phi_0|\hat{\mathbb{T}}\left[\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)\right]|\Phi_0\rangle \\ + \quad (-i)\int_{-\infty}^{\infty} dt_1 \langle\Phi_0|\hat{\mathbb{T}}\left[\hat{H}_{\rm I,1}(t_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)\right]|\Phi_0\rangle + \cdots \ , \end{aligned}$$

The first term of this expression is the one-body Green's function of a system of non-interacting particles, which we call G^0. The presence of $\delta(t_1 - t_1')$ allows us to insert an integral on t_1'. Therefore, we can write

$$\begin{aligned} iG^{\rm num}(x,y) &= iG^0(x,y) + (-i)\int_{-\infty}^{\infty} dt_1 \langle\Phi_0|\hat{\mathbb{T}}\Big[\frac{1}{2}\int d^3x_1 \int d^3x_1' \hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x_1') \\ &\quad \hat{V}(\mathbf{x}_1,\mathbf{x}_1')\delta(t_1-t_1')\hat{\psi}_{\rm I}(x_1')\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)\Big]|\Phi_0\rangle + \cdots \\ &= iG^0(x,y) \\ &+ (-i)\frac{1}{2}\int d^4x_1 \int d^4x_1' \, V(\mathbf{x}_1,\mathbf{x}_1')\delta(t_1-t_1') \\ &\quad \langle\Phi_0|T\left[\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x_1')\hat{\psi}_{\rm I}(x_1')\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)\right]|\Phi_0\rangle + \cdots \ . \end{aligned} \tag{12.8}$$

The evaluation of the above equation is done by using the techniques presented in the Chapter 6. In order to use the Wick's theorem it is necessary to define the contraction between two field operators. This is quite straightforward since the field operators can be expressed in terms of creation and destruction operators. We have shown that for these operators the anti-commutation properties are preserved in each picture. In the specific case of the interaction picture we have

$$\hat{a}_{{\rm I},k}(t) = \hat{a}_k e^{-i\omega_k t} \ ; \ \hat{a}^+_{{\rm I},k}(t) = \hat{a}^+_k e^{i\omega_k t} \ . \tag{12.9}$$

The field operators are expressed in terms of creation and destruction operators as

$$\hat{\psi}^+_{\rm I}(x) = \sum_k \phi^*_k(\mathbf{x})\hat{a}^+_{{\rm I},k} \ ; \ \hat{\psi}_{\rm I}(x) = \sum_k \phi_k(\mathbf{x})\hat{a}_{{\rm I},k} \ . \tag{12.10}$$

where the $\phi_k(\mathbf{x})$ is a single-particle wave function. We can express the contraction as

$$\begin{aligned} \hat{\psi}^+_{\rm I}(x)\hat{\psi}_{\rm I}(y) &= \sum_k\sum_{k'} \phi^*_k(\mathbf{x})\phi_{k'}(\mathbf{y})\hat{a}^+_{{\rm I},k}(t_x)\hat{a}_{{\rm I},k'}(t_y) \\ &= \sum_k\sum_{k'} \phi^*_k(\mathbf{x})e^{-i\omega_k t_x}\phi_{k'}(\mathbf{y})e^{i\omega_{k'}t_y}\hat{a}^+_k\hat{a}_{k'} \\ &= \sum_k\sum_{k'} \phi^*_k(\mathbf{x})e^{-i\omega_k t_x}\phi_{k'}(\mathbf{y})e^{i\omega_{k'}t_y}\left\{\hat{\mathbb{T}}[\hat{a}^+_k\hat{a}_{k'}] - \hat{\mathbb{N}}[\hat{a}^+_k\hat{a}_{k'}]\right\} \\ &= \hat{\mathbb{T}}[\hat{\psi}^+_{\rm I}(x)\hat{\psi}_{\rm I}(y)] - \hat{\mathbb{N}}[\hat{\psi}^+_{\rm I}(x)\hat{\psi}_{\rm I}(y)] \ , \end{aligned}$$

therefore

$$\begin{aligned}
& \overline{\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}}(y) = \langle\Phi_0|\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)|\Phi_0\rangle \\
= \; & \langle\Phi_0|\hat{\mathbb{T}}[\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)]|\Phi_0\rangle - \langle\Phi_0|\hat{\mathbb{N}}[\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)]|\Phi_0\rangle \\
= \; & \langle\Phi_0|\hat{\mathbb{T}}[\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)]|\Phi_0\rangle = iG^0(x,y) \ . \qquad (12.11)
\end{aligned}$$

The calculation of Eq. (12.8) requires the use of the Wick's theorem, therefore the calculation of contractions which, as we have shown above, can be expressed in terms of unperturbed Green's function. This means that the Green's function of an interacting system can be expressed as perturbative expansion in terms of Green's functions of non-interacting particles.

12.1 Goldstone-Feynman diagrams

We consider the perturbative expansion (12.8) of the numerator of the one-body Green's function truncated at the first order

$$\begin{aligned}
& iG^{(1),\rm num}(x,y) = iG^0(x,y) + \\
& (-i)\frac{1}{2}\int d^4x_1 \int d^4x'_1 \, \hat{\mathcal{U}}(x_1,x'_1)\langle\Phi_0|\hat{\mathbb{T}}\left[\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)\right]|\Phi_0\rangle \ .
\end{aligned}$$

Let's apply the Wick's theorem

$$\begin{aligned}
& \langle\Phi_0|\hat{\mathbb{T}}\left[\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)\right]|\Phi_0\rangle \qquad (12.12) \\
= \; & \langle\Phi_0|\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)|\Phi_0\rangle \\
+ \; & \langle\Phi_0|\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)|\Phi_0\rangle \\
+ \; & \langle\Phi_0|\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)|\Phi_0\rangle \\
+ \; & \langle\Phi_0|\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)|\Phi_0\rangle \\
+ \; & \langle\Phi_0|\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)|\Phi_0\rangle \\
+ \; & \langle\Phi_0|\hat{\psi}^+_{\rm I}(x_1)\hat{\psi}^+_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x_1)\hat{\psi}_{\rm I}(x)\hat{\psi}^+_{\rm I}(y)|\Phi_0\rangle \ .
\end{aligned}$$

In terms of unperturbed Green's function the above equation can be written as

$$\begin{aligned}
& iG^{(1),\rm num}(x,y) = iG^0(x,y) + (-i)\frac{1}{2}\int d^4x_1 \int d^4x'_1 \, \hat{\mathcal{U}}(x_1,x'_1) \\
\Big\{ \; & [iG^0(x,y)][-iG^0(x_1,x_1)][-iG^0(x'_1,x'_1)] \\
- \; & [iG^0(x,y)][-iG^0(x_1,x'_1)][-iG^0(x'_1,x_1)] \\
+ \; & [-iG^0(x,x_1)][-iG^0(x_1,x'_1)][iG^0(x'_1,y)] \\
- \; & [-iG^0(x,x_1)][-iG^0(x'_1,x'_1)][iG^0(x_1,y)] \\
+ \; & [-iG^0(x,x'_1)][-iG^0(x'_1,x_1)][iG^0(x_1,y)] \\
- \; & [-iG^0(x,x'_1)][-iG^0(x_1,x_1)][iG^0(x'_1,y)] \; \Big\} \ . \qquad (12.13)
\end{aligned}$$

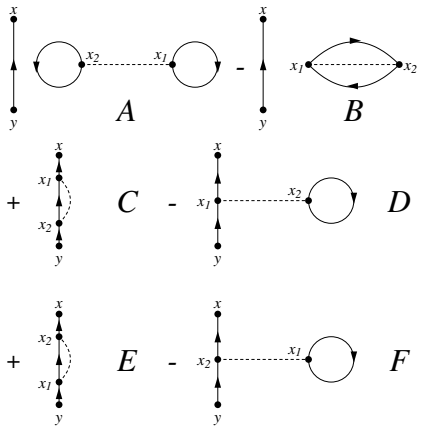

Figure 12.1:

Also in this case the use of a graphical representation is convenient. The unperturbed one-body Green's function $G^0(x, y)$ is represented by an oriented line going from y to x, since $t_x > t_y$. The interaction is represented by a dashed line. The various terms of the perturbative expansion (12.13) are described by the diagrams presented in Fig. 12.1.

The A and B terms of Fig. 12.1 are sub-units composed by unlinked diagrams. The numerator of the Green's function can be described as indicated in Fig. 12.2, i.e. by the product of two blocks of different kinds of diagrams. The first kind is composed by all the linked diagrams containing the points x and y. These diagrams are represented in the left bracket of the figure and they are multiplied by those contained in the right bracket where the x and y points do not appear. This latter set of terms is identical to that

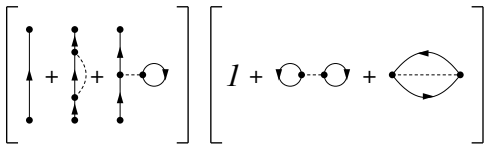

Figure 12.2:

of the denominator which does not contain the x and y points. For this reason the Green's function can be expressed only in terms of linked diagrams containing the x e y coordinates. Diagrams topologically equal, for example C and E as well as D and F, in Fig. 12.1, give identical contribution.

The one-body Green's function in configuration space depends on two coordinated. For translationally invariant systems it is convenient to use the Fourier transform of this function, defined in the momentum-energy space, since it depends on a single, four-dimensional, variable.

$$G(x,y) = \frac{1}{(2\pi)^4}\int d^4k\, e^{ik\cdot(x-y)}\tilde{G}(\mathbf{k},\omega) \ , \tag{12.14}$$

$$\tilde{G}(k) = \int d^4(x-y)\, e^{-ik\cdot(x-y)}G(x,y) \ . \tag{12.15}$$

where we defined $d^4k \equiv d^3k\, d\omega$ and $k\cdot x = \omega t \ - \mathbf{k}\cdot\mathbf{x}$. We obtain an analogous expression for G^0.

For instantaneous interactions depending only on the difference between the coordinates of the two interacting particles, we obtain

$$\hat{\mathcal{U}}(x,y) = \frac{1}{(2\pi)^4}\int d^4k\, e^{-ik\cdot(x-y)}\tilde{\hat{\mathcal{U}}}(k) = \frac{1}{(2\pi)^3}\int d^3k\, e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\tilde{\hat{V}}(\mathbf{k})\delta(t_x - t_y) \ . \tag{12.16}$$

By inserting these definitions in the expression of the Green's function it is possible to define the Fourier transform of expressions which can be viewed as Goldstone-Feynman diagrams. The interesting feature of this representation in momentum space is that the momentum is conserved at each vertex.

12.2 Dyson's equation and Self-energy

The expression (12.5) indicates that the Green's function of the interacting system is composed by the unperturbed Green's function plus all the linked diagrams which can be inserted between the coordinates x e y. The mathematical expression of the above observation is

$$G(x,y) = G^0(x,y) + \int d^4x_1 \int d^4x_1'\, G^0(x,x_1)\underline{\hat{\Sigma}}(x_1,x_1')G^0(x_1',y) \ , \tag{12.17}$$

which defines the quantity $\underline{\hat{\Sigma}}$ called **self-energy**.

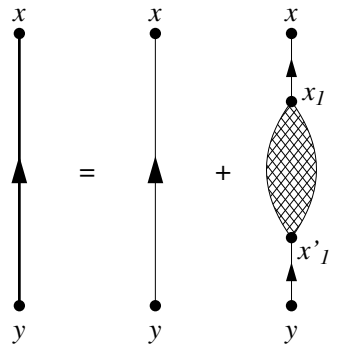

Figure 12.3: Graphical representation of the self-energy.

The graphical representation of this expression is given in Fig. 12.3. The thicker oriented line indicates the Green's function G of the interacting system, while the thinner lines indicates the Green's function G^0 of the non-interacting system. The blob represents the self-energy $\underline{\hat{\Sigma}}$.

From the point of view of the calculation it is more convenient to use the proper self-energy. In the perturbative expansions there are diagrams which can be separated by cutting a line representing G^0. For

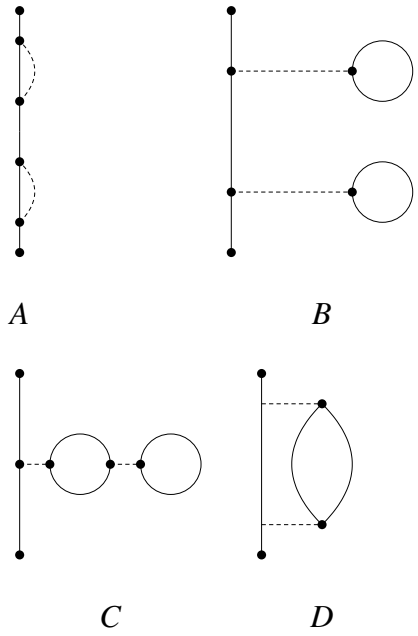

Figure 12.4: The proper insertions of the interaction lines are those of the C and D diagrams.

example, these are the diagrams A and B of Fig. 12.4. There are diagrams which cannot be separated in autonomous parts, as example the C and D diagrams of the figure.

The **proper self-energy** is defined as the sum of all the diagrams which cannot be separated. Clearly the self-energy can be obtained by summing all the possible proper self-energy insertions. In Fig. 12.5 the blob with two sets of dashed lines indicates the full self-energy, while the blobs with a set of single dashed lines the proper self-energies. The mathematical expression of this idea is expressed as

$$\underline{\hat{\Sigma}}(x_1,x_1') = \hat{\Sigma}(x_1,x_1') + \int d^4x_2 \int d^4x_2'\, \hat{\Sigma}(x_1,x_2)G^0(x_2,x_2')\hat{\Sigma}(x_2',x_1')$$
$$+ \int d^4x_2 \int d^4x_2' \int d^4x_3 \int d^4x_3'\, \hat{\Sigma}(x_1,x_2)G^0(x_2,x_2')\hat{\Sigma}(x_2',x_3)G^0(x_3,x_3')\hat{\Sigma}(x_3',x_1') + \cdots \ .$$

By inserting this definition of proper self-energy in Eq. (12.17) we obtain

$$G(x,y) = G^0(x,y) + \int d^4x_1 \int d^4x_1'\, G^0(x,x_1)\hat{\Sigma}(x_1,x_1')G^0(x_1',y)$$
$$+ \int d^4x_1 \int d^4x_1' \int d^4x_2 \int d^4x_2'\, G^0(x,x_1)\hat{\Sigma}(x_1,x_1')G^0(x_1',x_2)\hat{\Sigma}(x_2,x_2')G^0(x_2',y)$$
$$+ \cdots \ . \tag{12.18}$$

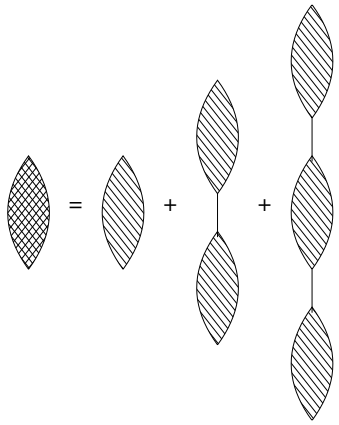

Figure 12.5: The self-energy can be rewritten as a sum of terms of proper self-energy insertions.

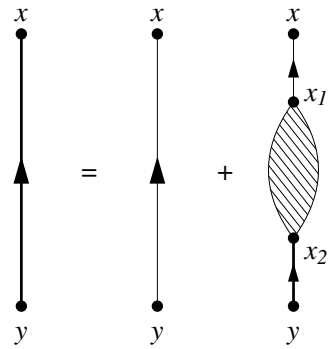

Figure 12.6: Graphical representation of the Dyson's equation.

This expression can be written as

$$G(x,y) = G^0(x,y) + \int d^4x_1 \int d^4x_1' \, G^0(x,x_1)\hat{\Sigma}(x_1,x_1')G(x_1',y) \ . \tag{12.19}$$

and it is known in the literature as **Dyson's equation**. Its graphical representation is shown in Fig. 12.6.

In this equation it is possible to carry out perturbative expansion of both Green's function and also of the self-energy. The possibility is evident for the Green's function. For $\hat{\Sigma}$, it is worth to consider the C diagram of Fig. 12.4. In this diagram the first order in the interaction contains a single loop; the complete diagrams is at the second order.

The Dyson's equation assumes a simpler expression when it is referred to a infinite and homogeneous system of fermions. In this case, we can define

$$G(x,y) = \frac{1}{(2\pi)^4}\int d^4k e^{-ik\cdot(x-y)}\tilde{G}(k) \ \text{ and } \ \hat{\Sigma}(x,y) = \frac{1}{(2\pi)^4}\int d^4k e^{-ik\cdot(x-y)}\tilde{\hat{\Sigma}}(k) \ . \tag{12.20}$$

By inserting these expressions in the Dyson's equation (12.19), and by using the conservation of the four-momentum k, we obtain

$$G(x,y) = \frac{1}{(2\pi)^4}\int d^4k e^{-ik\cdot(x-y)}\left[\tilde{G}^0(k) + \tilde{G}^0(k)\tilde{\hat{\Sigma}}(k)\tilde{G}(k)\right] \ , \tag{12.21}$$

therefore, the expression of the Dyson's equation in momentum space is

$$\tilde{G}(k) = \left[\tilde{G}^0(k) + \tilde{G}^0(k)\tilde{\hat{\Sigma}}(k)\tilde{G}(k)\right] \ , \tag{12.22}$$

from which

$$\tilde{G}(k) = \frac{\tilde{G}^0(k)}{1-\tilde{G}^0(k)\tilde{\hat{\Sigma}}(k)} = \frac{1}{[\tilde{G}^0(k)]^{-1} - \tilde{\hat{\Sigma}}(k)} \ . \tag{12.23}$$

Since

$$\tilde{G}^0(\mathbf{k},\omega) = \left[\frac{\Theta(k-k_{\rm F})}{\omega-\omega_k+i\eta} + \frac{\Theta(k_{\rm F}-k)}{\omega-\omega_k-i\eta}\right] \ , \tag{12.24}$$

we obtain

$$[\tilde{G}^0(k)]^{-1} = \omega - \omega_k \ , \tag{12.25}$$

and then

$$\tilde{G}(k) = \frac{1}{\omega-\omega_k-\tilde{\hat{\Sigma}}(k)} \ . \tag{12.26}$$

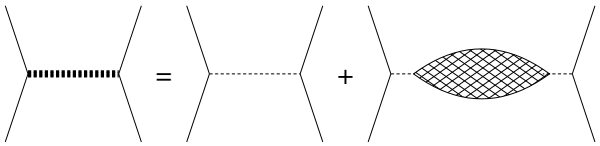

Figure 12.7:

In analogy to what we have done to obtain the Dyson's equation we can treat the interaction. Fig. 12.7 shows how it is possible to consider the interaction between two generic particle, or hole, lines by defining the *polarization operator* $\underline{\hat{\Pi}}$

$$\hat{u}(x,y) = \hat{u}_0(x,y) + \int d^4x_1 \int d^4x_1' \, \hat{u}_0(x,x_1)\underline{\hat{\Pi}}(x_1,x_1')\hat{u}_0(x_1',y) \ . \tag{12.27}$$

The above equation indicates that the interaction between two particles in the medium is composed by the *bare* interaction, that in vaccuum $\hat{u}_0$, plus all the terms related to the medium polarization, which we describe in terms of virtual particle-hole excitations. The polarization operator $\underline{\hat{\Pi}}$ contains all these excitations.

We present in Fig. 12.8 two of the possible diagrams contained in the polarization operator $\underline{\hat{\Pi}}$. The diagram A belongs to the kind of diagrams defined as proper diagrams since they cannot be separated by cutting an interaction line. The diagram B has three interaction lines, but it is possible to cut the second line and separate it in proper diagrams.

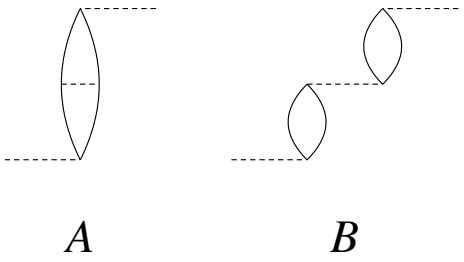

Figure 12.8:

In analogy to what we have done for the self-energy, we can describe the interaction in terms of proper diagrams, by defining a *proper polarization operator* $\hat{\underline{\Pi}}$ as the one containing only proper diagrams

$$\begin{aligned}
&\hat{\underline{\Pi}}(x_1,x_1') = \hat{\Pi}(x_1,x_1') + \int d^4x_2 \int d^4x_2'\, \hat{\Pi}(x_1,x_2)\hat{u}_0(x_2,x_2')\hat{\Pi}(x_2',x_1') \\
+ &\int d^4x_2 \int d^4x_2' \int d^4x_3 \int d^4x_3'\, \hat{\Pi}(x_1,x_2)\hat{u}_0(x_2,x_2')\hat{\Pi}(x_2',x_3)\hat{u}_0(x_3,x_3')\hat{\Pi}(x_3',x_1') + \cdots \\
= &\hat{\Pi}(x_1,x_1') + \int d^4x_2 \int d^4x_2'\, \hat{\Pi}(x_1,x_2)\hat{u}_0(x_2,x_2')\hat{\underline{\Pi}}(x_2',x_1') \ . \qquad (12.28)
\end{aligned}$$

Therefore

$$\begin{aligned}
\hat{u}(x,y) &= \hat{u}_0(x,y) + \int d^4x_1 \int d^4x_1'\, \hat{u}_0(x,x_1)\hat{\Pi}(x_1,x_1')\hat{u}_0(x_1',y) \\
&+ \int d^4x_1 \int d^4x_1' \int d^4x_2 \int d^4x_2'\, \hat{u}_0(x,x_1)\hat{\Pi}(x_1,x_2)\hat{u}_0(x_2,x_2')\hat{\Pi}(x_2',x_1')\hat{u}_0(x_1',y) + \cdots \\
&= \hat{u}_0(x,y) + \int d^4x_1 \int d^4x_1'\, \hat{u}_0(x,x_1)\hat{\Pi}(x_1,x_1')\hat{u}(x_1',y) \ . \qquad (12.29)
\end{aligned}$$

which is the analogous of the Dyson's equation for the interaction.

Also in this case, for translational invariant systems, therefore infinite and homogeneous, it is convenient to define the Fourier transforms of $\hat{u}$ and $\hat{\underline{\Pi}}$ which we indicate simply by inserting the dependence on the four-vector k:

$$\hat{u}(k) = \hat{u}_0(k) + \hat{u}_0(k)\hat{\underline{\Pi}}(k)\hat{u}_0(k) \qquad (12.30)$$

$$\hat{u}(k) = \hat{u}_0(k) + \hat{u}_0(k)\hat{\Pi}(k)\hat{u}(k) \ . \qquad (12.31)$$

From the second equation, above, we obtain an expression for $\hat{u}(k)$

$$\hat{u}(k) = \frac{\hat{u}_0(k)}{1 - \hat{u}_0(k)\hat{\Pi}(k)} \equiv \frac{\hat{u}_0(k)}{\hat{\mathcal{K}}(k)} \quad , \qquad (12.32)$$

where the last expression defines the dielectric function $\hat{\mathcal{K}}$ which modifies the bare interaction $\hat{u}_0$ for the presence of the medium.

12.3 Hartree - Fock

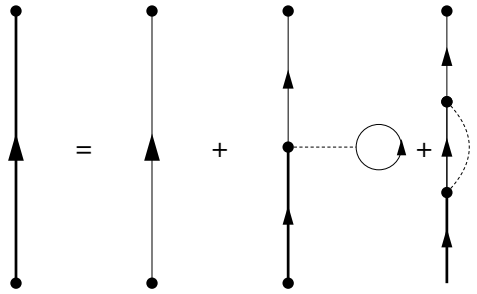

Figure 12.9: First order of the perturbation expansion of the Green's function described in terms of the Dyson's equation.

The first step to the solution of the Dyson's equation (12.19) consists in considering only the insertion of a single interaction line. Diagrammatically this approximation is described in Fig. 12.9. A slightly

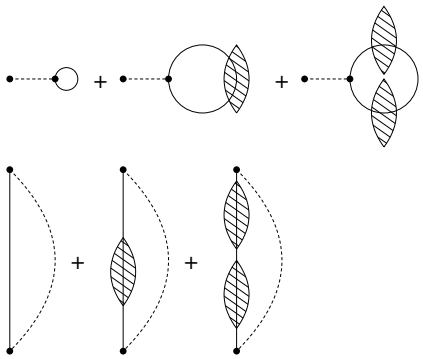

Figure 12.10: Self-energy insertions in the diagrams of Fig. 12.9.

more elaborated approximation consists in considering all the possible self-energy insertions in the Green's function lines of the two terms of Fig. 12.9. The results of this infinite number of self-energy insertions is graphically represented in Fig. 12.11.

Let's consider the Dyson's equation (12.19)

$$G(x,y) = G^0(x,y) + \int d^4x_1 \int d^4x_1' G^0(x,x_1)\hat{\Sigma}(x_1,x_1')G(x_1',y) \ .$$

In the approximation presented in Fig. 12.9 the self-energy can be expressed as

$$\hbar\hat{\Sigma}^{(I)}(x_1,x_1') = -i\left[\delta^4(x_1-x_1')\int d^4x_2 \hat{\mathcal{U}}(x_1,x_2)G^0(x_2,x_2) - \hat{\mathcal{U}}(x_1,x_1')G^0(x_1,x_1')\right] \ . \qquad (12.33)$$

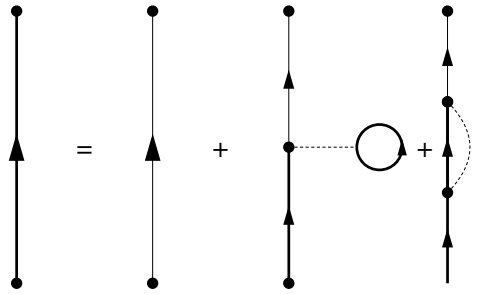

Figure 12.11: Representation of the HF approximation in the Dyson's equation.

and, in the approximationn of Fig. 12.11 as

$$\hbar\hat{\Sigma}^{(II)}(x_1,x_1') = -i\left[\delta^4(x_1-x_1')\int d^4x_2\hat{\mathcal{U}}(x_1,x_2)G(x_2,x_2) - \hat{\mathcal{U}}(x_1,x_1')G(x_1,x_1')\right] \ . \tag{12.34}$$

The HF approximation does not include diagrams such as those presented in Fig. 12.12. As usual, the hamiltonian $\hat{H}$ has been separated in $\hat{H}_0$ and $\hat{H}_1$. The unperturbed Green's function G^0 is defined with respect to the $\hat{H}_0$ eigensates. If the hamiltonian $\hat{H}$ is time independent, the interaction $\hat{\mathcal{U}}$ can be written as:

$$\hat{\mathcal{U}}(x_1,x_1') = \hat{V}(\mathbf{x}_1,\mathbf{x}_1')\delta(t_1-t_1') \ .$$

We define the Fourier transforms about the time variable

$$G(\mathbf{x}t,\mathbf{x}'t') = \frac{1}{2\pi}\int d\omega e^{-i\omega(t-t')}\tilde{G}(\mathbf{x},\mathbf{x}',\omega) \ , \tag{12.35}$$

$$G^0(\mathbf{x}t,\mathbf{x}'t') = \frac{1}{2\pi}\int d\omega e^{-i\omega(t-t')}\tilde{G}^0(\mathbf{x},\mathbf{x}',\omega) \ , \tag{12.36}$$

$$\hat{\Sigma}(\mathbf{x}t,\mathbf{x}'t') = \hat{\Sigma}(\mathbf{x},\mathbf{x}')\delta(t-t') = \frac{1}{2\pi}\int d\omega e^{-i\omega(t-t')}\hat{\Sigma}(\mathbf{x},\mathbf{x}') \ . \tag{12.37}$$

The Dyson's equation in mixed representation is

$$\tilde{G}(\mathbf{x},\mathbf{y},\omega) = \tilde{G}^0(\mathbf{x},\mathbf{y},\omega) + \int d^3x_1\int d^3x_1'\,\tilde{G}^0(\mathbf{x},\mathbf{x}_1,\omega)\hat{\Sigma}(\mathbf{x}_1,\mathbf{x}_1')\tilde{G}(\mathbf{x}_1',\mathbf{y},\omega) \ . \tag{12.38}$$

In the approximation (II) the self-energy becomes

$$\begin{aligned}&\hbar\hat{\Sigma}^{(II)}(x_1,x_1') = \hbar\hat{\Sigma}^{(II)}(\mathbf{x}_1,\mathbf{x}_1')\delta(t_1-t_1') = -i\delta(t_1-t_1')\\ &\times\left[\delta^3(\mathbf{x}_1-\mathbf{x}_1')\int d^4x_2\hat{V}(\mathbf{x}_1-\mathbf{x}_2)\frac{1}{2\pi}\int d\omega e^{-i\omega(t_2-t_2^+)}\tilde{G}(\mathbf{x}_2,\mathbf{x}_2,\omega)\right.\\ &\left.-\hat{V}(\mathbf{x}_1-\mathbf{x}_1')\frac{1}{2\pi}\int d\omega e^{-i\omega(t_1-t_1^+)}\tilde{G}(\mathbf{x}_1,\mathbf{x}_1',\omega)\right] \ .\end{aligned} \tag{12.39}$$

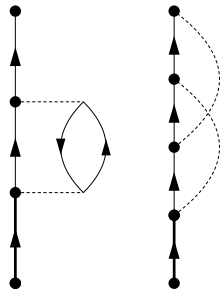

Figure 12.12: Example of diagrams not contained in the HF approximation.

In the above equation $t^+ > t$. We shall use this property to properly define the step function.
As usual, the symbol $\phi_j^0(\mathbf{r})$ is used to indicate the single particle wave functions of the one-body hamiltonian $\hat{H}_0$

$$\hat{H}_0 = \sum_j h_j \ ; \ \hat{h}_j \phi_j^0(\mathbf{r}) = \left[-\frac{\hbar^2 \nabla^2}{2m} + \hat{\mathcal{W}}(\mathbf{r}) \right] \phi_j^0(\mathbf{r}) = \epsilon_j \phi_j^0(\mathbf{r}) \ , \tag{12.40}$$

where $\hat{\mathcal{W}}(\mathbf{r})$ is the MF potential. We use the basis formed by these single-particle states to express the field operators in the interaction picture

$$\hat{\psi}_{\rm I}(\mathbf{x},t) = \sum_k \hat{a}_{{\rm I},k}(t) \phi_k^0(\mathbf{x}) \ ; \ \hat{\psi}_{\rm I}^+(\mathbf{x},t) = \sum_k \hat{a}_{{\rm I},k}^+(t) (\phi_k^0(\mathbf{x}))^* \ . \tag{12.41}$$

Therefore

$$\begin{aligned}
& iG^0(\mathbf{x}t,\mathbf{x}'t') = \langle \Phi_0 | \hat{\mathbb{T}} \left[\hat{\psi}_{\rm I}(\mathbf{x},t) \hat{\psi}_{\rm I}^+(\mathbf{x}',t') \right] | \Phi_0 \rangle \\
& = \langle \Phi_0 | \sum_k \hat{a}_k e^{-i\omega_k t} \phi_k^0(\mathbf{x}) \sum_{k'} \hat{a}_{k'}^+ e^{i\omega_{k'} t'} (\phi_{k'}^0(\mathbf{x}'))^* | \Phi_0 \rangle \Theta(t-t') \Theta(\omega_k - \epsilon_{\rm F}) \\
& - \langle \Phi_0 | \sum_{k'} \hat{a}_{k'}^+ e^{i\omega_{k'} t'} (\phi_{k'}^0(\mathbf{x}'))^* \sum_k \hat{a}_k e^{-i\omega_k t} \phi_k^0(\mathbf{x}) | \Phi_0 \rangle \Theta(t'-t) \Theta(\epsilon_{\rm F} - \omega_k) \\
& = \sum_k \phi_k^0(\mathbf{x}) (\phi_k^0(\mathbf{x}'))^* e^{-i\omega_k (t-t')} \left[\Theta(t-t') \Theta(\omega_k - \epsilon_{\rm F}) - \Theta(t'-t) \Theta(\epsilon_{\rm F} - \omega_k) \right] \ ,
\end{aligned} \tag{12.42}$$

where we defined $\omega_k = \epsilon_k/\hbar$, and used

$$\langle \Phi_0 | \hat{a}_k \hat{a}_{k'}^+ | \Phi_0 \rangle = \delta_{k'k} \Theta(\omega_k - \epsilon_{\rm F}) \ ; \ \langle \Phi_0 | \hat{a}_{k'}^+ \hat{a}_k | \Phi_0 \rangle = \delta_{k'k} \Theta(\epsilon_{\rm F} - \omega_k) \ . \tag{12.43}$$

By considering the integral representation of $\Theta(t-t')$, see Eq. (11.45), we obtain

$$\tilde{G}^0(\mathbf{x},\mathbf{x}',\omega) = \sum_k \phi_k^0(\mathbf{x}) (\phi_k^0(\mathbf{x}'))^* \left[\frac{\Theta(\epsilon_k - \epsilon_{\rm F})}{\omega - \omega_k + i\eta} + \frac{\Theta(\epsilon_{\rm F} - \epsilon_k)}{\omega - \omega_k - i\eta} \right] \ . \tag{12.44}$$

With the ϕ^0 obtained from Eq. (12.40), we can calculate the G^0 which can be used to activate an iterative procedure implying the Dyson's equation (12.38) and the self-energy equation (12.39).
It possible to search for G an expression analogous to that of Eq. (12.44) where the ϕ^0 are substituted by generic ϕ eigenstates of a new hamiltonian and related to the previous single-particle wave functions by a unitary transformation (see the discussion in Sect. 9.2.2). The Green's function has the following expression

$$\tilde{G}(\mathbf{x},\mathbf{x}',\omega) = \sum_k \phi_k(\mathbf{x}) \phi_k^*(\mathbf{x}') \left[\frac{\Theta(\epsilon_k - \epsilon_{\rm F})}{\omega - \omega_k + i\eta} + \frac{\Theta(\epsilon_k - \epsilon_{\rm F})}{\omega - \omega_k - i\eta} \right] \ . \tag{12.45}$$

By inserting this expression in Eq. (12.39) we encounter integrals of the type

$$\frac{1}{2\pi i}\int d\omega \frac{e^{i\omega|t-t^+|}}{\omega-\omega_k+i\eta}=0 \;\; ; \;\; \frac{1}{2\pi i}\int d\omega \frac{e^{i\omega|t-t^+|}}{\omega-\omega_k-i\eta}=\Theta(-|t-t^+|) \;\; , \tag{12.46}$$

therefore we obtain the expressions

$$\hat{\Sigma}^{(II)}(x_1,x_1')=\hat{\Sigma}^{(II)}(\mathbf{x}_1,\mathbf{x}_1')\delta(t_1-t_1') \tag{12.47}$$

$$\begin{aligned}\hbar\hat{\Sigma}^{(II)}(\mathbf{x}_1,\mathbf{x}_1') &= -i\Big[\delta^3(\mathbf{x}_1-\mathbf{x}_1')\int d^3x_2\hat{V}(\mathbf{x}_1-\mathbf{x}_2)i\sum_k \phi_k(\mathbf{x}_2)\phi_k^*(\mathbf{x}_2)\Theta(\epsilon_{\rm F}-\epsilon_k)\\ &-i\hat{V}(\mathbf{x}_1-\mathbf{x}_1')\sum_k\phi_k(\mathbf{x}_1)\phi_k^*(\mathbf{x}_1')\Theta(\epsilon_{\rm F}-\epsilon_k)\Big]\\ &= \delta^3(\mathbf{x}_1-\mathbf{x}_1')\int d^3x_2\hat{V}(\mathbf{x}_1-\mathbf{x}_2)\rho(\mathbf{x}_2)-\hat{V}(\mathbf{x}_1-\mathbf{x}_1')\sum_k\phi_k(\mathbf{x}_1)\phi_k^*(\mathbf{x}_1')\Theta(\epsilon_{\rm F}-\epsilon_k) \;\; ,\end{aligned} \tag{12.48}$$

where we used the expression of the expression of the density in the MF model

$$\rho(\mathbf{x})=\sum_k^{\epsilon_{\rm F}}\phi_k(\mathbf{x})\phi_k^*(\mathbf{x}) \;\; . \tag{12.49}$$

We define the operator

$$\hat{\mathcal{L}}\equiv\hbar\omega-\hat{H}_0=\hbar\omega+\frac{\hbar^2\nabla^2}{2m}-\hat{\mathcal{W}}(\mathbf{x}) \;\; , \tag{12.50}$$

and we apply it to the unperturbed Green's function

$$\begin{aligned}\hat{\mathcal{L}}\,\tilde{G}^0(\mathbf{x}_1,\mathbf{x}_1',\omega) &= \sum_k(\hbar\omega-\epsilon_k^0)\phi_k^0(\mathbf{x}_1)\phi_k^{0,*}(\mathbf{x}_1')\left[\frac{\Theta(\epsilon_k^0-\epsilon_{\rm F}^0)}{\omega-\omega_k+i\eta}+\frac{\Theta(\epsilon_{\rm F}^0-\epsilon_k^0)}{\omega-\omega_k-i\eta}\right]\\ &= \hbar\sum_k\phi_k^0(\mathbf{x}_1)\phi_k^{0,*}(\mathbf{x}_1')\left[\Theta(\epsilon_k^0-\epsilon_{\rm F}^0)+\Theta(\epsilon_{\rm F}^0-\epsilon_k^0)\right]=\hbar\delta^3(\mathbf{x}_1-\mathbf{x}_1') \;\; ,\end{aligned} \tag{12.51}$$

where we used the completeness of the ϕ^0, and $\omega_k=\epsilon_k^0/\hbar$. The previous expression indicates that the action of the operator $\hat{\mathcal{L}}$ is analogous to the multiplication by $(\tilde{G}^0)^{-1}$. I apply this operator to the Dyson's equation

$$\begin{aligned}\hat{\mathcal{L}}\,\tilde{G}(\mathbf{x}_1,\mathbf{x}_1',\omega) &= \hat{\mathcal{L}}\,\tilde{G}^0(\mathbf{x}_1,\mathbf{x}_1',\omega)+\int d^3x_2\int d^3x_2'\,\hat{\mathcal{L}}\,\tilde{G}^0(\mathbf{x}_1,\mathbf{x}_2,\omega)\hat{\Sigma}(\mathbf{x}_2,\mathbf{x}_2')\,\tilde{G}(\mathbf{x}_2',\mathbf{x}_1',\omega)\\ &= \hbar\delta^3(\mathbf{x}_1-\mathbf{x}_1')+\int d^3x_2'\hat{\Sigma}(\mathbf{x}_1,\mathbf{x}_2')\,\tilde{G}(\mathbf{x}_2',\mathbf{x}_1',\omega) \;\; .\end{aligned} \tag{12.52}$$

By making explicit the expression of $\hat{\mathcal{L}}$ we obtain

$$\begin{aligned}&\left[\hbar\omega+\frac{\hbar^2\nabla_1^2}{2m}-\hat{\mathcal{W}}(\mathbf{x}_1)\right]\sum_k\phi_k(\mathbf{x}_1)\phi_k^*(\mathbf{x}_1')\left[\frac{\Theta(\epsilon_k-\epsilon_{\rm F})}{\omega-\omega_k+i\eta}+\frac{\Theta(\epsilon_{\rm F}-\epsilon_k)}{\omega-\omega_k-i\eta}\right]\\ &= \hbar\delta^3(\mathbf{x}_1-\mathbf{x}_1')+\int d^3\mathbf{x}_2\,\hat{\Sigma}(\mathbf{x}_1,\mathbf{x}_2)\sum_k\phi_k(\mathbf{x}_2)\phi_k^*(\mathbf{x}_1')\left[\frac{\Theta(\epsilon_k-\epsilon_{\rm F})}{\omega-\omega_k+i\eta}+\frac{\Theta(\epsilon_{\rm F}-\epsilon_k)}{\omega-\omega_k-i\eta}\right]\end{aligned} \tag{12.53}$$

By multiplying by $\phi_j(\mathbf{x}_1')$ and integrating on $\mathbf{x}_1'$, for the orthonormality properties of the ϕ_k the sum disappear and we obtain the equation

$$\begin{aligned}&\left[\hbar\omega+\frac{\hbar^2\nabla_1^2}{2m}-\hat{\mathcal{W}}(\mathbf{x}_1)\right]\phi_j(\mathbf{x}_1)\left[\frac{\Theta(\epsilon_j-\epsilon_{\rm F})}{\omega-\omega_j+i\eta}+\frac{\Theta(\epsilon_{\rm F}-\epsilon_j)}{\omega-\omega_j-i\eta}\right]\\ &= \hbar\phi_j(\mathbf{x}_1)+\int d^3\mathbf{x}_2\,\hat{\Sigma}(\mathbf{x}_1,\mathbf{x}_2)\phi_j(\mathbf{x}_2)\left[\frac{\Theta(\epsilon_j-\epsilon_{\rm F})}{\omega-\omega_j+i\eta}+\frac{\Theta(\epsilon_{\rm F}-\epsilon_j)}{\omega-\omega_j-i\eta}\right] \;\; .\end{aligned} \tag{12.54}$$

By multiplying by $\omega - \omega_j \equiv \omega - \epsilon_j/\hbar$ we obtain

$$\left[-\frac{\hbar^2\nabla_1^2}{2m} + \hat{\mathcal{W}}(\mathbf{x}_1)\right]\phi_j(\mathbf{x}_1) + \int d^3\mathbf{x}_2'\,\hat{\Sigma}(\mathbf{x}_1,\mathbf{x}_2')\phi_j(\mathbf{x}_2) = \epsilon_j\phi_j(\mathbf{x}_1)\ , \tag{12.55}$$

and by inserting Eq. (12.48)

$$\begin{aligned}&\left[-\frac{\hbar^2\nabla_1^2}{2m} + \hat{\mathcal{W}}(\mathbf{x}_1)\right]\phi_j(\mathbf{x}_1) + \int d^3\mathbf{x}_2\,\hat{V}(\mathbf{x}_1-\mathbf{x}_2)\rho(\mathbf{x}_2)\phi_j(\mathbf{x}_1)\\ -\ &\int d^3\mathbf{x}_2\,\hat{V}(\mathbf{x}_1-\mathbf{x}_2)\sum_k \phi_k(\mathbf{x}_1)\phi_k^*(\mathbf{x}_2)\phi_j(\mathbf{x}_2)\Theta(\epsilon_{\rm F}-\epsilon_k) = \epsilon_j\phi_j(\mathbf{x}_1)\ .\end{aligned} \tag{12.56}$$

which is the traditional form of expressing the HF equations, (see Sect. 9.2.2).

12.4 Bethe-Salpeter equation

In the calculation of the Green's function with the Dyson equation as indicate in Fig. 12.13, each single term of the perturbative sum remains finite only if the potential remains finite. In general, the presence of a strongly repulsive core in the bare interaction between two particles makes each term of the sum much greater than the value which has to be evaluated. This is the same kind of problem discussed in Chapter 8 for the calculation of the energy of the system, tackled by using the Bruekner's theory.

Each thin line of Fig. 12.13 indicates the Green's function G^0, which can be described in terms of single-particle wave functions ϕ_k, as indicated by the Eqs. (12.44) and (12.45). This means that each intersection between a dashed and a continuous line implies the product $\hat{V}\phi_k$ between microscopic interaction and unperturbed wave function. As discussed in Chapter 8 this product is not finite for potentials going to infinity. By using a strategy analogous to that presented in Chapt. 8, we build an effective interaction by summing an infinite set of diagrams such as the product $\hat{V}^{\rm eff}\phi_k$ is finite.

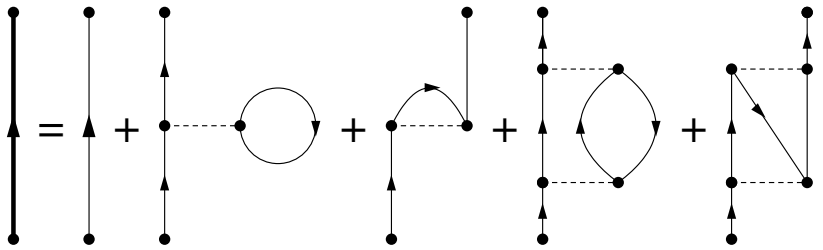

Figure 12.13:

We consider all the interactions linking the particle lines. This approximation, called of *ladder diagrams* is presented, for the first three terms in Fig. 12.14. We remark that the *ladder approximation* sums all the, infinite, interaction terms linked to the particle line. This restriction is necessary since in the interaction process the fermion modifies its state. Since the hole states are all occupied the use of the particle state avoids problems with the Pauli exclusion principle.

We consider the interaction term between two particles as represented by the diagrams in the higher part of Fig. 12.15, and indicate it as $\hat{\Sigma}_{\rm L}$ where with sub-index L, we indicate the ladder approximation.

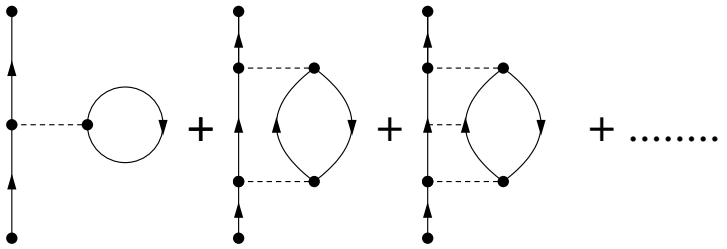

Figure 12.14:

The expression of the interaction can be written as

$$\begin{aligned}
&\hat{\Sigma}_{\rm L}(x_1,x_1') = \hat{u}(x_1,x_1') + \hat{u}(x_1,x_1')\int d^4x_2 \int d^4x_2'\, G^0(x_1,x_2)\hat{u}(x_2,x_2')G^0(x_2',x_1') \\
+ \quad & \hat{u}(x_1,x_1')\int d^4x_2 \int d^4x_2' \int d^4x_3 \int d^4x_3' \\
& G^0(x_1,x_2)\hat{u}(x_2,x_2')G^0(x_2,x_3)\hat{u}(x_3,x_3')G^0(x_3',x_2')G^0(x_2',x_1') + \cdots \\
= \quad & \hat{u}(x_1,x_1')\Big\{1 + \int d^4x_2 \int d^4x_2'\, G^0(x_1,x_2)\hat{u}(x_2,x_2')\Big[1 + \\
& \int d^4x_3 \int d^4x_3' G^0(x_2,x_3)\hat{u}(x_3,x_3')\Big(1+\cdots\Big)G^0(x_3',x_2')\Big]G^0(x_2',x_1')\Big\} \ . \qquad (12.57)
\end{aligned}$$

The above expression iterates the same integration kernel. By considering the expansion at all the orders, we obtain the expression

$$\hat{\Sigma}_{\rm L}(x_1,x_1') = \hat{u}(x_1,x_1')\left[1 + \int d^4x_2 \int d^4x_2'\, G^0(x_1,x_2)\hat{\Sigma}_{\rm L}(x_2,x_2')G^0(x_2',x_1')\right] \ , \qquad (12.58)$$

whose graphical representation is given by the diagrams of the lower part of Fig. 12.15. Eq. (12.58) is known as **Bethe-Salpeter equation** even though, in reality, is the ladder approximation of the Bethe-Salpeter equation.

Also in this equation there are products between the microscopic, bare, potential $\hat{u}$ and the non-interacting Green's function G^0. However, these terms are multiplied by $\hat{\Sigma}_{\rm L}$ which make the integrand finite.

The above the Bethe-Salpeter equation is expressed in terms of G^0, but it is possible to use a G obtained by a HF calculation.

12.5 Random Phase Approximation

It is possible to formulate an equation similar to the Dyson's equation (12.19) also for the two-body Green's function. We consider here only the two-body Green's functions describing the time evolution of a particle-hole pair. For this situation, the analogous to the Dyson's equation is:

$$\begin{aligned}
& G(x_1,x_2,x_3,x_4) = G^0(x_1,x_2,x_3,x_4) \\
+ \quad & \int d^4y_1\, d^4y_2\, d^4y_3\, d^4y_4\, G^0(x_1,x_2,y_1,y_2)\underline{\hat{\mathcal{K}}}(y_1,y_2,y_3,y_4)G^0(y_3,y_4,x_3,x_4) \ , \qquad (12.59)
\end{aligned}$$

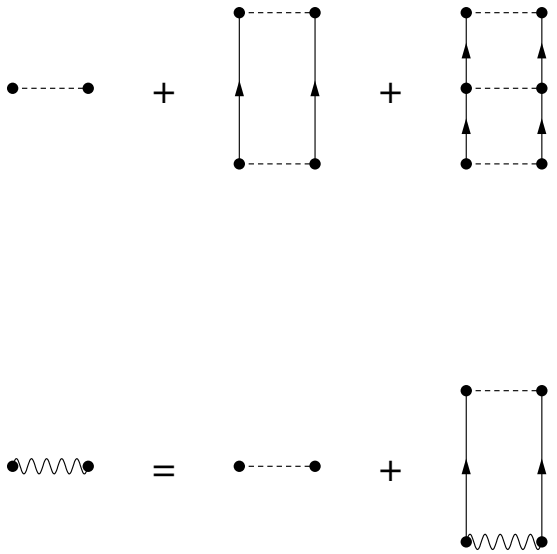

Figure 12.15:

where the term $\underline{\hat{\mathcal{K}}}$ contains all the linked diagrams which can be inserted between particle and hole lines.

Also in this case it is possible to define proper, irreducible, diagrams. In Fig. 12.17 the diagram A is reducible since it is possible to cut the external particle and hole lines generating two diagrams already present in the perturbative expansion of the two-body Green's function. On the contrary, this is not possible for the B diagram which is called irreducible, or proper. By considering the insertion of only proper diagrams Eq. (12.59) can be formally rewritten as

$$\begin{aligned} & G(x_1,x_2,x_3,x_4) = G^0(x_1,x_2,x_3,x_4) \\ + & \int d^4y_1\, d^4y_2\, d^4y_3\, d^4y_4\, G^0(x_1,x_2,y_1,y_2)\hat{\mathcal{K}}(y_1,y_2,y_3,y_4)G(y_3,y_4,x_3,x_4) \ , \end{aligned} \tag{12.60}$$

where the kernel $\hat{\mathcal{K}}$ contains the insertion of all the irreducible diagrams.

The Random Phase Approximation (RPA) consists in considering, in the previous equation, instead of the $\hat{\mathcal{K}}$ the interaction $\hat{u}$ depending only by two coordinates

$$\hat{\mathcal{K}}^{\rm RPA}(y_1,y_2,y_3,y_4) = \hat{u}(y_1,y_4)\left[\delta(y_1-y_2)\delta(y_3-y_4) - \delta(y_1-y_3)\delta(y_2-y_4)\right] \ , \tag{12.61}$$

therefore

$$\begin{aligned} G^{\rm RPA}(x_1,x_2,x_3,x_4) &= G^0(x_1,x_2,x_3,x_4) \\ &+ \int d^4y_1\, d^4y_2\, G^0(x_1,x_2,y_1,y_1)\hat{u}(y_1,y_2)G^{\rm RPA}(y_2,y_2,x_3,x_4) \\ &- \int d^4y_1\, d^4y_2\, G^0(x_1,x_2,y_1,y_2)\hat{u}(y_1,y_2)G^{\rm RPA}(y_1,y_2,x_3,x_4) \ , \end{aligned} \tag{12.62}$$

where we separated the direct and the exchange terms. The graphical representation of the above equation is given Fig. 12.19.

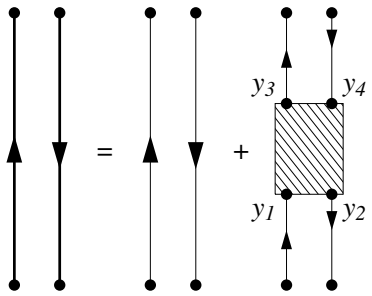

Figure 12.16: Graphical representation of Eq. (12.59). The dashed part represents the kernel $\overline{\mathscr{K}}$.

Let's consider the expression of the two-body Green's function in Lehmann representation Eq. (11.79). Since $|\Psi_n\rangle$ and $\langle\Psi_n|$ indicate the same excited state the terms

$$\langle\Psi_0|a_{k_1}a^+_{k_2}|\Psi_n\rangle\langle\Psi_n|a_{k_3}a^+_{k_4}|\Psi_0\rangle \ ,$$

imply

$$\delta_{k_2,k_3}\theta(k_2-k_F)\delta_{k_4,k_1}\theta(k_4-k_F) \ .$$

For this reason it is possible to define the Fourier transforms of the two-body Green's function, and also of the interaction kernel, depending on two momenta

$$G(x_1,x_2,x_3,x_4) = (2\pi)^{-8}\int d^4k_1\, d^4k_2 e^{-ik_1(x_1-x_4)}e^{ik_2(x_2-x_3)}\tilde{G}(k_1,k_2) \ , \tag{12.63}$$

$$\hat{\mathscr{K}}(x_1,x_2,x_3,x_4) = (2\pi)^{-8}\int d^4k_1\, d^4k_2 e^{-ik_1(x_1-x_4)}e^{ik_2(x_2-x_3)}\tilde{\hat{\mathscr{K}}}(k_1,k_2) \ . \tag{12.64}$$

By inserting these definitions in Eq. (12.60), and using the RPA assumption (12.62) on the kernel, we obtain an expression of the Dyson's equation for the RPA in momentum space. A long calculation, even though does not present difficulties, shows that by considering the direct term only of Eq. (12.62), the equation assumes a purely algebraic aspect

$$\tilde{G}^{\mathrm{RPA,D}}(k_1,k_2) = \tilde{G}^0(k_1,k_2) + \tilde{G}^0(k_1,k_2)\tilde{\hat{U}}(k_1-k_2=q)\tilde{G}^{\mathrm{RPA,D}}(k_1,k_2) \ . \tag{12.65}$$

The exchange term cannot be factorized in a simple algebraic expression.

By considering only the direct term, the RPA assumes the so-called ring diagrams approximation, and the expression of the two-body Green's function in this approximation is

$$\tilde{G}^{\mathrm{RPA,D}}(k_1,k_1+q) = \tilde{G}^0(k_1,k_1+q) + \tilde{G}^0(k_1,k_1+q)\tilde{\hat{U}}(q)\tilde{G}^{\mathrm{RPA,D}}(k_1,k_1+q) \tag{12.66}$$

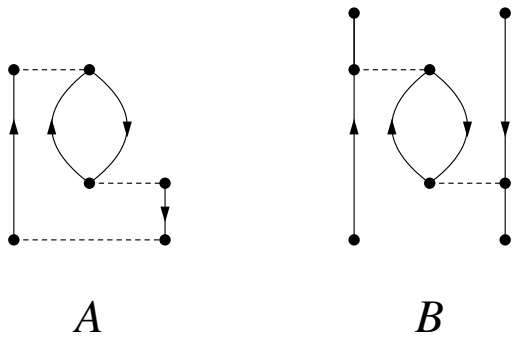

Figure 12.17: The A diagram is reducible while the B diagram is irreducible (proper).

$$\tilde{G}^{\mathrm{RPA,D}}(k_1, k_1+q)\left[1-\tilde{G}^0(k_1, k_1+q)\tilde{\hat{U}}(q)\right] = \tilde{G}^0(k_1, k_1+q) \tag{12.67}$$

$$\tilde{G}^{\mathrm{RPA,D}}(k_1, k_1+q) = \frac{\tilde{G}^0(k_1, k_1+q)}{1-\tilde{G}^0(k_1, k_1+q)\tilde{\hat{U}}(q)} \tag{12.68}$$

This expression is commonly used to calculated the linear response to an external probe for infinite fermion systems.

The RPA obtained by using the two-body Green's function seems to be a completely different theory with respect that presented in Chapter 10. As it has been done for HF theory, also in this case it is possible to obtain the RPA formulae presented in Chapter 10 starting from Eq. (12.62). The calculation is quite long and cumbersome. The key point which allows the identification of the two-formulations of the RPA is the following correspondences between the X and Y RPA amplitudes of Sect. 10.3.2 and the transition amplitudes of the two-body Green's function in Lehmann representation Eq. (11.79). The relations are:

$$X_{mi} = \langle\Psi_0|\hat{a}_m\hat{a}_i^+|\Psi_n\rangle \quad ; \quad X^*_{mi} = \langle\Psi_n|\hat{a}_i\hat{a}_m^+|\Psi_n\rangle \tag{12.69}$$

$$Y_{mi} = \langle\Psi_0|\hat{a}_i\hat{a}_m^+|\Psi_n\rangle \quad ; \quad Y^*_{mi} = \langle\Psi_n|\hat{a}_m\hat{a}_i^+|\Psi_0\rangle \tag{12.70}$$

$$\tag{12.71}$$

where $|\Psi_n\rangle$ and $|\Psi_0\rangle$ are, respectively, RPA excited and ground states.

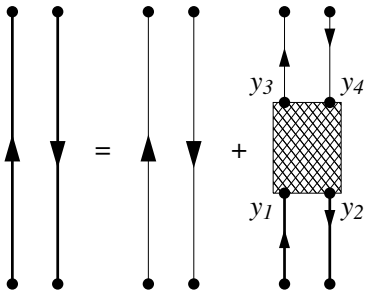

Figure 12.18: Graphical representation of Eq. (12.60). The doubly dashed part represent the proper kernel $\hat{\mathcal{K}}$.

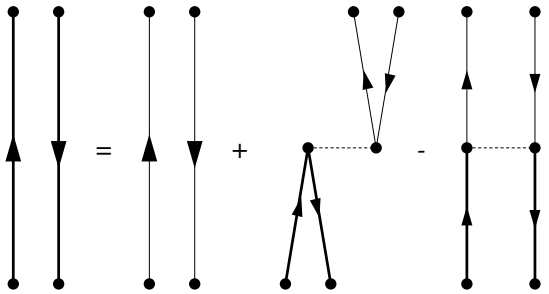

Figure 12.19:

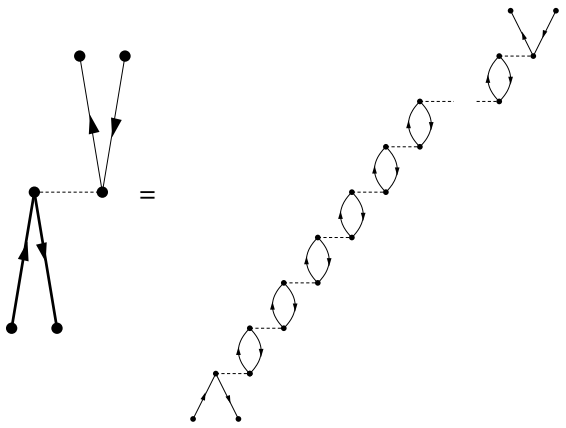

Figure 12.20: Graphical representation of the ring diagrams approximation of the RPA.

Part IV

Theories inspired to Statistical Mechanics

Chapter 13

Correlated Basis Function theory

13.1 Introduction

In the previous chapters we have pointed out that, in the description of many-body systems, a naif application of perturbation theories has to be avoided because of the strongly repulsive core of the bare particle-particle interaction.

In part III, by using language and terminology inspired to Quantum Field Theory, we have shown how this problem can be tackled. The interaction between particles in medium is modified with respect to that in vacuum. The Brueckner's theory, Chapter. 8, is a typical example how to produce this kind of effective interaction which is defined by Eq.(8.2).

A different approach to the many-body problem comes from the Statistical Mechanics. In this case the focus is not on the interaction, but rather on the wave function describing the relative motion of the interacting pair of particles. The situation is exemplified in Fig. 8.1, where ϕ indicates the unperturbed wave function of the two interacting particles whose overlap with the potential produces the large values of the matrix elements which hinder the application of the perturbation theory. By multiplying ϕ by a function, called *correlation function*, which prevents the two particles to get too close, it is possible to avoid the problem of the strongly repulsive core. This is the basic idea of the *Correlated Basis Function* (CBF). The language is completely different from that used in Part III. The treatment is the correlation function.

The starting point of the CBF theory is the search for solutions of the many-body Schrödinger equation by using the variational principle (see Appendix A). The equation to be solved is

$$\delta E[\Psi_{\rm T}] = \delta \frac{<\Psi_{\rm T}|\hat{H}|\Psi_{\rm T}>}{<\Psi_{\rm T}|\Psi_{\rm T}>} = 0 \ , \tag{13.1}$$

where $\hat{H}$ is the hamiltonian describing the system of interacting particles, and $|\Psi_{\rm T}\rangle$ is a many-body trial wave function. In the specific case of the CBF theory, the search for the minimum is carried out on all the wave functions which can be expressed as

$$\Psi_{\rm T}(1,...,A) = F(1,...,A)\Phi(1,....,A) \ , \tag{13.2}$$

where $|\Phi\rangle$ is the state describing the system of non-interacting particles. In the fermionic case $|\Phi\rangle$ is a Slater determinant, while for bosonic systems is a symmetrized product of single particle wave functions.

The second assumption of the theory, usually called Jastrow's anstatz, is that the many-body corre-

lation function F can be written as a product of two-body correlation functions

$$F(1, ..., A) = \prod_{j>i=1}^{A} f(r_{ij}) \ , \tag{13.3}$$

where $\hat{f}(r_{ij})$ is a function of the distance between the i and j particles composing the system.

These assumptions are the same adopted in the VMC approach presented in Sect. 4.2. The difference between these two theories is in methods used to calculate the expectation value of the hamiltonian in Eq. (13.1). In the case of VMC the expectation value is obtained by using the Monte Carlo multidimensional integration techniques, see Chapter 4. In the CBF case it used a cluster expansion proposed by Mayer and Mayer to describe liquids within the traditional statistical Mechanics [May40]. The particles, correlated by the function f, generates clusters. The CBF theory, after a topological study of the various clusters succeed in formulating a set of integral equation which sum in closed form all the clusters of a certain type. For bosonic systems this set of equations is called Hypernetted Chain (HNC). The extension of the theory to the fermionic case is far from being trivial and has been formulated at the beginning of the 70's of the last century [Fan74].

Even though our interest is in fermion systems, we introduce first the CBF theory for the bosonic case where the formulation is simpler and it will be used to clarify the essential points of the theory. After that, we shall discuss the extension to fermionic system which has to account for the Pauli exclusion principle.

13.2 Bosons

Let's consider a system of A bosons, with zero spin for simplicity, contained in a volume $\mathcal{V}$. The thermodynamics limit is obtained by considering both A and $\mathcal{V}$ going to infinity but maintaining finite the particle density $\rho = A/\mathcal{V}$. The system is homogeneous and has translational invariance, therefore the particle density is a constant. The wave function describing this system can be expressed as

$$\Phi(x_1, x_2, \ldots, x_A) = \hat{\mathcal{S}}\Big(\phi_1(x_1) \cdots \phi_A(x_A)\Big) \ , \tag{13.4}$$

where $\hat{\mathcal{S}}$ is an operator which symmetrizes the total wave function for the exchange of two particles. In the previous equation, $\phi_i(x_i)$ indicates the single particle wave functions generated by a translational invariant mean-field model. We called x_i the generalized coordinates of the i-th particle, that is in addition to the space coordinates also spin, and eventually isospin and other quantum numbers which can characterize the particle.

In this description of the system ground state, all the bosons occupy the same single particle state, that of minimal energy. In analogy to the case presented in Sect. 2.3, the single particle wave functions are eigenstates of the momentum $\mathbf{p} = \hbar\mathbf{k}$, and they can be expressed as:

$$\phi_j(x_j) = \frac{1}{\sqrt{\mathcal{V}}} \, e^{i\mathbf{k}_j \cdot \mathbf{r}_j} \ . \tag{13.5}$$

In this case, the generalized coordinate x corresponds to $\mathbf{r}$. The density of the system can be obtained by using the equations (13.4) and (13.5),

$$\rho_0(x) = A\phi^*(x)\phi(x) = \frac{A}{\mathcal{V}} = \rho \ . \tag{13.6}$$

which is a constant, as expected.

As we have already anticipated the idea is to solve the Schrödinger equation by using the variational principle with the trial wave function (13.2) where the correlation function is given by the expression (13.3).

In the calculation of the energy functional (13.1) it is very convenient the use of a quantity called two-body distribution function (TBDF) defined as:

$$\begin{aligned} g(x_1,x_2) &= \frac{A(A-1)\int dx_3\dots dx_A \Psi_{\rm T}^*(x_1,x_2,\dots,x_A)\Psi_{\rm T}(x_1,x_2,\dots,x_A)}{\rho^2\int dx_1dx_2\dots dx_A \Psi_{\rm T}^*(x_1,x_2,\dots,x_A)\Psi_{\rm T}(x_1,x_2,\dots,x_A)} \\ &= \frac{A(A-1)\int dx_3\dots dx_A F^2(x_1,x_2,\dots,x_A)|\Phi(x_1,x_2,\dots,x_A)|^2}{\rho^2\int dx_1dx_2\dots dx_A F^2(x_1,x_2,\dots,x_A)|\Phi(x_1,x_2,\dots,x_A)|^2} \ , \end{aligned} \tag{13.7}$$

where the fact that F is a real scalar function has been used. The expectation value of every two-body operator, such as the interaction, is given by integrating the product of the operator and the TBDF on the two coordinates x_1 e x_2:

$$< \hat{\mathcal{O}} >= \frac{1}{2}\rho^2 \int dx_1dx_2\, g(x_1,x_2)\, \hat{\mathcal{O}}(x_1,x_2) \ . \tag{13.8}$$

The use of the TBDF allows us to separate the evaluation of the many-body effects independently of the operator $\mathcal{O}(x_1,x_2)$ which has to be considered. In case of a bosonic system we have that

$$|\Phi|^2 = \prod_{i=1}^{A}\phi^*(x_i)\phi(x_i) = \frac{\rho_0(x_1)}{A}\frac{\rho_0(x_2)}{A}\cdots\frac{\rho_0(x_A)}{A} = \frac{\rho^A}{A^A} \tag{13.9}$$

where in the last equivalence we used the fact that the system is homogeneous.

By using the equations (13.4), (13.5), (13.6) and the expressions (13.2) and (13.3), the numerator and the denominator of Eq. (13.7) can be written, respectively, as

$$\mathcal{N} = (A-1)\frac{\rho^{A-2}}{A^{A-1}}\int dx_3dx_4...dx_A \prod_{i<j} f^2(r_{ij}) \ , \tag{13.10}$$

where we also included the term $1/\rho^2$, and

$$\mathcal{D} = \frac{\rho^A}{A^A}\int dx_1dx_2...dx_A \prod_{i<j} f^2(r_{ij}) \ . \tag{13.11}$$

The cluster expansion is obtained by defining an new function $h(r_{ij})$

$$f^2(r_{ij}) = 1 + h(r_{ij}) \ . \tag{13.12}$$

and inserting it in the Jastrow's ansatz of the many-body correlation function,

$$\prod_{i<j} f^2(r_{ij}) = \prod_{i<j}(1+h(r_{ij})) = (1+h(r_{12}))(1+h(r_{13}))\cdots(1+h(r_{23}))\cdots \tag{13.13}$$

The cluster expansion consists in grouping the terms containing the same number of h-functions

$$\prod_{i<j} f^2(r_{ij}) = 1 + \sum_{i<j}^{A} h(r_{ij}) + \sum_{i<j,k<l} h(r_{ij})h(r_{kl}) + \cdots \tag{13.14}$$

A convenient method to analyze the structure of the various terms of Eq. (13.14) consists in using the graphical representation introduced by Mayer [May40]. In this representation, the coordinates x which are integrated are called **internal points** and are they are represented by black circles. The h-functions are indicated by dashed lines.

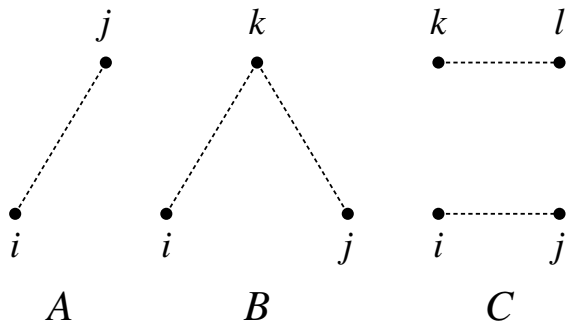

Figure 13.1: Graphical representation of some terms contributing to Eq. (13.15). The dashed lines indicate the h-functions, the black points indicate the internal points which are intergrated.

Let's first consider the denominator $\mathcal{D}$, Eq. (13.11), which can be written as

$$\mathcal{D} = \frac{\rho^A}{A^A} \int dx_1 dx_2 ... dx_A \qquad \Big[1 + \sum_{i<j} h(r_{ij}) + 3 \sum_{i<j<k} h(r_{ik}) h(r_{jk}) + \sum_{i<j<k<l} h(r_{ij}) h(r_{kl}) + \dots \Big] \, . \tag{13.15}$$

The first sum of Eq. (13.15) is represented by the diagram A of Fig. 13.1. A single h-function relating the i and j points.

The second sum of Eq. (13.15) is represented by the diagram B. In this case the point k is shared with the two h-functions of the sum. The total contribution of this term is:

$$\frac{1}{2} \frac{(A-1)(A-2)}{A^2} \rho^3 \int dx_i dx_j dx_k h(r_{ik}) h(r_{jk}) \, , \tag{13.16}$$

where the factor $(A-1)(A-2)$ takes care of the fact that, in the sums, the indexes i, j and k are limited by the condition $i < k < j$.

The third sum of Eq. (13.15) contains two h-functions, as the second one, but these functions involve four different points. The contribution of this term is represented by the C diagram of Fig. 13.1, and it is given by the expression

$$\frac{A!}{4!(A-4)!} \frac{\rho^4}{A^4} \int dx_i dx_j dx_k dx_l h(r_{ij}) h(r_{kl}) \, . \tag{13.17}$$

The global contribution of this equation is given by the product of two separated integrals, a first one on x_i and x_j and a second one on x_k and x_l.

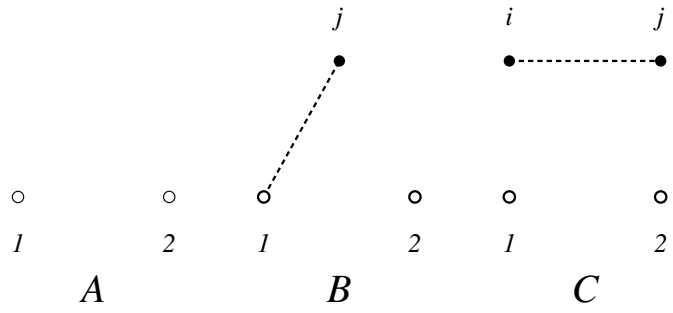

Figure 13.2: Graphical representation of some terms contributing to Eq. (13.18).

Let's consider now the numerator, defined in Eq. (13.10). In this case, there is no integration on two coordinates, which have been identified with the 1 and 2 indexes. In the product of the correlation functions it is convenient to factorize the $f^2(r_{12})$ term outside the integral. By using the expansion (13.12) we obtain the expression

$$\begin{aligned} n &= f^2(r_{12})\frac{(A-1)}{A}\left[1+2\frac{\rho}{A}(A-2)\sum_{j>2}\int dx_j h(r_{1j})\right. \\ &\left. +\frac{(A-2)(A-3)}{2}\frac{\rho^2}{A^2}\sum_{j>i>2}\int dx_i dx_j h(r_{ij})+\ldots\right]. \end{aligned} \tag{13.18}$$

For the description of the numerator a new graphical symbol has to be included. The points 1 and 2 which are not integrated, called **external points**, are indicated by white circles as it is shown in Fig. 13.2, where the terms of lower order in the expansion of Eq. (13.18) are represented.

The uncorrelated term is represented by the A diagram. In the equation a correlation function $f^2(r_{12})$ is present, and it is unserstood in the graphical representation. The B diagram represents the first sum of Eq. (13.18), where the h-function connects an external point with an internal one. Also the second sum of the Eq. (13.18) contains a single h-functions, but, in this case, it connects only internal points. The contribution of this term is represented by the C diagram of Fig. 13.2. The points 1 and 2 can be interchanged and this produces the factor 2 of the second term, and, in general, doubles the contribution of each kind of diagram.

The numerator and denominator of the TBDF (13.7) are expressed by the Eqs. (13.15) and (13.18) as sum of terms characterized by the number of the h-functions and by that of internal and external points. Each term of these sums forms a cluster of particles, linked by the h-functions of the correlation, and it can be described by a diagram.

Let's make a topological classification of the various diagrams.

a) *Linked and unliked diagrams*
From the graphical point of view the unlinked diagrams are easily identified since they are composed by separated parts, as, for example, the diagrams C of Figs. 13.1 and 13.2. From the mathematical point of view, we have already seen that the contribution of this type of diagrams is obtained by multiplying the integrals which describe by the separated parts of the diagrams. For example, for the diagram C of Fig.

13.1 we have that

$$\frac{A!}{4!(A-4)!}\frac{\rho^4}{A^4}\int\int dr_i dr_j dr_k dr_l h(r_{ij})h(r_{kl}) =$$
$$\frac{1}{4!}(1-\frac{6}{A}+\frac{11}{A^2}-\frac{6}{A^3})\rho^2\int dr_i dr_j h(r_{ij})\cdot\rho^2\int dr_k dr_l h(r_{kl}) \quad .$$

The linked diagrams cannot be expressed as products of independent parts, for example the diagram B of Fig.13.1.

The parts of the unlinked diagrams which do not contain the two external points are present in the set of the diagrams of the denominator.

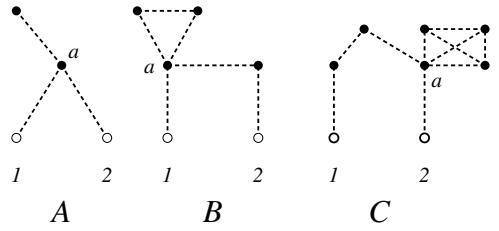

Figure 13.3: Examples of reducible diagrams in the numerator of the TBDF, Eq. (13.18).

b) *Reducible diagrams*
The linked diagrams of Fig.13.3 have the property of being *reducible*. From the graphical point of view these type of diagrams are characterized by the presence of, at least, one internal point linking the part of the diagram containing the external points with a part containing only internal point. For the translational invariance of the system, the contribution of these two parts can be factorized. In bosonic systems the unlinked diagrams and also the reducible ones can be expressed as products of a term containing external points time one, or more, terms containing only internal points.

The factorized part of these diagrams which does not contain external points can be simplified, up to $1/A$ order by the diagrams of the denominator. The proof of this property is presented in Ref. [Fan74].

By summarizing the situation, we can state that in the expression (13.7) of the TBDF, the diagrams of the denominator cancel the factorized contributions of the unlinked and reducible diagrams present in the numerator. For this reason the TBDF can be expressed as sum of linked and irreducible diagrams, all containing the external points 1 and 2:

$$g(r_{12}) = f^2(r_{12})\sum_{\text{all orders}} Y_{irr}(r_{12}) = f^2(r_{12})\left(1+S(r_{12})+C(r_{12})\right) \ . \tag{13.19}$$

The translational invariance of the system implies that the TBDF depends only on the relative distance of the two external points r_{12}.

In Eq. (13.19) we have already made explicit the fact that the irreducible diagrams can be further classified in *simple* and *composite* which have been, respectively, indicated with $S(r_{12})$ and $C(r_{12})$.

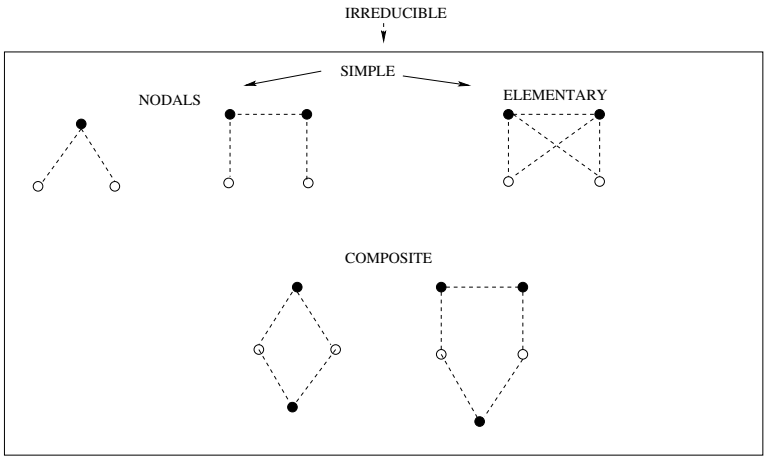

Figure 13.4: Examples of irreducible diagrams, classified as composite and simple. The latter ones are classified as nodal and elementary.

c) *Simple and composite diagrams*
The composite diagrams are formed by parts which are connected only trough the two external points, as indicated in Fig. 13.4. These composite diagrams can be expressed in terms of simple diagrams. Since there is not integration on the external points, the contribution of a composite diagram is given by the product of the simple diagrams connected to the external points.

Let's call $S^2(r_{12})$ the contribution given by the sum of all the composite diagrams formed by the product of only two simple diagrams, as in the case of the composite diagrams of Fig. 13.4. Since the exchange of all the particles of a sub-diagram with those of the other one produces the same composite diagram it is necessary to multiply $S^2(r_{12})$ by a factor $1/2$ to avoid double counting. In the box it is clarified how this $1/2$ factor comes out by considering the diagrams of Fig. (13.5).

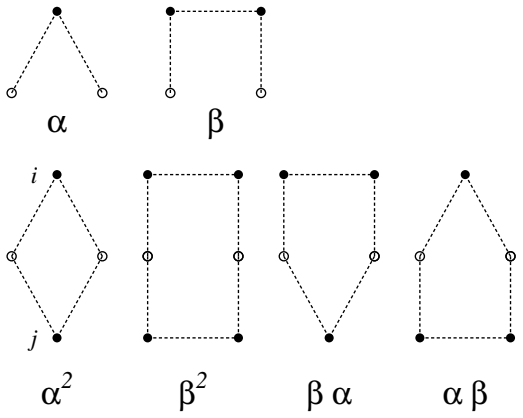

Figure 13.5: Example of formation of composite diagrams starting from simple diagrams.

Let's suppose to build composite diagrams with the two α and β diagrams of Fig. 13.5. The contribution of the diagrams obtained by iterating twice α e β is given by $(\alpha+\beta)^2 = \alpha^2 + \beta^2 + 2\alpha\beta$. The diagrams α^2 and β^2 have symmetry 1/2. In the evaluation of the numerator (13.18) it necessary to insert this factor since by interchanging the i and j indexes one obtains the same contribution. On the other hand, the sums of Eq. (13.18) are limited with $j > i$ and this implies that only one of the two topologically identical terms appears. The same idea is valid for the β^2 diagram. For example the expression for α^2 is

$$\sum_{i>j} \int dx_i h(r_{1i}) h(r_{i2}) \int dx_j h(r_{1j}) h(r_{j2}) = \frac{1}{2} \sum_{i,j} \int dx_i h(r_{1i}) h(r_{i2}) \int dx_j h(r_{1j}) h(r_{j2}) \ .$$

Also the sum in the last two diagrams must be multiplied by 1/2 since the limits on the sums require that only one of the two diagram contributes.

The same reasoning can be repeated for every composite diagram formed by two simple diagrams.

The same procedure can be used to build composite diagrams with n simple diagrams. The symmetry properties used to obtain the 1/2 factor for $S^2(r_{12})$ are valid for each $S^n(r_{12})$ and require the presence of a $1/n!$ factor to avoid double counting. The total sum of the composite diagrams can be expressed in terms of simple diagrams as:

$$C(r_{12}) = \frac{S^2(r_{12})}{2!} + \frac{S^3(r_{12})}{3!} + \frac{S^4(r_{12})}{4!} + \dots \ . \tag{13.20}$$

By using this result, the TBDF, Eq. (13.19), can be rewritten as:

$$\begin{aligned} g(r_{12}) &= f^2(r_{12}) \left[1 + S(r_{12}) + \frac{S^2(r_{12})}{2!} + \frac{S^3(r_{12})}{3!} + \dots \right] \\ &= f^2(r_{12}) \exp[S(r_{12})] \ , \end{aligned} \tag{13.21}$$

where the lst equality appears since the system has an infinite number of particles.

The above equation expresses the TBDF only in terms of simple diagrams which can be classified as nodal or elementary, sometime called bridge, diagrams.

d) *Nodal and elementary (bridge) diagrams*
In a nodal diagram there is at least one point where all the paths going from one external point to the other ones have to pass. These special internal points are called nodes. Diagrams without nodes are called elementary. Some example of nodal and elementary diagrams is presented in Fig. 13.4.

The situation of the calculation of the TBDF can be summarized by stating that there is no contribution of unliked and reducible diagrams, while that of the composite diagrams can be expressed as infinite sum of simple diagrams as indicated by Eq. (13.21). By calling $N(r_{12})$ the contribution of all the nodal diagrams, and $E(r_{12})$ that of the elementary diagrams, the TBDF can be expressed as:

$$g(r_{12}) = f^2(r_{12}) \exp[N(r_{12}) + E(r_{12})] \tag{13.22}$$

$$\begin{aligned} &= [1 + h(r_{12})] [1 + N(r_{12}) + E(r_{12}) + \dots] \\ &= 1 + N(r_{12}) + X(r_{12}) \ . \end{aligned} \tag{13.23}$$

This equation defines the diagrams contained in $X(r_{12})$, which are normally called non-nodal since they do not have nodes.

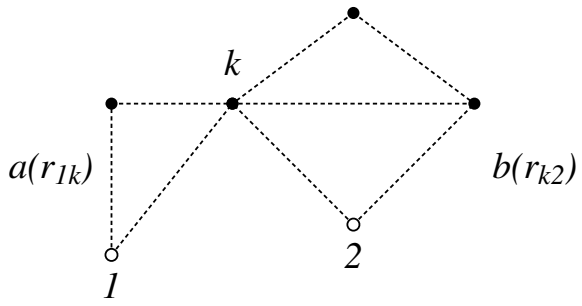

Figure 13.6: Example of nodal diagram. The contribution of the part of the diagram to the left hand side of the node k is called $a(r_{1k})$ and that to the right hand side as $b(r_{k2})$.

A nodal diagram can be considered as composed by parts which are connected in the nodal point. For this reason, each nodal diagram can be obtained by integrating the two, or more, functions representing the contributions of the various parts of the diagram. Let's consider, as example, the nodal diagram of Fig. 13.6 which has 1 and 2 as external points and k as a node. The contributions of the two parts of the diagrams are called $a(r_{1k})$ and $b(r_{k2})$ and the total contribution to the TBDF (13.19) of this diagram is:

$$\int d\mathbf{r}_k a(r_{ik}) b(r_{kj}) \rho(r_k) = \rho \int d\mathbf{r}_k a(r_{ik}) b(r_{kj}) \equiv \Big(a(r_{ik}) \Big| \rho(\mathbf{r}_k) b(r_{kj}) \Big) \ , \tag{13.24}$$

where the density $\rho(\mathbf{r}_k)$ has been associated to the integration point $\mathbf{r}_k$ to have the correct normalization. Because of the homogeneity and the translational invariance property of the bosonic system we are considering the density is constant, therefore it has been factorized outside the integral. The last term defines the symbol $\Big(\Big| \Big)$ which indicate the folding product on the $\mathbf{r}_k$ point.

The global contribution $N(r_{12})$ of all the nodal diagrams between the points 1 and 2 can be obtained as folding product in the node $\mathbf{r}_k$ of all the irreducible diagrams which can be built between 1 and k and between k and 2:

$$N(r_{12}) = \Big(X(r_{1k}) \Big| \rho(\mathbf{r}_k) [N(r_{k2}) + X(r_{k2})] \Big) \ . \tag{13.25}$$

Each nodal diagram has, at least, one node, and every path between the external points 1 and 2 must go through all the nodes of the diagram. The above equation indicates that the part of the diagram between 1 and the first node k, which is a non-nodal diagram, must be folded in $\mathbf{r}_k$ with
i) a non-nodal diagram, and this generates a diagram with a single node,
ii) a nodal diagram, and this produces a diagram with more than one node.
The folding of $N(r_{ik})$ with $N(r_{kj})$ would generate diagrams already present in $N(r_{ij})$ and, therefore, it is not considered.

The set of equations (13.22), (13.23) and (13.25) are known as HyperNetted Chain equations (HNC). Eq. (13.22) expresses the TBDF in terms of simple diagrams by summing, in closed form, the composite diagrams, and Eq. (13.25) calculates the contribution of all the nodal diagrams. No closed expression to calculate the elementary diagrams is available. They have to be included one by one. The calculations of TBDM without the contribution of the of the elementary diagrams are called HNC/0. When the contribution of the simplest elementary diagram, that shown in Fig. 13.4, is included the calculation of the TBDF is named HNC/4, since this diagram involves four particles.

The HNC equation are solved by using an iterative procedure. The input required by the calculation is the correlation function $f(r_{12})$. Starting from the ansatz $N(r_{12}) = E(r_{12}) = 0$, which implies $X(r_{12}) = f^2(r_{12}) - 1$, one obtains a new set of nodal diagrams by using Eq. (13.25). With this new set of nodal diagrams one calculates $g(r_{12})$ with Eq. (13.22) which allows the evaluation of the non-nodal $X(r_{12})$ diagrams by means of Eq. (13.23) which are used again in Eq. (13.25) to calculate a new set of nodal diagrams. The procedure continues up to when convergence is reached.

The solution of the HNC provides the TBDF which is used to obtain the energy value (13.1) with the l'hamiltonian

$$\hat{H} = -\sum_{i=1}^{A} \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j=1}^{A} \hat{V}_{ij} \ . \tag{13.26}$$

The expectation value of the energy is calculated by using the trial wave function

$$\Psi_{\rm T}(1,\ldots,A) = F(1,\ldots,A)\Phi(1,\ldots,A) = \mathcal{S}\Big(\prod_{i<j} f_{ij}\Big)\Phi(1,\ldots,A) \ . \tag{13.27}$$

The calculation of the contribution of the two-body potential term V_{ij} is straightforward, as indicated by Eq. (13.8). The evaluation of the kinetic energy term is more involved. The procedure commonly adopted separates the contribution in three parts

$$\langle T\rangle \equiv T_\phi + T_F - T_{c.m.} \ . \tag{13.28}$$

The first part is a term where the derivatives act on the mean-field wave function Φ

$$T_\phi \equiv -\frac{\hbar^2}{4m}\left(< \Phi^* F^2 \sum_{i=1}^{A} \nabla_i^2 \Phi > - < \sum_{i=1}^{A} (\nabla_i \Phi^*)\cdot F^2 \nabla_i \Phi) > \right) , \tag{13.29}$$

the second part is a term where the derivatives act on the correlation function

$$T_F \equiv -\frac{\hbar^2}{4m} < \Phi^* \Big[F\Big(\sum_{i=1}^{A} \nabla_i^2 F\Big) - \sum_{i=1}^{A} (\nabla_i F)^2 \Big] \Phi > , \tag{13.30}$$

and the third part is a term giving the center of mass contribution:

$$T_{c.m.} = -\frac{\hbar^2}{2mA} < \Psi_{\rm T}^* \Big(\sum_{i=1}^{A} \nabla_i \Big)^2 \Psi_{\rm T} > \ . \tag{13.31}$$

In the previous equations the symbol <> indicates

$$< X >= \frac{\int dx_1,\ldots,dx_A X(x_1,\ldots,x_A)}{< \Psi_{\rm T}|\Psi_{\rm T} >} \ . \tag{13.32}$$

The term T_F is handled in analogous manner of the two-body term of the interaction $\hat{V}_{ij}$ and inserted in Eq. (13.8). The evaluation of the other terms is more complicated, but it does not present special problems.

13.3 Fermions

In the description of a fermionic system it is necessary to consider the Pauli exclusion principle. The extension of the theory HNC to these systems is called Fermi HyperNetted Chain (FHNC). In this case, the mean-field wave function Φ (13.2) is a Slater determinant of single particle wave functions ϕ_a.

The expression of the TBDF (13.7) contains the squared module of the uncorrelated wave function. The $|\Phi|^2$ can be expressed as:

$$|\Phi(1,2,\ldots,A)|^2 = \begin{vmatrix} \rho_0(x_1,x_1) & \rho_0(x_1,x_2) & \ldots & \rho_0(x_1,x_A) \\ \rho_0(x_2,x_1) & \rho_0(x_2,x_2) & \ldots & \rho_0(x_2,x_A) \\ \vdots & \vdots & \ddots & \vdots \\ \rho_0(x_A,x_1) & \rho_0(x_A,x_2) & \ldots & \rho_0(x_A,x_A) \end{vmatrix} , \tag{13.33}$$

were the elements of the above determinant have been defined as:

$$\rho_0(x_i,x_j) = \sum_a \phi_a^*(x_i)\phi_a(x_j) \ . \tag{13.34}$$

The sum is carried out on all the occupied single-particle states, which for the ground state are all the states below the Fermi surface. Eq. (13.34) defines the uncorrelated One-Body Density Matrix (OBDM) which is the basic ingredient of the calculation od the TBDF in fermionic system.

A fundamental property of the OBDM, due to the orthonormality of the single-particle wave functions, is:

$$\int dx_j \rho_0(x_i,x_j)\rho_0(x_j,x_k) = \rho_0(x_i,x_k) \ , \tag{13.35}$$

where the integral sign indicates the integration on the space coordinate and also the sum on the third components of spin, and eventually, of isospin.

The sub-determinants are defined as:

$$\Delta_p(1,...,p) = \begin{vmatrix} \rho_0(x_1,x_1) & \rho_0(x_1,x_2) & \ldots & \rho_0(x_1,x_p) \\ \rho_0(x_2,x_1) & \rho_0(x_2,x_2) & \ldots & \rho_0(x_2,x_p) \\ \vdots & \vdots & \ddots & \vdots \\ \rho_0(x_p,x_1) & \rho_0(x_p,x_2) & \ldots & \rho_0(x_p,x_p) \end{vmatrix} \quad p \le A \ . \tag{13.36}$$

For the property (13.35) of the OBDM, the sub-determinants have the following property

$$\int dx_{p+1}\Delta_{p+1}(1,....,p+1) = (A-p)\Delta_p(1,...,p) \ , \tag{13.37}$$

and, by iterating

$$\int dx_{p+1}...dx_A\Delta_A(1,....,A) = (A-p)!\Delta_p(1,...,p) \ . \tag{13.38}$$

This implies that:

$$\Delta_p = 0 \ , \qquad \text{if} \qquad p > A \ . \tag{13.39}$$

As example, we show these propertied in the Δ_3 case.

$$\Delta_3(1,2,3) \quad = \quad \begin{vmatrix} \rho_0(x_1,x_1) & \rho_0(x_1,x_2) & \rho_0(x_1,x_3) \\ \rho_0(x_2,x_1) & \rho_0(x_2,x_2) & \rho_0(x_2,x_3) \\ \rho_0(x_3,x_1) & \rho_0(x_3,x_2) & \rho_0(x_3,x_3) \end{vmatrix}$$

$$
\begin{aligned}
&= \rho(x_1,x_1)\begin{vmatrix} \rho_0(x_2,x_2) & \rho_0(x_2,x_3) \\ \rho_0(x_3,x_2) & \rho_0(x_3,x_3) \end{vmatrix} \\
&- \rho(x_1,x_2)\begin{vmatrix} \rho_0(x_2,x_1) & \rho_0(x_2,x_3) \\ \rho_0(x_3,x_1) & \rho_0(x_3,x_3) \end{vmatrix} \\
&+ \rho(x_1,x_3)\begin{vmatrix} \rho_0(x_2,x_1) & \rho_0(x_2,x_2) \\ \rho_0(x_3,x_1) & \rho_0(x_3,x_2) \end{vmatrix} .
\end{aligned}
$$

For the normalization of the OBDM and the property (13.35) we obtain

$$
\begin{aligned}
\int d^3r_3\,\Delta_3(1,2,3) &= \rho(x_1,x_1)\rho(x_2,x_2)A - \rho(x_1,x_1)\rho(x_1,x_2) \\
&- \rho(x_1,x_2)\rho(x_2,x_1)A + \rho(x_1,x_2)\rho(x_2,x_1) \\
&+ \rho(x_2,x_1)\rho(x_1,x_2) - \rho(x_1,x_1)\rho(x_2,x_2) \\
&= (A-1)\rho(x_1,x_1)\rho(x_2,x_2) - (A-1)\rho(x_2,x_1)\rho(x_1,x_2) \\
&= (A-1)\begin{vmatrix} \rho_0(x_1,x_1) & \rho_0(x_1,x_2) \\ \rho_0(x_2,x_1) & \rho_0(x_2,x_2) \end{vmatrix}
\end{aligned}
$$

The property (13.39) is extremely useful in the application of the cluster expansion techniques in finite fermionic systems. It is worth to remark that these properties of the OBDM and of the sub-determinants depend only on the orthonormality of the single-particle wave functions, and not on their expression. For this reason they are valid for both infinite and finite fermion systems.

Also in the fermionic case the cluster expansion is analyzed in terms of diagrams. It is necessary to include a new graphical symbol to consider the fact that particles of the system are correlated not only by the $h(r_{ij})$-function, which takes into account the so-called *dynamical correlation*, but also by the Pauli exclusion principle, usually referred to as *statistical correlation*. This last fact is inserted in the OBDM $\rho_0(x_i,x_j)$ which, in the calculation of the TBDF, forms closed loops which do not overlap. The graphical symbol adopted to indicate the OBDM is an oriented line joining the x_i and x_j points.

As in the bosonic case there is no limit for the number of dynamical correlation lines which can join a single point. On the contrary, the Pauli exclusion principle implies that a point can be reached by two statistical lines or by none. Only the external points have a possibility of being reached by a single statistical line.

By using the trial wave function (13.2) with the Jastrow ansatz (13.3) and the definition (13.12) of the h-function the TBDF (13.7) can be written as:

$$
g(x_1,x_2) = \frac{A(A-1)\int dx_3....dx_A(1+\sum_{i<j}h_{ij}+\sum_{i<j<k}h_{ij}h_{jk}+....)|\Phi(x_1,....,x_A)|^2}{\rho^2\int dx_1....dx_A(1+\sum_{i<j}h_{ij}+\sum_{i<j<k}h_{ij}h_{jk}+....)|\Phi(x_1,....,x_A)|^2} , \tag{13.40}
$$

where $h_{ij} \equiv h(r_{ij})$.

By using the definition of sub-determinant (13.36) the numerator, $\mathcal{N}$, and the denominator, $\mathcal{D}$, of the previous equation can be expressed as sums of terms characterized by the number of h-functions:

$$
\mathcal{N} = \frac{A(A-1)}{\rho^2}f^2(r_{12})\int dx_3....dx_A\left(1+\sum_{i<j}h_{ij}+\sum_{i<j<k}h_{ij}h_{jk}+....\right)\Delta_A , \tag{13.41}
$$

$$
\mathcal{D} = \int dx_1....dx_A\left(1+\sum_{i<j}h_{ij}+\sum_{i<j<k}h_{ij}h_{jk}+....\right)\Delta_A . \tag{13.42}
$$

The expressions of $\mathcal{n}$ and $\mathcal{D}$ can be rewritten by grouping the terms with the same number of points p, this set of term is indicated by $X^{(p)}(1,2,3,..,p)$. For example,

$$X^{(3)}(1,2;i) = h_{1i} + h_{2i} + h_{1i}h_{2i} \ .$$

By using this convention, the TBDF can be written as

$$\begin{aligned} g(x_1,x_2) = \quad = \quad & \frac{A(A-1)}{\rho^2} f^2(r_{12}) \int dx_3 ... dx_A \Delta_A \left[1 + \sum_{p=3}^{A} \frac{(A-2)!}{(p-2)!(A-p)!} X^{(p)}(1,2;\ldots,p) \right] \\ & \left[\int dx_1 ... dx_A \Delta_A \left(1 + \sum_{p=2}^{A} \frac{A!}{p!(A-p)!} X^{(p)}(1,\ldots,p) \right) \right]^{-1} . \end{aligned}$$

The factorial terms multiplying the $X^{(p)}$ functions take care of the fact that each permutation of the internal points do not modify the value of the diagram.

By using the property (13.38) it is possible to integrate the above expression of the TBDF on all the coordinates which are not reached by the correlations, i.e. those which are not present in the $X^{(p)}$ functions. This procedure leads to the following expressions of numerator and denominator of the TBDF

$$\mathcal{n} = A! \frac{f^2(r_{12})}{\rho^2} \sum_{p=2}^{A} \frac{1}{(p-2)!} \int dx_3 ... dx_p X^{(p)}(1,2;...,p) \Delta_p(1,...,p) \, , \tag{13.43}$$

$$\mathcal{D} = A! \sum_{p=0}^{A} \frac{1}{p!} \int dx_1 ... dx_p X^{(p)}(1,...,p) \Delta_p(1,...,p) \ . \tag{13.44}$$

It is possible to formally extend up to infinity the upper limits of the two sums of the previous expressions by using the property (13.39) of the sub-determinants.

In analogy to the bosonic case, at this point of the calculation a topological classification of the various diagrams contained in $\mathcal{n}$ and $\mathcal{D}$ is required.

a) *Linked and unlinked diagrams*
The definition of linked and unlinked diagrams is analogous to that used for the bosonic case, with the novelty that now the links to the external point can be obtained either by a dynamical correlation line (a dashed line) or by a statistical correlation line (a continuous oriented line). The mathematical expression of the unlinked diagram show a factorization of the integrals containing the external points and those without them. The sum of this latter type of diagrams is exactly the sum of the diagrams of the denominator which simplify. The TBDF can be expressed by considering only the linked diagrams $\mathcal{L}_n(1,2,i_3,...,i_n)$

$$g(x_1,x_2) = g(r_{12}) = \frac{f^2(r_{12})}{\rho^2} \left[\Delta_2(1,2) + \sum_{p=3}^{\infty} \frac{1}{(p-2)!} \int dx_3 ... dx_p \, \mathcal{L}_p(1,2;...,p) \right] . \tag{13.45}$$

b) *Reducible diagrams*
In the bosonic systems the contribution of the reducible diagrams is canceled by the denominator up to $1/A$ factor. In the fermionic system this contribution is exactly zero in infinite systems. The point is illustrated in Fig. 13.7. The two reducible diagrams shown in the upper part of the diagram differ only for the presence of a statistical loop in the right diagrams. In an infinite system the statistical

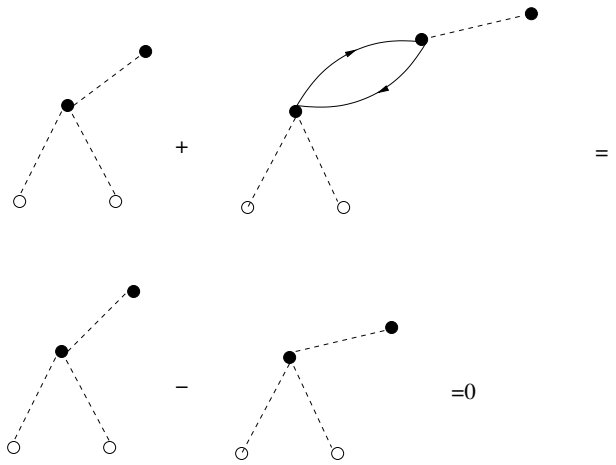

Figure 13.7: Example of cancellation of two FHNC reducible diagrams The statistical loop in the higher part introduces a minus sign and, therefore, the total contribution of the two diagrams is zero.

loop contributes with a -1 factor. Therefore, the contribution of the diagram with an additional loop is identical to that of the other diagram but with a different global sign. As indicated in lower part of the figure the total contribution is zero. In an infinte system to each reducible diagram is associated another diagram with an additional statistical loop.

In finite fermionic systems the contribution of the reducible diagrams is not zero. The sum of the parts which develop out of the reduction point produces a factor which is the correlated one-body density of system. By including this vertex correction in the reduction points the reducible diagrams are included in the counting of the simple diagrams.

c) *Simple and composite diagrams*
As in the case of the bosonic system, the composite diagrams are construced by joining simple diagrams in the external points. Of course, one has to consider the role of the statistical correlations, but also in this case the contribution of the composite diagrams is obtained by summing the simple diagrams classified in nodal and elementary.

d) *Nodal and elementary*
The definition of nodal and elementary diagrams is analogous to that of the bosonic case, but both dynamical and statistical correlations are considered. The presence of statistical correlation does not allows the formulation of a single integral equation for the calculation of all the nodal diagrams, as it happened in Eq. (13.25). It is, however, possible to formulate a system of linked integral equations which describe the contributions of the nodal diagrams classified by the type of correlation reaching the external points.

The graphical examples of the various types of diagrams required to obtain the different integral equations are shown in Fig. 13.8. In the A and B diagrams, the external points are reached by dynamical correlations only. For this reason they are identified with the *dd* (dynamical-dynamical) sub-indexes. The C and D diagrams have dynamical correlations reaching the point 1 and two statistical correlations reaching the point 2. The sub-indexes identifying the diagrams are *de* (dynamical-exchange). The E and F diagrams are indicated as *ee* (exchange-exchange) since in both cases the external points are reached by statistical lines. It convenient to define diagrams which are reached by a statistical correlation starting from 1 and arriving to 2 and forming an open ring. These diagrams are called *cc* (cyclic-cyclic) and do

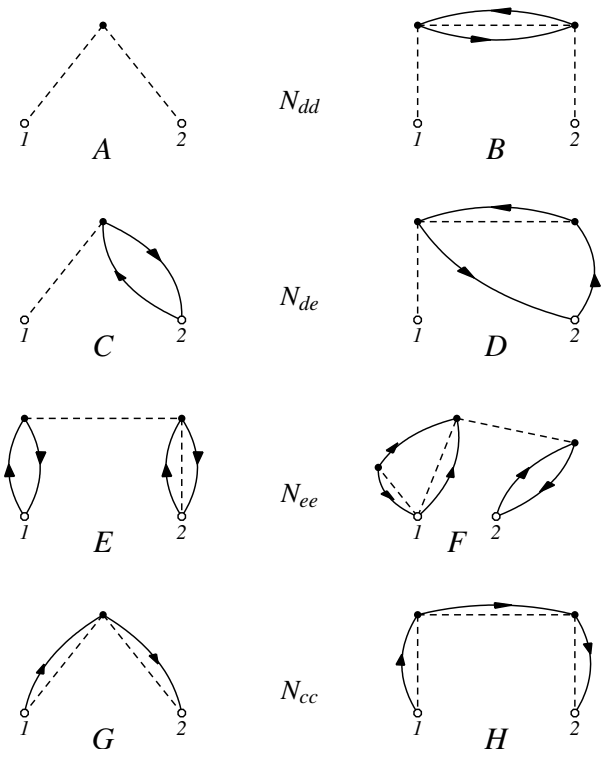

Figure 13.8: The variou tyopes of nodal diagrams required by the FHNC equations. The sub-indexes classify the diagrams with respect to the type of correlation reaching the external points 1 and 2.

not directly contribute to the calculation of the TBDF.

As in the bosonic case, see Eq. (13.25), also in the present case, the total contribution of the nodal diagrams can be obtained by carrying out a folding integral of the various terms of the diagrams in the nodal point. In the fermionic systems the Pauli exclusion principle prohibits the folding between diagrams of the same type. For example a diagram of e type can be folded only by diagrams of type d in that point.

Let's indicate with N the sum of all the nodal diagrams and with X that of the non-nodal irreducible ones. Clearly, N e X are identified by the sub-indexes dd, de, ee e cc. For the nodal diagrams it is possible to write the following set of equations

$$\begin{aligned}
N_{dd}(r_{12}) &= \Big(X_{dd}(r_{13}) + X_{de}(r_{13})|\rho(\mathbf{r}_3)[N_{dd}(r_{32}) + X_{dd}(r_{32})]\Big) \\
&+ \Big(X_{dd}(r_{13})|\rho(\mathbf{r}_3)[N_{ed}(r_{32}) + X_{ed}(r_{32})]\Big) \ , \\
N_{de}(r_{12}) &= \Big(X_{dd}(r_{13}) + X_{de}(r_{13})|\rho(\mathbf{r}_3)[N_{de}(r_{32}) + X_{de}(r_{32})]\Big) \\
&+ \Big(X_{dd}(r_{13})|\rho(\mathbf{r}_3)[N_{ee}(r_{32}) + X_{ee}(r_{32})]\Big) \ , \\
N_{ee}(r_{12}) &= \Big(X_{ed}(r_{13}) + X_{ee}(r_{13})|\rho(\mathbf{r}_3)[N_{de}(r_{32}) + X_{de}(r_{32})]\Big) \\
&+ \Big(X_{ed}(r_{13})|\rho(\mathbf{r}_3)[N_{ee}(r_{32}) + X_{ee}(r_{32})]\Big) \ ,
\end{aligned}$$

$$N_{cc}(r_{12}) = \Big(X_{cc}(r_{13})|\rho(\mathbf{r}_3)[N_{cc}(r_{32}) + X_{cc}(r_{32}) - \ell(k_F r_{32})/\nu]\Big) \ . \tag{13.46}$$

The equations for the non-nodal diagrams are:

$$\begin{aligned}
X_{dd}(r_{12}) &= g_{dd}(r_{12}) - N_{dd}(r_{12}) - 1 \ , \\
X_{de}(r_{12}) &= g_{dd}(r_{12})[N_{de}(r_{12}) + E_{de}(r_{12})] - N_{de}(r_{12}) \ , \\
X_{ee}(r_{12}) &= g_{dd}(r_{12})\{N_{ee}(r_{12}) + E_{ee}(r_{12}) + [N_{de}(r_{12} + E_{de}(r_{12})]^2 \\
&\quad -\nu[N_{cc}(r_{12}) + E_{cc}(r_{12}) - \frac{1}{\nu}\ell(k_F r_{12})]^2\} - N_{ee}(r_{12}) \ , \\
X_{cc}(r_{12}) &= g_{dd}(r_{12})[N_{cc}(r_{12}) + E_{cc}(r_{12}) - \frac{1}{\nu}\ell(k_F r_{12})] \\
&\quad - \ N_{cc}(r_{12}) + \frac{1}{\nu}\ell(k_F r_{12}) \ .
\end{aligned} \tag{13.47}$$

The partial definitions of the TBDF are:

$$\begin{aligned}
g_{dd}(r_{12}) &= f^2(r_{12}) e^{N_{dd}(r_{12}) + E_{dd}(r_{12})} \ , \\
g_{de}(r_{12}) &= N_{de}(r_{12}) + X_{de}(r_{12}) \ , \\
g_{ed}(r_{12}) &= g_{de}(r_{12}) \ , \\
g_{ee}(r_{12}) &= N_{ee}(r_{12}) + X_{ee}(r_{12}) \ , \\
g_{cc}(r_{12}) &= N_{cc}(r_{12}) + X_{cc}(r_{12}) - \frac{1}{\nu}\ell(k_F r_{12}) \ .
\end{aligned} \tag{13.48}$$

The total TBDF is obtained by summing the partial terms

$$g(r_{12}) = g_{dd}(r_{12}) + g_{ed}(r_{12}) + g_{de}(r_{12}) + g_{ee}(r_{12}) \tag{13.49}$$

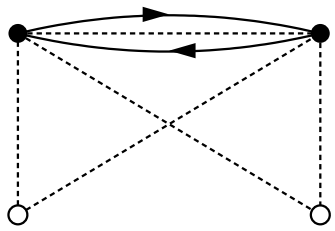

Figure 13.9: Four-points elementary diagram.

The system of Eqs. (13.46), (13.47), (13.48) and (13.49) form the Fermi HyperNetted Chain (FHNC) equations. As in the case of the bosonic HNC equations, also the FHNC allows the calculation of all the composite and nodal diagrams in closed form. Also in this case, the elementary diagrams, such as that of Fig. 13.9, are excluded and they have to be calculated one by one.

Also in this case the FHNC equations are solved by using an iterative procedure analogous to that adopted for the solution of the HNC equations. After the TBDF has been obtained the energy of the system is calculated following the same paths outlined for the bosonic case.

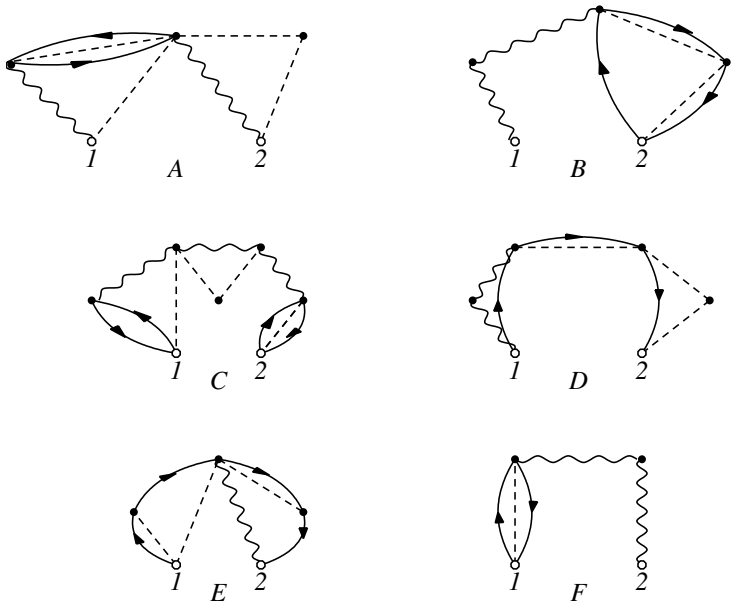

Figure 13.10: Examples of the FHNC/SOC diagrams. The wavy lines represent operator dependent correlations.

The FHNC theory has been applied to the fermionic liquid helium. It is the case where the helium atoms are composed by ^{3}He nuclei and not ^{4}He. The properties of the fermionic liquid helium are rather different from those of the bosonic case, since the two liquids follows two different quantum statistics. The interaction in both cases is the purely scalar Coulomb interaction as discussed in Sect. 3.4.

The nuclear interaction is much more complex, as discussed in Sect. 3.3, the FHNC approach presented so far is not adequate to handle all the different aspects of the problem. For this reason in nuclear systems the Jastrow's ansatz (13.3) is modified by adding correlation terms depending on the operators used to describe the nuclear hamiltonian (3.1)

$$\mathcal{F}(1,...,A) = \mathcal{S}\Big(\prod_{j>i=1}^{A} F_{ij}\Big) = \mathcal{S}\Big(\prod_{j>i=1}^{A}\sum_{p=1}^{6} f_p(r_{ij})\hat{O}_{ij}^p\Big) \ . \tag{13.50}$$

with the operators defined as

$$\hat{O}_{ij}^{p=1,6} = \hat{\mathbb{I}}, \hat{\boldsymbol{\tau}}_i\cdot\hat{\boldsymbol{\tau}}_j, \hat{\boldsymbol{\sigma}}_i\cdot\hat{\boldsymbol{\sigma}}_j, (\hat{\boldsymbol{\sigma}}_i\cdot\hat{\boldsymbol{\sigma}}_j)(\hat{\boldsymbol{\tau}}_i\cdot\hat{\boldsymbol{\tau}}_j), \hat{S}_{ij}, \hat{S}_{ij}(\hat{\boldsymbol{\tau}}_i\cdot\hat{\boldsymbol{\tau}}_j) \ . \tag{13.51}$$

The step (13.12) defining the h-function had a universal value because the correlation was a scalar function. Now it is necessary to consider that the various terms of the correlation do not necessarily commute with the terms of the hamiltonian and neither between them. This fact does not allow the formulation of equations which sum in closed form all the diagrams of a certain type. It is necessary to introduce an approximation.

It is possible to sum in a closed form diagrams containing chains of operator-dependent correlations which have only one correlation between two points, as in the diagrams of Fig. 13.10. This approximation is called of Single Operator Chain (SOC). The FHNC/SOC theory with the inclusion of the elementary diagram of Fig. 13.9 is the most elaborated theory of CBF type used in nuclear physics. This theoretical

framework is adequate to treat hamiltonians with two-body interactions only. The insertion of three-body forces is not included in the diagrammatic expansion scheme of the FHNC, but, analogously to the elementary diagrams, is inserted by considering the single diagrams.

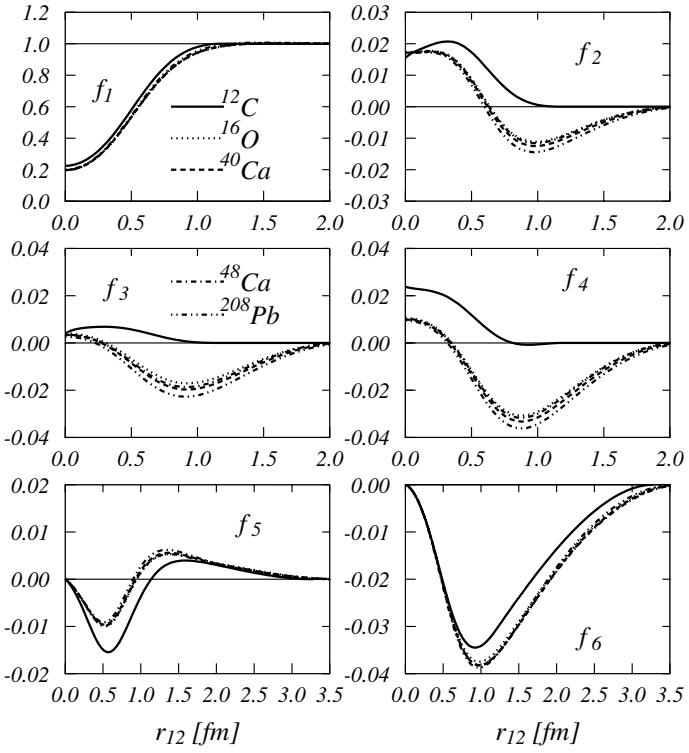

Figure 13.11: Correlations obtained in variational FHNC/SOC in the various operator channels for various doubly magic nuclei [Ari07].

We show in Fig. 13.11 the correlation functions f_p obtained in a variational FHNC/SOC calculations for some doubly-magic nuclei. The different panels present the correlation functions of the various operator channels. The most important correlations are the scalar ones which are, usually, one order of magnitude larger than those in the other channels.

13.3.1 Infinite nuclear matter

As example of application of the CBF theory we discuss here some results obtained for nuclear matter. The system under study has translational invariance and constant nucleonic density defined by the sum $\rho = \rho_{\rm p} + \rho_{\rm n}$ of the, constant, proton and neutron densities. The energy per nucleon $e = E/A$ is traditionally written in power expansion with respect to the asymmetry parameter $\delta = (\rho_{\rm n} - \rho_{\rm p})/\rho$, i.e.

$$e(\rho,\delta) \,=\, e(\rho,0) \,+\, e_{\rm sym}(\rho)\,\delta^2 \,+\, \mathcal{O}(\delta^4)\,. \tag{13.52}$$

Around the minimum of symmetric nuclear matter, $\delta = 0$, at the saturation density ρ_0, the two coefficients are expanded in powers of the parameter $\epsilon = (\rho - \rho_0)/(3\,\rho_0)$.

	exp	AFDMC	CBF	D1M	SLy5	DDME2
ρ_0	0.16 ± 0.01	0.16	0.16	0.16	0.16	0.15
$e(\rho_0, 0)$	-16.0 ± 0.1	-16.00	-16.00	-16.01	-15.98	-16.13
B	220 ± 30	276	269	217	228	278
$e_{\rm sym}(\rho_0)$	30-35	31.3	33.94	29.45	32.66	33.20
$\mathcal{L}$	88 ± 25	60.10	58.08	25.41	48.38	54.74

Table 13.1: Properties of infinite nuclear matter obtained with different types of calculations. The saturation density ρ_0 is expressed in fm^{-3}. All the other quantities in MeV. The Monte Carlo results are those of Ref. [Gan10], those of the CBF theory from Ref. [Akm98]. The other results from [Co12].

For the symmetric nuclear matter we obtain

$$e(\rho, 0) \, = \, a_V \, + \, \frac{1}{2} K_V \, \epsilon^2 \, + \, \ldots \, , \tag{13.53}$$

where the term of first order in ϵ, related to te first derivative with respect to ρ, is zero since $e(\rho, 0)$ has a minimum for $\rho = \rho_0$. In the quadratic term, related to the second derivative, the coeffient, defined as

$$B \, = \, 9\rho_0^2 \, \left. \frac{\partial^2 e(\rho, 0)}{\partial \rho^2} \right|_{\rho=\rho_0} \tag{13.54}$$

is called compression modulus, see Eq. (2.60).

The second coefficient of Eq. (13.52), called symmetry energy, is expanded as

$$e_{\rm sym}(\rho) \, = \, a_{\rm sym} \, + \, \mathcal{L} \, \epsilon \, + \, \ldots \, . \tag{13.55}$$

with the coefficient

$$\mathcal{L} \, = \, 3\rho_0 \, \left. \frac{\partial e_{\rm sym}(\rho)}{\partial \rho} \right|_{\rho=\rho_0} \, . \tag{13.56}$$

Table 13.1 shows the values of these quantities calculated with different theories at the value of the saturation density ρ_0. The comparison is done with empirical values (exp). The values obtained with the CBF theory [Akm98] are compared with those obtained by a calculation of Auxiliary Field Diffusion Monte Carlo (AFDMC) [Gan10], both of them are using the same microscopic interaction of phenomenological type. The other results are obtained in HF calculations with different effective interactions.

The values of the saturation densities and of the minimal energy agree within variation of 2% and 0.4%, respectively. Other variables have similar values in other calculations. The major differences are present in the values of $\mathcal{L}$.

The equation of state for pure neutronic matter (a), symmetric nuclear matter (b), and symmetry energy (c) are shown in Fig. 13.12. All the calculations show a good agreement at the saturation point of symmetric nuclear matter. There are remarkable differences away from this point.

What it is interesting is the close similarity between the CBF e AFDMC results.

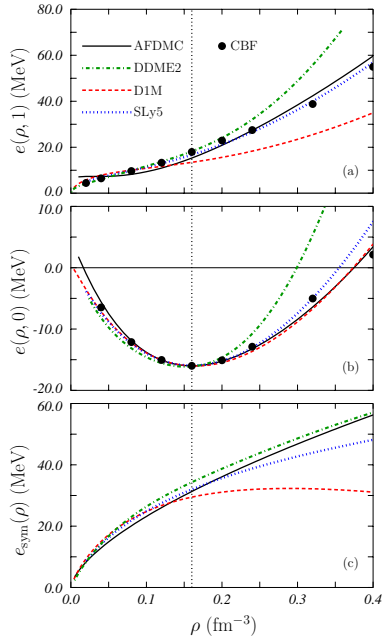

Figure 13.12: Equation of state for pure neutron matter (a), symmetric neutron matter (b) and symmetry eneregy The black points show the CBF results [Akm98], the black lines those of the AFDMC [Gan10] and the other lines different HF results [Co12].

Chapter 14

Unitary correlation operator method

Around the 90's of the last century, mainly in the framework of the theoretical nuclear physics, and more in general, in that of the many-body problem, a great attention on the short-range correlations has been addressed. Among the various proposals of treating these type of correlation it is particularly interesting the Unitary Correlation Operator Method (UCOM) [Fel98] which emphasizes the duality in the interpretation of the correlations.

14.1 The Unitary Correlation Operator

Let's consider the Schrödinger equation with the full hamiltonian containing a microscopic interaction (Cap. 3),

$$\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle \quad . \tag{14.1}$$

Let's define an operator $\hat{C}$ such as its action on a MF state generates the eigenstate of the hamiltonian $\hat{H}$,

$$|\Psi_n\rangle = \hat{C}(\hat{H},\{\Phi\})\,|\Phi_n\rangle \quad , \tag{14.2}$$

where we made explicit the dependence of the $\hat{C}$ operator on both the hamiltonian $\hat{H}$ and also on the single-particle wave functions generated by a MF hamiltonian and forming the Slater determinant $|\Phi_n\rangle$.

Since both the set of $|\Phi_n\rangle$ states and also that of the eigenstates of $\hat{H}$, $|\Psi_n\rangle$, form complete bases, the $\hat{C}(\hat{H},\{\Phi\})$ operator can be formally expressed as

$$\hat{C}(\hat{H},\{\Phi\}) = \sum_k |\Psi_k\rangle\,\langle\Phi_k| \tag{14.3}$$

showing that $\hat{C}$ is a unitary operator which diagonalizes the hamiltonian $\hat{H}$. In fact we can write

$$\begin{aligned}\langle\Psi_k|\hat{H}|\Psi_n\rangle &= \langle\Phi_k|\hat{C}^+\hat{H}\hat{C}|\Phi_n\rangle = \langle\Phi_k|\sum_i |\Phi_i\rangle\,\langle\Psi_i|\,\hat{H}\sum_j |\Psi_j\rangle\,\langle\Phi_j|\Phi_n\rangle \\ &= \sum_{ij}\langle\Phi_k|\Phi_i\rangle\,E_i\delta_{ij}\,\langle\Phi_j|\Phi_n\rangle = \sum_{ij} E_i\delta_{ij}\delta_{ik}\delta_{jn} = E_n\delta_{kn} \quad .\end{aligned} \tag{14.4}$$

Since the $\hat{C}$ is unitary, the correlated state $|\Psi_n\rangle$ (14.2) has the same normalization of the MF state $|\Phi_n\rangle$. The structure of the equations (14.2) and (13.2) defining the correlations respectively in UCOM and in CBF is the same. However the Jastrow's ansatz (13.3) on the expression of the correlation in CBF does not produce a unitary operator, for this reason it is necessary a specific treatment to obtain the

proper normalization of the wave function. On the contrary, the correlation in UCOM is defined such as to ensure the unitarity property.

The second step of Eq. (14.4) can be viewed as a change of the eigenstate of $\hat{H}$, or as a change of the operator $\hat{H}$

$$\langle\Psi_k|\hat{H}|\Psi_n\rangle = \langle\Phi_k|\hat{C}^+\hat{H}\hat{C}|\Phi_n\rangle = \langle\Phi_k|\hat{H}^{\rm eff}|\Phi_n\rangle \quad , \tag{14.5}$$

with the obvious definition of the effective hamiltonian $\hat{H}^{\rm eff}$. This is what we meant in the introduction of the chapter with duality in the interpretation of the correlation effects.

We pointed out how the unitarity of the correlation operator is an essential requirement of the model. A unitary operator can be described as

$$\hat{C} = e^{-i\hat{G}} \tag{14.6}$$

where $\hat{G}$ is a hermitian operator whose properties are listed here below. Since we are considering a fermionic system the number of particles is conserved by the action of the operator. The $\hat{G}$ is invariant for the exchange of two-particles since the antisymmetry is present in the Slater determinant $|\Phi\rangle$. In addition, G must be at least a two-body operator, or more complicated, since a one-body operator would produced a unitary transformation of the set of single-particle states generating another Slater determinant completely equivalent for what concerns the calculation of observables.

The operator $\hat{G}$ can be expressed as

$$\hat{G} = \sum_{i<j} \hat{g}(i,j) + \cdots \quad , \tag{14.7}$$

where $\hat{g}(i,j)$ is an operator acting on the fermions i and j, and $\cdots$ indicates the eventual presence of operators acting on more than two particles. Each correlated operator

$$\underline{\hat{B}} = \hat{C}^+\hat{B}\hat{C} = \hat{C}^{-1}\hat{B}\hat{C} = e^{i\hat{G}}\hat{B}e^{-i\hat{G}} \quad , \tag{14.8}$$

is an overlap of zero-, one-, two-, three- ... $A-$body operators.

It is convenient the use of a notation which allows the identification of a $n-$body operator which cannot be written as a sum of simpler operators, for this reason called irreducible:

$$\hat{B}^{[n]}_A = \sum_{i_1<\cdots<i_n}^{A} \hat{b}^{[n]}(i_1,i_2,\cdots,i_n) \quad , \tag{14.9}$$

where $\hat{b}^{[n]}(i_1,i_2,\cdots,i_n)$ is an operator acting on n of the A particles forming the system. If $n > A$ then $\hat{b}^{[n]}_A = 0$. In this notation, the hamiltonian composed by the kinetic energy and by a two-body potential is expressed as

$$\hat{H} \equiv \hat{H}_A = \hat{T}^{[1]}_A + \hat{V}^{[2]}_A = \sum_{i}^{A} \hat{t}^{[1]}(i) + \sum_{i<j}^{A} \hat{v}^{[2]}(i,j) \quad . \tag{14.10}$$

The absence of the upper index $[n]$ indicates that the operator is sum of operators acting on different numbers of particles.

The expression of a correlated operator in terms of irreducible operators can be written as

$$\underline{\hat{B}} \equiv \underline{\hat{B}}_A = \hat{C}^{-1}_A\hat{B}_A\hat{C}_A = \sum_{n=1}^{A} \hat{B}^{[n]}_A \quad , \tag{14.11}$$

where

$$\underline{\hat{B}}^{[n]}_A = \sum_{i_1<\cdots<i_n}^{A} \underline{\hat{b}}^{[n]}(i_1,i_2,\cdots,i_n) \quad . \tag{14.12}$$

From the above definitions we obtain the expression

$$\hat{\underline{b}}^{[n]} \equiv \hat{\underline{B}}_n - \sum_{k=1}^{n-1} \hat{\underline{B}}_n^{[k]} = \hat{C}_n^{-1}\hat{B}_n\hat{C}_n - \sum_{k=1}^{n-1}\sum_{i_1<\cdots<i_k}^{n} \hat{\underline{b}}^{[k]}(i_1,\cdots,i_k) \ . \tag{14.13}$$

The first $\hat{\underline{b}}^{[n]}$ term different from zero, is related to the number of particles connected by the $\hat{B}$ operator. For one-body operators $n = 1$, for two-body operators $n = 2$, etc..

We shall consider, henceforth, a generator $\hat{G}$ composed by two-body operators only. This means that we neglect the terms indicated by the points in the expression (14.7).

The kinetic energy term is described as

$$\hat{\underline{T}}_A \equiv \hat{C}_A^+\hat{T}_A\hat{C}_A = \sum_{n=1}^{A} \hat{\underline{T}}_A^{[n]} \ . \tag{14.14}$$

The first term, $n = 1$, is the MF kinetic energy

$$\hat{\underline{T}}_A^{[1]} = \sum_{i}^{A} \hat{\underline{t}}^{[1]}(i) = \sum_{i}^{A} \hat{t}^{[1]}(i) = \hat{T}_A^{[1]} \ . \tag{14.15}$$

The second term, $n = 2$, is obtained by considering Eq. (14.12),

$$\hat{\underline{T}}_A^{[2]} = \sum_{i<j} \hat{\underline{t}}^{[2]}(i,j) \ , \tag{14.16}$$

where

$$\hat{\underline{t}}^{[2]}(i,j) = \hat{c}(i,j)^{-1}\Big(\hat{t}^{[1]}(i) + \hat{t}^{[1]}(j)\Big)\hat{c}(i,j) - \Big(\hat{t}^{[1]}(i) + \hat{t}^{[1]}(j)\Big) \ , \tag{14.17}$$

with

$$\hat{c}(i,j) = \exp\{-i\hat{g}^{[2]}(i,j)\} \ . \tag{14.18}$$

This means that, for each pair i and j, the two-body part is the difference between the correlated term and uncorrelated one.

For the third term of Eq. (14.14), $n = 3$, we have that

$$\hat{\underline{T}}_A^{[3]} = \sum_{i<j<k} \hat{\underline{t}}^{[3]}(i,j,k) \ , \tag{14.19}$$

where

$$\begin{aligned} \hat{\underline{t}}^{[3]}(i,j) &= \hat{c}(i,j,k)^{-1}\Big(\hat{t}^{[1]}(i) + \hat{t}^{[1]}(j) + \hat{t}^{[1]}(k)\Big)\hat{c}(i,j,k) \\ &- \Big(\hat{\underline{t}}^{[2]}(i,j) + \hat{\underline{t}}^{[2]}(i,k) + \hat{\underline{t}}^{[2]}(j,k)\Big) - \Big(\hat{t}^{[1]}(i) + \hat{t}^{[1]}(j) + \hat{t}^{[1]}(k)\Big) \ , \end{aligned} \tag{14.20}$$

with the definition

$$\hat{c}(i,j,k) = \exp\Big\{ - i\Big(\hat{g}^{[2]}(i,j) + \hat{g}^{[2]}(i,k) + \hat{g}^{[2]}(j,k)\Big)\Big\} \ . \tag{14.21}$$

Also in this case, the correlated contribution is obtained by subtracting the uncorrelated two-body and one-body terms.

We use the same approach to descrive the two-body interaction term. In this case te first term different from zero is $n = 2$, therefore

$$\hat{\underline{V}}_A \equiv \hat{C}_A^+\hat{V}_A\hat{C}_A = \sum_{n=2}^{A} \hat{\underline{V}}_A^{[n]} \ , \tag{14.22}$$

where

$$\hat{\underline{V}}_A^{[2]} = \sum_{i<j} \hat{\underline{v}}^{[2]}(i,j) \ , \tag{14.23}$$

with

$$\hat{\underline{v}}^{[2]}(i,j) = \hat{c}(i,j)^{-1} \hat{v}^{[2]}(i,j) \hat{c}(i,j) \ , \tag{14.24}$$

and

$$\hat{\underline{V}}_A^{[3]} = \sum_{i<j<k} \hat{\underline{v}}^{[3]}(i,j,k) \ , \tag{14.25}$$

where we defined

$$\begin{aligned} \hat{\underline{v}}^{[3]}(i,j) &= \hat{c}(i,j,k)^{-1} \Big(\hat{v}^{[2]}(i,j) + \hat{v}^{[2]}(i,k) + \hat{v}^{[2]}(j,k) \Big) \hat{c}(i,j,k) \\ &- \Big(\hat{\underline{v}}^{[2]}(i,j) + \hat{\underline{v}}^{[2]}(i,k) + \hat{\underline{v}}^{[2]}(j,k) \Big) \end{aligned} \tag{14.26}$$

14.2 Representation as coordinates transformation

We express here the action of the operator $\hat{c}(i,j)$ in coordinate space. The relative coordinate and momentum of the identical fermions i and j are defined as

$$\mathbf{r} = \mathbf{r}(i) - \mathbf{r}(j) \ \text{ and } \ \hat{\mathbf{q}} = \frac{1}{2}(\hat{\mathbf{p}}(i) - \hat{\mathbf{p}}(j)) \ . \tag{14.27}$$

where the momenta are operators in coordinate space. The generator $\hat{g}(i,j) \equiv \hat{g}(\mathbf{r}, \hat{\mathbf{q}})$, Eq. (14.7), can be defined with a symmetric and hermitian form as

$$\hat{g}(\mathbf{r}, \hat{\mathbf{q}}) = \frac{1}{2} \left\{ \left(\hat{\mathbf{q}} \cdot \frac{\mathbf{r}}{r} \right) s(r) + s(r) \left(\frac{\mathbf{r}}{r} \cdot \hat{\mathbf{q}} \right) \right\} \ \text{ with } \ r \equiv |\mathbf{r}| \ , \tag{14.28}$$

where $s(r)$ is s suitable scalar function. The unitary operator $\hat{c}(\mathbf{r}, \mathbf{q})$ moves the relative position of the interacting pair of particles from $\mathbf{r}$ at about $\mathbf{r} + s(r)\mathbf{r}/r$. The idea is that of defining the function $s(r)$ such as the particles remains always far from the region of the strongly repulsive core of the potential.

In coordinate representation, by expressing $\hat{\mathbf{q}}$ in operator terms, the action of the generator $g(\mathbf{r}, \hat{\mathbf{q}})$ on the wave function $\langle \mathbf{r}|\phi\rangle$ describing the relative motion of the two-independent particles is

$$\frac{1}{\hbar} \langle \mathbf{r}|\hat{g}|\phi\rangle = -i \left(\frac{1}{2} \frac{\partial s(r)}{\partial r} + \frac{s(r)}{r} + s(r) \frac{\partial}{\partial r} \right) \langle \mathbf{r}|\phi\rangle = -i \frac{1}{r\sqrt{s(r)}} \, s(r) \frac{\partial}{\partial r} r\sqrt{s(r)} \, \langle \mathbf{r}|\phi\rangle \ . \tag{14.29}$$

For the correlation operator we obtain

$$\frac{1}{\hbar} \langle \mathbf{r}|\hat{c}|\phi\rangle = \exp\left(\frac{-1}{r\sqrt{s(r)}} \, s(r) \frac{\partial}{\partial r} r\sqrt{s(r)} \right) \langle \mathbf{r}|\phi\rangle = \frac{1}{r\sqrt{s(r)}} \, \exp\left(-s(r) \frac{\partial}{\partial r} \right) r\sqrt{s(r)} \, \langle \mathbf{r}|\phi\rangle \ . \tag{14.30}$$

The last step can be verified by making a power expansion of the exponential.
It is convenient to make a change of variables

$$s(r) \frac{\partial}{\partial r} \to \frac{\partial}{\partial y} \ . \tag{14.31}$$

We call the transformations between y e r, and viceversa, as $Y(r)$ and $R(y)$ respectively

$$r \xrightarrow{Y} y = Y(r) \ ; \ y \xrightarrow{R} r = R(y) \ , \tag{14.32}$$

and, by construction

$$R\Big(Y(r)\Big) = r \;\; ; \;\; Y\Big(R(y)\Big) = y \;\; . \tag{14.33}$$

From the definition (14.31) we obtain the following equations

$$\frac{\partial}{\partial r} Y(r) = \frac{1}{s(r)} \;\; ; \;\; \frac{\partial}{\partial y} R(y) = s\Big(R(y)\Big) \;\; ; \;\; y = \int^{R(y)} \frac{d\xi}{s(\xi)} \;\; . \tag{14.34}$$

We rewrite Eq. (14.30) in terms of y and $R(y)$

$$\begin{aligned} \langle R(y)\frac{\mathbf{r}}{r}|c|\phi\rangle &= \frac{1}{R(y)\sqrt{s\Big(R(y)\Big)}} \exp\left(-\frac{\partial}{\partial y}\right) R(y)\sqrt{s\Big(R(y)\Big)}\, \langle R(y)\frac{\mathbf{r}}{r}|\phi\rangle \\ &= \frac{R(y-1)}{R(y)} \sqrt{\frac{s\Big(R(y-1)\Big)}{s\Big(R(y)\Big)}}\, \langle R(y-1)\frac{\mathbf{r}}{r}|\phi\rangle \;\; . \end{aligned} \tag{14.35}$$

The action of the exponential term consists in exchanging $y \to y-1$ and in maintaining the direction of $\mathbf{r}$. We rewrite this transformation in terms of r

$$\langle \mathbf{r}|c|\phi\rangle = \frac{R(Y(r)-1)}{r} \sqrt{\frac{s\Big(R(Y(r)-1)\Big)}{s(r)}}\, \langle R(Y(r)-1)\frac{\mathbf{r}}{r}|\phi\rangle \;\; , \tag{14.36}$$

and it inverse relation

$$\langle \mathbf{r}|c^{-1}|\phi\rangle = \frac{R(Y(r)+1)}{r} \sqrt{\frac{s\Big(R(Y(r)+1)\Big)}{s(r)}}\, \langle R(Y(r)+1)\frac{\mathbf{r}}{r}|\phi\rangle \;\; . \tag{14.37}$$

Since the transformations appear only as $R(Y(r) \pm 1)$ we define the symbol

$$R_\pm(r) \equiv R\Big(Y(r) \pm \Big) \;\; ; \;\; R'_\pm(r) = \frac{\partial}{\partial r} R_\pm(r) = \frac{s\Big(R_\pm(r)\Big)}{s(r)} \;\; . \tag{14.38}$$

therefore

$$\langle \mathbf{r}|\hat{c}|\phi\rangle = \frac{R_-(r)}{r}\sqrt{R'_-(r)}\, \langle R_-(r))\frac{\mathbf{r}}{r}|\phi\rangle \;\; ; \;\; \langle \mathbf{r}|\hat{c}^{-1}|\phi\rangle = \frac{R_+(r)}{r}\sqrt{R'_+(r)}\, \langle R_+(r))\frac{\mathbf{r}}{r}|\phi\rangle \;\; . \tag{14.39}$$

The correlated relative distance can be expressed as

$$\underline{\mathbf{r}} = \hat{c}^{-1}\, \mathbf{r}\, \hat{c} = R_+(r)\frac{\mathbf{r}}{r} \;\; . \tag{14.40}$$

Analoguosly, the radial part of the momentum transforms as

$$\underline{\hat{q}}_r = \hat{c}^{-1}\, \hat{q}_r\, c = \frac{1}{\sqrt{R'_+(r)}} \frac{1}{r} \hat{q}_r r \frac{1}{\sqrt{R'_+(r)}} \;\; . \tag{14.41}$$

with

$$\langle r|\hat{q}_r|\phi\rangle = \langle r|\frac{\mathbf{r}}{r}\cdot\hat{\mathbf{q}}|\phi\rangle = -i\hbar\frac{\partial}{\partial r}\, \langle r|\phi\rangle \;\; . \tag{14.42}$$

The correlated angular momentum is the same as the uncorrelated one

$$\underline{\hat{\mathbf{l}}} = \hat{c}^{-1}\, \hat{\mathbf{l}}\, \hat{c} = \hat{c}^{-1}\, (\mathbf{r}\times\hat{\mathbf{q}})\, \hat{c} = \hat{\mathbf{l}} \;\; . \tag{14.43}$$

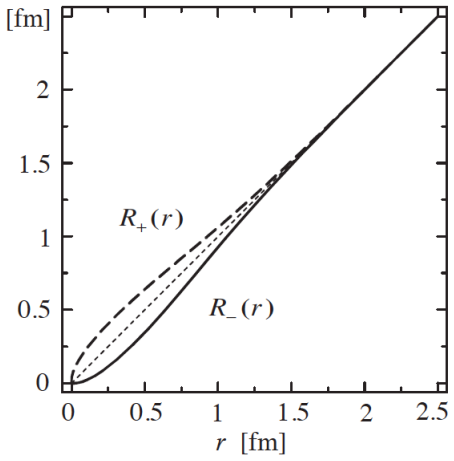

Figure 14.1: Example of transformation of coordinates $R_+(r)$ and of its inverse $R_-(r)$ due to the short-range correlations. The uncorrelated transformation is indicated by the dotted line which is diagonal.

From the transformation presented above, it is possible to deduce the fact that, in coordinate space, the action of every correlated operator $\underline{\hat{b}}(\mathbf{r})$ can be described as that of uncorrelated operator evaluated at a different distance

$$\underline{\hat{b}}(\mathbf{r}) \equiv \hat{c}^{+}\,\hat{b}(\mathbf{r})\,\hat{c} = \hat{c}^{-1}\,\hat{b}(\mathbf{r})\,\hat{c} = \hat{b}\left(R_+(r)\frac{\mathbf{r}}{r}\right) \tag{14.44}$$

This general description must be adapted to the physical situation under study. This means to find a convenient coordinate transformation to describe the physical problem under investigation. There are properties which $R_+(r)$ must have: it has to increase monotonically and must be differentiable in the full dominion. Since the repulsive core of the potential is limited to short relative distances, the effect of the short-range correlation is that of modifying the structure of the uncorrelated wave functions only in the surroundings of the repulsive core. For a nuclear system, Fig. 14.1 shows that $R_+(r)$ is larger than the diagonal, the correlated case, up to about 1.5 fm. After that distance the two transformations coincide. This indicates that the effect of the transformation is that of moving away the interacting particles when they are at relative distances within the repulsive core.

14.3 The correlated hamiltonian

We use the expression of the correlation operators in the coordinate space to write the various terms of the correlated hamiltonian. The easiest term is the two-body term (14.24). In case of purely scalar two-body interaction we obtain

$$\underline{\hat{v}}^{[2]}(i,j) = v\big(R_+(r_{ij})\big) \ , \tag{14.45}$$

where r_{ij} is the distance between the i and j particles.

For the kinetic energy, there is a contribution of the uncorrelated term, as indicated by Eq. (14.15)

$$\tilde{t}^{[1]}(i) = t^{[1]}(i) \tag{14.46}$$

The calculation of the two-body term (14.15) of the kinetic energy is presented here below

---

The total kinetic energy of the fermion pair i e j is given by

$$\hat{t}(i)+\hat{t}(j)=\frac{\hat{\mathbf{q}}_{ij}^2}{m}+\frac{1}{4m}\Big(\hat{\mathbf{p}}(i)+\hat{\mathbf{p}}(j)\Big)^2 \;\text{ with }\; \hat{\mathbf{q}}_{ij}=\frac{1}{2}\Big(\hat{\mathbf{p}}(i)-\hat{\mathbf{p}}(j)\Big)\;. \tag{14.47}$$

Since the correlation term $\hat{g}^{[2]}(i,j)$ commutes with the center of mass, only the term related to the relative momentum is correlated

$$\hat{c}^{-1}\Big(\hat{t}(i)+\hat{t}(j)\Big)\hat{c}=\frac{1}{m}\hat{c}^{-1}\hat{\mathbf{q}}_{ij}^2\hat{c}+\frac{1}{4m}\Big(\hat{\mathbf{p}}(i)+\hat{\mathbf{p}}(j)\Big)^2\;. \tag{14.48}$$

We separate $\hat{\mathbf{q}}_{ij}$ in a radial and angular part

$$\hat{\mathbf{q}}_{ij}^2=\hat{q}_{r\,ji}^{+}\,\hat{q}_{r\,ji}+\frac{\hat{\mathbf{l}}_{ij}^2}{r_{ij}^2}\;\;,\;\;\text{where}\;\;\hat{q}_r=\frac{\mathbf{r}}{r}\cdot\mathbf{q}\;\;\text{and the angular momentum}\,,\;\;\hat{\mathbf{l}}=\mathbf{r}\times\hat{\mathbf{q}}\;\;. \tag{14.49}$$

By using the expressions (14.41) and (14.43) we obtain

$$\begin{aligned}\hat{c}^{-1}\hat{\mathbf{q}}_{ij}^2\hat{c} &= \frac{r_{ij}}{\sqrt{R'_+(r_{ij})}}\hat{q}_{r\,ji}^{+}\frac{1}{r_{ij}^2R'_+(r_{ij})}\hat{q}_{r\,ji}\frac{r_{ij}}{\sqrt{R'_+(r_{ij})}}+\frac{\hat{\mathbf{l}}_{ij}^2}{\Big(R_+(r_{ij})\Big)^2}\\ &\equiv \hat{q}_{r\,ji}^{+}\frac{1}{\Big(R'_+(r_{ij})\Big)^2}\hat{q}_{r\,ji}+\frac{\hat{\mathbf{l}}_{ij}^2}{\Big(R_+(r_{ij})\Big)^2}+m\underline{\hat{u}}^{[2]}(i,j)\end{aligned} \tag{14.50}$$

with the definition

$$\underline{\hat{u}}^{[2]}(i,j)\equiv\frac{1/m}{\Big(R'_+(r_{ij})\Big)^2}\left[2\frac{R''_+(r_{ij})}{r_{ij}R'_+(r_{ij})}-\frac{5}{4}\left(\frac{R''_+(r_{ij})}{R'_+(r_{ij})}\right)^2+\frac{1}{2}\frac{R'''_+(r_{ij})}{R'_+(r_{ij})}\right] \tag{14.51}$$

By considering terms up to the second order in the correlation we can express the hamiltonian as

$$\begin{aligned}\underline{\hat{H}}^{[1]}+\underline{\hat{H}}^{[2]} &= \sum_i^A t(i)\\ &+ \sum_{i<j}^A\left[q_{r\,ij}^{+}\frac{1}{2\mu_r(r_{ij})}q_{r\,ij}+\frac{\mathbf{l}_{ij}^2}{2\mu_r(r_{ij})r_{ij}^2}\right]\\ &+ \sum_{i<j}^A\Big[\tilde{u}^{[2]}(i,j)+\tilde{v}^{[2]}(i,j)\Big]\end{aligned} \tag{14.52}$$

The first term is the uncorrelated kinetic energy, followed by a two-body term depending on the relative momentum of the two interacting particles. The last term of the expression includes a two-body part coming from the kinetic energy and by the correlated interaction. The latter ones is modified in a way that does not present any more the strongly repulsive core.

The calculation continues by evaluating the minimum of the expectation value of this hamiltonian following the variational principle

$$E(\Phi,R_\pm)=\langle\Phi|\hat{C}^{+}(R_-)\hat{H}\hat{C}(R_-)|\Phi\rangle\simeq\langle\Phi|\underline{\hat{H}}^{[1]}+\underline{\hat{H}}^{[2]}|\Phi\rangle \tag{14.53}$$

The variational quantities in the search for the minimum of the energy functional are the coordinate transformation $R_\pm$, and the set of single-particle wave functions defining the IPM state $|\Phi\rangle$.

The symbol $\simeq$ in Eq. (14.53) is due the fact that we considered terms up to two-body in the expression of the correlated hamiltonian. Since the definition of $\hat{C}$ (14.7) involves the presence of operators of any order, up to A, this truncation implies an approximation in the use of the variational principle. Formally, the search for the minimum is a sub-space of the Hamilton space, leads to an energy value greater than the exact eigenvalue of the chosen hamiltonian (see Appendix A). However, in the present case, the hamiltonian is modified, since some part is neglected. The contribution of the neglected parts can increase or decrease the energy eiegenvalue, which is not any more an upper limit to the results.

Clearly, it is possible to go beyond the limit of two-body terms by considering terms od higher order, for example tree-body terms

$$\hat{C} = \exp\left(-i \sum_{i<j} \hat{g}^{[2]}(i,j) - i \sum_{i<j<k} \hat{g}^{[3]}(i,j,k) \right) \quad . \tag{14.54}$$

All the procedure must be reconsidered by including the new term. The equations are rather complicated, and usually the three-body terms are approximated.

14.4 Spin, and isospin, dependent correletions

All the presentation done so far has used purely scalar expressions of the correlation. The complexity of the nuclear interaction requires that the correlations depend also by the spin and the isospin of the interacting nucleons. For this purpose the generator of the unitary correlation operator is decomposed in four different channels.

$$\hat{g}^{[2]}\big(\mathbf{r}, \hat{\mathbf{q}}, \hat{\boldsymbol{\sigma}}(i), \hat{\boldsymbol{\sigma}}(j), \hat{\boldsymbol{\tau}}(i), \hat{\boldsymbol{\tau}}(j)\big) = \sum_{ST}^{\{0,1\}} \hat{g}^{[2]}_{ST}(\mathbf{r}, \hat{\mathbf{q}}) \hat{\Pi}_S \otimes \hat{\Pi}_T \quad , \tag{14.55}$$

where we indicated with the symbol $\hat{\Pi}$ the spin and isospin projection operators

$$\hat{\Pi}_{S=0} = \frac{1}{4}\big(1 - \hat{\boldsymbol{\sigma}}(i) \cdot \hat{\boldsymbol{\sigma}}(j)\big) \quad ; \quad \hat{\Pi}_{S=1} = \frac{1}{4}\big(3 + \hat{\boldsymbol{\sigma}}(i) \cdot \hat{\boldsymbol{\sigma}}(j)\big) \tag{14.56}$$

$$\hat{\Pi}_{T=0} = \frac{1}{4}\big(1 - \hat{\boldsymbol{\tau}}(i) \cdot \hat{\boldsymbol{\tau}}(j)\big) \quad ; \quad \hat{\Pi}_{T=1} = \frac{1}{4}\big(3 + \hat{\boldsymbol{\tau}}(i) \cdot \hat{\boldsymbol{\tau}}(j)\big) \quad . \tag{14.57}$$

The unitary correlation operator is

$$\hat{C}_A = \exp\left(-i \sum_{i<j} \hat{g}^{[2]}(\mathbf{r}_{ij}, \hat{\mathbf{q}}_{ij}, \hat{\boldsymbol{\sigma}}(i), \hat{\boldsymbol{\sigma}}(j), \hat{\boldsymbol{\tau}}(i), \hat{\boldsymbol{\tau}}(j) \right) \quad . \tag{14.58}$$

Also in this case, a truncation to the two-body terms is adopted $\hat{c} \equiv \hat{C}_2$, therefore

$$\hat{c} = \exp\left(-i \sum_{ST}^{\{0,1\}} \hat{g}^{[2]}_{ST}(\mathbf{r}, \hat{\mathbf{q}}) \hat{\Pi}_S \otimes \hat{\Pi}_T \right) = \sum_{ST}^{\{0,1\}} \exp\left(-i \hat{g}^{[2]}_{ST}(\mathbf{r}, \hat{\mathbf{q}}) \right) \hat{\Pi}_S \otimes \hat{\Pi}_T \quad . \tag{14.59}$$

By using the projectors $\hat{\Pi}_{S,T}$ it is possible to express the correlation operator as a sum of four, commuting, correlation operators, one for each channel. With respect to the case of purely scalar correlation, there are four correlation functions $R_+(r)$ to be determined. Usually the $R_\pm(r)$ are expressed by functions containing parameters, and the search for the minimum is done by changing the values of these parameters.

In nuclear physics, UCOM has been applied by using relatively simple two-body potentials. For some nuclei, Fig. 14.2 compares the results obtained with UCOM with those obtained with other microscopic calculations, these latter ones are indicated by the arrows.

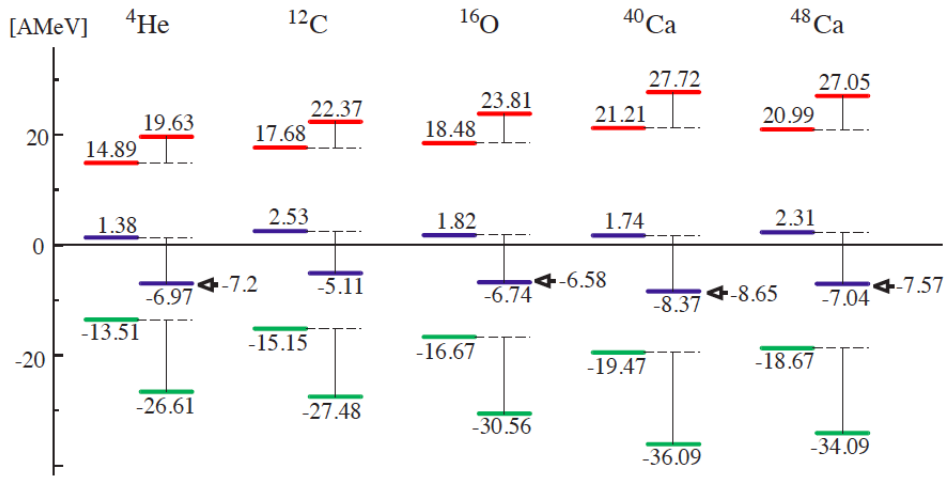

Figure 14.2: Energie per nucleon obtained with UCOM for some nuclei by using a spin dependent potential. The results on the left hand sides are obtained without correlations, while those on the right hand sides with correlations. The red lines indicate the kinetic energies, the green ones the potential energies and the blues lines the total energies. The values indicated by the arrows show the results obtained with other microscopic calculations, Yakubowski for ^{4}He and CBF for other nuclei.

Chapter 15

The Coupled Cluster Method

We presented the CBF theory in Chapt. 13 and the UCOM in Chapt. 14, where the solution of the problem of the strongly repulsive core of the microscopic interactions is concentrated on the definition of the short-range correlation. The language used in these two theories is completely different from that proposed in the Part III of these notes. From the linguistic point view, the Coupled Cluster Method (CCM) is a bridge between the two languages used so far. From the physics point of view it is an approach strictly related to the Statistical Mechanics even though it adopts the concepts of particle and hole states taken from Field Theory. The essential point is that, also in this case, the basic quantity of the theory is the correlation function, which in this case, is described in terms of particle-hole excitations.

15.1 The many-body state in the CCM

In the description of the many-body system, each eigenstate $|\Psi\rangle$ of the total hamiltonian $\hat{H}$ can be expressed as linear combination of Slater determinants formed by single-particle states obtained in the IPM framework (Cap. 2). By using the language presented in Chapter 5, each Slater determinant is characterized by a certain number of particle-hole $(p-h)$ excitations. Obviously, the Slater determinant describing the IPM ground state does not have any excitation of this type. There are Slater determinant containing one-particle one-hole $(1p-1h)$ excitations, states with $(2p-2h)$, and so on, up to consider excitations with $Ap-Ah$.

A way of describing this situation is that of defining operators indicating the number of p-h excitations. For example, for $1p-1h$ we have the operator

$$\hat{S}_1 = \sum_{ph} Z_{ph} \hat{a}_p^+ \hat{a}_h \quad , \tag{15.1}$$

for $2p-2h$ the operator

$$\hat{S}_2 = \frac{1}{(2!)^2} \sum_{p_1 h_1 p_2 h_2} Z_{p_1 h_1 p_2 h_2} \hat{a}_{p_1}^+ \hat{a}_{p_2}^+ \hat{a}_{h_2} \hat{a}_{h_1} \tag{15.2}$$

and for $3p-3h$ the operator

$$\hat{S}_3 = \frac{1}{(3!)^2} \sum_{p_1 h_1 p_2 h_2} Z_{p_1 h_1 p_2 h_2 p_3 h_3} \hat{a}_{p_1}^+ \hat{a}_{p_2}^+ \hat{a}_{p3}^+ \hat{a}_{h_3} \hat{a}_{h_2} \hat{a}_{h_1} \tag{15.3}$$

and so on. The determination of the values of the Z coefficients is the aim of the CCM which uses the variational principle.

Since the hamiltonian includes the two-body interaction term, the simplest type of excitation induced by the hamiltonian is given by the action of $\hat{S}_2$ on the IPM ground state $|\Phi_0\rangle$. This action produces a $\hat{S}_2 |\Phi\rangle$ component of the eigenstate $|\Psi\rangle$ of the total hamiltonian $\hat{H}$. This component considers those states where the two fermions occupying the h_1 and h_2 states below the Fermi surface are promoted such as to occupy the p_1 and p_2 states above the Fermi surface. It is possible to conceive states where this happens without the intervention of the residual interaction of the hamiltonian. This means that the excitations of $2p-2h$ pairs is done independently one of the other one. The simplest case of this type is that of a Slater determinant with $4p-4h$ excitations where the two pairs of $2p-2h$ excitations are not related among them. In general, the components of the total wave function described by excitations of this type are described by applying m-times the $\hat{S}_2$ operator. In this case, the component of the total wave function is

$$\frac{1}{m!}\hat{S}_2^m |\Phi_0\rangle \quad ,$$

where the $1/m!$ term takes care of the double counting. The total contribution of $2m$-particles and $2m-$holes is:

$$\sum_{m=0}^{\infty} \frac{1}{m!}\hat{S}_2^m |\Phi_0\rangle = e^{\hat{S}_2} |\Phi_0\rangle \quad . \tag{15.4}$$

Obviously, for $m > A/2$ there are not excitations, therefore the sum is, in fact, truncated. However, it is convenient to formally express the contribution of the various $p-h$ excitations by using exponential expressions.

The contribution to the total wave function of $3p-3h$ independent excitations is

$$\frac{1}{p!}\hat{S}_3^p |\Phi_0\rangle \quad .$$

The contribution of a set of m $2p-2h$ and p $3p-3h$ excitations all independent of each other is

$$\frac{1}{m!p!}\hat{S}_3^p \hat{S}_2^m |\Phi_0\rangle \quad .$$

Since the excitations are independent of each other, the operators $\hat{S}_2$ and $\hat{S}_3$ commutes. This means that all the indexes p and h identifying the creation and destruction operators are different from each other. By expressing everything in terms of infinite sums we obtain for the total contribution the expression

$$e^{\hat{S}_2+\hat{S}_3} |\Phi_0\rangle \quad ,$$

and systematically continuing with $np-nh$ excitations we arrive to the expression

$$e^{\hat{S}_2+\hat{S}_3+\cdots+\hat{S}_A} |\Phi_0\rangle \quad .$$

In the interaction between the various particle clusters it is possible to excite also $1p-1h$ states. For this reason, it is possible to write

$$|\Psi\rangle = e^{\hat{S}} |\Phi_0\rangle \quad \text{with} \quad \hat{S} = \sum_{n=1}^{A} \hat{S}_n \quad . \tag{15.5}$$

A different method to describe the same kind of physics is that of expressing the $\hat{H}$ eigenstate as

$$|\Psi\rangle = \left(1 + \sum_{n=1}^{A} \hat{F}_n\right) |\Phi_0\rangle \quad , \tag{15.6}$$

with the definition

$$\hat{F}_n \equiv \frac{1}{(n!)^2} \sum_{p_1 \cdots p_n, h_1 \cdots h_n} \Lambda_{p_1 \cdots p_n, h_1 \cdots h_n} \hat{a}^+_{p_1} \cdots \hat{a}^+_{p_n} \hat{a}_{h_n} \cdots \hat{a}_{h_1} \quad , \tag{15.7}$$

where the amplitudes Λ are numbers.

The two operators $\hat{S}_n$ and $\hat{F}_n$ describe the same state in terms excitations of $np-nh$ type. The relation between these two pictures is

$$\begin{aligned}
\hat{F}_1 &= \hat{S}_1 \\
\hat{F}_2 &= \hat{S}_2 + \frac{1}{2}\hat{S}_1^2 \\
\hat{F}_3 &= \hat{S}_3 + \hat{S}_2\hat{S}_1 + \frac{1}{6}\hat{S}_1^3 \\
\hat{F}_4 &= \hat{S}_4 + \hat{S}_3\hat{S}_1 + \frac{1}{2}\hat{S}_2^2 + \frac{1}{2}\hat{S}_2\hat{S}_1^2 + \frac{1}{24}\hat{S}_1^4 \\
\hat{F}_5 &= \cdots
\end{aligned}$$

These expressions clarify the difference between these two types of operators. The operators $\hat{S}_n$ describe connected clusters of $np-nh$ excitations, while the operators $\hat{F}_n$ describe all the possible $np-nh$ excitations, also those induced by non-connected excitations clusters.

15.2 The CCM equations

We obtain here a set of equations which allows the determination of the amplitudes Z of the equations (15.1, 15.2, 15.3). We write the Schrödinger equation, and express the wave function by using Eq. (15.5)

$$E_0 \left|\Psi_0\right\rangle = \hat{H} \left|\Psi_0\right\rangle = \hat{H} e^{\hat{S}} \left|\Phi_0\right\rangle \quad . \tag{15.8}$$

We consider the overlap of this equation on states of the type

$$\begin{aligned}
&\left\langle\Phi_0\right| \hat{a}^+_{h_1} \hat{a}_{p_1} \\
&\left\langle\Phi_0\right| \hat{a}^+_{h_2} \hat{a}^+_{h_1} \hat{a}_{p_1} \hat{a}_{p_2} \\
&\left\langle\Phi_0\right| \hat{a}^+_{h_3} \hat{a}^+_{h_2} \hat{a}^+_{h_1} \hat{a}_{p_1} \hat{a}_{p_2} \hat{a}_{p_3} \qquad .
\end{aligned} \tag{15.9}$$

It is convenient to rewrite the $\hat{S}$ operators by using the expression

$$\hat{S} = \sum_{n \neq 0} \mathcal{S}_n \hat{C}^+_n \tag{15.10}$$

where the $\mathcal{S}_n$ are numbers, and the $\hat{C}^+_n$ operator represents the set of the n pairs of creation and destruction operators which characterize it

$$\hat{C}^+_n = \hat{a}^+_{p_1} \cdots \hat{a}^+_{p_I} \hat{a}_{h_I} \cdots \hat{a}_{h_1} \quad . \tag{15.11}$$

Let's multiply the Schrödinger equation, on the left hand side, by $e^{-\hat{S}}$

$$e^{-\hat{S}} \hat{H} e^{\hat{S}} \left|\Phi_0\right\rangle = e^{-\hat{S}} \hat{H} \left|\Psi_0\right\rangle = e^{-\hat{S}} E_0 \left|\Psi_0\right\rangle = e^{-\hat{S}} E_0 e^{\hat{S}} \left|\Phi_0\right\rangle = E_0 \left|\Phi_0\right\rangle \quad , \tag{15.12}$$

and, therefore, by projecting on the $\left\langle\Phi_0\right|$ state we have

$$E_0 = \langle\Phi_0| e^{-\hat{S}} \hat{H} e^{\hat{S}} |\Phi_0\rangle = \langle\Phi_0| \hat{H} e^{\hat{S}} |\Phi_0\rangle \quad . \tag{15.13}$$

The last equality has been obtained by considering that

$$\langle\Phi_0|\, e^{-\hat{S}} = \langle\Phi_0| \sum_{n=0}^{\infty} \frac{(\hat{S}_n)^n}{n!} = \langle\Phi_0|\, \hat{S}_0 = \langle\Phi_0| \quad , \tag{15.14}$$

because $\hat{S}_{n>0}$ contains creation operators above the Fermi surface such as $\langle\Phi_0|\, \hat{a}_p^+ = 0$.

By projecting the eiegenvalue equation (15.12) on states containing particles and holes, such as those indicated in Eq. (15.9), we encounter equations of the type

$$\langle\Phi_0|\hat{C}_n e^{-\hat{S}} \hat{H} e^{\hat{S}}|\Phi_0\rangle = 0 \;\text{ with }\; n > 0 \;\; . \tag{15.15}$$

The expressions (15.15) indicates a set of connected equations related to different number of particle-hole excitations, indicated by the operator $\hat{C}_n$.

It is possible to express the operator term of Eq. (15.12) as a set of connected commutators

$$\begin{aligned} e^{-\hat{S}} \hat{H} e^{\hat{S}} &= \hat{H} + [\hat{H}, \hat{S}] + \frac{1}{2!}\big[[\hat{H}, \hat{S}], \hat{S}\big] + \frac{1}{3!}\Big[\big[[\hat{H}, \hat{S}], \hat{S}\big], \hat{S}\Big] + \cdots \\ &= \hat{H} + \sum_n \mathcal{S}_n [\hat{H}, \hat{C}_n^+] + \frac{1}{2} \sum_{n,m} \mathcal{S}_n \mathcal{S}_m \big[[\hat{H}, \hat{C}_n^+], \hat{C}_m^+\big] + \cdots \end{aligned} \tag{15.16}$$

This expression inserted in Eq. (15.15) generates a system of equations whose unknown are the amplitudes $\mathcal{S}_n$.

The expression (15.16) has an infinite number of terms. In reality one has to realize that, in the calculation of the expectation value with respect to $|\Phi_0\rangle$ there is a truncation of the sum. This can be understood by considering that the $\hat{C}_n^+$ commutes $[\hat{C}_n^+, \hat{C}_m^+] = 0$. This implies that, in the evaluation of the contractions only those indexes relating the free indexes of the hamiltonian with the fixed ones of the C_n^+ operators, are different from zero. For this reason the series is naturally truncated. For example, for a hamiltonian containing only two-body terms, i.e. a two-body interaction, the sum ends with commutators up to the fourth order:

$$\begin{aligned} &\langle\Phi_0|\hat{C}_n \hat{H}|\Phi_0\rangle + \sum_m \mathcal{S}_m \langle\Phi_0|\hat{C}_n [\hat{H}, \hat{C}_m]|\Phi_0\rangle \\ &+\frac{1}{2!} \sum_{m,p} \mathcal{S}_m \mathcal{S}_p \langle\Phi_0|\hat{C}_n \big[[\hat{H}, \hat{C}_m^+], \hat{C}_p^+\big]|\Phi_0\rangle \\ &+\frac{1}{3!} \sum_{m,p,q} \mathcal{S}_m \mathcal{S}_p \mathcal{S}_q \langle\Phi_0|\hat{C}_n \Big[\big[[\hat{H}, \hat{C}_m^+], \hat{C}_p^+\big], \hat{C}_q^+\Big]|\Phi_0\rangle \\ &+\frac{1}{4!} \sum_{m,p,q,r} \mathcal{S}_m \mathcal{S}_p \mathcal{S}_q \mathcal{S}_r \langle\Phi_0|\hat{C}_I \Big[\Big[\big[[\hat{H}, \hat{C}_m^+], \hat{C}_p^+\big], \hat{C}_q^+\Big], \hat{C}_r^+\Big]|\Phi_0\rangle = 0 \end{aligned} \tag{15.17}$$

This because the two-body term of the hamiltonian contains four creation and destruction operators, and it is necessary a $\hat{C}^+$ to saturate the creation and destruction operators of the $\hat{C}$ applyed to $\langle\Phi_0|$.

Once the number of $p-h$ excitations defining the bra state, that is $\hat{C}_I$, has been defined, the expression (15.17) indicates a closed, and finite, set of connected equations whose unknows are the $\mathcal{S}_n$, strictly related to the Z amplitudes of Eqs. (15.1, 15.2, 15.3).

15.3 Approximations

The computational scheme presented in the previous sections requires the calculation of Eq. (15.13) to obtain the ground state energy. This calculation can be done by solving Eqs. (15.17) which give the $\mathcal{S}_n$

amplitudes. If in Eq. (15.10) only the $\hat{C}_1$ and $\hat{C}_2$ operators are chosen, then the following equations must be solved

$$\sum_{ph} \langle \Phi_0 | \hat{a}_h^+ \hat{a}_p e^{-\hat{S}} \hat{H} e^{\hat{S}} | \Phi_0 \rangle = 0 \ , \tag{15.18}$$

and

$$\sum_{p_1 h_1 p_2 h_2} \langle \Phi_0 | \hat{a}_{h_2}^+ \hat{a}_{h_1}^+ \hat{a}_{p_2} \hat{a}_{p_1} e^{-\hat{S}} \hat{H} e^{\hat{S}} | \Phi_0 \rangle = 0 \ . \tag{15.19}$$

The computational cost of this calculation scales as the square of the number of the hole states and the fourth power of the particle states. The solutions obtained in this manner are not satisfactory, and it is necessary to improve the approximation inserted in the truncation of the sum of Eq. (15.10). On the other hand, the use of C_3 requires a very heavy computational cost scaling with the cube of the number of hole states, and the fifth power of the particle states.

For this reason, in actual calculation it is adopted a different strategy. Let's define an eigenvalue problem related to the bra state as

$$\langle \Phi_0 | \, \hat{\Lambda} e^{-\hat{S}} \hat{H} e^{\hat{S}} = E_0 \langle \Phi_0 | \, \hat{\Lambda} \ , \tag{15.20}$$

where $\hat{\Lambda}$ is an operator, called of de-excitation, defined as:

$$\hat{\Lambda} = \hat{\mathbb{I}} + \sum_{I>0} \hat{\Lambda}_I \hat{C}_I = \hat{\mathbb{I}} + \sum_{ph} \lambda_{ph} \hat{a}_h^+ \hat{a}_p + \sum_{p_1 h_1 p_2 h_2} \lambda_{p_1 p_2 h_1 h_2} \hat{a}_{h_2}^+ \hat{a}_{h_1}^+ \hat{a}_{p_2} \hat{a}_{p_1} \cdots \ , \tag{15.21}$$

where the λ are numbers. Since

$$\langle \Phi_0 | \hat{C}_{I>0} | \Phi_0 \rangle = 0 \ ,$$

the result of Eq. (15.20) is trivial

$$\langle \Phi_0 | \, \Lambda e^{-\hat{S}} \hat{H} e^{\hat{S}} = \langle \Phi_0 | \, e^{-\hat{S}} \hat{H} e^{\hat{S}} = \langle \Phi_0 | \, E_0 = E_0 \langle \Phi_0 | \, \Lambda \ .$$

The idea is to consider the eigenvalue equation (15.20) and to project it on $\hat{C}_n^+ | \Phi_0 \rangle$ states

$$\langle \Phi_0 | \Lambda (e^{-\hat{S}} \hat{H} e^{\hat{S}} - E_0) \hat{C}_n^+ | \Phi_0 \rangle = 0 \ \text{ with } \ n > 0 \ . \tag{15.22}$$

At this point, the problem is solved in two steps. First the CCM equations (15.17) are solved, and then the (15.18) and (15.19) in case of truncation up to C_2. Once the aplitudes $\mathcal{S}_1$ and $\mathcal{S}_2$ have been obtained, the Eqs. (15.22) are solved to obtain the Λ_n, in the present case one has to consider Λ_1 and Λ_2 only.

15.4 Excited states

The most common application of the CCM concern the ground state of the many-body system. On the other hand, it is possible to consider, in the CCM framework, a set of equations which describe the excited states. Essentially, it is matter of reformulating the CCM equations in such a way to rewrite them as the equation of motion described in Chapter (10.1). In analogy to what has been done there, let's define an operator $\hat{Q}_\nu^+$ which generates the excited states of the system.

$$| \Psi_\nu \rangle = \hat{Q}_\nu^+ | \Psi_0 \rangle = \hat{Q}_\nu^+ e^{\hat{S}} | \Phi_0 \rangle \ , \tag{15.23}$$

where ν indicates the quantum numbers which identify the excited state. The Schrödinger equations which must be satisfied are:

$$\hat{H} | \Psi_\nu \rangle = \hat{H} \hat{Q}_\nu^+ | \Psi_0 \rangle = \hat{H} \hat{Q}_\nu^+ e^{\hat{S}} | \Phi_0 \rangle = E_\nu | \Psi_\nu \rangle = E_\nu \hat{Q}_\nu^+ e^{\hat{S}} | \Phi_0 \rangle \tag{15.24}$$

$$\hat{H} | \Psi_0 \rangle = \hat{H} e^{\hat{S}} | \Phi_0 \rangle = E_0 e^{\hat{S}} | \Phi_0 \rangle \ . \tag{15.25}$$

Let's multiply by $e^{-\hat{S}}$ the first equation

$$e^{-\hat{S}}\hat{H}\left|\Psi_\nu\right\rangle = e^{-\hat{S}}\hat{H}\hat{Q}_\nu^+ e^{\hat{S}}\left|\Phi_0\right\rangle e^{-\hat{S}}E_\nu\hat{Q}_\nu^+ e^{\hat{S}}\left|\Phi_0\right\rangle = E_\nu\hat{Q}_\nu^+ e^{-\hat{S}}e^{\hat{S}}\left|\Phi_0\right\rangle = E_\nu\hat{Q}_\nu^+\left|\Phi_0\right\rangle \quad ,$$

and by $\hat{Q}_\nu^+ e^{-\hat{S}}$ the second equation

$$\hat{Q}_\nu^+ e^{-\hat{S}}\hat{H}\left|\Psi_0\right\rangle = \hat{Q}_\nu^+ e^{-\hat{S}}\hat{H}e^{\hat{S}}\left|\Phi_0\right\rangle = E_0\hat{Q}_\nu^+ e^{-\hat{S}}e^{\hat{S}}\left|\Phi_0\right\rangle = E_0\hat{Q}_\nu^+\left|\Phi_0\right\rangle \quad ,$$

where we used the fact that $[\hat{Q}_\nu^+, S] = 0$. By subtracting the second equation from the first one, and using the commutation between $\hat{Q}_\nu^+$ and $\hat{S}$, we obtain

$$\left(e^{-\hat{S}}\hat{H}e^{\hat{S}}\hat{Q}_\nu^+ - \hat{Q}_\nu^+ e^{-\hat{S}}\hat{H}e^{\hat{S}}\right)\left|\Phi_0\right\rangle = (E_\nu - E_0)\hat{Q}_\nu^+\left|\Phi_0\right\rangle \quad . \tag{15.26}$$

Eq. (15.26) can be rewritten as

$$[\hat{H}_{\rm eff}, \hat{Q}_\nu^+]\left|\Phi_0\right\rangle \equiv \left[e^{-\hat{S}}\hat{H}e^{\hat{S}}, \hat{Q}_\nu^+\right]\left|\Phi_0\right\rangle = (E_\nu - E_0)\hat{Q}_\nu^+\left|\Phi_0\right\rangle \equiv \omega_\nu\hat{Q}_\nu^+\left|\Phi_0\right\rangle \tag{15.27}$$

with the obvious definition of the effective hamiltonian $\hat{H}_{\rm eff}$ and of the excitation energy ω_ν. This equation is analogous to Eq. (10.3) which is the base of the equation of motion.

15.5 Applications

The CCM calculations are very complicated, also from the numerical point of view. The application of the method are limited to relatively simple systems, with very well defined simmetries.

The parameters to be considered to define the problems are the choice of C_n, i.e. the number of $p-h$ to be considered. This choice sets the configuration space, specifically the number of particle states, those above the Fermi surface. On the basis of these choices the CCM calculations are catalogued with different acronyms. Unfortunately each research field has its own way of making this catalogue, and this create some problem in comparing calculations carried out in different fields.

We summarize here below some important points of the results obtained which are, in any case, in continuous evolution, this is also related to the advances of the computer facilities.

Systems interacting with Coulomb interaction
In this case the hamiltonian is well defined and it contains only the two-body scalar term of Coulomb type. The electronic properties of simple atoms and molecules are evaluated. The results obtained by restricting to the $\hat{C}_2$ choice compare well with to those obtained with the GFMC. The differences between binding energies, and also ionization energies, of some molecules studied are of 1-2 %. The comparison with the experimental value has differences of the same order of magnitude.

Nuclear systems
The comparison between CCM results and those obtained with other microscopic calculations has been done for spherical systems and for nuclear interactions which exclude tensor and spin-orbit terms. For the few-body system ^{4}He the differences between the binding energies calculated with GFMC and with CCM with approximations related to $\hat{C}_2$, are of about 6% circa. The other system studied is the ^{16}O nucleus. In this case the theoretical results of reference is obtained with FHNC-1. The differences are strictly related to the approximations used to deal the $\hat{C}_2$ choice. With an approximation there are differences of about 20%, with another approximation the differences are even smaller than 1%. This only means that FHNC-1 and the approximation chosen for the CCM calculations describe the same physics. There are recent calculations for Ca isotopes carried out with microscopic interactions taken from effective field theories which are extremely promising in the comparison with experimental data.

He atoms drops
A very useful system to verify the validity of the many-body theories is that of the He drops. Is is matter of constructing many-body systems where the fundamental particles are helium atoms. The system can be bosonic in case the nuclei of the helium atoms are ^{4}He, or fermionic in case they are ^{3}He. The interaction is purely scalar and contains a repulsive core, as discussed in Chapter 3.4. It is interesting to study how these system get bound as a function of the particle numbers.

	N	VMC	CCM
He_4	20	- 30.44	- 32.73
	40	- 93.44	- 98.17
He_3	20	4.12	3.44
	40	- 1.44	- 2.55

Table 15.1: Binding energies in K, for bosonic systems, He_4, and fermionic systems, He_3, of helium atoms. Adapted from [Nav02].

We show in Tab. 15.1 the comparison between the CCM results and those obtained with VMC. The relative differences between the results of the two calculations are smaller for the bosonic than for the fermionic systems. The bosonic system are more bound than the fermionic ones. The fermionic system with 20 atoms is not bound while it is bound that with 40 particles.

Part V

Phenomenological theories

Chapter 16

Effective theories

The aim of the theories so far presented was the solution of the Schrödinger equation with microscopic hamiltonians, those presented in Chapter 3 which contain interaction tailored to reproduce the properties of two-body, and, eventually, also three-body, systems. Since these interactions have a strongly repulsive core at small interacting distances, these theories developed different non-perturbative methods to handle this feature of the interaction.

In the theories inspired to the Quantum Field Theory, the approach consists in transforming the microscopic interaction and build another interaction where the repulsive core is not present any more. For example, in Brueckner's theory this goal is acheived by summing all the ladder diagrams, see Chapter 8. In theories inspired to the Statistical Mechanics, such as CBF, the problem of the repulsive core is tackled by using a correlation functions which inhibits the two interacting particles to get too close to each other. In all these approaches the hamiltonian is a quantity external to the theory which is developed independently of its form.

The effective theories tackle the many-body problem by using a different point of view. The idea is to find an effective hamiltonian which, working on a sub-space of the full Hilbert space, is able to reproduce the same eigenvalues of the true hamiltonian. This means that the equation

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle \ , \tag{16.1}$$

is substituted by the equation

$$\hat{H}^{\rm eff}|\Psi_n^{\rm eff}\rangle = E_n|\Psi_n^{\rm eff}\rangle \ . \tag{16.2}$$

Formally, we can find the relation between $\hat{H}$ and $\hat{H}^{\rm eff}$ by using the separation of the hamiltonian in two parts $\hat{H} = \hat{H}_0 + \hat{H}_1$, and by considering the projection operator $\hat{P}$ on the $\hat{H}_0$ eigenstates, and the operator $\hat{Q}$ which is its complement

$$\hat{P}^2 = \hat{P} \ ; \ \hat{Q}^2 = \hat{Q} \ ; \ \hat{Q} = \hat{\mathbb{I}} - \hat{P} \ ; \ \hat{P}\hat{Q} = 0 \ , \tag{16.3}$$

where

$$\hat{H}_0\hat{P}|\Psi_n\rangle = E_n^0\hat{P}|\Psi_n\rangle \Rightarrow \hat{P}\hat{H}_0|\Psi_n\rangle = E_n^0\hat{P}|\Psi_n\rangle \ , \tag{16.4}$$

since $\hat{P}$ and $\hat{H}_0$ commute. Eq. (16.1) can be rewritten as

$$\hat{H}_1|\Psi_n\rangle = (E_n - \hat{H}_0)|\Psi_n\rangle \ , \tag{16.5}$$

and by multiplying to the left hand side $\hat{P}$, we obtain

$$\begin{aligned} \hat{P}\hat{H}_1|\Psi_n\rangle &= \hat{P}(E_n - \hat{H}_0)|\Psi_n\rangle = (E_n - \hat{H}_0)\hat{P}|\Psi_n\rangle \\ \hat{P}\hat{H}_1(\hat{P}+\hat{Q})|\Psi_n\rangle &= (E_n - \hat{H}_0)\hat{P}|\Psi_n\rangle \\ \hat{P}\hat{H}_1\hat{Q}|\Psi_n\rangle &= (E_n - \hat{H}_0 - \hat{P}\hat{H}_1)\hat{P}|\Psi_n\rangle \ . \end{aligned} \tag{16.6}$$

Working in analogous manner, and by multiplying on the left hand side by $\hat{Q}$, we have

$$\hat{Q}\hat{H}_1\hat{P}|\Psi_n\rangle = (E_n - \hat{H}_0 - \hat{Q}\hat{H}_1)Q|\Psi_n\rangle \ . \tag{16.7}$$

By using the properties of these two operators, we can rewrite the two equations as

$$\begin{aligned} (\hat{P}\hat{H}_1\hat{Q})\hat{Q}|\Psi_n\rangle &= (E_n - \hat{H}_0 - \hat{P}\hat{H}_1\hat{P})\hat{P}|\Psi_n\rangle & (16.8)\\ (\hat{Q}\hat{H}_1\hat{P})\hat{P}|\Psi_n\rangle &= (E_n - \hat{H}_0 - \hat{Q}\hat{H}_1\hat{Q})\hat{Q}|\Psi_n\rangle \ . & (16.9) \end{aligned}$$

We obtain $Q|\Psi_n\rangle$ from Eq. (16.9) and we substitute it in Eq. (16.8), the result is

$$\begin{aligned} (\hat{P}\hat{H}_1\hat{Q})\frac{1}{E_n - \hat{H}_0 - \hat{Q}\hat{H}_1\hat{Q}}(\hat{Q}\hat{H}_1\hat{P})\hat{P}|\Psi_n\rangle &= (E_n - \hat{H}_0 - \hat{P}\hat{H}_1\hat{P})\hat{P}|\Psi_n\rangle \\ \left[\hat{H}_0 + \hat{P}\left(\hat{H}_1 + \hat{H}_1\hat{Q}\frac{1}{E_n - \hat{H}_0\hat{Q}\hat{H}_1\hat{Q}}\hat{Q}\hat{H}_1\right)\hat{P}\right]\hat{P}|\Psi_n\rangle &= E_n\hat{P}|\Psi_n\rangle \ . \end{aligned} \tag{16.10}$$

This equation has the structure of Eq. (16.2) and it is possible to identify the effective interaction with the term

$$\hat{V}^{\text{eff}} = \hat{P}\left(\hat{H}_1 + \hat{H}_1\hat{Q}\frac{1}{E_n - \hat{H}_0\hat{Q}\hat{H}_1\hat{Q}}\hat{Q}\hat{H}_1\right)\hat{P} \ . \tag{16.11}$$

A first consideration is that the effective interaction depends on the energy E_n. A second consideration, more important in the present context, is that the effective interaction depends on $\hat{P}$, or how the hamiltonian is separated. The effective interaction is strictly related to the theory where it is used. Every theory has its own effective interaction.

The derivation presented above has a purely formal value to show how, in principle, it is possible to rigorously define the effective theories and relate them to the microscopic theories. From the practical point of view, finding the solution of these equations is as complicated as to solve directly the original Schrödinger equation.

The problem is tackled with phenomenological approaches, by using interactions containing parameters whose values are chosen such that the theory can reproduce selected empirical data of the many-body system under investigation. Clearly the aim of the theory is to make predictions on different quantities whit respect to those used to define the interaction. These phenomenological effective interactions have different characteristics with respect to the microscopic ones, especially they do not have the strongly repulsive core at short distances. In general, the effective theories tackle, and solve, the many-body problem in a much simpler manner than the microscopic theories. For this reason they are widely used in the comparison with the experimental data, especially if the systems to be described are very complex, that is without evident symmetries. Effective interactions are widely used in mean-field approaches such as HF and DFT. The connection between effective and microscopic theories is a very active research field.

Chapter 17

The Fermi liquid theory

17.1 Introduction

One of the effective theories of major success is that of the Fermi liquids formulated by L. V. Landau at the end of the 50's of last century and perfected by other authors, mainly of the Russian school. The basic idea is that a system of interacting particles can be described by a set of non-interacting quasi-particles. This step is far from being trivial. It is possible to add a particle to a set of non-interacting quasi-particles with the only condition that the state of the new particle must be above the Fermi surface. This system will remain stable. When the interaction is switched on the added fermion can induce particle-hole ($p-h$) excitations which will conduct the system to decay in a new ground state. Also the energy of the added fermion will be modified, and this case can be interpreted as the state of the added fermion is unstable and decays. The idea that all the states of non-interacting fermions can be transformed in quasi-particle states, i.e. dressed by the interaction, is wrong. On the other hand, if the energy of the added fermion is very closed to the Fermi energy, the Pauli exclusion principle blocks the possibility of decaying since the density of the accessible final states is very small, if not even zero. Therefore, it is plausible to assume that those states closed to the Fermi surface can be described in terms of quasi-particle states.

The theory of the Fermi liquids was originally formulated by Landau to describe infinite fermionic systems, especially the fermionic liquid helium, composed by fermionic atoms since their nuclei are those of the isotope ^{3}He. The Landau theory is an excellent example of effective theory and its success pushed towards its extension to treat finite systems and atomic nuclei.

17.2 Adiabatic continuity

The basic idea of the Fermi liquid theory is the possibility of transforming a many-body system of non-interacting particles in a system of interacting particles by adiabatically switching on the interaction. We have already used this trick in Sect. 6.4 as a theoretical-mathematical expedient to link the two systems. In the case of Fermi liquid theory the assumption has a more phenomenological ground, therefore it deserves a deeper discussion in order to define better the validity and its limits.

To clarify better the situation, we consider a one-dimensional toy model, where the particles interact with a potential which allows a factorization of the time and space dependent terms

$$\hat{V}(x,t) = -V_0(t)V_x(x) \ , \tag{17.1}$$

The depth of the potential changes with the time between the initial value $V_0(1)$ and the final one $V_0(2)$.

The single-particle Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}\phi(x,t) = \hat{H}(t)\phi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}(x,t)\right)\phi(x,t) \ . \tag{17.2}$$

If we assume that $V_0(t)$ changes its value in a sensitive manner with respect to the initial value, and also with respect to the kinetic energy, much more slowly of the changes of the particle the wave function, we can search for an adiabatic solution which consider $V_0(t)$ as a constant

$$\phi_{\rm adia}(x,t) \simeq \phi_{V_0(t)}(x)e^{-\frac{i}{\hbar}E_{V_0(t)}t} \ , \tag{17.3}$$

where $E_{V_0(t)}$ is the eigenvalue of the time independent Schrödinger equation of which $\phi_{V_0(t)}(x)$ is eigenstate

$$\hat{H}(t)\,\phi_{V_0(t)}(x) = E_{V_0(t)}\,\phi_{V_0(t)}(x) \ . \tag{17.4}$$

By inserting the expression (17.3) in Eq. (17.2) we obtain

$$i\hbar\frac{\partial}{\partial t}\phi_{\rm adia}(x,t) = \hat{H}(t)\phi_{\rm adia}(x,t) = E_{V_0(t)}\,\phi_{\rm adia}(x,t) + i\hbar\left(\frac{\partial\phi_{\rm adia}(x,t)}{\partial V_0(,t)}\right)\left(\frac{\partial V_0(t)}{\partial t}\right) \ . \tag{17.5}$$

The assumption that the expression (17.3) is eigenstate of the hamiltonian becomes more valid the smaller becomes the second term of the expression, in other words, when the derivative of $V_0(t)$ with respect to the time becomes small. If the rate of changes of $V(t)$ is sufficiently small with respect to the times involved in the study, it is possible to reach the final value $V_0(2)$ by making small changes of the solution, starting from $V_0(1)$ up to when the new value is reached. The essential point is that this procedure does not allows discontinuities. For example, if the initial state is a bound state, also the final one must be a bound state. There is no possibility to reach a final state which contains particles in the continuum, a ionized atomic state, for example. The same can be said for the phase transitions, which cannot be described by this procedure.

17.3 The concept of quasi-particle

The properties of fermionic system with translational invariance, called Fermi gas, have been presented in Sect. 2.3. The single-particle wave functions are plane waves characterized by a wave number $\mathbf{k}$ related to momentum by the relation $\mathbf{p} = \hbar\mathbf{k}$, Eq. (2.40). The eigenstates of this system are Slater determinant formed by plane waves. In order to define the eigenstate of this system it is sufficient to indicate which eigenstates of $\mathbf{k}$ are occupied. For this reason, it is convenient to use the distribution function $n(k)$, which indicates the probability density of finding a fermion with module of $\mathbf{k}$ between k and $k+dk$. The distribution function depends only on the module of the wave vector for the isotropy of the medium. In the ground state the distribution function is $n(k) = \Theta(k_{\rm F}-k)$ where $k_{\rm F}$ is the Fermi wave number and Θ the step function.

The distribution function $n(k)$ for the ground state of the Fermi gas is shown in Fig.17.1.

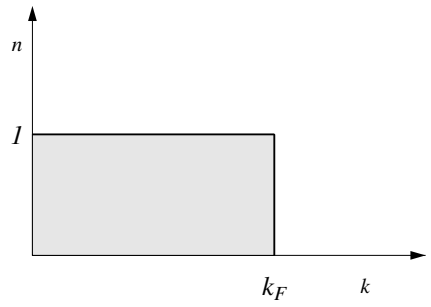

Figure 17.1: Distribution function $n(k)$ for the Fermi gas ground state.

By using the language of Chapter 5, we can say that the excited states of this system are generated by the creation of particle-hole, $(p-h)$, pairs. The description of excited states whose excitation energies are smaller with respect to the total energy of the system is done by considering small fluctuations $\delta n(k)$ of the distribution

$n(k)$ of the ground state. The ground state energy is modified by these fluctuations by the value

$$\delta E = \sum_k \frac{\hbar^2 k^2}{2m} \delta n(k) \ . \tag{17.6}$$

The single particle energy is obtained as functional derivative of the energy $\delta E/\delta n(k) = \hbar^2 k^2/2m$. Since removing a particle, i.e. creating a hole state, reduces the value of the total energy, then $\delta n(k)$ must be negative. Obviously, the contrary is valid for the creation of a particle.

These are considerations referred to a gas of non-interacting fermions. The situation is more complicated when the interaction between fermions becomes active. The idea of Landau is to go from the description of a system of non-interacting fermions, which we shall call Fermi gas henceforth, to that of interacting fermion system, which we shall call real system, by adiabatically switching on the interaction. In this procedure there is the assumption that the evolution of the Fermi gas ground state leads to the ground state of the real system. It is worth to notice that this assumption does not exclude that in the real system some states can be formed, but they disappear when the interaction is switched off.

Let's add to the Fermi gas a particle with $k > k_{\rm F}$, and then let's switch on the interaction. In this way a state of the real system has been obtained. We can say that we added a *quasi-particle* with wave number k to the ground state of the real system. In analogy, we call *quasi-hole* of wave number $k < k_{\rm F}$ the situation where a fermion is removed by the Fermi gas and then the interaction is activated.

There are properties of the system described by operators which commute with the hamiltonian and they are the same in the Fermi gas and the real system; for example the number of particles, the electric charge, the current, the spin. For this reason, the quasi-particles can be characterized by quantum numbers indicating the particles momentum $\mathbf{p}$, spin, electric charge, etc.

The description of the excitations of a real system in terms of creation and destruction of quasi-particles is restricted to a limited time window. The times of these excitations must be shorter than those required by the system to return in its ground state. Since this latter effect is due to the elastic scattering of the quasi-particles, we can say that the time required by the excitation of a quasi-particle pair must be smaller of the typical time required by the elastic scattering of the quasi-particles. On the other hand, these times must be sufficiently long to ensure that the quasi-particle has a defined energy in agreement with the energy-time relation $\Delta E \Delta t \geq \hbar$.

For what we have outlined above, the quasi-particles conserve all the particle quantum numbers, therefore also the feature of being fermions. For this reason, the quasi-particle momentum distribution in the real system is represented by Fig. 17.1, and the notion of Fermi surface remains valid also for the quasi-particles. The excitation of the system is measured by the deviation

$$\delta n(k) = n(k) - n^0(k) \tag{17.7}$$

where $n^0(k)$ indicates the quasi-particle distribution of the ground state, represented in Fig. 17.1.

The notion of quasi-particle is valid only when the values of $\delta n(k)$ are remarkably different from zero for $k \simeq k_{\rm F}$. The statement that the real system is composed by quasi-particles filling all the states up to the Fermi surface, is wrong. The quasi-particles is an elementary excitation of the real system for states which are close to the ground state. This means that the excitation energy is much smaller than the binding energy. The Fermi liquid theory does not provide information on the system ground state but it aims to a description of small fluctuation around it.

In this theory, the energy of the system E is assumed to be a functional of the momentum distribution function $n(k)$. In the Fermi gas this energy is the sum of the kinetic energies of the single particle, as it is described by Eq. (17.6). For a real system the situation is more complicated. If $n^0(k)$ is modified by

a quantity $\delta n(k)$, the variation of the energy up to the first order is given by

$$\delta E = \sum_k \epsilon_k \, \delta n(k) \ , \tag{17.8}$$

this expression defines

$$\epsilon_k = \delta E / \delta n(k) \ . \tag{17.9}$$

For $k > k_{\rm F}$, ϵ_k this is the variation of the energy when a particle is added, therefore it is the energy of the quasi-particle. The definition of ϵ_k is related to the energy fluctuation of the total energy of the system. In this theory, it is not possible to obtain information on the total energy of the system which is not the sum of the quasi-particle energies. This because, once a particle with k is added, the energy of the system changes, and the energy of a new particle $\epsilon_{k'}$ cannot be obtained by using (17.9) whose variation is done with respect to the old state which did not contain the particle k.

For $k = k_{\rm F}$, ϵ_k is the energy acquired by adding one particle to the Fermi surface. The new state is the ground state of the system with $A + 1$ particles. We can write the equation

$$\epsilon_{k_{\rm F}} = E_0(A+1) - E_0(A) \equiv \mu \ , \tag{17.10}$$

where $\mu = \partial E_0 / \partial A$ is, by definition, the chemical potential.

The expression of the energy variation (17.8) is valid up to the first order. This allows a description of situations dominated by excitations of a single quasi-particle. In general, this is not sufficient since the density of quasi-particle is so large that it is not possible to neglect their interaction. This indicates the need to go beyond the first order, and to consider also the second one

$$\delta E = \sum_k \epsilon_k^0 \, \delta n(k) + \frac{1}{2} \sum_k \sum_{k'} f(k,k') \delta n(k) \delta n(k') \ . \tag{17.11}$$

where the $f(k,k')$ term which describes the interaction between the quasi-particles is defined as the second functional derivative, with the property $f(k,k') = f(k',k)$. We called ϵ_k^0 the quasi-particle energy in absence of interaction.

Up to now, we did not considered the presence of quasi-particle spin. The quasi-particles have the fermion characteristics, and we treat the spin $1/2$ case, by indicating with s its third component. In this case, the system is not any more homogeneous since the spin orientation defines a direction in the space. For this reason all the quantities which we have previously defined as dependent on k only, must be considered dependent on $\mathbf{k}$ and s, and the sums on k becomes sums on $\mathbf{k}$ and $s = \pm 1/2$. Specifically, we have that $f(k,k') \to f(\mathbf{k},s;\mathbf{k}',s')$ and the symmetry properties become

$$f(\mathbf{k},s;\mathbf{k}',s') = f(-\mathbf{k},-s;-\mathbf{k}',-s') = f(\mathbf{k},-s;\mathbf{k}',-s') = f(\mathbf{k}',s';\mathbf{k},s) \ . \tag{17.12}$$

Once $\mathbf{k}$ and $\mathbf{k}'$ have been defined, the only differences between the f functions are due to the fact that the directions of the spins of the two interacting particles are parallel or anti-parallel. For this reason, it is convenient to define symmetric and antisymmetric terms of the interaction as

$$f(\mathbf{k},s;\mathbf{k}',s) = f^s(\mathbf{k},\mathbf{k}') + f^a(\mathbf{k},\mathbf{k}') \ , \tag{17.13}$$

$$f(\mathbf{k},s;\mathbf{k}',-s) = f^s(\mathbf{k},\mathbf{k}') - f^a(\mathbf{k},\mathbf{k}') \ . \tag{17.14}$$

The f^a and f^s terms depend only on the $\mathbf{k}$ and $\mathbf{k}'$ vectors, which means on the modules of the two vectors and on the relative angle. For this reason, they can be expanded in power of Legendre polynomials P_l:

$$f^{s(a)}(\mathbf{k},\mathbf{k}') = f^{s(a)}(k,k',cos\theta) = \sum_l f_l^{s(a)}(k,k') P_l(\cos\theta) \ . \tag{17.15}$$

Since the quasi-particles are defined on the Fermi surface one has $k = k' = k_{\rm F}$, therefore it is possible to eliminate the dependence on modules of the wave numbers in the f_l. The dimensions of these coefficients are those of an energy. It is common practice the use of dimensionless coefficients obtained by multiplying the f_l by the density of states at the Fermi surface

$$F_l \equiv \rho_\epsilon(\epsilon_{\rm F}) f_l = \frac{\mathcal{V}\mathcal{D}}{2\pi^2}\frac{k_{\rm F}}{\hbar^2} m^* f_l \ , \tag{17.16}$$

where we used the expression (2.64) of the density of states

$$\rho_\epsilon(\epsilon_{\rm F}) = \frac{\mathcal{V}\mathcal{D}}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\epsilon_{\rm F}^{1/2} = \frac{\mathcal{V}\mathcal{D}}{2\pi^2}\frac{m^*}{\hbar^2}k_{\rm F} \ . \tag{17.17}$$

The quantities $\mathcal{V}$ and $\mathcal{D}$, defined in Chapter 2.3, are, respectively, the volume of the system and the fermions degeneration, which in this chapter we consider to be only that due to the spin, therefore $\mathcal{D} = 2$. Since we are talking of quasi-particles we indicated with m^* their effective mass.

The usefulness of the theory is due to the fact that only few F_l are required to obtain a good description of the fermionic system under study. The values of F_l are determined by reproducing few empirical data. With these few parameters the theory provides predictions on other independent observables.

17.4 Equilibrium properties

17.4.1 Effective mass and specific heat

The velocity of the quasi-particle can be defined by using analogies with the free particles. In the latter case the single-particle energies are the kinetic energies $mv^2/2$. In this analogy, we can define one cartesian component, α, of the velocity as

$$(v_k)_\alpha = \frac{1}{\hbar}\frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\alpha} \ , \tag{17.18}$$

and, therefore, for an isotropic system, we have that

$$|\mathbf{v}_k| \equiv v_{\mathbf{k}} = \frac{\hbar k}{m^*} \tag{17.19}$$

In principle m^* depends on k, but, as we have already discussed, the quasi-particles are defined on the Fermi surface, therefore m^* has a single, well defined value. The empirical datum used to select the value of m^* is the specific heat per unit of volume, defined as variation of the internal energy of the system with respect to the temperature, Eq. (2.72), divided by the volume

$$c_v = \frac{1}{\mathcal{V}} C_v = \frac{1}{\mathcal{V}}\frac{\partial E}{\partial T} \ . \tag{17.20}$$

We consider temperature variations such as $T/T_{\rm F} \ll 1$. The energy fluctuations of the energy can be expressed as

$$\delta E = \sum_{\mathbf{k},s} \epsilon_{k,s}\delta n(\mathbf{k}, s) \ . \tag{17.21}$$

An increase of the temperature generates an increase of the quasi-particle number above the Fermi surface of the order $\delta n(\mathbf{k}, s)$. In principle there is also an increase of the energy E due to the interaction between quasi-particles but this is of the order of $(T/T_F)^3$ and, by the assumption done above, it is negligible.

Because of Eq. (17.21), we can calculate the specific heat of a real system can be calculated as that of system of non-interacting quasi-particles. The calculation of Sect. 2.3 is repeated keeping in mind that

we are handling quasi-particles, instead of particles, therefore, the effective mass m^* has to be considered. We use the expression (2.74) and obtain

$$c_v = \frac{1}{\mathcal{V}} C_v = \frac{1}{\mathcal{V}} \mathrm{k}_\mathrm{B}^2 T \rho_\epsilon(\epsilon_\mathrm{F}) \frac{\pi^2}{3} = \frac{1}{2} \mathcal{D} \frac{m^* k_\mathrm{F}}{3} \mathrm{k}_\mathrm{B}^2 T \tag{17.22}$$

where we considered the expression (17.17) of the density of states. The value of the effective mass of the quasi-particles can be obtained by measuring the specific heat of a system of interacting fermions.

17.4.2 Sound speed and compressibility

In the appendix C.3 we show that the relation between speed of sound v_s in a fluid and the compression modulus B is

$$v_s = \sqrt{\frac{B}{m\rho}} \; . \tag{17.23}$$

We calculate the compression modulus by using the definition of Eq. (2.60)

$$B = \frac{1}{K} = -\mathcal{V} \frac{\partial P}{\partial \mathcal{V}} \; . \tag{17.24}$$

Since the pressure is related to the variation of the energy with respect to the variation of the volume, it is necessary to calculate the energy variations. We assume that the ground state energy E depends on a function $\mathcal{F}$ of the particle density as

$$E = \mathcal{V} \mathcal{F}(\rho) = \mathcal{V} \mathcal{F} \left(\frac{A}{\mathcal{V}} \right) \; . \tag{17.25}$$

Since

$$\frac{\partial \rho}{\partial \mathcal{V}} = A \left(\frac{-1}{\mathcal{V}^2} \right) = \frac{-1}{\mathcal{V}} \rho \; , \tag{17.26}$$

the pressure can be expressed as

$$P = -\frac{\partial E}{\partial \mathcal{V}} = -\left[\mathcal{F} - \rho \frac{\partial \mathcal{F}}{\partial \rho} \right] \; , \tag{17.27}$$

and, therefore, the variation of the pressure becomes

$$\begin{aligned} \frac{\partial P}{\partial \mathcal{V}} &= -\left[\frac{\partial \mathcal{F}}{\partial \rho} \frac{\partial \rho}{\partial \mathcal{V}} - \frac{\partial \rho}{\partial \mathcal{V}} \frac{\partial \mathcal{F}}{\partial \rho} - \rho \frac{\partial}{\partial \rho} \left(\frac{\partial \mathcal{F}}{\partial \rho} \right) \frac{\partial \rho}{\partial \mathcal{V}} \right] \\ &= -\frac{\rho^2}{\mathcal{V}} \frac{\partial^2 \mathcal{F}}{\partial \rho^2} \; , \end{aligned} \tag{17.28}$$

and the compression modulus is

$$B = \rho^2 \frac{\partial^2 \mathcal{F}}{\partial \rho^2} \; . \tag{17.29}$$

I use the expression (17.25) in the definition of chemical potential

$$\mu = \frac{\partial E}{\partial A} = \frac{\partial}{\partial A} \left[\mathcal{V} \mathcal{F} \right] = \frac{\partial \mathcal{F}}{\partial \rho} \; . \tag{17.30}$$

The variation of the chemical potential is

$$\frac{\partial \mu}{\partial A} = \frac{\partial}{\partial \rho} \left(\frac{\partial \mathcal{F}}{\partial \rho} \right) \frac{\partial \rho}{\partial A} = \frac{\partial^2 \mathcal{F}}{\partial \rho^2} \frac{1}{\mathcal{V}} \; . \tag{17.31}$$

By using the expression of the second derivative of $\mathcal{F}$ in the expression (17.29) we obtain

$$B = A\rho \frac{\partial \mu}{\partial A} \ , \tag{17.32}$$

and for the sound speed

$$v_s^2 = \frac{B}{m\rho} = \frac{A}{m}\frac{\partial \mu}{\partial A} \ . \tag{17.33}$$

The Fermi liquid theory provides the expression of $\partial A/\partial \mu$. In the box here below we show that A is related to the variation of $n(k)$ by the expression

$$dA = \sum_{\mathbf{k},s} \delta n(\mathbf{k}, s) = \sum_{\mathbf{k},s} \delta(\epsilon_k - \mu)\, \hbar v_k \, dk \ . \tag{17.34}$$

Let's derive Eq. (17.34).

$$\delta n(\mathbf{k}, s) = -\frac{dn^0(\mathbf{k}, s)}{d\epsilon_k}\frac{\partial \epsilon_k}{\partial k} dk \ . \tag{17.35}$$

At the end the calculation of the variation we shall make the limit $k \to k_{\rm F}$.

The variation of the single-particle energy can be written as

$$d\epsilon_k = d\left(\frac{\hbar^2 k^2}{2m}\right) = \hbar \frac{\hbar k}{m}\, dk = \hbar \frac{m v_k}{m} dk = \hbar v_k dk \ . \tag{17.36}$$

Let's consider now the variation of $n^T(k, s)$ for an excited state, and for $T > 0$. Since the system is composed by fermions, the expression of $n^T(\mathbf{k}, s)$ is that of a Fermi-Dirac distribution

$$n^T(\mathbf{k}, s) = \left[\exp\left(\frac{\epsilon - \mu}{{\rm k_B} T}\right) + 1\right]^{-1} \ , \tag{17.37}$$

therefore

$$\frac{d\, n^T(\mathbf{k}, s)}{d\epsilon} = \frac{-\frac{1}{{\rm k_B} T} \exp\left[(\epsilon - \mu)/({\rm k_B} T)\right]}{\left\{\exp\left[(\epsilon - \mu)/({\rm k_B} T)\right] + 1\right\}^2} \ . \tag{17.38}$$

In the limit $T \to 0$, therefore for the ground state, the Fermi-Dirac distribution becomes a step function Θ. For the property of the Dirac distribution δ, $d\Theta/dx = \delta(x)$, we can write

$$\lim_{T \to 0} \frac{d\, n^T(\mathbf{k}, s)}{d\epsilon} = -\delta(\epsilon - \mu) \ , \tag{17.39}$$

therefore, on the Fermi surface the expression is

$$\delta n(\mathbf{k}_{\rm F}, s) = \delta(\epsilon_{\rm F} - \mu) \hbar v_{k_{\rm F}} dk_{\rm F} \ . \tag{17.40}$$

A quasi-particle added to the system on top to the new Fermi energy must have an energy $\epsilon(\mu + d\mu)$ satisfying

$$d\mu = \epsilon(\mu + d\mu) - \epsilon(\mu) = \hbar v_{k_{\rm F}} dk_{\rm F} + \sum_{\mathbf{k}', s'} f(\mathbf{k}, s; \mathbf{k}', s') \delta n(\mathbf{k}', s') \tag{17.41}$$

By using the expression (17.40) we have that

$$\frac{\partial \mu}{\partial \mu} = 1 = \hbar v_{k_{\rm F}} \frac{\partial k_{\rm F}}{\partial \mu} + \sum_{\mathbf{k}', s} f(\mathbf{k}, s; \mathbf{k}', s) \delta(\epsilon_{k'} - \mu) \hbar v_{k'} \frac{\partial k'}{\partial \mu} \ . \tag{17.42}$$

The calculation of the sum on $\mathbf{k}'$ and s' is presented in the box.

The sum on $\mathbf{k}'$ is transformed by using the conventions presented in Sect. 2.3.

$$\begin{aligned}
&\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k'}-\mu)\hbar v_{k'}\frac{\partial k'}{\partial \mu} \\
= &\sum_{s'}\frac{\mathcal{V}}{(2\pi)^3}\int d^3k'\, f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k'}-\mu)\hbar v_{k'}\frac{\partial k'}{\partial \mu} \\
= &\frac{\mathcal{V}}{(2\pi)^3}\sum_{s'}\int dk'k'^2\int_{-1}^{1} d(\cos\theta)\int_0^{2\pi} d\phi f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k'}-\mu)\hbar v_{k'}\frac{\partial k'}{\partial \mu}\ .
\end{aligned}$$

Since the variation between ϵ_{k_F} and μ is very small, we can write, by considering that we are describing a system of quasi-particles of effective mass m^*

$$\epsilon_k-\mu|_{k=k_\mathrm{F}} \simeq d\epsilon_k|_{k=k_\mathrm{F}} = d\left(\frac{\hbar^2 k}{2m^*}\right)_{k=k_\mathrm{F}} = \frac{\hbar^2 k_\mathrm{F}}{m^*}dk_\mathrm{F} \simeq \frac{\hbar^2 k_\mathrm{F}}{m^*}(k-k_\mathrm{F})\ ,$$

for the properties of Dirac's δ distribution

$$\delta(ax)=\frac{1}{|a|}\delta(x)\ ,$$

we can substitute in the integral

$$\delta(\epsilon'_k-\mu)=\frac{m^*}{\hbar^2 k_\mathrm{F}}\delta(k'-k_\mathrm{F})\ \ ,$$

which becomes

$$\begin{aligned}
&\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k'}-\mu)\hbar v_{k'}\frac{\partial k'}{\partial \mu} \\
= &\frac{\mathcal{V}2\pi}{(2\pi)^3}\sum_{s'}\int dk'k'^2\int_{-1}^{1} d(\cos\theta) f(\mathbf{k},s;\mathbf{k}',s')\frac{m^*}{\hbar^2 k_\mathrm{F}}\delta(k'-k_\mathrm{F})\hbar v_{k'}\frac{\partial k'}{\partial \mu} \\
= &\frac{\mathcal{V}}{4\pi^2}\frac{m^* {k_\mathrm{F}}^2}{\hbar^2 k_\mathrm{F}}\hbar v_{k_\mathrm{F}}\frac{\partial k_\mathrm{F}}{\partial \mu}\int_{-1}^{1} d(\cos\theta)\left[f(\mathbf{k}_\mathrm{F},s;\mathbf{k}_\mathrm{F},s)+f(\mathbf{k},s;\mathbf{k}_\mathrm{F},-s)\right]\ .
\end{aligned}$$

Let's use the expressions (17.13) and (17.14) of the f function and consider that, since on the Fermi surface the interaction depends only on the angle between $\mathbf{k}$ e $\mathbf{k}'$ whose modules are k_F, we can use the expansion in Legendre polynomials (17.15). We obtain the equation

$$\begin{aligned}
&\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k'}-\mu)\hbar v_{k'}\frac{\partial k'}{\partial \mu} \\
= &\frac{\mathcal{V}}{4\pi^2}\frac{m^*}{\hbar^2}k_\mathrm{F}\hbar v_{k_\mathrm{F}}\frac{\partial k_\mathrm{F}}{\partial \mu}\int_{-1}^{1} d(\cos\theta)\, 2\sum_l f_l^s(k_\mathrm{F},k_\mathrm{F})P_l(\cos\theta)\ .
\end{aligned}$$

Because of the orthogonality of the Legendre polynomials

$$\int_{-1}^{1} dx\, P_l(x) = 2\delta_{l,0}\ ,$$

we obtain

$$\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k'}-\mu)\hbar v_{k'}\frac{\partial k'}{\partial \mu} = \frac{\mathcal{V}}{\pi^2}\frac{m^*\, k_\mathrm{F}}{\hbar^2}\hbar v_{k_\mathrm{F}}\frac{\partial k_\mathrm{F}}{\partial \mu}f_0^s(k_\mathrm{F},k_\mathrm{F})\ .$$

We insert the result of the box in Eq. (17.42) and use the expression (17.17) of the density of states, and the definition (17.16) of the dimensionless Landau coefficients

$$\begin{aligned} 1 &= \hbar v_{k_F} \frac{\partial k_\mathrm{F}}{\partial \mu} + \frac{\mathcal{V}}{\pi^2} \frac{m^* k_\mathrm{F}}{\hbar^2} \hbar v_{k_\mathrm{F}} \frac{\partial k_\mathrm{F}}{\partial \mu} f_0^s(k_\mathrm{F}, k_\mathrm{F}) \\ &= \hbar v_{k_F} \frac{\partial k_\mathrm{F}}{\partial \mu} + \rho_\epsilon(\epsilon_\mathrm{F}) f_0^s(k_\mathrm{F}, k_\mathrm{F}) \hbar v_{k_F} \frac{\partial k_\mathrm{F}}{\partial \mu} = \hbar v_{k_F} \frac{\partial k_\mathrm{F}}{\partial \mu} \left[1 + F_0^s\right] \ . \end{aligned} \tag{17.43}$$

From Eq. (17.34) we obtain

$$\frac{\partial A}{\partial \mu} = \sum_{\mathbf{k},s} \delta(\epsilon_k - \mu)\, \hbar v_k \frac{\partial k}{\partial \mu} \tag{17.44}$$

Let's use the definition (17.33) of speed of sound and consider that the sum on $\delta(\epsilon_k - \mu)$ is the density of states ρ_ϵ. We have that

$$\frac{A}{m v_s^2} = \frac{\rho_\epsilon(\epsilon_\mathrm{F})}{1 + F_0^s} \ , \tag{17.45}$$

from where

$$v_s^2 = \frac{A}{m} \frac{\pi^2 \hbar^2}{\mathcal{V} m^* k_\mathrm{F}} (1 + F_0^s) = \frac{\pi^2 \hbar^2}{m m^* k_\mathrm{F}}\, \rho\, (1 + F_0^s) = \frac{\pi^2 \hbar^2}{m m^* k_\mathrm{F}} \left(\frac{{k_\mathrm{F}}^3}{3\pi^2}\right) (1 + F_0^s) = \frac{\hbar^2 {k_\mathrm{F}}^2}{3 m m^*} (1 + F_0^s) \ . \tag{17.46}$$

It is remarkable the simultaneous presence of two masses, the mass of the particle m and that of the quasi-particle m^*. The former mass is inserted because of the definition of mass density of the fluid, as in traditional Statistical Mechanics. The latter one is the quasi-particle effective mass which takes care that the interaction between particles modifies the density of states. Clearly, the particle interaction enters in the expression of the speed of sound also with the term F_0^s. When all the other variables are kept constant, if the interaction is repulsive, i.e. $F_0^s > 0$, the speed of sound increases. On the other hand, values of $F_0^s < -1$ generate imaginary sound speeds. In this case, the density fluctuations sums and generate instability in the system.

17.4.3 Magnetic susceptibility

Another observable used to determine the values of the free parameters of the Fermi liquid theory is the magnetic suscettibility χ_M. In presence of a magnetic field $\mathbf{H}$, a particle modifies its energy by the quantity $-g\mu_\mathrm{B} s|\mathbf{H}|$, where g is the Landé factor, which we take equal to 2, and $\mu_\mathrm{B} = e\hbar/mc$ the Bohr magneton. We call $s = 1/2$ the case where the fermion spin is parallel to the direction of the magnetic field $\mathbf{H}$, and $s = -1/2$ the opposite case.

In a real gas, the change of the energy implies also a change of the momentum distribution $n(\mathbf{k}, s)$. In the system there are particles with both values of s. If the system is in equilibrium, the value of the chemical potential μ has to be the same for all the particles, independently of the value of s, or, in other words, the energy required to add a particle has to be the same. Since the particles with $s = -1/2$ have acquired energy in presence of the magnetic field $\mathbf{H}$ the value of the Fermi energy is lowered by a factor δk_F with respect to the case without magnetic field. For the particles $s = 1/2$ the situation changes with opposite sign, there is an increase of δk_F of the Fermi surface.

Taking care of the isotropy of the system, therefore $n(\mathbf{k}, s) = n(k, s)$, the variation of the momentum distribution is given by

$$\delta n(k, s) = -\left(\frac{\partial n(k, s)}{\partial k}\right)_{k = k_\mathrm{F}} \delta k_\mathrm{F} = -\left[-\delta(k - k_\mathrm{F})\right](2s) \delta k_\mathrm{F} \ . \tag{17.47}$$

The Dirac δ distribution is generated by the fact that, in the ground state, $n(k, s)$ is a step function of k, and, therefore, its derivative is the δ of Dirac (see the box in Sect.17.4.2). The term $2s = \pm 1$ takes care of the increase, or of the lowering, of the Fermi surface due to the presence of the magnetic field.

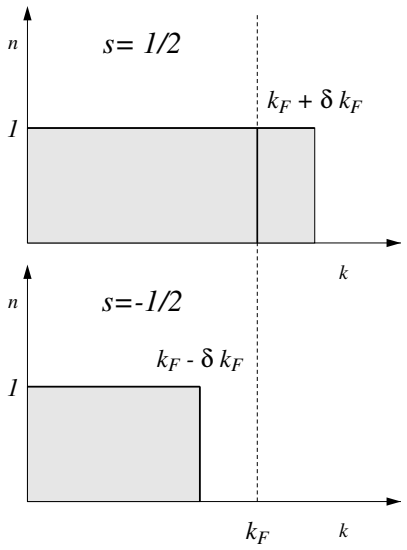

Figure 17.2: Variation of the Fermi surface due to the presence of the magnetic field $\mathbf{H}$.

The variation of the quasi-particle energy is given by

$$\delta\epsilon_{k_{\rm F}} = -g\mu_{\rm B}s|\mathbf{H}| + (2s)\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta n(\mathbf{k}',s') \ , \tag{17.48}$$

the term $2s = \pm 1$ is inserted since $s = 1/2$ and $s = -1/2$ give different contributions. Let's search for a solution of the type

$$\delta\epsilon_{k_{\rm F}} = -\eta s|\mathbf{H}| \ , \tag{17.49}$$

where η is a constant to be defined. We consider that

$$\frac{d\epsilon_k}{d|\mathbf{k}|} = \frac{\hbar^2|\mathbf{k}|}{m^*} \ , \tag{17.50}$$

therefore

$$\delta k_{\rm F} = \left|\frac{d\epsilon_k}{d|\mathbf{k}|}\right|^{-1}_{k=k_{\rm F}} |\delta\epsilon_{k_{\rm F}}| = \frac{m^*}{\hbar^2 k_{\rm F}}\eta\frac{1}{2}|\mathbf{H}| \ , \tag{17.51}$$

for $s = 1/2$.

We sum on $\mathbf{k}'$ and s', and we have to consider that the momentum distributions $n(k,s)$ (17.47) are different for the fermions with spin parallel or antiparallel to the magnetic field direction. The calculation is done with the same strategy used for the evaluation of the speed of sound. In the present case, we use the definition of the antisymmetric interaction of Eqs. (17.13) and (17.14), and the expansion in Legendre polynomials (17.15). In this manner, we obtain the following expressions

$$\begin{aligned}
& (2s)\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta n(\mathbf{k}',s') \\
= \ & (2s)\sum_{s'=\pm 1/2}\frac{\mathcal{V}}{(2\pi^3)}\int d^3k' f(\mathbf{k},s,\mathbf{k}',s')\delta(k'-k_{\rm F})(2s')\left[\frac{m^*}{\hbar^2 k_{\rm F}}\eta\frac{1}{2}|\mathbf{H}|\right] \\
= \ & \frac{\mathcal{V}}{(2\pi^3)}(2\pi)(2s)\int dk' k'^2\delta(k'-k_{\rm F})\int_{-1}^{1} d(\cos\theta) 2f^a(k,k',\cos\theta)\left[\frac{m^*}{\hbar^2 k_{\rm F}}\eta\frac{1}{2}|\mathbf{H}|\right] \\
= \ & \frac{\mathcal{V}}{2\pi^2}s\left[\frac{m^*}{\hbar^2 k_{\rm F}}\eta|\mathbf{H}|\right]{k_{\rm F}}^2\int_{-1}^{1} d(\cos\theta)\sum_l f^a_l(k,k')P_l(\cos\theta) \\
= \ & \frac{\mathcal{V}}{2\pi^2}s\frac{m^*}{\hbar^2 k_{\rm F}}\eta|\mathbf{H}|{k_{\rm F}}^2 f^a_0 2 = F^a_0 s\eta|\mathbf{H}|
\end{aligned}$$

By using this result in Eq. (17.48) we obtain

$$\delta\epsilon_{k_{\rm F}} = -\eta s|\mathbf{H}| = -g\mu_{\rm B}s|\mathbf{H}| + F^a_0 s\eta|\mathbf{H}| \ , \tag{17.52}$$

from which we have

$$\eta\left[1+F^a_0\right] = g\mu_{\rm B} \ ; \ \eta = \frac{g\mu_{\rm B}}{1+F^a_0} \ . \tag{17.53}$$

The magnetization energy per unit of volume is given by the product of the magnetic suscettibility $\chi_{\rm M}$ and the module of he magnetic field $|\mathbf{H}|$. This corresponds to the sum of the variations of the

quasi-particle energies which have magnetic field $gs\mu_{\rm B}$, due to the change of the momentum distribution $n(\mathbf{k},s)$.

$$\begin{aligned} M &= \frac{1}{\mathcal{V}}\chi_{\rm M}|\mathbf{H}| = \frac{1}{\mathcal{V}}\sum_{\mathbf{k},s} gs\mu_{\rm B}\delta n(\mathbf{k},s) \\ &= \frac{1}{\mathcal{V}}g\mu_{\rm B}\sum_{s} s\frac{\mathcal{V}}{(2\pi^3)}\int d^3k\delta(k-k_{\rm F})\left[\frac{m^*}{\hbar^2 k_{\rm F}}(2s)\eta\frac{1}{2}|\mathbf{H}|\right] \\ &= g\mu_{\rm B}\frac{1}{4\pi^2}\frac{m^*k_{\rm F}}{\hbar^2}\eta|\mathbf{H}| \ . \end{aligned}$$

The magnetic suscettibility per unit of volume is

$$\frac{1}{\mathcal{V}}\chi_{\rm M} = \frac{M}{|\mathbf{H}|} = \frac{m^*k_{\rm F}}{4\pi^2\hbar^2}\frac{(g\mu_{\rm B})^2}{1+F_0^a} \tag{17.54}$$

The values of the fundamental parameters of the theory of Landau, effective mass, scalar and spin-dependent parts of the interaction f, are selected by using their relations with empirical quantities, specific heat, speed of sound, magnetic suscettibility. There is the possibility to relate these parameters to more fundamental properties of the hamiltonian [Pin66, Abr75, Gro91, Bru04]. In any case, the main interest of the theory is to make predictions on phenomena not directly related to the observable quantities used to determine the effective mass and the interaction.

17.5 Excitations

17.5.1 Transport equation

In this section, we shall present a description of the response of fermionic fluid excited by compression waves, in the framework of the Fermi liquid theory.

Let's consider a system containing some non homogeneous parts which are treated as small units in local equilibrium. These parts are small in comparison with the total dimensions of the system, but they are sufficiently large to contain a number of fermions sufficient to define a momentum distribution function $n_{\mathbf{k},s}(\mathbf{r},t)$, where $\mathbf{r}$ is the vector defining the position of the sub-unit.

The presence of a quantity defined by the precise knowledge of the mometum $\hbar\mathbf{k}$ and of the position $\mathbf{r}$ violates the Heisenberg uncertainty principle. The present description is valid only if the phenomena under study are macroscopic. In other words, energy and momenta of the excitation must be much smaller than those characterizing the particles, as well as the distances into play are much larger than those between the basic particles composing the system. For example in the treatment of liquid helium phenomena these assumptions are verified since the typical helium binding energies are much smaller of the excitation energies of the helium atoms.

Let's assume that the external perturbation which, locally, changes the density of the system has a harmonic behaviour with frequency $\hbar\omega$ and transfers to the system a momentum $\mathbf{q}$. The momentum distribution of the fermion system subject to this perturbation can be expressed as

$$n_{\mathbf{k},s}(\mathbf{r},t) = n^0_{\mathbf{k},s} + \delta n_{\mathbf{k},s}(\mathbf{r},t) = n^0_{\mathbf{k},s} + \delta n_{\mathbf{k},s}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{r}-\hbar\omega t)} \ , \tag{17.55}$$

where $n^0_{\mathbf{k},s}$ is the momentum distribution of the system in absence of perturbation. The approach is valid for energy much smaller than the chemical potential $\omega << \mu$. We can express the energy fluctuations at

the time t as

$$E(t) = E_0 \quad + \quad \sum_{\mathbf{k},s} \int d^3r\, \epsilon_{k,s}\, \delta n_{\mathbf{k},s}(\mathbf{r},t) + \quad \frac{1}{2} \sum_{\mathbf{k},s,\mathbf{k}',s} \int\int d^3r d^3r' f(\mathbf{r},\mathbf{k},s;\mathbf{r}',\mathbf{k}',s') \delta n_{\mathbf{k},s}(\mathbf{r},t) \delta n_{\mathbf{k}',s}(\mathbf{r}',t) \ . \tag{17.56}$$

We make some assumption on the properties of the interaction between the particles. A first one, already used in the previous expression, is that the interaction does not depend on the time. The second one, is related to the Galilean invariance: we assume that the interaction depends only on the distance $\mathbf{r} - \mathbf{r}'$ between the particles. Finally, we assume that the interaction is short-ranged, in the sense presented in Chapter 3. This last assumption is not valid for the Coulomb interaction. The charged Fermi liquid must be treated differently [Pin66].

Let's consider an extremely short-ranged interaction by assuming

$$f(\mathbf{r},\mathbf{k},s;\mathbf{r}',\mathbf{k}',s') = f(\mathbf{k},s;\mathbf{k}',s')\delta(\mathbf{r}-\mathbf{r}') \ , \tag{17.57}$$

therefore, the second term of Eq. (17.56) can be written as

$$\int\int d^3r d^3r' f(\mathbf{r},\mathbf{k},s;\mathbf{r}',\mathbf{k}',s') \delta n_{\mathbf{k},s}(\mathbf{r},t) \delta n_{\mathbf{k}',s'}(\mathbf{r}',t) = \int d^3r f(\mathbf{k},s;\mathbf{k}',s') \delta n_{\mathbf{k},s}(\mathbf{r},t) \delta n_{\mathbf{k}',s'}(\mathbf{r},t) \ , \tag{17.58}$$

and

$$E(t) = E_0 + \int d^3r \delta E(\mathbf{r},t) \ , \tag{17.59}$$

with

$$\delta E(\mathbf{r},t) = \sum_{\mathbf{k},s} \epsilon_{k,s} \delta n_{\mathbf{k},s}(\mathbf{r},t) + \frac{1}{2} \sum_{\mathbf{k},s,\mathbf{k}',s} f(\mathbf{k},s;\mathbf{k}',s') \delta n_{\mathbf{k},s}(\mathbf{r},t) \delta n_{\mathbf{k}',s'}(\mathbf{r},t) \ . \tag{17.60}$$

The local excitation energy of the quasi-particle is defined as

$$\tilde{\epsilon}_{\mathbf{k},s}(\mathbf{r},t) \equiv \frac{\partial E(\mathbf{r},t)}{\partial n_{\mathbf{k},s}(\mathbf{r},t)} = \epsilon_{k,s} + \sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s') \delta n_{\mathbf{k}',s'}(\mathbf{r},t) \ . \tag{17.61}$$

In the approach of Landau the gas of quasi-particle gas is considered as a classic gas following the Maxwell-Boltzmann statistics. Each particle, whose energy is $\tilde{\epsilon}_{\mathbf{k},s}$, is described by a classical hamiltonian. Let's consider a volume $d\mathbf{r}\ d\mathbf{k}$ in the six-dimensional phase space and apply to the $n_{\mathbf{k},s}(\mathbf{r},t)$ distribution the transport equation (D.24)

$$\mathcal{J}(n_{\mathbf{k},s}(\mathbf{r},t)) = \frac{\partial n_{\mathbf{k},s}(\mathbf{r},t)}{\partial t} + \nabla_{\mathbf{r}} n_{\mathbf{k},s}(\mathbf{r},t) \cdot \nabla_{\mathbf{p}} \tilde{\epsilon}_{\mathbf{k},s}(\mathbf{r},t) - \nabla_{\mathbf{p}} n_{\mathbf{k},s}(\mathbf{r},t) \cdot \nabla_r \tilde{\epsilon}_{\mathbf{k},s}(\mathbf{r},t) \ . \tag{17.62}$$

This expression is immediately identifiable with Eq. (D.24) by considering that $\nabla_{\mathbf{p}} \tilde{\epsilon}_{\mathbf{k},s} = \mathbf{v}_{\mathbf{k},s}$ and $-\nabla_{\mathbf{r}} \tilde{\epsilon}_{\mathbf{k},s}(\mathbf{r},t) = \mathbf{F}$. Let's explicitly write Eq. (17.62) by using Eqs. (17.55) and (17.61)

$$\begin{aligned}
\mathcal{J}(n_{\mathbf{k},s}(\mathbf{r},t)) &= \frac{\partial n_{\mathbf{k},s}(\mathbf{r},t)}{\partial t} + \nabla_{\mathbf{r}} \delta n_{\mathbf{k},s}(\mathbf{r},t) \cdot \nabla_{\mathbf{p}} \tilde{\epsilon}_{\mathbf{k},s}(\mathbf{r},t) \\
&- \left\{ \nabla_{\mathbf{p}} [n^0_{\mathbf{k},s} + \delta n_{\mathbf{k},s}(\mathbf{r},t)] \cdot \nabla_{\mathbf{r}} [\epsilon_{k,s} + \sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s') \delta n_{\mathbf{k}',s'}(\mathbf{r},t)] \right\} \\
= \quad & \frac{\partial n_{\mathbf{k},s}(\mathbf{r},t)}{\partial t} + \nabla_{\mathbf{r}} \delta n_{\mathbf{k},s}(\mathbf{r},t) \cdot \mathbf{v}_{\mathbf{k},s} - \left[\nabla_{\mathbf{p}} n^0_{\mathbf{k},s} + \nabla_{\mathbf{p}} \delta n_{\mathbf{k},s}(\mathbf{r},t) \right] \cdot \sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s') \nabla_{\mathbf{r}} \delta n_{\mathbf{k}',s'}(\mathbf{r},t) \\
\simeq \quad & \frac{\partial n_{\mathbf{k},s}(\mathbf{r},t)}{\partial t} + \nabla_{\mathbf{r}} \delta n_{\mathbf{k},s}(\mathbf{r},t) \cdot \mathbf{v}_{\mathbf{k},s} - \nabla_{\mathbf{p}} n^0_{\mathbf{k},s} \cdot \sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s') \nabla_{\mathbf{r}} \delta n_{\mathbf{k}',s'}(\mathbf{r},t)
\end{aligned} \tag{17.63}$$

where we considered that $\nabla_{\mathbf{r}}\epsilon_{k,s} = 0$ since $\epsilon_{k,s}$ is constant and, in the last step, we neglected the second order terms in $\delta n_{\mathbf{k}}$. The first two terms describe a flux of quasi-particles which move independently from each other. The last term, which includes the interaction, can be though as the flux of the particles of the ground state drifted by the interaction with the non homogeneous parts of the system. Without these non homogeneous parts, δn would be constant, therefore, this term would be zero.

17.5.2 Continuity equation

Let's consider the case when the collision integral $\mathcal{I}$ is negligible. This implies that the number of quasi-particle collisions which brings them out of the counting of $n_{\mathbf{k},s}$ is very small. At zero temperature we have that

$$\nabla_{\mathbf{p}} n^0_{\mathbf{k},s} = -\mathbf{v}_{k,s}\delta(\epsilon_{k,s} - \mu) \ , \tag{17.64}$$

and we remember that the values of $\mathbf{p} = \hbar\mathbf{k}$ which have to be considered are closed to the Fermi surface. By inserting this expression in Eq. (17.63) we obtain

$$\frac{\partial n_{\mathbf{k},s}(\mathbf{r},t)}{\partial t} + \mathbf{v}_k\delta(\epsilon_{k,s} - \mu)\cdot\nabla_{\mathbf{r}}\left[\delta n_{\mathbf{k},s}(\mathbf{r},t) + \sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta n_{\mathbf{k}',s'}(\mathbf{r},t)\right] = 0 \ . \tag{17.65}$$

An equation describing the motion of all the particles of the system is obtained by summing on all the values of $\mathbf{k}$ and s.

$$\begin{aligned}
&\sum_{\mathbf{k},s}\frac{\partial n_{\mathbf{k},s}(\mathbf{r},t)}{\partial t} + \sum_{\mathbf{k},s}\mathbf{v}_{k,s}\cdot\nabla_{\mathbf{r}}\left[\delta n_{\mathbf{k},s}(\mathbf{r},t) + \delta(\epsilon_{k,s}-\mu)\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta n_{\mathbf{k}',s'}(\mathbf{r},t)\right] \\
= \ & \frac{\partial}{\partial t}\sum_{\mathbf{k}} n_{\mathbf{k},s}(\mathbf{r},t) + \sum_{\mathbf{k},s}\nabla_{\mathbf{r}}\delta n_{\mathbf{k},s}(\mathbf{r},t)\cdot\mathbf{v}_{k,s} + \sum_{\mathbf{k},s,\mathbf{k}',s'}\delta(\epsilon_{k,s}-\mu)f(\mathbf{k},s;\mathbf{k}',s')\nabla_{\mathbf{r}}\delta n_{\mathbf{k}',s'}(\mathbf{r},t)\cdot\mathbf{v}_{k,s} \\
= \ & \frac{\partial}{\partial t}\sum_{\mathbf{k},s} n_{\mathbf{k},s}(\mathbf{r},t) + \sum_{\mathbf{k},s}\nabla_{\mathbf{r}}\delta n_{\mathbf{k},s}(\mathbf{r},t)\cdot\mathbf{v}_{k,s} + \sum_{\mathbf{k},s,\mathbf{k}',s'}\delta(\epsilon_{k',s'}-\mu)f(\mathbf{k},s;\mathbf{k}',s')\nabla_{\mathbf{r}}\delta n_{\mathbf{k},s}(\mathbf{r},t)\cdot\mathbf{v}_{k',s'} \\
= \ & \frac{\partial}{\partial t}\sum_{\mathbf{k}} n_{\mathbf{k},s}(\mathbf{r},t) + \nabla_{\mathbf{r}}\cdot\sum_{\mathbf{k},s}\delta n_{\mathbf{k},s}(\mathbf{r},t)\left[\mathbf{v}_{k,s} + \sum_{\mathbf{k}',s'}\delta(\epsilon_{k',s'}-\mu)f(\mathbf{k},s;\mathbf{k}',s')\mathbf{v}_{k',s'}\right] \\
= \ & \frac{\partial\rho(\mathbf{r},t)}{\partial t} + \nabla\cdot\mathbf{J}(\mathbf{r},t) = 0 \ ,
\end{aligned} \tag{17.66}$$

where we have defined

$$\rho(\mathbf{r},t) = \sum_{\mathbf{k},s} n_{\mathbf{k},s}(\mathbf{r},t) \ , \tag{17.67}$$

and

$$\mathbf{J}(\mathbf{r},t) = \sum_{\mathbf{k},s}\delta n_{\mathbf{k},s}(\mathbf{r},t)\left[\mathbf{v}_{k,s} + \sum_{\mathbf{k}',s'}\delta(\epsilon_{k',s'}-\mu)f(\mathbf{k},s;\mathbf{k}',s')\mathbf{v}_{\mathbf{k}',s'}\right] \equiv \sum_{\mathbf{k},s}\delta n_{\mathbf{k},s}(\mathbf{r},t)\mathbf{j}_{\mathbf{k},s} \ . \tag{17.68}$$

In the above calculation the properties $f(\mathbf{k},s;\mathbf{k}',s') = f(\mathbf{k}',s';\mathbf{k},s)$ and $|\delta n_{\mathbf{k}',s'}(\mathbf{r},t)| = |\delta n_{\mathbf{k},s}(\mathbf{r},t)|$ have been taken into account. We also have to considered that the variations are always done on the Fermi surface, therefore, $|\mathbf{k}| = |\mathbf{k}'| = k_{\mathrm{F}}$.

Eq. (17.66) is evidently a continuity equation, and describes the conservation of the number of particles of the system. The current generated by the quasi-particle motion is

$$\mathbf{j}_{\mathbf{k},s} = \mathbf{v}_{k,s} + \sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k',s'}-\mu)\mathbf{v}_{k',s'} \tag{17.69}$$

In absence of interaction, the current would correspond to $\mathbf{v}_{k,s}$ as it would be in a classical treatment. The second term appears since we are describing an interacting system. Adding a particle to the system, in addition to the trivial contribution of the current generated by $\mathbf{v}_{k,s}$, there is the contribution due to the interaction of the quasi-particle with all the other ones. This second terms, is sometime called *drag current* as to describe the fact that the medium is dragged by the quasi-particle added to the system.

In an infinite system, with translational invariance, we can use the relation (17.19) in Eq. (17.69) to relate the effective mass of the quasi-particle to the bare mass

$$\frac{\hbar k}{m} = \frac{\hbar k}{m^*} + \sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k,s}-\mu)\mathbf{v}_{k',s'} \tag{17.70}$$

The calculation of the sum is presente in the box.

In this calculation the sum is transformed into an integral by using the conventions presented in Sect. 2.3. We consider the z-axis parallel to $\mathbf{k}$ without losing in generality We indicate with θ the angle between $\mathbf{k}$ and $\mathbf{k}'$ and $v_{k,s} = |\mathbf{v}_{k|,s}$.

$$\begin{aligned}
&\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta(\epsilon_{k'}-\mu)v_{k',s'}\cos\theta \\
= &\sum_{s'} \frac{\mathcal{V}}{(2\pi)^3}\int d^3k'\, f(\mathbf{k},s;\mathbf{k}',s)\frac{m^*}{\hbar^2 k}\delta(k'-k_{\mathrm{F}})v_{k',s'}\cos\theta \\
= &\frac{\mathcal{V}}{(2\pi)^3}\sum_{s'}\int dk' k'^2 \int_{-1}^{1} d(\cos\theta)\int_0^{2\pi} d\phi\, f(\mathbf{k},s;\mathbf{k}',s)\frac{m^*}{\hbar^2 k}\delta(k'-k_{\mathrm{F}})v_{k',s'}P_1(\cos\theta) \\
= &\frac{\mathcal{V}}{(2\pi)^3}(2)(2\pi)\frac{m^*}{\hbar^2 k_{\mathrm{F}}}{k_{\mathrm{F}}}^2 v_{k_{\mathrm{F}}}\int_{-1}^{1} d(\cos\theta)\sum_l f_l^s P_l(\cos\theta)P_1(\cos\theta) \\
= &\frac{\mathcal{V}m^* k_{\mathrm{F}}}{2\pi^2}\sum_l f_l^s \int_{-1}^{1} dx P_l(x)P_1(x) = F_1^s\frac{1}{2}\frac{2}{3}\delta_{l,1}v_k = \frac{1}{3}v_k F_1^s
\end{aligned}$$

where we have considered that $v_{k_{\mathrm{F}},1/2} = v_{k_{\mathrm{F}},-1/2} = v_{k_{\mathrm{F}}}$

$$\frac{\hbar k}{m} = \frac{\hbar k}{m^*} + \frac{1}{3}F_1^s v_k = \frac{\hbar k}{m^*}\left(1+\frac{F_1^s}{3}\right) \tag{17.71}$$

therefore

$$\frac{m^*}{m} = 1 + \frac{F_1^s}{3} \tag{17.72}$$

Since the value of m^* is related to the specific heat, see Sect. 17.4.1, this relation gives new information on the interaction $f(\mathbf{k},s;\mathbf{k}',s')$. We remark that for $F_1^s \leq -3$ the system becomes unstable since negative masses would be obtained.

17.5.3 Collective excitations

The external perturbation of the system is harmonic ad has momentum $\mathbf{q}$ and energy ω. The variation (17.55) of the distribution can be expressed as

$$n_{\mathbf{k},s}(\mathbf{r},t) = n^0_{\mathbf{k},s} + \delta n_{\mathbf{k},s}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{r}-\hbar\omega t)} \tag{17.73}$$

By inserting this expression in the transport equation (17.63) we obtain

$$\begin{aligned} & \frac{\partial}{\partial t}\left[\delta n_{\mathbf{k},s}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\right] + \nabla_{\mathbf{r}}\left[\delta n_{\mathbf{k},s}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\right]\cdot\mathbf{v}_{k,s} \\ - \quad & \nabla_{\mathbf{p}} n^0_{\mathbf{k},s}\cdot\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\nabla_{\mathbf{r}}\left[\delta n_{\mathbf{k}',s'}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\right] = 0 \ . \end{aligned} \tag{17.74}$$

and therefore

$$(\mathbf{q}\cdot\mathbf{v}_{k,s}-\omega)\delta n_{\mathbf{k},s}(\mathbf{q},\omega) - \nabla_{\mathbf{p}} n^0_{\mathbf{k},s}\cdot\mathbf{q}\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta n_{\mathbf{k}',s'}(\mathbf{q},\omega) = 0 \ . \tag{17.75}$$

and also

$$(\mathbf{q}\cdot\mathbf{v}_{k,s}-\omega)\delta n_{\mathbf{k},s}(\mathbf{q},\omega) + \mathbf{v}_{k,s}\cdot\mathbf{q}\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')\delta n_{\mathbf{k}',s'}(\mathbf{q},\omega) = 0 \ . \tag{17.76}$$

Since for Eq. (17.64) $\delta(\epsilon_p-\mu) = \delta(k-k_{\rm F})m^*/\hbar^2 k_{\rm F}$ we can rewrite the variation $\delta n_{\mathbf{k},s}$ as

$$\delta n_{\mathbf{k},s}(\mathbf{q},\omega) = \delta(k-k_{\rm F})v_{k_{\rm F}}u_{\mathbf{k},s} \ , \tag{17.77}$$

and, then, we obtain the equation

$$(\mathbf{q}\cdot\mathbf{v}_{k,s}-\omega)u_{\mathbf{k},s}(\mathbf{q},\omega) + \mathbf{v}_{k,s}\cdot\mathbf{q}\sum_{\mathbf{k}',s'} f(\mathbf{k},s;\mathbf{k}',s')u_{\mathbf{k}',s'}(\mathbf{q},\omega) = 0 \ . \tag{17.78}$$

Without loss of generality, we defined the z in the direction of $\mathbf{q}$. We indicate with θ the angle between $\mathbf{q}$ and $\mathbf{k}$ and with θ' the angle between $\mathbf{k}'$ and $\mathbf{q}$. We use the symbols q, k, k' to indicate the modules of the relative vectors. Since everything happens at the Fermi surface $k = k' = k_{\rm F}$, the interaction depends only on the angle between the two vectors $\mathbf{k}$ and $\mathbf{k}'$, therefore

$$f(\mathbf{k},s;\mathbf{k}',s') \equiv f[\cos(\theta-\theta');s,s'] = \frac{\pi^2\hbar^2}{\mathcal{V}m^*}F[\cos(\theta-\theta');s,s'] \ , \tag{17.79}$$

where we used the definition (17.64) of F. We transform the sums in Eq. (17.78) as integrals following the conventions of Sect. 2.3, and obtain

$$(qv_{k_{\rm F},s}\cos\theta-\omega)u(\theta,\phi,\sigma) + qv_{k_{\rm F},s}\frac{\cos\theta}{8\pi}\sum_{s'}\int_0^{2\pi}d\phi'\int_{-1}^{1}d(\cos\theta')F[\cos(\theta-\theta');s,s']u(\theta',\phi',\sigma') = 0 \ . \tag{17.80}$$

In analogy to what has been done for the interaction in the Eqs. (17.13) and (17.14) we separate u in a symmetric and antisymmetric parts of the spin

$$u(\theta,\phi,\pm 1/2) = u^s(\theta,\phi) \pm u^a(\theta,\phi) \ . \tag{17.81}$$

We insert these definitions in Eq. (17.80), we divide by $qv_{k_{\rm F},s}$ and by using the new variable $\xi \equiv \omega/qv_{k_{\rm F},s}$ we obtain two independent equations for the unknowns u^s and u^a.

$$(\cos\theta-\xi)u^s(\theta,\phi) + \frac{\cos\theta}{4\pi}\int_0^{2\pi}d\phi'\int_{-1}^{1}d(\cos\theta')F^s[\cos(\theta-\theta')]u^s(\theta',\phi') = 0 \tag{17.82}$$

$$(\cos\theta-\xi)u^a(\theta,\phi) + \frac{\cos\theta}{4\pi}\int_0^{2\pi}d\phi'\int_{-1}^{1}d(\cos\theta')F^a[\cos(\theta-\theta')]u^a(\theta',\phi') = 0 \tag{17.83}$$

A formal solution of these equations can be obtained by expanding the $u^{s,a}(\theta,\phi)$ in spherical harmonics $Y_{l,\mu}(\theta,\phi)$. The independence of the known terms of the angle ϕ indicates that one obtains independent equations each of them characterized by the quantum number μ. This means that it is possible to classify the solutions by following the value of μ. Longitudinal solutions are those for $\mu = 0$, transverse solutions are those for $\mu = 1$, quadrupole solutions those for $\mu = 2$, etc..

The most interesting excitation mode is the longitudinal one for the symmetric solution. This situation describe a density compression mode which propagates in the **q** direction and which involves all the particles independently of their spin direction. It is an excitation mode very similar to that of the traditional sound propagation in classical systems. For this reason it is called *zero sound* opposite to the *first sound* which is that traditional mode described in the hydrodynamical regime.

Qe present here a simple model to describe the zero sound. Let's assume that the interaction is independent of θ and θ', therefore, in expansion in terms of Lagrange polynomials $F^s[\cos(\theta-\theta')]$, only the term F_0^s remains. By inserting this interaction in Eq. (17.82), and working out the integrals we obtain

$$(\cos\theta - \xi)u^s(\theta,\phi) + \frac{\cos\theta}{2}F_0^s\int_{-1}^{1} d(\cos\theta')u^s(\theta',\phi') = 0 \quad . \tag{17.84}$$

We search for a solution of type

$$u^s(\theta,\phi) = C\frac{\cos\theta}{\xi - \cos\theta} \tag{17.85}$$

where C is a constant. By inserting this solution in Eq. (17.84) we obtain

$$\frac{\xi}{2}\log\frac{\xi+1}{\xi-1} = \frac{1}{F_0^s} \tag{17.86}$$

The integral to be calculated is

$$\int_{-1}^{1} d(\cos\theta)\frac{\cos\theta}{\xi-\cos\theta} \quad .$$

Since

$$\int dx\,\frac{x}{\xi - x} = -\left[x + \xi\log(x-\xi)\right] + \text{costante} \quad ,$$

Eq. (17.84) becomes

$$(\cos\theta - \xi)C\frac{\cos\theta}{\xi-\cos\theta} + \frac{\cos\theta}{2}F_0^s C\left\{\xi[\log(\xi+1) - \log(\xi-1)]\right\} = 0 \quad ,$$

from which we obtain Eq. (17.86).

In case of a repulsive interaction $F_0^s > 0$ there is always a real solution with $\xi > 1$. This corresponds to a wave without damping. The phase velocity is greater than v_{k_F}. If there is a weak attraction between the quasi-particles $-1 < F_0^s < 0$, Eq. (17.86) has a complex solution which represents a damped oscillation. If $F_0^s < -1$ the zero sound oscillation is unstable, i. e. it is not formed.

It is relevant to analyze the differences between zero and first sound in order to clarify their physics content. There are two aspects to be considered. The first one is the interaction between the particles, and the second one their elastic collisions. Both effects are present in a realistic description of the system. The zero sound appears when the interaction dominates, while the first sound is present when the role of the elastic collisions becomes dominant.

The first sound propagates since the perturbation, due to a local change of the density, has an oscillation frequency $\hbar\omega$ much smaller than that of the elastic collisions between quasi-particles. Since

the number of these collisions is large for each oscillation, it is possible to reach a local thermal equilibrium in a macroscopic part of the system, large if compared to the interparticle distance, but localized. This perturbation moves in the systems as a consequence of the particle collisions, phenomenon which quenches the amplitude since it transfers energy from the localized region to the full system. If the temperature increases also the propagation speed increases since it increases the number of elastic collisions. Also the effect of the quenching increases. From the mathematical point of view this situation is described by the transport equation (17.63) where the collision integral plays an important role.

The opposite physical conditions are those which allows the formation, and propagation, of the zero sound. The oscillation frequency $\hbar\omega$ is much larger of the frequency of the elastic collisions between the particles. In this situation the interaction between quasi-particles, which is active at times much smaller than ω^{-1}, and to the typical average times of elastic collisions, dominates. The zero sound propagates since the particles are correlated by their interaction. The number of elastic collisions is relatively small for each oscillation and the perturbation is not damped. In the zero temperature limit there are not elastic collisions and the zero sound propagates indefinitely. In obtaining the solution for the zero sound propagation we used the transport equation (17.63) by neglecting the collision integral.

The transition between these two collective modes of sound propagation happens in a situation where $\hbar\omega$ is comparable with the frequency of the elastic collisions. In this case, there is no zero sound since the collisions are numerous enough to immediately damp the oscillation. On the other hand, the collisions are too few to thermalize and produce a collective motion. There is no first sound propagation.

The existence of zero sound was predicted by Landau at the end of the 50's of the last century, and experimentally identified in 1966 in the fermionic liquid helium [Abe66]. The experiment was carried out by analyzing the absorption of sound waves with different frequencies at a fixed temperature, and by identifying the presence of the three physical regimes above described, first sound, transition region and zero sound.

Part VI

Appendices

Appendix A

Variational principle

Let's consider a system composed by many fermions and described by the hamiltonian $\hat{H}$. The corresponding Schrödinger equation is

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \ , \tag{A.1}$$

where $|\Psi\rangle$ is the eigenstate describing the system. We consider only the ground state of the system. We shall show that, by considering the energy of the system as functional of Ψ, the search for its minimum, i.e. the solution of the equation

$$\delta E[\Psi] = \delta \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 0 \ , \tag{A.2}$$

corresponds to the solution of the Schrödinger equation (A.1).

The definition of energy (A.2) can be written as

$$E[\Psi]\,\langle\Psi|\Psi\rangle = \langle\Psi|\hat{H}|\Psi\rangle \ , \tag{A.3}$$

By doing the variation we obtain

$$\begin{aligned}
\delta E[\Psi]\langle\Psi|\Psi\rangle &+ E[\Psi]\delta\left(\langle\Psi|\Psi\rangle\right) = \delta\left(\langle\Psi|\hat{H}|\Psi\rangle\right) \\
\delta E[\Psi]\langle\Psi|\Psi\rangle &= \delta\left(\langle\Psi|\hat{H}|\Psi\rangle\right) - E[\Psi]\delta\left(\langle\Psi|\Psi\rangle\right) \\
\delta E[\Psi] &= \frac{1}{\langle\Psi|\Psi\rangle}\left[\delta\left(\langle\Psi|\hat{H}|\Psi\rangle\right) - E[\Psi]\delta\left(\langle\Psi|\Psi\rangle\right)\right] = 0 \ .
\end{aligned}$$

This term is zero if the part between squared brackets is zero

$$\delta\left(\langle\Psi|\hat{H}|\Psi\rangle\right) - E[\Psi]\delta\left(\langle\Psi|\Psi\rangle\right) = 0 \ , \tag{A.4}$$

and, since E is a number,

$$\langle\delta\Psi|\hat{H} - E|\Psi\rangle + \langle\Psi|\hat{H} - E|\delta\Psi\rangle = 0 \ . \tag{A.5}$$

Since Ψ is a complex function, the variation of $\langle\Psi|$ is independent of that of $|\Psi\rangle$. This because the real and the imaginary parts of $|\Psi\rangle$ vary independently from each other. This can be seen by substituting in (A.5) $|i\delta\Psi\rangle$ to $|\delta\Psi\rangle$.

$$-i\langle\delta\Psi|\hat{H} - E|\Psi\rangle + i\langle\Psi|\hat{H} - E|\Psi\delta\rangle = i\left[-\langle\delta\Psi|\hat{H} - E|\Psi\rangle + \langle\Psi|\hat{H} - E|\Psi\delta\rangle\right] = 0 \ . \tag{A.6}$$

Since the equations (A.5) and (A.6) must be verified at the same time, one has

$$\langle \delta\Psi|\hat{H} - E|\Psi\rangle = 0 \quad \text{e} \quad \langle \Psi|\hat{H} - E|\delta\Psi\rangle = 0 \ . \tag{A.7}$$

Since $|\delta\Psi\rangle$ is arbitrary the previous equations are always satisfied if

$$[H - E]\,|\Psi\rangle = 0 \ , \tag{A.8}$$

which is the Schrödinger equation (A.1).

Let's consider now a trial wave function $|\Phi\rangle$

$$|\Phi\rangle = \sum_{n=0}^{\infty} D_n |\Psi_n\rangle \tag{A.9}$$

expressed as linear combination of eaigenstates of $\hat{H}$

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle \tag{A.10}$$

where the D_n are complex numbers.

The energy functional can be expressed as

$$\begin{aligned} E[\Phi] &= \frac{\langle\Phi|\hat{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \frac{\displaystyle\sum_{n,n'}\langle\Psi_{n'}|D^*_{n'}\hat{H}D_n|\Psi_n\rangle}{\displaystyle\sum_{n,n'}\langle\Psi_{n'}|D^*_{n'}D_n|\Psi_n\rangle} \\ &= \frac{\displaystyle\sum_{n,n'} D^*_{n'}D_n\langle\Psi_{n'}|\hat{H}|\Psi_n\rangle}{\displaystyle\sum_{n,n'} D^*_{n'}D_n\langle\Psi_{n'}|\Psi_n\rangle} = \frac{\displaystyle\sum_{nn'} D^*_{n'}D_nE_n\delta_{n,n'}}{\displaystyle\sum_{n}|D_n|^2} \geq \frac{\displaystyle\sum_{n}|D_n|^2E_0}{\displaystyle\sum_{n}|D_n|^2} = E_0 \ . \end{aligned} \tag{A.11}$$

This inequality shows how the energy obtained by searching for the minimum of the energy functional in a subspace of trial wave functions gives an energy value larger than the correct ground state eigenvalue of the $\hat{H}$ hamiltonian.

Appendix B

Creation and destruction operators in angular momentum coupling

In this appendix, we consider the definition of fermion creation and destruction operators in case one it is concerned to exploit the spherical symmetry of the system.

In case of a one-body hamiltonian with spherical symmetry and spin-orbit interaction, the quantum numbers characterizing the single particle wave function are: the principal quantum number n, the quantum number l related to orbital angular momentum, j related to the total angular momentum and also m, the projection of j on the quantisation axis z. In the following we shall not explicitly write the dependence on n and l.

The action of the creation operators is:

$$\hat{a}^+_{j,m}|0\rangle = |jm\rangle \tag{B.1}$$

which indicates that the $\hat{a}^+_{j,m}$ puts a particle on the $|jm\rangle$ state. All the states with the same j have the same energy this is $2j+1$ degeneracy. For this reason it is necessary to specify also m.

The $2j+1$ components of $\hat{a}^+_{j,m}$ behave such as to form an irreducible spherical tensor [Edm57] satisfying the equations

$$\left[\hat{J}_z, \hat{a}^+_{j,m}\right] = m\hat{a}^+_{j,m} \tag{B.2}$$

$$\left[\hat{J}_\pm, \hat{a}^+_{j,m}\right] = \left[j(j+1) - m(m\pm 1)\right]^{1/2} \hat{a}^+_{j,m\pm 1}, \tag{B.3}$$

where we indicated with $J_\pm$ and J_z the spherical components of the generalized angular momentum of the system.

One of the properties characterizing the irreducible spherical tensor of rank k is that its $2k+1$ components transform in those of its hermitian conjugate as:

$$\left(\hat{T}^k_q\right)^+ = \left(\hat{T}^k_{-q}\right)(-)^q \ . \tag{B.4}$$

This means that the conjugate of $\hat{a}^+_{j,m}$, i.e. $\hat{a}_{j,m}$, is not a component of an irreducible spherical tensor, while the operator

$$\tilde{\hat{a}}_{j,m} = (-)^{j+m} a_{j,-m} \ , \tag{B.5}$$

satifies this requirement.

It is useful to use operators which are irreducible spherical tensor in the description of system with rotational invariance. For this reason, the use of $\tilde{\hat{a}}_{j,m}$ is preferred with respect to $\hat{a}_{j,m}$. The anticommutation properties are:

$$\left\{\hat{a}^+_{j,m}, \hat{a}^+_{j,m'}\right\} = 0 \qquad \left\{\tilde{\hat{a}}_{j,m}, \tilde{\hat{a}}_{j',m'}\right\} = 0 \tag{B.6}$$

$$\left\{\tilde{\hat{a}}_{j,m}, \hat{a}^+_{j',m'}\right\} = (-)^{j+m}\delta_{j,j'}\delta_{-m,m'} \tag{B.7}$$

It is possible to create a state composed by many particles by iteratively apply $a^+_{j,m}$ to the vacuum state and by using the rules of the angular momentum coupling. For example, the creation operator of two particles becomes:

$$\hat{A}^+(j_1 j_2; JM) = \frac{1}{(1+\delta_{j_1 j_2})^{1/2}} \left[\hat{a}^+_{j_1} \otimes \hat{a}^+_{j_2}\right]^J_M \tag{B.8}$$

where we have defined:

$$\left[\hat{a}^+_{j_1} \otimes \hat{a}^+_{j_2}\right]^J_M = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | JM\rangle \hat{a}^+_{j_1,m_1}\hat{a}^+_{j_2,m_2} \tag{B.9}$$

where $\langle j_1 m_1 j_2 m_2 | JM\rangle$ is a Clebsch-Gordan coefficient. The destruction operator for a particle pair becomes:

$$\tilde{\hat{A}}(j_1 j_2; JM) = (-)^{J+M}\left[\hat{A}^+(j_1 j_2; J-M)\right]^+ = -\frac{1}{(1+\delta_{j_1 j_2})^{1/2}}\left[\tilde{\hat{a}}_{j_1} \otimes \tilde{\hat{a}}_{j_2}\right]^J_M \tag{B.10}$$

and the operator creating a particle-hole pair is:

$$\hat{U}(j_1 j_2; JM) = [\hat{a}^+_{j_1} \otimes \tilde{\hat{a}}_{j_2}]^J_M \tag{B.11}$$

When $j_1 = j_2$, the two particles are identified by $m_1 \neq m_2$ therefore, since the above equations include a sum on the m_1 and m_2 it is necessary to divide by $\sqrt{2}$ since there is a double counting of identical configurations. For example, the configuration where the the particle 1 has m_1 and that of particle 2 m_2, is identical to that where the particle 1 has m_2 and particle 2 m_1.

Appendix C

Speed of sound in fluids

In this appendix, we obtain the expression for the speed of sound in a classical fluid. The derivation is quite standard [Blu06]. We consider classical fluids, non quantum fluids, and combine continuity and Euler equations.

We call $\mathbf{u}(\mathbf{r}, t)$ the local velocity of an infinitesimal mass of fluid, and ρ_{m} the mass density, related to the number density by the relation $\rho_{\mathrm{m}} = m\rho$ where m is the mass of the particle whose ρ represents the probability that it is present in a unitary volume.

C.1 Continuity equation

The mass of a fluid which, in the unit of time, goes out from a closed surface S is given by

$$\int_S \rho_{\mathrm{m}}\, \mathbf{u} \cdot d\mathbf{S} \ . \tag{C.1}$$

This is a surface integral and the direction of $d\mathbf{S}$ is given by a vector orthogonal to plane touching the infinitesimal surface element. The loss of flux implies a lowering of the fluid density in the volume contained by the surface S

$$\int_S \rho_{\mathrm{m}}\, \mathbf{u} \cdot d\mathbf{S} = -\frac{\partial}{\partial t} \int_V \rho_{\mathrm{m}}\, dV \tag{C.2}$$

where the integral in the right hand side is a volume integral.

This is the continuity equation expressed in the integral form. We obtain a differential expression of this equation by applying the divergence theorem to the term of left hand side

$$\int_S \rho_{\mathrm{m}}\, \mathbf{u} \cdot d\mathbf{S} = \int_V \rho_{\mathrm{m}}\, \nabla \cdot \mathbf{u} dV = -\int_V \frac{\partial \rho_{\mathrm{m}}}{\partial t}\, dV \ , \tag{C.3}$$

where we have inverted the order of the integration and differentiation operations in the last integral. By equating the two integrands we obtain

$$\nabla \cdot (\rho_{\mathrm{m}} \mathbf{u}) = -\frac{\partial \rho_{\mathrm{m}}}{\partial t} \ , \tag{C.4}$$

where $\rho_{\mathrm{m}}\mathbf{u}$ is commonly called current density. The one-dimensional expression is

$$\frac{\partial (\rho_{\mathrm{m}} u)}{\partial x} = -\frac{\partial \rho_{\mathrm{m}}}{\partial t} \ . \tag{C.5}$$

C.2 Euler equation

In a fluid, the rate of change of a vector property $\mathbf{X}(\mathbf{r}, \mathbf{t})$ depending on the position and on the time t is described by a **convective** derivative which is a total derivative with respect to the time.

$$\frac{D\mathbf{X}}{Dt} = \frac{\partial \mathbf{X}}{\partial t} + \sum_{i=1}^{3} \frac{\partial \mathbf{X}}{\partial x_i}\frac{\partial x_i}{\partial t} = \frac{\partial \mathbf{X}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{X} \ . \tag{C.6}$$

We consider an infinitesimal element of the fluid. The external force acting on this element is given by the convective derivative of the velocity $\mathbf{u}$. This force induce a gradient on the pressure generated by the considered element on the other parts of the fluid. The pressure gradient per mass units is given by the equation

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho_{\mathrm{m}}}\nabla P \ , \tag{C.7}$$

where the $-$ sign is due the fact that the force is external to the volume considered and a positive force induces a negative pressure gradient.

By writing the explicit expression of the convective derivative we obtain

$$-\frac{1}{\rho_{\mathrm{m}}}\nabla P = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} \ , \tag{C.8}$$

and in one dimension we have

$$-\frac{1}{\rho_{\mathrm{m}}}\frac{\partial P}{\partial x} = \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} \ . \tag{C.9}$$

C.3 Velocity of the sound

Let's consider a situation where the sound propagates in a specific direction. We use the one-dimensional expressions of the continuity and Euler equations. The latter one can be written as

$$u\frac{\partial \rho_{\mathrm{m}}}{\partial x} + \rho_{\mathrm{m}}\frac{\partial u}{\partial x} = -\frac{\partial \rho_{\mathrm{m}}}{\partial t} \ . \tag{C.10}$$

We divide by ρ_{m} and use the variable $s = (\delta\rho_{\mathrm{m}})/\rho_{\mathrm{m}}$

$$u\frac{\partial s}{\partial x} + \frac{\partial u}{\partial x} = -\frac{\partial s}{\partial t} \ . \tag{C.11}$$

We consider sound waves with small amplitudes. This means that the density changes are on small distance scale with repect to the fluid dimensions, and therefore those of the sound propagation. The quadratic terms in u are negligible, and also the term where the fluid velocity u multiplies the density variation $\delta s/\delta x$. By using these approximations, the previous equation becomes

$$\frac{\partial u}{\partial x} = -\frac{\partial s}{\partial t} \tag{C.12}$$

and the Euler equation

$$-\frac{1}{\rho_{\mathrm{m}}}\frac{\partial P}{\partial x} = \frac{\partial u}{\partial t} \tag{C.13}$$

By using the definition of compression modulus (2.60) we have

$$B = -\mathcal{V}\frac{\partial P}{\partial \mathcal{V}} = -\frac{A}{\rho_{\mathrm{m}}}\frac{\partial P}{\left(-\frac{\mathcal{V}}{\rho_{\mathrm{m}}}\partial\rho_{\mathrm{m}}\right)} = \rho_{\mathrm{m}}\frac{\partial P}{\partial \rho_{\mathrm{m}}} \ , \tag{C.14}$$

from which $\delta P = B\delta s$, We can express the equation (C.13) as

$$\frac{\partial u}{\partial t} = -\frac{B}{\rho_{\rm m}}\frac{\partial s}{\partial x} \ . \tag{C.15}$$

We insert the expression of δu obtained by this equation in (C.12), and obtain

$$\frac{B}{\rho_{\rm m}}\frac{\partial^2 s}{\partial x^2} = \frac{\partial^2 s}{\partial t^2} \ . \tag{C.16}$$

Possible solutions of this equation are

$$s \propto e^{i(kx-\omega t)} \ , \tag{C.17}$$

which inserted in (C.16) gives the relation

$$\frac{B}{\rho_{\rm m}}k^2 = \omega^2 \ . \tag{C.18}$$

Therefore, the speed of propagation of the sound wave is

$$v_s = \frac{\omega}{k} = \sqrt{\frac{B}{\rho_{\rm m}}} \ . \tag{C.19}$$

Appendix D

Boltzmann transport equation

In this appendix we provide a derivation of the classical transport equation of Boltzmann. In this derivation the the motion of a single particle is described by the three components of its position $\mathbf{r}$ and by the three components of its velocity $\mathbf{v}$. The goal is to find the variations of the distribution function $f(\mathbf{r}, \mathbf{v}, t)$. The number of particles which, at the time t, are in the infinitesimal volume $d\mathcal{V}$ of the six dimensional phase space described by $\mathbf{r}$ and $\mathbf{v}$ is given by $f(\mathbf{r}, \mathbf{v}, t)$. In other words, is if A is the particle number, the probability of finding a particle in the volume $d\mathcal{V}$ at the time t is given by $(1/A)f(\mathbf{r}, \mathbf{v}, t)$.

The distribution function defines completely the state of the system. For example, the particle local density $\rho(\mathbf{r}, t)$, whatever is their velocity, is obtained by integrating on the velocities

$$\rho(\mathbf{r}, t) = \int d^3v \, f(\mathbf{r}, \mathbf{v}, t) \ . \tag{D.1}$$

Let's consider the case where there are not collisions among the particles. External forces, whose vector sum, at the time t, is given by $\mathbf{F}(\mathbf{r}, t)$, are acting on the system. The time variation of position and velocity of the individual particle is given by

$$\mathbf{r}' = \mathbf{r}(t + dt) = \mathbf{r}(t) + \mathbf{v}(t)dt \ , \tag{D.2}$$

$$\mathbf{v}' = \mathbf{v}(t + dt) = \mathbf{v}(t) + \frac{\mathbf{F}(\mathbf{r}, t)}{m} dt \ . \tag{D.3}$$

The distribution function describing, at the time t, the system in a volume $d\mathcal{V}$ evolves at the time $t + dt$ both because it explicitly depends on time, but also because of the variation of $\mathbf{r}$ e $\mathbf{v}$. We can write the new distribution function as

$$f(\mathbf{r}', \mathbf{v}', t + dt) = f(\mathbf{r}', \mathbf{v}', t)dt + \frac{\partial f}{\partial t} dt + \sum_{i=1}^{3} \frac{\partial f}{\partial x_i} \dot{x_i} dt + \sum_{i=1}^{3} \frac{\partial f}{\partial v_i} \dot{v_i} dt \ , \tag{D.4}$$

where the dot on the letter indicates the time partial derivative. We can define the total derivative as

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \sum_{i=1}^{3} \frac{\partial f}{\partial x_i} \dot{x_i} + \sum_{i=1}^{3} \frac{\partial f}{\partial v_i} \dot{v_i} \ , \tag{D.5}$$

or in vector form

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot (\nabla_{\mathbf{r}} f) + \frac{1}{m} \mathbf{F} \cdot (\nabla_{\mathbf{v}} f) \ , \tag{D.6}$$

where the subscripts indicate that the gradients are calculated with respect to the coordinates or to the velocities.

In a collisionless situation and for conservative external forces, i.e. independent of the velocities, there is a conservation of the particle flux in the volume $d\mathcal{V}$. This statement can be expressed in terms of current conservation

$$\frac{\partial f}{\partial t} + \nabla(f\mathbf{v}) = 0 \ , \tag{D.7}$$

which in the six-dimensional **r v** space becomes

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} \frac{\partial (f\dot{x_i})}{\partial x_i} + \sum_{i=1}^{3} \frac{\partial (f\dot{v_i})}{\partial v_i} = 0 \ . \tag{D.8}$$

Therefore

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} \left[\frac{\partial f}{\partial x_i}\dot{x_i} + f\frac{\partial \dot{x_i}}{\partial x_i} \right] + \sum_{i=1}^{3} \left[\frac{\partial f}{\partial v_i}\dot{v_i} + f\frac{\partial \dot{v_i}}{\partial v_i} \right] = 0 \ , \tag{D.9}$$

and

$$\frac{Df}{Dt} + f\sum_{i=1}^{3} \left(\frac{\partial \dot{x_i}}{\partial x_i} + \frac{\partial \dot{v_i}}{\partial v_i} \right) = 0 \ . \tag{D.10}$$

Since the hamiltonian is conservative, the Hamilton equations are valid

$$\dot{x_i} = \frac{\partial H}{\partial p_i} = \frac{\partial H}{m\partial v_i} \ , \tag{D.11}$$

$$-\dot{p_i} = -m\dot{v_i} = \frac{\partial H}{\partial x_i} \ , \tag{D.12}$$

$$\frac{\partial \dot{x}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\frac{\partial H}{m\partial v_i} \right] = \frac{1}{m}\left[\frac{\partial^2 H}{\partial v_i \partial x_i} \right] = \frac{\partial}{\partial v_i}\left[\frac{1}{m}\frac{\partial H}{\partial x_i} \right] = -\frac{\partial \dot{v_i}}{\partial v_i} \ . \tag{D.13}$$

Therefore

$$\frac{Df}{Dt} = 0 \ . \tag{D.14}$$

The presence of collision between the particle modifies Eq. (D.14) as

$$\frac{Df(\mathbf{r}, \mathbf{v}, t)}{Dt} = \Delta^+ - \Delta^- \ , \tag{D.15}$$

where we indicated with Δ^- the lowering of the value of f because of the particles that, in the physical volume $dV = d\mathbf{r}$, after the collision have a velocity different from $\mathbf{v}$, and with Δ^+ the increase of the value of f because of the particle which have initially a value of the velocity different from $\mathbf{v}$, and then, after collision have a velocity between $\mathbf{v}$ and $\mathbf{v} + d\mathbf{v}$ values. All this changes happen in the unit of time.

Let's make some assumptions to evaluate these two terms.

1. The mean free path of each particle is much larger than its dimensions.

2. Short-range interactions.

3. Binary collisions. Collisions betwee three, or even more particles are negligible.

4. Only elastic collisions.

We evaluate first Δ^-. Let's consider a particle with velocity $\mathbf{v}$ having a collision with another particle of initial velocity $\mathbf{w}$. We call $\mathbf{v}'$ and $\mathbf{w}'$ the velocities after the collision. Since we assumed that the collision is elastic, because of the momentum and kinetic energy conservation we obtain,

$$\begin{aligned} \mathbf{v}+\mathbf{w} &= \mathbf{v}'+\mathbf{w}' && \text{(D.16)} \\ \mathbf{v}^2+\mathbf{w}^2 &= (\mathbf{v}')^2+(\mathbf{w}')^2 \ . && \text{(D.17)} \end{aligned}$$

The modules of the relative velocities $\mathbf{V}=\mathbf{v}-\mathbf{w}$ e $\mathbf{V}'=\mathbf{v}'-\mathbf{w}'$ do not change

$$|\mathbf{V}|=|\mathbf{V}'| \ . \tag{D.18}$$

We call $\sigma_{\mathbf{v},\mathbf{w}\to\mathbf{v}',\mathbf{w}'}$ the elastic cross section of this collision which is invariant under time reversal, $t\to -t$, therefore,

$$\sigma_{\mathbf{v},\mathbf{w}\to\mathbf{v}',\mathbf{w}'}=\sigma_{\mathbf{v}',\mathbf{w}'\to\mathbf{v},\mathbf{w}} \ , \tag{D.19}$$

this means that, once the relative velocity value is selected $|\mathbf{V}|$ the cross section depends only on the incoming and outgoing directions, in other words on the solid angle Ω where the particles are scattered. In the specific case of unpolarized particles, such as those without spin, the cross section depends only on the angle θ between incoming and outgoing directions. Therefore, we have

$$\int d^3v'd^3w'\sigma_{\mathbf{v},\mathbf{w}\to\mathbf{v}',\mathbf{w}'}=\int d\Omega\sigma(\Omega) \ . \tag{D.20}$$

The number of molecules that, because of the collisions, in the unit of time, goes from $(\mathbf{v},\mathbf{w})$ to $(\mathbf{v}',\mathbf{w}')$ is proportional to the cross section and also the flux, therefore to the relative speed $\mathbf{v}-\mathbf{w}$, and to the joint probability of finding a particle with velocity $\mathbf{v}$ and another one with velocity $\mathbf{w}$. We make now a new assumption: the joint probability is the product of the two individual probabilities. This means to neglect the correlations, i.e. to consider the motion of each particle independent of the presence of the other particles. This probability is, therefore, the product of $f(\mathbf{r},\mathbf{v},t)$ times $f(\mathbf{r},\mathbf{w},t)$ wich we write as $f_\mathbf{v}f_\mathbf{w}$. Putting together all the assumptions we obtain

$$\Delta^-=\int d^3w\,d^3v'\,d^3w'\,|\mathbf{v}-\mathbf{w}|\sigma_{\mathbf{v},\mathbf{w}\to\mathbf{v}',\mathbf{w}'}f_\mathbf{v}f_\mathbf{w} \ . \tag{D.21}$$

The path to obtain Δ^+ is similar. One has to substitute $\mathbf{v}$ and $\mathbf{w}$ with $\mathbf{v}'$ and $\mathbf{w}'$ respectively

$$\Delta^+=\int d^3w\,d^3v'\,d^3w'\,|\mathbf{v}'-\mathbf{w}'|\sigma_{\mathbf{v}',\mathbf{w}'\to\mathbf{v},\mathbf{w}}f_{\mathbf{v}'}f_{\mathbf{w}'} \ . \tag{D.22}$$

By considering the invariance of the relative velocity module (D.18) the time reversal invariance (D.19), the relation (D.20) between cross section, we can write the transport equation (D.15) as

$$\begin{aligned} \frac{Df}{Dt} &= \int d^3w\,d^3dv'\,d^3w'\,|\mathbf{v}-\mathbf{w}|\sigma_{\mathbf{v}',\mathbf{w}'\to\mathbf{v},\mathbf{w}}(f_{\mathbf{v}'}f_{\mathbf{w}'}-f_\mathbf{v}f_\mathbf{w}) \\ &= \int d^3w\,d\Omega\,|\mathbf{v}-\mathbf{w}|\sigma(\Omega)(f_{\mathbf{v}'}f_{\mathbf{w}'}-f_\mathbf{v}f_\mathbf{w}) \ , && \text{(D.23)} \end{aligned}$$

and in the more extended expression

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot(\nabla_\mathbf{r}f)+\frac{1}{m}\mathbf{F}\cdot\nabla_\mathbf{v}f=\int d^3w\,d\Omega\,|\mathbf{v}-\mathbf{w}|\sigma(\Omega)(f_{\mathbf{v}'}f_{\mathbf{w}'}-f_\mathbf{v}f_\mathbf{w}) \ . \tag{D.24}$$

The right hand side of this equation is usually called collision integral, $\mathcal{J}(f)$.

Appendix E

Acronyms

AFDMC	Auxilary Field Diffusion Monte Carlo (Sect. 4.4)
CCM	Coupled Cluster Method (Chapter 15)
CBF	Correlated Basis Function (Chapter 13)
DFT	Density Functional Theory (Sect. 9.3)
FG	Fermi Gas (Chapter 2.3)
FHNC	Fermi Hypernetted Chain (Sect. 13.3)
GFMC	Green Function Monte Carlo (Chapter 4.3)
HF	Hartree-Fock (Sect. 12.3 e 9.2)
HNC	Hypernetted Chain (Sect. 13.2)
IPM	Independent Particle Model (Chapter 2)
KS	Khon-Sham (Sect. 9.3.2)
MF	Mean-Field (Chapter 2)
QBA	Quasi Boson Approximation (Sect. 10.3.2)
OBDM	One-body density matrix (Sect. 13.3)
ONR	Occupation number representation (Chapter 5)
QBA	Quasi Boson Approximation (Sect. 10.3)
QCD	Quantum Chromodynamics
QED	Quantum Electrodynamics
RPA	Random Phase Approximation (Sect. 12.5 e Cap. 10)
TBDF	Two-body distribution function (Sect. 13.2)
TDA	Tamm Dankoff Approximation (Sect. 10.2)
VMC	Variational Monte Carlo (Chapter 4.2)
UCOM	Unitary Correlation Operator Method (Chapter 14)

Appendix F

Symbols

This is a list of symbols whose meaning is the same in all the chapters of the book

$\hat{a}$, $\hat{a}^+$	Creation and destruction operators (Chapter 5)
A	Number of particles
E	Energy of the interacting particles system
$\mathcal{E}$	Energy of the non-interacting particles system
G	Green's function (Chapters 8 and 11)
$\mathcal{G}$	Effecttive interaction from Brueckner's theory (Chapter 8)
$\hat{h}$	Single-particle hamiltonian (Chapter 2)
$\hat{H}$	Total hamiltoniana (Chapter 2)
$\hat{H}_0$	One-body hamiltonian, of mean-field (Chapter 2)
$\hat{H}_1$	Perturbative term, interaction term, of the hamiltonian H (Chapter 2)
$\hat{\mathbb{I}}$	The identity operator.
$\hat{\mathbb{N}}$	Normal ordered product operator (Chapter 5)
$\hat{T}$	Kinetic energy operator of the hamiltonian (Chapter 2)
$\hat{\mathbb{T}}$	Time ordered product operator (Chapter 5)
$\hat{V}$	Interaction Potential (Chapter 2)
$\mathcal{V}$	Volume of the system (Chapter 2)
Y_{lm}	Spherical harmonics (Chapter 2)
$\mathcal{Y}_{ljm}$	Spin spherical harmonics (Chapter 2)
Φ	Eigenstate of H_0, mean-field state, Slater determinant for fermions (Chapter 2)
ϕ_i	Single-particle wave function eigenstate of h (Chapter 2)
Ψ	Eigenstate of H (Chapter 2)
ψ , ψ^+	Field operators (Chapter 5)
ρ	Number density of the particles (Chapter 2)
ρ_ϵ	Density of states (Chapter 2)
Σ	Self-energy (Chapter 12).
Ω	Polar angular coordinates (Chapter 2)
Z	atomic number

Bibliography

[Abe66] W. R. Abel, A. C. Anderson, J. C. Wheatley, Phys. Rev. Lett. 17 (1966) 74.

[Abr75] A. A. Abrikosov, L. P. Gorkov, I. E. Dzyaloshinski, Methods of quantum field theory in statistical physics, Dover, New York (1975).

[Akm98] A. Akmal, V. R. Pandharipande, D. G. Ravenhall, Phys. Rev. C 58 (1998) 1804.

[Ahr75] J. Ahrens et al., Nucl. Phys. A 251 (1975) 479.

[Ari07] F. Arias de Saavedra, C. Bisconti, G. Co' and A. Fabrocini Phys. Rep. 450 (2007) 1.

[Ash76] N. W. Ashcroft and N. D. Mermin, Solid State Physics, Saunders, Orlando, (1976).

[Blu06] S. J. Blundell, K. M. Blundell, Concepts in Thermal Physics, Oxford University Press, Oxford (2006).

[Boh53] D. Bohm, D. Pines, Phys. Rev. 92 (1953) 609.

[Bru04] H. Bruus, K. Flensbeg, Many-body Quantum Theory in Condensed Matter Physics, Oxford Univ. Press, Oxford (2004).

[Car15] J. Carlson, S. Gandolfi, F. Pederiva, S. C. Pieper, R. Schiavilla, K.E. Schmidt, R.B. Wiringa Rev. Mod. Phys. 87 (2015).

[Co12] G. Co', V. De Donno, P. Finelli, M. Grasso, M. Anguiano, A. M. Lallena, C. Giusti, A. Meucci, F. D. Pacati, Phys. Rev. C 85 (2012) 024322.

[Coe77] C. Cohen-Tannoudji, B. Diu, F. Laloë, Quantum Mechanics, John Wiley, New York (1977).

[Day67] B. D. Day, Rev. Mod. Phys., 39 (1967) 719.

[Don11] V. De Donno, G. Co', M. Anguiano, A. M. Lallena, Phys. Rev. C 83 (2011) 044324

[Edm57] A. R. Edmonds, Angular momentum in quantum mechanics, Princeton University Press, Princeton (1957)

[Fan74] S. Fantoni, S. Rosati, Nuov. Cim. A 20 (1974) 179.

[Fel98] H. Feldmeier, T. Neff, R. Roth, J. Schnack, Nucl. Phys. A 632 (1988) 61.

[Fet71] A. L. Fetter and J. D. Walecka, Quantum theory of many–particle systems, Mc Graw–Hill, New York (1971), anche Dover, New York (2003).

[Gan10] S. Gandolfi, A. Y. Illarionov, S. Fantoni, J. C. Miller, F. Pederiva, K. E. Schmidt, Mont. Not. R. Astron. Soc. 404 (2010) L35.

[Gro91] E. K. U. Gross, E. Runge and O. Heinonen, Many-particle theory, Adam Hilger, Bristol (1991).

[Goo85] D. L. Goodstein, States of matter, Dover, New York (1985).

[Kit80] C. Kittel, H. Kroemer, Thermal Physics, W. H. Freeman, New York (1980).

[Kit86] C. Kittel, Introduction to Solid State Physics, John Wiley, New York (1986).

[Kra88] K. Krane, Introductory Nuclear Physics, John Wiley & sons, New York (1988).

[Mar67] N. H. March, W. H. Young and S. Sampanthar, The many-body problem in quantum mechanics, Cambridge University Press, Cambridge (1967), anche, Dover, New York (1995).

[Mat67] R. D. Mattuck, A guide to Feynmann diagrams in the many–body problem, Mc Graw–Hill, New York (1967), anche Dover, New York (1992).

[May40] J. E. Mayer, M. G. Mayer, Statistical Mechanics, Wiley, New York (1940).

[Mes61] A. Messiah, Quantum Mechanics, North Holland, Amsterdam (1961), anche, Dover, New York (2014).

[Nav02] J. Navarro, R. Guardiola, I. Moliner, The Coupled Cluster Method and its applications, in Introduction to modern methods of quantum many-body theory and their applications, A. Fabrocini, S. Fantoni, E. Krotsheck Eds., World Scientific, Singapore (2002), p. 121.

[Pin66] D. Pines, P. Nozières, The theory of Quantum Liquids, Benjamin, New York (1966).

[Pry66] J. A. Pryde, The liquid state, Hutchinson, London (1966)

[Rin80] P. Ring, P. Schuck, The nuclear many-body problem, Springer (Berlino) 1980.

[Sch92] K. E. Schmidt, D. E. Ceperley, Monte Carlo Techniques for Quantum Fluids, Solids and Droplets, in The Monte Carlo Method in Condensed Matter Physics, ed. K. Binder, Topics in Applied Physics, Vol 71, Springer-Verlag, (1992).

[Sla29] J. C. Slater, Phys. Rev. 34 (1929) 1293.

[Suh07] J. Suhonen, From nucleons to nucleus, Springer (Berlino) 2007.

[Tho61] D. J. Thouless, Nucl. Phys. 22 (1961) 78.

Index