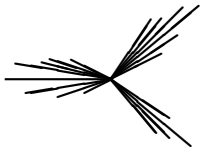

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DISSERTAÇÃO DE MESTRADO IFT–D.013/09

Evaluation of the partition function of fermions using Grassmann coherent states without path integrals

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Resumo

A presente dissertação tem como objetivo principal fazer uma revisão sobre o uso de estados coerentes para calcular a função de partição gran canônica de sistemas fermiônicos, sem empregar integrais de trajetória. Após discutir um método de cálculo baseado numa expansão de altas temperaturas, formulamos uma teoria de perturbação otimizada empregando campos auxiliares via transformação de Hubbard-Stratonovich. Aproximações não perturbativas tradicionais de campo médio tipo Hartree-Fock e de BCS são obtidas em ordem zero da teoria de pertubação otimizada. Correções não perturbativas à aproximação de ordem zero são implementadas usando uma expansão em potências de uma interação modificada, em que os efeitos dos campos médios são subtraídos da interação original do Hamiltoniano da teoria.

Palavras Chaves: Estados coerentes, Integrais de trajetória, Férmions, Álgebra de Grassmann, Transformação de Hubbard-Stratonovich, Teoria de perturbação otimizada

Áreas do conhecimento: Física Nuclear, Teoria de Campos e Partículas Elementares, Física da Matéria Condensada

Abstract

The primary aim of the dissertation is to review the use of coherent states for the calculation of the grand canonical partition function for fermion systems, without employing path integrals. After discussing a calculational method based on a high temperature expansion, we formulate an optimized perturbation theory employing external fields via the Hubbard-Stratonovich transformation. Traditional non-perturbative mean field approximations like Hartree-Fock and BCS are obtained in zeroth order in the optimized perturbation theory. Non-perturbative corrections to the zeroth order approximation are implemented through a power series expansion of a modified interaction,where the effects of the mean fields are subtracted from the original interaction of the Hamiltonian of the theory.

Índice

Capítulo 1

Introduction

The present dissertation is primarily a review on the use of coherent states in the evaluation of the quantum grand canonical partition function of a many-particle system at finite temperature. The main focus of the dissertation are systems of spin-1/2 fermions. The grand canonical partition function is the fundamental quantity in the mathematical treatment of many-body systems from which all physical quantities can be derived [1, 2]. However, it can scarcely be calculated in closed form, a fact that is not surprising in view of the intractability of the many-body problem. On the other hand, there is great activity on the development of efficient numerical methods for calculating the partition function non-perturbatively. Monte Carlo methods have been central to such methods, in particular in the context of quantum field theory problems. The basic strategy of the Monte Carlo (MC) [3] method in field theory is to express the trace over field configurations in terms of a path integral so that the problem is reduced to the evaluation of a multidimensional integral using importance sampling [4]. Path integral formulations of fermion quantum fields involve the use of anti-commuting Grassmann variables [5], providing a very useful tool for implementing covariant perturbation theory calculations in gauge theories [6] and super-symmetric field theories [7]. However, this approach is problematic for nonperturbative approaches like the MC method. For models (or theories) involving boson-fermion couplings, like Quantum Electrodynamics (QED) and Quantum Chromodynamics (QCD), invariably the application of the MC method involves a formal, exact integration over the Grassmann variables in favor of determinants that depend only on the boson fields. For models involving only fermion fields the application of the MC method involves the use of a Hubbard-Stratonovich transformation [8]. This method introduces auxiliary boson fields so that the self-interacting part of the interaction becomes quadratic so that the Grassmann variables representing fermion fields can be integrated. Again this leads to determinants that involve only boson fields. In many cases the resulting

determinants can be rewritten as path integrals over additional boson fields and the problem is then reduced to the evaluation of multidimensional integrals over boson degrees of freedom. The problem with this approach is that the resulting determinants are in general complex (when not complex, they might not be positive) and the use of a MC approach becomes very inefficient or even inapplicable. This problem of a non-positive determinant is known in the literature as the *sign problem*.

An alternative to the path integral formulation of the grand canonical partition function is the direct evaluation of the trace over Grassmann variables. A particularly interesting novel approach in this direction was introduced a few years ago by Thomaz and collaborators [9]. The method is based on the high temperature expansion of the Boltzmann factor in the partition function and makes use of the coherent-state representation of the trace [1]. Each term of the expansion is evaluated exactly exploiting the anti-commuting nature of the Grassmann numbers. This novel method builds on previous experience in calculating the high-temperature expansion of the partition function of an anharmonic fermionic oscillator on a lattice [10] and of the one-dimensional Hubbard model [11]. Crucial to the method are two results obtained by Thomaz and collaborators in two separate publications. First, Charret, de Souza and Thomaz [12] have shown that the moments of a Gaussian Grassmann multi-variable integral are related to the co-factors of the matrix of the Gaussian exponential. This result is important because the expansion of the Boltzmann factor requires the evaluation of a trace of multiple products of operators. The trace of a product of operators can be expressed in terms of matrix elements in a coherent-state representation and this leads to a multi-variable integral over Grassmann numbers. Second, I.C. Charret, Corrêa Silva, S.M. de Souza, O. Rojas Santos, and M.T. Thomaz [13] have shown that the matrix related to the co-factors mentioned above can be diagonalized analytically through a similarity transformation. This result is valid for any dimensionality of the matrix and is model independent, in that it depends only on the kinematical aspects of the approach. This was a tremendous achievement, since despite the closed form of the result of the multidimensional Grassmann integral in terms of co-factors, their explicit evaluation is still a formidable task.

In the present dissertation we review this approach developed by Thomaz and collaborators. We name this approach the *Niterói method*. In addition to reviewing the method, we indicate further developments beyond the high temperature expansion of the Boltzmann factor. In particular we make the case for using the method in the context of improving mean field type of approximations through the combined use of the Hubbard-Stratonovich transformation and the ideas of *optimized perturbation theory* (OPT) [14]. Specifically, the high temperature expansion of the

partition function can be re-summed in the case of a quadratic Hamiltonian, i.e. for an Hamiltonian that involves the product of only two field operators. On the other hand, a mean-field type of approximation is a non-perturbative method that is able to bring the full Hamiltonian, which in general involves the product of four field operators, into a quadratic form through a regrouping of the operators. Examples includes the well known Hartree-Fock and BCS approximation schemes [1, 2]. Initially we show explicitly that known mean field type of approximations can be obtained trivially within the Niteói method. In addition, we show that one can reproduce standard formulas for perturbative corrections to the mean field approximations within the same method. As is well known, perturbative corrections to mean field approximations, like with all kinds of perturbative calculations, become very involved when higher order corrections are needed. We propose an approach in that the high order corrections can be calculated in the context of OPT – also known in some contexts as the δ-expansion Ref. [15], or optimized δ-expansion [16]. A more complete list of references on this subject can be found in Ref. [17].

We envisage application of the proposed method in different fields. One immediate application is in the context of atomic fermionic gases [18]. The field of fermionic gases is witnessing explosive interest, both in theoretical and experimental contexts, and can be considered as a natural follow up of the first experimental realizations of atomic Bose-Einstein condensates [19]. The first atomic experimental observation of atomic Fermi gases occurred in 2003 [20] and others followed very soon afterwards [21]. Good review articles is Ref. [22] and a more complete list of references and discussions on recent experimental developments can be found at the sites mentioned in Refs. [24][25]. The excitement on the subject is due to the possibility of exploring and manipulating experimentally matter composed of particles with no classical analogue. Contrary to bosons, fermions cannot be described in terms of the dynamical dynamical variables like position and momentum, they require new dynamical variables that are not of common use in Physics, like Grassmann variables.

Another interesting aspect of Fermi systems is what became known as the *unitarity limit*. This is meant to be a limit in which much of the phenomena happening in such systems are well described by assuming point-like fermions interacting very strongly through very short-ranged interactions – the unitarity limit is realized when the scattering length characterizing the interaction strength is much larger than the inter-particle spacing, so that the only scale relevant in the problem is the scattering length. Such systems are encountered in different fields of physics [23], like in nuclear physics in the context of the low-energy properties of the atomic nucleus and the structure of neutron stars, in astro-particle physics in studies related to quark-

gluon plasma of the early Universe, in condensed matter physics in the context of strongly correlated electron systems. Theoretical developments closely related to these subjects and to the main theme of the present dissertation can be found in Refs. [26]-[29]. These references deal with the use of coherent states in the combined framework of path integrals and the Hubbard-Stratonovich transformation, mainly in context of lattice formulations.

We believe that our proposed method has interest beyond pure academics. A major contemporary goal in the physics of atomic Fermi gases is to go beyond the framework of mean field physics to access manifestations of strong interactions and correlations. The experimental possibility of tuning the interaction using external magnetic fields through Feshbach resonances [18] is a powerful experimental tool to control physics beyond mean field and provides excellent opportunities to test and understand applicability limits of traditional approximation schemes. Moreover, we also believe that our proposed method can be extended to more ambitious situations of quantum field theory, like to lattice QCD [30] [31]. Here we envisage the applications in the strong coupling limit of the theory, a subject with renewed recent interest [32] [33]. The strong coupling expansion of the QCD action resembles in many respects the high temperature expansion and so the Niterói method should be of direct applicability.

A natural question that might arise is, why one would give up the possibility of obtaining an exact result and use, instead, an approximate scheme like OPT? The exact result is actually a formal one, in that one still needs to perform Monte Carlo simulations to integrate over the auxiliary scalar fields. An exact, numerical result is of course preferred, but in many cases it does not bring understanding of the basic processes responsible for observed features of the system. It is hoped that through an expansion in a modified interaction one can capture most of the physics relevant to the problem and that a milder, or even no sign problem arises – of course this we will only know with explicit calculations. Also, it is important to understand how correlations affect the zeroth-order mean field results, and a systematic expansion that builds such correlations might be very useful for the insight one can get from this. And finally, comparison with an exact solution will allow to measure the quality of such an approximate scheme.

The dissertation is organized as follows. In the next Chapter we review the second-quantization formalism as employed in the context of non-relativistic quantum many-body theory. The discussion is didactic and an effort is made to present explicit derivation of important results. In Chapter 3, we review the use of coherent states for calculating traces over fermionic variables. We also discuss the path integral representation of the partition function using coherent states. The Niterói

method is discussed with detail in Chapter 4. As in the previous Chapters, our discussion is deliberately didactic and detailed derivations are given whenever possible and adequate. In Chapter 5 we present applications of the Niterói method to simple problems. Initially, we consider the illustrative case of the free Fermi gas and afterwards we consider mean field type of approximations to the interacting non-relativistic Fermi gas. In Section 5.3 we discuss how to obtain the well known results of perturbation theory on the top of the mean field approximation. In Section 5.4 we propose to use the Niterói method in connection with the Hubbard-Stratonovich [8] transformation to implement high order optimized perturbation theory [14]-[17] to improve on the mean field approximation. The aim here is to set up the approach and no attempt is made to obtain explicit evaluations of high order corrections, since this would require an specific model and some numerical work. This would extrapolate the scope of the present dissertation and therefore we leave these issues for future work. Our Conclusions and Perspectives are presented in Chapter 6. The dissertation contains also five Appendices, where we collect some demonstrations cited in the main text.

Capítulo 2

Second Quantization Formalism

In the present Chapter we will present a very short review on the basics of the second quantization formalism for a system of identical particles. At the cost of being sometimes pedantic, our approach is deliberately didactic, in that we make an effort to present explicit derivation of important results. Our discussion here is strongly based on the book of Negele and Orland [1]. We will start discussing the quantum mechanical description of many-particle systems making use of single-particle basis states. Next the formalism of second quantization and the Fock space is discussed. Finally, the important issue of changing representation is presented, with emphasis on the change from the coordinate representation to the momentum representation.

2.1 Many-particle bases

Let $\mathcal{H}$ be a Hilbert space for one particle and $\{|\alpha_i\rangle\}$ a basis of dimension D. Let us assume that the basis is orthonormal,

$$\langle\alpha_i|\alpha_j\rangle = \delta_{ij}\,, \tag{2.1}$$

and complete

$$\sum_{i=1}^{D} |\alpha_i\rangle\langle\alpha_i| = I. \tag{2.2}$$

We denote the space for N particles by

$$\mathcal{H}^N \equiv \mathcal{H} \otimes \cdots N \text{ times} \cdots \otimes \mathcal{H}. \tag{2.3}$$

For $|\psi_N\rangle$ a vector of $\mathcal{H}^N$, it has to satisfy in the configuration space the condition

$$\langle\psi_N|\psi_N\rangle = \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_N |\psi_N(\mathbf{r}_1, \cdots, \mathbf{r}_N)|^2 < \infty. \tag{2.4}$$

A basis for this space can be taken as the external product of one-particle basis

$$|\alpha_{i_1} \cdots \alpha_{i_N}) \equiv |\alpha_{i_1}\rangle \otimes \cdots \otimes |\alpha_{i_N}\rangle. \tag{2.5}$$

It is easily proved that this basis is orthonormal

$$(\alpha_{i_1}\cdots\alpha_{i_N}|\alpha_{j_1}\cdots\alpha_{j_N}) = \delta_{i_1 j_1}\cdots\delta_{i_N j_N}, \tag{2.6}$$

and complete

$$\sum_{\{i\}=1}^{D} |\alpha_{i_1}\cdots\alpha_{i_N})(\alpha_{i_1}\cdots\alpha_{i_N}| = I, \tag{2.7}$$

where $\{i\}$ denotes all the indices i.

For a system of identical particles, it is known that only completely symmetric or antisymmetric states are observed in nature

$$\psi(\mathbf{r}_{P1},\cdots,\mathbf{r}_{PN}) = \varsigma^P \psi(\mathbf{r}_1,\cdots,\mathbf{r}_N), \tag{2.8}$$

where $\{\mathbf{r}_{P1},\cdots,\mathbf{r}_{PN}\}$ denotes a permutation of the indices $\mathbf{r}_1,\cdots,\mathbf{r}_N$; ς is equal to 1 for bosons and -1 for fermions; and the exponent P of ς indicates the parity of the permutation. In this expression we have dropped the subindex N in the wave function. If a state vector $|\psi_1\cdots\psi_N\rangle$ is symmetric or antisymmetric under a permutation of particles, it belongs to a Hilbert space of bosons (particles with integer spin) $\mathcal{H}_+^{\mathcal{N}}$ or to a Hilbert space of fermions (particles with half integer spin) $\mathcal{H}_-^{\mathcal{N}}$, respectively. As we shall see in the following, the restriction to symmetric or antisymmetric states implies restrictions on many-body observables.

It is useful to define a *symmetrization operator* S_+ and a *antisymmetrization operator* S_- as

$$S_\varsigma|\psi_1\rangle\otimes\cdots\otimes|\psi_N\rangle \equiv \frac{1}{N!}\sum_P \varsigma^P |\psi_{P1}\rangle\otimes\cdots\otimes|\psi_{PN}\rangle, \tag{2.9}$$

where the factor $1/N!$ is conveniently introduced so that S_ς is also a projection operator, i.e.

$$\begin{aligned}
S_\varsigma^2|\psi\rangle &= \frac{1}{N!^2}\left(\sum_{P'_{even}} + \varsigma\sum_{P'_{odd}}\right)\left(\sum_{P_{even}} + \varsigma\sum_{P_{odd}}\right)|\psi\rangle \\
&= \frac{1}{N!^2}\left[\sum_{P'_{even}P_{even}} + \sum_{P'_{odd}P_{odd}} + \varsigma\left(\sum_{P'_{even}P_{odd}} + \sum_{P'_{odd}P_{even}}\right)\right]|\psi\rangle \\
&= \frac{1}{N!^2}\left[\frac{N!}{2}\sum_{P_{even}} + \frac{N!}{2}\sum_{P_{even}} + \varsigma\left(\frac{N!}{2}\sum_{P_{odd}} + \frac{N!}{2}\sum_{P_{odd}}\right)\right]|\psi\rangle \\
&= \frac{1}{N!}\left(\sum_{P_{even}} + \varsigma\sum_{P_{odd}}\right)|\psi\rangle \\
&= S_\varsigma|\psi\rangle.
\end{aligned} \tag{2.10}$$

The operators S_ς are hermitian, as can be verified by comparing its matrix elements with the ones of its hermitian conjugated. Explicitly, the matrix elements of S_ς are

given by

$$\begin{aligned}(\alpha_{i_1}\cdots\alpha_{i_N}|S_\varsigma\alpha_{j_1}\cdots\alpha_{j_N}) &= \langle\alpha_{i_1}|\otimes\cdots\otimes\langle\alpha_{i_N}|\frac{1}{N!}\sum_P\varsigma^P|\alpha_{j_{P1}}\rangle\otimes\cdots\otimes|\alpha_{j_{PN}}\rangle \\ &= \frac{1}{N!}\sum_P\varsigma^P\langle\alpha_{i_1}|\alpha_{j_{P1}}\rangle\cdots\langle\alpha_{i_N}|\alpha_{j_{PN}}\rangle \\ &= \frac{1}{N!}\sum_P\varsigma^P\delta_{i_1,j_{P1}}\cdots\delta_{i_N,j_{PN}}, \qquad (2.11)\end{aligned}$$

while the matrix elements of $S_\varsigma^\dagger$ are given by

$$\begin{aligned}(\alpha_{i_1}\cdots\alpha_{i_N}|S_\varsigma^\dagger\alpha_{j_1}\cdots\alpha_{j_N}) &= (\alpha_{i_1}\cdots\alpha_{i_N}S_\varsigma|\alpha_{j_1}\cdots\alpha_{j_N}) \\ &= \frac{1}{N!}\sum_{P'}\varsigma^{P'}\langle\alpha_{P'i_1}|\alpha_{j_1}\rangle\cdots\langle\alpha_{P'i_N}|\alpha_{j_N}\rangle \\ &= \frac{1}{N!}\sum_{P'}\varsigma^{P'}\delta_{P'i_1,j_1}\cdots\delta_{P'i_N,j_N}\,. \qquad (2.12)\end{aligned}$$

Since the sum over P' runs through all the permutations , we can make $P'=P^{-1}$

$$(\alpha_{i_1}\cdots\alpha_{i_N}|S_\varsigma^\dagger\alpha_{j_1}\cdots\alpha_{j_N}) = \frac{1}{N!}\sum_P\varsigma^{P^{-1}}\delta_{P^{-1}i_1,j_1}\cdots\delta_{P^{-1}i_N,j_N}, \qquad (2.13)$$

and this proves that both expressions are equal term by term, then

$$S_\varsigma = S_\varsigma^\dagger. \qquad (2.14)$$

A basis for the symmetric or antisymmetric $\mathcal{H}_\varsigma^{\mathcal{N}}$ spaces is

$$\begin{aligned}|\alpha_{i_1}\cdots\alpha_{i_N}\} &\equiv S_\varsigma|\alpha_{i_1}\cdots\alpha_{i_N}) \qquad (2.15)\\ &= \frac{1}{N!}\sum_P\varsigma^P|\alpha_{Pi_1}\rangle\otimes\cdots\otimes|\alpha_{Pi_N}\rangle. \qquad (2.16)\end{aligned}$$

It should be noticed that this basis is over complete, since it has non-independent elements

$$|\alpha_{i_1}\alpha_{i_2}\alpha_{i_3}\cdots\alpha_{i_N}\} = \varsigma|\alpha_{i_2}\alpha_{i_1}\alpha_{i_3}\cdots\alpha_{i_N}\}. \qquad (2.17)$$

The orthogonality of this basis follows from the two properties of S_ς we have just demonstrated, namely $S_\varsigma^2 = S_\varsigma$ and $S_\varsigma^\dagger = S_\varsigma$,

$$\begin{aligned}\{\alpha_{i_1}\cdots\alpha_{i_N}|\alpha_{j_1}\cdots\alpha_{j_N}\} &= (\alpha_{i_1}\cdots\alpha_{i_N}|S_\varsigma^\dagger S_\varsigma\alpha_{j_1}\cdots\alpha_{j_N}) \\ &= (\alpha_{i_1}\cdots\alpha_{i_N}|S_\varsigma^2\alpha_{j_1}\cdots\alpha_{j_N}) \\ &= (\alpha_{i_1}\cdots\alpha_{i_N}|S_\varsigma\alpha_{j_1}\cdots\alpha_{j_N}) \\ &= \frac{1}{N!}\sum_P\varsigma^P(\alpha_{i_1}\cdots\alpha_{i_N}|\alpha_{Pj_1}\cdots\alpha_{Pj_N}) \\ &= \frac{1}{N!}\sum_P\varsigma^P\delta_{i_1,Pj_1}\cdots\delta_{i_N,Pj_N}\,, \qquad (2.18)\end{aligned}$$

this is zero if $\{\alpha_i\} \neq \{\alpha_j\}$. For the non-zero case and for fermions one can't have repeated states, so we are going to have just one permutation that doesn't vanish

$$\{\alpha_{i_1} \cdots \alpha_{i_N} | \alpha_{j_1} \cdots \alpha_{j_N}\} = \frac{(-1)^P}{N!}, \tag{2.19}$$

instead, for bosons, if the α_k are repeated n_{α_k} times so that $\sum_{k=1}^{D} n_{\alpha_k} = N$, one has

$$\{\alpha_{i_1} \cdots \alpha_{i_N} | \alpha_{j_1} \cdots \alpha_{j_N}\} = \frac{n_{\alpha_1}! \cdots n_{\alpha_D}!}{N!}. \tag{2.20}$$

Summarizing both cases

$$\{\alpha_{i_1} \cdots \alpha_{i_N} | \alpha_{j_1} \cdots \alpha_{j_N}\} = \frac{\varsigma^P n_{\alpha_1}! \cdots n_{\alpha_D}! \delta_{\{i\},\{j\}}}{N!}. \tag{2.21}$$

The closure of this basis is

$$\sum_{\{i\}=1}^{D} |\alpha_{i_1} \cdots \alpha_{i_N}\}\{\alpha_{i_1} \cdots \alpha_{i_N}| = S_\varsigma. \tag{2.22}$$

To see why one has the symmetrizer operator appearing on the r.h.s., note that

$$\begin{aligned} \sum_{\{i\}=1}^{D} |\alpha_{i_1} \cdots \alpha_{i_N}\}\{\alpha_{i_1} \cdots \alpha_{i_N}| &= S_\varsigma \sum_{\{i\}=1}^{D} |\alpha_{i_1} \cdots \alpha_{i_N})(\alpha_{i_1} \cdots \alpha_{i_N}| S_\varsigma^\dagger \\ &= S_\varsigma I S_\varsigma^\dagger \\ &= S_\varsigma^2 \\ &= S_\varsigma, \end{aligned} \tag{2.23}$$

where we have used the completeness of the non symmetrized states and the properties $S_\varsigma^2 = S_\varsigma$ and $S_\varsigma^\dagger = S_\varsigma$. If we think this thoroughly, S_ς is actually the identity in the symmetrized spaces, since when one applies this operator to any symmetrized vector we obtain the same vector. In the future when we will mention the identity I in a symmetric space context we would be referring to S_ς. We can express S_ς in the original, unsymmetrized basis as

$$\begin{aligned} S_\varsigma &= S_\varsigma I \\ &= S_\varsigma \sum_{\{i\}=1}^{D} |\alpha_{i_1} \cdots \alpha_{i_N})(\alpha_{i_1} \cdots \alpha_{i_N}| \\ &= \frac{1}{N!} \sum_{\{i\}=1}^{D} \sum_P \varsigma^P |\alpha_{i_{P1}} \cdots \alpha_{i_{PN}})(\alpha_{i_1} \cdots \alpha_{i_N}|, \end{aligned} \tag{2.24}$$

or

$$\begin{aligned} S_\varsigma &= I S_\varsigma \\ &= \sum_{\{i\}=1}^{D} |\alpha_{i_1} \cdots \alpha_{i_N})(\alpha_{i_1} \cdots \alpha_{i_N}| S_\varsigma \\ &= \frac{1}{N!} \sum_{\{i\}=1}^{D} \sum_P \varsigma^P |\alpha_{i_1} \cdots \alpha_{i_N})(\alpha_{i_{P1}} \cdots \alpha_{i_{PN}}|. \end{aligned} \tag{2.25}$$

Finally to normalize the orthogonal basis we use the result in Eq. (2.21) and define the final basis

$$\begin{aligned} |\alpha_{j_1}\cdots\alpha_{j_N}\rangle &\equiv \sqrt{\frac{N!}{n_{\alpha_1}!\cdots n_{\alpha_D}!}}|\alpha_{i_1}\cdots\alpha_{i_N}\} \\ &= \frac{1}{\sqrt{N!n_{\alpha_1}!\cdots n_{\alpha_D}!}}\sum_P \varsigma^P|\alpha_{Pi_1}\cdots\alpha_{Pi_N}). \end{aligned} \tag{2.26}$$

The orthonormality expressed in this basis is

$$\langle\alpha_{i_1}\cdots\alpha_{i_N}|\alpha_{j_1}\cdots\alpha_{j_N}\rangle = \varsigma^P\delta_{\{i\}\{j\}}; \tag{2.27}$$

and the completeness is

$$\sum_{\{i\}=1}^{D}\frac{n_{\alpha_1}!\cdots n_{\alpha_D}!}{N!}|\alpha_{i_1}\cdots\alpha_{i_N}\rangle\langle\alpha_{i_1}\cdots\alpha_{i_N}| = S_\varsigma. \tag{2.28}$$

It is important to notice the different notation used to denote the several many-particle basis we have discussed: the general many-particle state $|\alpha_{j_1}\cdots\alpha_{j_N})$, the symmetrized orthogonal state $|\alpha_{j_1}\cdots\alpha_{j_N}\}$, and finally, the symmetrized and orthonormal state $|\alpha_{j_1}\cdots\alpha_{j_N}\rangle$.

2.2 Many-body operators

Let us consider a many-particle observable $\widehat{O}$. We are going to use a physical condition to know what property a symmetric operator should have. Using the fact that a permutation operator (P) is a unitary operator

$$\begin{aligned} \langle\psi_1\cdots\psi_N|\widehat{O}_\zeta|\psi_1\cdots\psi_N\rangle &= \langle\psi_{P1}\cdots\psi_{PN}|\widehat{O}_\zeta|\psi_{P1}\cdots\psi_{PN}\rangle \\ &= \langle\psi_1\cdots\psi_N|P^\dagger\widehat{O}_\zeta P|\psi_1\cdots\psi_N\rangle, \end{aligned} \tag{2.29}$$

that is,

$$\widehat{O}_\zeta = P^\dagger\widehat{O}_\zeta P. \tag{2.30}$$

In other words, a symmetrized operator has to be invariant under any permutation. If we write the operator using explicitly a basis

$$\widehat{O}_\zeta = \sum_{\{j,i\}}|\alpha_{j_1}\cdots\alpha_{j_N})O_{\{j,i\}}(\alpha_{i_1}\cdots\alpha_{i_N}|, \tag{2.31}$$

we can write the r.h.s. of Eq. (2.30) as

$$\begin{aligned} P^\dagger\widehat{O}_\zeta P &= \sum_{\{j,i\}}|P^{-1}\alpha_{j_1}\cdots\alpha_{j_N})O_{\{j,i\}}(\alpha_{i_1}\cdots\alpha_{i_N}P^\dagger| \\ &\quad \sum_{\{j,i\}}|\alpha_{P^{-1}j_1}\cdots\alpha_{P^{-1}j_N})O_{\{j,i\}}(\alpha_{P^{-1}i_1}\cdots\alpha_{P^{-1}i_N}|. \end{aligned}$$

Since the indices are dummy, we can reorder them so that

$$P^{\dagger}\widehat{O}_{\zeta}P = \sum_{\{j,i\}} |\alpha_{j_1}\cdots\alpha_{j_N})O_{\{Pj,Pi\}}(\alpha_{i_1}\cdots\alpha_{i_N}|. \tag{2.32}$$

Finally the condition for a symmetrized operator would be

$$O_{\{j,i\}} = O_{\{Pj,Pi\}}. \tag{2.33}$$

An operator $\widehat{O}^{(1)}$ is said to be an *one-body operator* when

$$\widehat{O}^{(1)} = \sum_{i=1}^{N} \widehat{O}_i, \tag{2.34}$$

i.e. it is a sum of operators that depend on one single-particle label only. One example of such an operator is the kinetic energy

$$\widehat{T} = \sum_{i=1}^{N} \frac{\widehat{\mathbf{p}}_i^2}{2m_i}. \tag{2.35}$$

The condition (2.33) for this type of operators defined with Eq. (2.34), impose that

$$\widehat{O}_i = \widehat{O}_j \tag{2.36}$$

for every $i, j = 1, ..., N$. But still each one acting in its own space.

Another class of operators we are going to consider in the present dissertation is the one formed by *two-body operators*, defined as

$$\widehat{O}^{(2)} = \sum_{i,j=1}^{N} \widehat{O}_{ij}, \tag{2.37}$$

i.e. it is a sum of operators that depend on two single-particle labels only. One example of such an operator is the interaction potential energy between two particles

$$\widehat{V} = \frac{1}{2}\sum_{i\neq j}^{N} \widehat{V}_{ij} = \sum_{i<j}^{N} \widehat{V}_{ij}. \tag{2.38}$$

Such a two-body operator is said to be *local* or *velocity independent* when it is diagonal in configuration space, that is the matrix element of the operator in a general two-particle state $|\mathbf{r}_i\mathbf{r}_j)$ is given by

$$(\mathbf{r}_1\mathbf{r}_2|\widehat{O}|\mathbf{r}_3\mathbf{r}_4) = \delta(\mathbf{r}_1 - \mathbf{r}_3)\,\delta(\mathbf{r}_2 - \mathbf{r}_4)\,O(\mathbf{r}_1, \mathbf{r}_2). \tag{2.39}$$

2.3 Creation and annihilation operators

For each single particle state $|\lambda_i\rangle$ of the space $\mathcal{H}$, we define a boson or fermion *creation operator* $a^\dagger_{\lambda_i}$ (we are not going to use a hat on these operators) that acts on a symmetrized vector state in the following way

$$a^\dagger_{\alpha_j}|\alpha_{j_N}\cdots\alpha_{j_1}\} \equiv |\alpha_j\alpha_{j_N}\cdots\alpha_{j_1}\}. \tag{2.40}$$

The action of $a^\dagger_{\lambda_i}$ on the N-particles state $|\alpha_{j_N}\cdots\alpha_{j_1}\}$ which belongs to the Hilbert space $\mathcal{H}^N_\zeta$ leads to a N+1-particles state $|\alpha_j\alpha_{j_N}\cdots\alpha_{j_1}\}$, which belongs to the Hilbert space $\mathcal{H}^{N+1}_\zeta$

$$a^\dagger_{\alpha_j} : \mathcal{H}^N_\zeta \to \mathcal{H}^{N+1}_\zeta. \tag{2.41}$$

The action of $a^\dagger_{\lambda_i}$ over a normalized state can be deduced as following

$$\frac{a^\dagger_{\alpha_j}|S_\zeta\alpha_{j_N}\cdots\alpha_{j_1})}{\sqrt{n_{\alpha_1}!\cdots n_{\alpha_j}!\cdots n_{\alpha_D}!(n_{\alpha_j}+1)}} = \frac{|S_\zeta\alpha_j\alpha_{j_N}\cdots\alpha_{j_1})}{\sqrt{n_{\alpha_1}!\cdots (n_{\alpha_j}+1)!\cdots n_{\alpha_D}!}}, \tag{2.42}$$

that is

$$a^\dagger_{\alpha_j}|\alpha_{j_N}\cdots\alpha_{j_1}\rangle = \sqrt{n_{\alpha_j}+1}\,|\alpha_j\alpha_{j_N}\cdots\alpha_{j_1}\rangle. \tag{2.43}$$

This leads to the definition of a vacuum state (a state with no particles) $|0\rangle$ such that

$$a^\dagger_{\alpha_i}|0\rangle = |\alpha_i\rangle. \tag{2.44}$$

This state has to be distinguished from the zero-norm state of the $\mathcal{H}$.

For the hermitian conjugated operator a_{α_j}, or *annihilation operator*

$$a_{\alpha_j} : \mathcal{H}^N_\zeta \to \mathcal{H}^{N-1}_\zeta, \tag{2.45}$$

one can deduce its action applying it over an N-particles basis, i.e.

$$a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\}. \tag{2.46}$$

Using the identity of $\mathcal{H}^{N-1}_\zeta$ on the r.h.s. of Eq. (2.46), one has that

$$a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\} = \frac{1}{(N-1)!}\sum_{\{k\}=1}^{D}|\alpha_{k_1}\cdots\alpha_{k_{N-1}}\}\{\alpha_{k_1}\cdots\alpha_{k_{N-1}}|a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\}. \tag{2.47}$$

Here we need $\{\alpha_{j_N}\cdots\alpha_{j_1}|a_{\alpha_j}$. This can be obtained considering the expression for the dual of Eq. (2.40),

$$\{\alpha_{j_N}\cdots\alpha_{j_1}|a_{\alpha_j} = \{\alpha_j\alpha_{j_N}\cdots\alpha_{j_1}|. \tag{2.48}$$

Using this in Eq. (2.47), one obtains

$$a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\} = \frac{1}{(N-1)!}\sum_{\{k\}=1}^{D}\{\alpha_j\alpha_{k_1}\cdots\alpha_{k_{N-1}}|\alpha_{i_1}\cdots\alpha_{i_N}\}|\alpha_{k_1}\cdots\alpha_{k_{N-1}}\}, \quad (2.49)$$

and using Eq. (2.21)

$$\begin{aligned} a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\} &= \frac{1}{(N-1)!}\sum_{\{k\}=1}^{D}\sum_{P}\varsigma^P\delta_{j,Pi_1}\delta_{k_1,Pi_2}\cdots\delta_{k_{N-1},Pi_N}|\alpha_{k_1}\cdots\alpha_{k_{N-1}}\} \\ &= \frac{1}{(N-1)!}\sum_{P}\varsigma^P\delta_{j,Pi_1}|\alpha_{Pi_2}\cdots\alpha_{Pi_N}\}. \end{aligned} \quad (2.50)$$

Next, we just need to expand the sum and the permutations inside each ket to obtain $(N-1)!$ terms for each permutation of the deltas, and we can sum all of them because of the property

$$\varsigma|\alpha_{i_3}\alpha_{i_2}\alpha_{i_4}\cdots\alpha_{i_N}\} = |\alpha_{i_2}\alpha_{i_3}\alpha_{i_4}\cdots\alpha_{i_N}\}. \quad (2.51)$$

After some algebra, we get

$$a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\} = \sum_{k=1}^{N}\varsigma^{k-1}\delta_{j,i_k}|\alpha_{i_1}\cdots\widehat{\alpha}_{i_k}\cdots\alpha_{i_N}\}, \quad (2.52)$$

where $\widehat{\alpha}_i$ denotes a state removed from the ket at the indicated position. For an orthonormal state, one has

$$a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\rangle = \frac{1}{\sqrt{n_{\alpha_j}}}\sum_{i=i_1}^{i_N}\varsigma^{i-1}\delta_{j,i}|\alpha_{i_1}\cdots\widehat{\alpha}_i\cdots\alpha_{i_N}\rangle. \quad (2.53)$$

The exchange symmetry of many-particle systems implies certain commutation properties for the creation and annihilation operators. Namely,

$$\begin{aligned} a^\dagger_{\alpha_j}a^\dagger_{\alpha_k}|\alpha_{i_1}\cdots\alpha_{i_N}\} &= |\alpha_j\alpha_k\alpha_{i_1}\cdots\alpha_{i_N}\} \\ &= \zeta|\alpha_k\alpha_j\alpha_{i_1}\cdots\alpha_{i_N}\} \\ &= \zeta a^\dagger_{\alpha_k}a^\dagger_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\}, \end{aligned} \quad (2.54)$$

or

$$a^\dagger_{\alpha_j}a^\dagger_{\alpha_k} - \zeta a^\dagger_{\alpha_k}a^\dagger_{\alpha_j} \equiv [a^\dagger_{\alpha_k}, a^\dagger_{\alpha_j}]_{-\zeta} = 0. \quad (2.55)$$

More explicitly, we have defined the commutator and the anticommutator as

$$\begin{aligned} [a^\dagger_{\alpha_k}, a^\dagger_{\alpha_j}]_- &= a^\dagger_{\alpha_k}a^\dagger_{\alpha_j} - a^\dagger_{\alpha_j}a^\dagger_{\alpha_k}, \\ [a^\dagger_{\alpha_k}, a^\dagger_{\alpha_j}]_+ &= a^\dagger_{\alpha_k}a^\dagger_{\alpha_j} + a^\dagger_{\alpha_j}a^\dagger_{\alpha_k}, \end{aligned} \quad (2.56)$$

Taking the hermitean conjugate of Eq. (2.55), one has

$$[a_{\alpha_k}, a_{\alpha_j}]_{-\zeta} = a_{\alpha_k}a_{\alpha_j} - \zeta a_{\alpha_j}a_{\alpha_k} = 0. \quad (2.57)$$

To obtain the (anti)commutator of a and $a^\dagger$, we apply them in sequence on the state $|\alpha_{i_1}\cdots\alpha_{i_N}\}$

$$\begin{aligned} a_{\alpha_j}a^\dagger_{\alpha_k}|\alpha_{i_1}\cdots\alpha_{i_N}\} &= a_{\alpha_j}|\alpha_k\alpha_{i_1}\cdots\alpha_{i_N}\} \\ &= \delta_{jk}|\alpha_{i_1}\cdots\alpha_{i_N}\} + \sum_{l=1}^{N}\varsigma^l\delta_{j,i_l}|\alpha_k\alpha_{i_1}\cdots\widehat{\alpha}_{i_l}\cdots\alpha_{i_N}\}, \end{aligned} \tag{2.58}$$

and

$$\begin{aligned} a^\dagger_{\alpha_k}a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\} &= a^\dagger_{\alpha_k}\sum_{l=1}^{N}\varsigma^{l-1}\delta_{j,i_l}|\alpha_{i_1}\cdots\widehat{\alpha}_{i_l}\cdots\alpha_{i_N}\} \\ &= \sum_{l=1}^{N}\varsigma^{l-1}\delta_{j,i_l}|\alpha_k\alpha_{i_1}\cdots\widehat{\alpha}_{i_l}\cdots\alpha_{i_N}\}. \end{aligned} \tag{2.59}$$

Using this last result into the first one

$$a_{\alpha_j}a^\dagger_{\alpha_k}|\alpha_{i_1}\cdots\alpha_{i_N}\} = \delta_{jk}|\alpha_{i_1}\cdots\alpha_{i_N}\} + \varsigma a^\dagger_{\alpha_k}a_{\alpha_j}|\alpha_{i_1}\cdots\alpha_{i_N}\}. \tag{2.60}$$

Therefore, we arrived at the result

$$[a_{\alpha_j}, a^\dagger_{\alpha_k}]_{-\zeta} = a_{\alpha_j}a^\dagger_{\alpha_k} - \zeta a^\dagger_{\alpha_k}a_{\alpha_j} = \delta_{\alpha_j\alpha_k}. \tag{2.61}$$

2.4 Fock space

Lets define the *Fock space* as the space in which the creation and annihilation operator act

$$\begin{aligned} \mathcal{H}_\zeta &\equiv \oplus_{N=0}^{\infty}\mathcal{H}_\zeta^N \\ &= \mathcal{H}_\zeta^0 \oplus \mathcal{H}_\zeta^1 \oplus \mathcal{H}_\zeta^2 \oplus \cdots, \end{aligned} \tag{2.62}$$

with

$$\mathcal{H}_\zeta^0 = \lambda|0\rangle. \tag{2.63}$$

A basis for this space can be the union of all the symmetrized basis, normalized

$$\{|0\rangle\} \cup \{|\alpha_i\rangle\} \cup \{|\alpha_{i_1}\alpha_{i_2}\rangle\} \cup \cdots, \tag{2.64}$$

or not normalized

$$\{|0)\} \cup \{|\alpha_i\}\} \cup \{|\alpha_{i_1}\alpha_{i_2}\}\} \cup \cdots. \tag{2.65}$$

These are in fact orthogonal basis, because every state in $\mathcal{H}_\zeta^N$ is orthogonal with every state in $\mathcal{H}_\zeta^{N'}$ with $N \neq N'$. We are not going to give a general proof of this, but the following example will suffice

$$\begin{aligned} \{\alpha_i|\alpha_j\alpha_k\} &= \langle 0|a_{\alpha_i}a^\dagger_{\alpha_j}a^\dagger_{\alpha_k}|0\rangle = \langle 0|\left(\delta_{\alpha_i\alpha_j} + \zeta a^\dagger_{\alpha_j}a_{\alpha_i}\right)a^\dagger_{\alpha_k}|0\rangle \\ &= \delta_{\alpha_i\alpha_j}\langle 0|a^\dagger_{\alpha_k}|0\rangle + \zeta\langle 0|a^\dagger_{\alpha_j}\left(\delta_{\alpha_i\alpha_k} + \zeta a^\dagger_{\alpha_k}a_{\alpha_i}\right)|0\rangle \\ &= \delta_{\alpha_i\alpha_j}\langle 0|a^\dagger_{\alpha_k}|0\rangle + \zeta\left(\delta_{\alpha_i\alpha_k}\langle 0|a^\dagger_{\alpha_j}|0\rangle + \zeta\langle 0|a^\dagger_{\alpha_j}a^\dagger_{\alpha_k}a_{\alpha_i}|0\rangle\right) \\ &= 0. \end{aligned} \tag{2.66}$$

The closure condition is going to be just the sum of the completeness relations of every $\mathcal{H}_\zeta^N$

$$\begin{aligned} I &= |0\rangle\langle 0| + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\{i\}=1}^{D} |\alpha_{i_1} \cdots \alpha_{i_N}\}\{\alpha_{i_1} \cdots \alpha_{i_N} S_\varsigma| \\ &= |0\rangle\langle 0| + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\{i\}=1}^{D} n_{\alpha_1}! \cdots n_{\alpha_D}! |\alpha_{i_1} \cdots \alpha_{i_N}\rangle\langle\alpha_{i_1} \cdots \alpha_{i_N}|. \end{aligned} \tag{2.67}$$

2.5 Change of representation

Let us consider a change of basis, from $\{|\alpha_i\rangle\}$ to a new basis $\{|\lambda_i\rangle\}$,

$$|\lambda_i\rangle = \sum_{j=1}^{D} \langle\alpha_j|\lambda_i\rangle |\alpha_j\rangle. \tag{2.68}$$

By definition, one has that

$$a_{\lambda_j}^\dagger |\lambda_{j_N} \cdots \lambda_{j_1}\} \equiv |\lambda_j \lambda_{j_N} \cdots \lambda_{j_1}\} \tag{2.69}$$

$$= \sum_{i=1}^{D} \langle\alpha_i|\lambda_j\rangle |\alpha_i \lambda_{j_N} \cdots \lambda_{j_1}\} \tag{2.70}$$

$$= \sum_{i=1}^{D} \langle\alpha_i|\lambda_j\rangle a_{\alpha_i}^\dagger |\lambda_{j_N} \cdots \lambda_{j_1}\}. \tag{2.71}$$

Therefore, the creation and annihilation operators behave under this change of transformation as

$$a_{\lambda_j}^\dagger = \sum_{i=1}^{D} \langle\alpha_i|\lambda_j\rangle a_{\alpha_i}^\dagger, \tag{2.72}$$

and

$$a_{\lambda_j} = \sum_{i=1}^{D} \langle\lambda_j|\alpha_i\rangle a_{\alpha_i}. \tag{2.73}$$

The commutation relation between a creation and annihilation operator in the new basis follows straightforwardly

$$\begin{aligned} [a_{\lambda_j}, a_{\lambda_k}^\dagger]_{-\zeta} &= \sum_{i=1}^{D} \langle\lambda_j|\alpha_i\rangle \sum_{l=1}^{D} \langle\alpha_l|\lambda_k\rangle [a_{\alpha_i}, a_{\alpha_l}^\dagger]_{-\zeta} \\ &= \sum_{i=1}^{D} \langle\lambda_j|\alpha_i\rangle \sum_{l=1}^{D} \langle\alpha_l|\lambda_k\rangle \delta_{\alpha_i \alpha_l} \\ &= \sum_{i=1}^{D} \langle\lambda_j|\alpha_i\rangle \langle\alpha_i|\lambda_k\rangle = \langle\lambda_j|\lambda_k\rangle = \delta_{\lambda_j \lambda_k}. \end{aligned} \tag{2.74}$$

The commutation relations between two annihilation operators and two creation operators are easily found to be zero, following exactly the same procedure as above

$$[a_{\lambda_j}, a_{\lambda_k}]_{-\zeta} = 0 [a_{\lambda_j}^\dagger, a_{\lambda_k}^\dagger]_{-\zeta} = 0. \tag{2.75}$$

As an example of change of representation, lets assume that we start with creation and annihilation operators in the momentum representation, i.e. these create or annihilate particles with defined momentum $\mathbf{p}$ (other quantum numbers might be added when needed), and want to change to creation and annihilation operators in the coordinate representation, where they create and annihilate particles at a definite position $\mathbf{r}$. This can be accomplished using Eq.'s (2.72) and (2.73)

$$\widehat{\psi}^\dagger(\mathbf{r}) = \sum_{\mathbf{p}} \langle \mathbf{p}|\mathbf{r}\rangle \, a^\dagger_{\mathbf{p}} = \sum_{\mathbf{p}} \phi^*_{\mathbf{p}}(\mathbf{r}) \, a^\dagger_{\mathbf{p}}, \tag{2.76}$$

and

$$\widehat{\psi}(\mathbf{r}) = \sum_{\mathbf{p}} \langle \mathbf{r}|\mathbf{p}\rangle \, a_{\mathbf{p}} = \sum_{\mathbf{p}} \phi_{\mathbf{p}}(\mathbf{r}) \, a_{\mathbf{p}}, \tag{2.77}$$

where, we have introduced the *field operators* $\widehat{\psi}^\dagger(\mathbf{r})$ and $\widehat{\psi}(\mathbf{r})$; and

$$\langle \mathbf{r}|\mathbf{p}\rangle = \phi_{\mathbf{p}}(\mathbf{r}) = \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{(2\pi\hbar)^{3/2}}. \tag{2.78}$$

As it can be seen these equations matches the well known Fourier Transform of functions.

The commutation relations of the field operators are given by

$$[\widehat{\psi}(\mathbf{r}), \widehat{\psi}(\mathbf{r}')] = 0, \tag{2.79}$$

$$[\widehat{\psi}^\dagger(\mathbf{r}), \widehat{\psi}^\dagger(\mathbf{r}')] = 0, \tag{2.80}$$

$$[\widehat{\psi}(\mathbf{r}), \widehat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'). \tag{2.81}$$

All operators of the theory can be written in terms of creation and annihilation operators. An easy way to express a general operator in terms of creation and annihilation operator is to use a basis in which the operator is diagonal. The expression of the operator in another basis, in which the operator is not diagonal, can be obtained by a change of representation. To help us do that, let us define the *number operator*

$$\widehat{n}_{\alpha_i} \equiv a^\dagger_{\alpha_i} a_{\alpha_i}. \tag{2.82}$$

This operator, when acting on a state $|\alpha_{i_1} \cdots \alpha_{i_N}\}$, gives the number of particles in state with quantum number α_i. This can be shown making use of Eqs. (2.52) and (2.40),

$$\begin{aligned}
\widehat{n}_{\alpha_j}|\alpha_{i_1} \cdots \alpha_{i_N}\} &= a^\dagger_{\alpha_j} \sum_{k=1}^{N} \varsigma^{k-1} \delta_{j,i_k} |\alpha_{i_1} \cdots \widehat{\alpha}_{i_k} \cdots \alpha_{i_N}\} \\
&= \sum_{k=1}^{N} \varsigma^{k-1} \delta_{j,i_k} |\alpha_j \alpha_{i_1} \cdots \widehat{\alpha}_{i_k} \cdots \alpha_{i_N}\} \\
&= \sum_{k=1}^{N} \delta_{j,i_k} |\alpha_{i_1} \cdots \alpha_{i_{k-1}} \alpha_j \alpha_{i_{k+1}} \cdots \alpha_{i_N}\} \\
&= n_{\alpha_j} |\alpha_{i_1} \cdots \alpha_{i_N}\}.
\end{aligned} \tag{2.83}$$

Naturally, the operator that counts all the particles is

$$\widehat{N} = \sum_{i=1}^{D} \widehat{n}_{\alpha_i} = \sum_{i=1}^{D} a^\dagger_{\alpha_i} a_{\alpha_i}. \tag{2.84}$$

For simplicity, let us consider first a one-body operator $\widehat{O}$, such that all the $\widehat{O}_i$, see Eq. (2.34), are equal and diagonal in the single particle basis $\{|\alpha_j\rangle\}$

$$\widehat{O}_i|\alpha_j\rangle = O_j|\alpha_j\rangle. \tag{2.85}$$

In an arbitrary element of this basis

$$\begin{aligned}
\widehat{O}|\alpha_{j_1}\cdots\alpha_{j_N}\} &= \sum_{i=1}^{N} \widehat{O}_i \frac{1}{\sqrt{N!}} \sum_P \varsigma^P |\alpha_{Pj_1}\rangle \otimes \cdots \otimes |\alpha_{Pj_N}\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_P \varsigma^P \sum_{i=1}^{N} \widehat{O}_i |\alpha_{Pj_1}\rangle \otimes \cdots \otimes |\alpha_{Pj_N}\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_P \varsigma^P \sum_{i=1}^{N} O_{Pj_i} |\alpha_{Pj_1}\rangle \otimes \cdots \otimes |\alpha_{Pj_N}\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_P \varsigma^P \sum_{k=1}^{D} n_{\alpha_k} O_k |\alpha_{Pj_1}\rangle \otimes \cdots \otimes |\alpha_{Pj_N}\rangle \\
&= \left(\sum_{k=1}^{D} n_{\alpha_k} O_k \right) |\alpha_{j_1}.\cdots\alpha_{j_N}\} \\
&= \sum_{k=1}^{D} O_k \widehat{n}_{\alpha_k} |\alpha_{j_1}\cdots\alpha_{j_N}\},
\end{aligned} \tag{2.86}$$

then

$$\widehat{O} = \sum_{k=1}^{D} O_k a^\dagger_{\alpha_k} a_{\alpha_k}\,. \tag{2.87}$$

Next, the transformation to another basis $|\{\lambda_i\rangle\}$ (in general of different dimension D')

$$\begin{aligned}
\widehat{O} &= \sum_{k=1}^{D} O_k \sum_{l=1}^{D} \delta_{kl} a^\dagger_{\alpha_l} a_{\alpha_k} = \sum_{k=1}^{D} O_k \sum_{l=1}^{D} \langle\alpha_l|\alpha_k\rangle a^\dagger_{\alpha_l} a_{\alpha_k} = \sum_{k,l=1}^{D} \langle\alpha_l|\widehat{O}_i|\alpha_k\rangle a^\dagger_{\alpha_l} a_{\alpha_k} \\
&= \sum_{k,l=1}^{D} \langle\alpha_l| \left(\sum_{p=1}^{D'} |\lambda_p\rangle\langle\lambda_p| \right) \widehat{O}_i \left(\sum_{q=1}^{D'} |\lambda_q\rangle\langle\lambda_q| \right) |\alpha_k\rangle a^\dagger_{\alpha_l} a_{\alpha_k} \\
&= \sum_{k,l=1}^{D} \sum_{p,q=1}^{D'} \langle\alpha_l|\lambda_p\rangle\langle\lambda_p|\widehat{O}_i|\lambda_q\rangle\langle\lambda_q|\alpha_k\rangle a^\dagger_{\alpha_l} a_{\alpha_k} \\
&= \sum_{p,q=1}^{D'} \langle\lambda_p|\widehat{O}_i|\lambda_q\rangle \sum_{l=1}^{D} \langle\alpha_l|\lambda_p\rangle a^\dagger_{\alpha_l} \sum_{k=1}^{D} \langle\lambda_q|\alpha_k\rangle a_{\alpha_k}.
\end{aligned} \tag{2.88}$$

Using Eqs. (2.72) and (2.73), one obtains finally

$$\widehat{O} = \sum_{p,q=1}^{D'} \langle\lambda_p|\widehat{O}_i|\lambda_q\rangle a^\dagger_{\lambda_p} a_{\lambda_q}\,. \tag{2.89}$$

For example in the configuration representation, one has

$$\widehat{O} = \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \, \langle \mathbf{r}_1 | \widehat{O}_i | \mathbf{r}_2 \rangle \, \widehat{\psi}^\dagger(\mathbf{r}_1) \widehat{\psi}(\mathbf{r}_2). \tag{2.90}$$

In the case of the kinetic energy operator,

$$\widehat{T} = \frac{\widehat{\mathbf{p}}^2}{2m}, \tag{2.91}$$

Eq. (2.90) becomes

$$\begin{aligned} \widehat{T} &= \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \, \langle \mathbf{r}_1 | \mathbf{r}_2 \rangle \, \frac{\hbar^2 \nabla^2_{\mathbf{r}_2}}{2m} \, \widehat{\psi}^\dagger(\mathbf{r}_1) \widehat{\psi}(\mathbf{r}_2) \\ &= \frac{\hbar^2}{2m} \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \, \delta(\mathbf{r}_1 - \mathbf{r}_2) \, \widehat{\psi}^\dagger(\mathbf{r}_1) \, \nabla^2_{\mathbf{r}_2} \, \widehat{\psi}(\mathbf{r}_2) \\ &= \frac{\hbar^2}{2m} \int d^3\mathbf{r} \, \widehat{\psi}^\dagger(\mathbf{r}) \, \nabla^2 \, \widehat{\psi}(\mathbf{r}). \end{aligned} \tag{2.92}$$

For a two body operator, we can do an analogous procedure (see Appendix A), obtaining the result

$$\widehat{O} = \sum_{r,s,t,u=1}^{D'} (\lambda_r \lambda_s | \widehat{O}_{ij} | \lambda_t \lambda_u) a^\dagger_{\lambda_r} a^\dagger_{\lambda_s} a_{\lambda_u} a_{\lambda_t}. \tag{2.93}$$

In the configuration representation, one will have

$$\widehat{O} = \int \left(\prod_{k=1}^{4} d^3\mathbf{r}_k \right) (\mathbf{r}_1 \mathbf{r}_2 | \widehat{O}_{ij} | \mathbf{r}_3 \mathbf{r}_4) \, \widehat{\psi}^\dagger(\mathbf{r}_1) \widehat{\psi}^\dagger(\mathbf{r}_2) \widehat{\psi}(\mathbf{r}_4) \widehat{\psi}(\mathbf{r}_3). \tag{2.94}$$

For a *local* or *velocity independent* operator, see Eq. (2.39), one has

$$\begin{aligned} \widehat{O} &= \int \left(\prod_{k=1}^{4} d^3\mathbf{r}_k \right) \delta(\mathbf{r}_1 - \mathbf{r}_3) \, \delta(\mathbf{r}_2 - \mathbf{r}_4) \, O(\mathbf{r}_1, \mathbf{r}_2) \, \widehat{\psi}^\dagger(\mathbf{r}_1) \widehat{\psi}^\dagger(\mathbf{r}_2) \widehat{\psi}(\mathbf{r}_4) \widehat{\psi}(\mathbf{r}_3) \\ &= \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \, O(\mathbf{r}_1, \mathbf{r}_2) \, \widehat{\psi}^\dagger(\mathbf{r}_1) \widehat{\psi}^\dagger(\mathbf{r}_2) \widehat{\psi}(\mathbf{r}_2) \widehat{\psi}(\mathbf{r}_1). \end{aligned} \tag{2.95}$$

Capítulo 3

Coherent states and Path Integrals at Finite Temperature

In the present Chapter we will present a review on the use of coherent states in the evaluation of the grand canonical partition function. We will show how these states can be used to obtain a path integral representation of the partition function. We will also show how they can be used to calculate directly the trace defining the partition function, without the use of path integrals.

In quantum statistical mechanics description of many-particle systems, the use of field theoretic methods in Fock space is common practice. In such a formulation, the use of the grand canonical ensemble is a natural choice, since in Fock space one deals with states with an indefinite number of particles. The sum over all the microstates can be written as the trace of the operator in the Fock space as

$$\begin{aligned} Z &= \sum_{\alpha} \langle \alpha | e^{-\beta\left(\widehat{H}-\mu\widehat{N}\right)} | \alpha \rangle \\ &= \operatorname{Tr} e^{-\beta\left(\widehat{H}-\mu\widehat{N}\right)}, \end{aligned} \tag{3.1}$$

where $|\alpha\rangle$ is representing an element of a symmetrized many particle basis. Z is the grand canonical partition function. All possible information on the macroscopic states of a many-body system can be derived in principle from Z.

It is striking the resemblance with the trace of the well known *evolution operator* of Quantum Mechanics

$$\operatorname{Tr} U = \operatorname{Tr} e^{-it\widehat{H}/\hbar}. \tag{3.2}$$

In the next Section we will briefly review the Feynman path integral in quantum mechanics. Although out of the main scope of the present dissertation, the subject is included here for two main reasons. First, to motivate the similarities between path integrals in quantum mechanics and in statistical mechanics. Second, to motivate future developments of the Niterói method to problems in quantum field theory, as will be discussed in a later Chapter in this dissertation.

3.1 Feynman path integral in quantum mechanics

The starting point of the Feynman path integral in quantum mechanics is the probability amplitude of finding a particle at position $\mathbf{r_f}$ at time t_f, knowing that it was at position $\mathbf{r_i}$ at t_f. Specifically, this probability amplitude is given by

$$U(\mathbf{r}_f, t_f; \mathbf{r}_i, t_i) \equiv {}_H\langle \mathbf{r}, t_f | \mathbf{r}, t_i \rangle_H = \langle \mathbf{r}_f | e^{-i(t_f - t_i)\widehat{H}/\hbar} | \mathbf{r}_i \rangle, \tag{3.3}$$

where the sub-index H in ${}_H\langle \mathbf{r}, t_f | \mathbf{r}, t_i \rangle_H$ means Heisenberg representation and $\widehat{H}$ is the hamiltonian of the particle

$$\begin{aligned} \widehat{H} &= H(\widehat{\mathbf{p}}, \widehat{\mathbf{r}}) \\ &= \frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}}). \end{aligned} \tag{3.4}$$

The next step is to divide the time interval $t_f - t_i$ into M equal parts

$$\epsilon \equiv \frac{t_f - t_i}{M}, \tag{3.5}$$

so that

$$t_n \equiv t_i + \epsilon\, n, \qquad n = 0, 1, \cdots, M-1. \tag{3.6}$$

and

$$U(\mathbf{r}_f, t_f; \mathbf{r}_i, t_i) = \langle \mathbf{r}_f | \left(e^{-i\epsilon \widehat{H}/\hbar} \right)^M | \mathbf{r}_i \rangle = \langle \mathbf{r}_f | e^{-i\epsilon \widehat{H}/\hbar}\, e^{-i\epsilon \widehat{H}/\hbar}\, \cdots\, e^{-i\epsilon \widehat{H}/\hbar} | \mathbf{r}_i \rangle. \tag{3.7}$$

Inserting $M-1$ closures between the exponentials

$$\begin{aligned} U(\mathbf{r}_f, t_f; \mathbf{r}_i, t_i) &= \langle \mathbf{r}_f | \left(e^{-i\epsilon \widehat{H}/\hbar} \right)^M | \mathbf{r}_i \rangle = \int \prod_{j=1}^{M-1} d^3\mathbf{r}_j \langle \mathbf{r}_f | e^{-i\epsilon \widehat{H}/\hbar} | \mathbf{r}_{M-1} \rangle \\ &\times \langle \mathbf{r}_{M-1} | e^{-i\epsilon \widehat{H}/\hbar} | \mathbf{r}_{M-2} \rangle \langle \mathbf{r}_{M-2} | \cdots | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | e^{-i\epsilon \widehat{H}/\hbar} | \mathbf{r}_i \rangle. \end{aligned} \tag{3.8}$$

Denoting $\mathbf{r}_0 \equiv \mathbf{r}_i$ and $\mathbf{r}_M \equiv \mathbf{r}_f$, the probability amplitude can be written in the more compact form

$$U(\mathbf{r}_f, t_f; \mathbf{r}_i, t_i) = \int \prod_{j=1}^{M-1} d^3\mathbf{r}_j \prod_{k=0}^{M-1} \langle \mathbf{r}_{k+1} | e^{-i\epsilon \widehat{H}/\hbar} | \mathbf{r}_k \rangle, \tag{3.9}$$

and one needs therefore to evaluate the matrix elements of the form

$$U(\mathbf{r}_{k+1}, \epsilon; \mathbf{r}_k, 0) = \langle \mathbf{r}_{k+1} | e^{-i\epsilon \widehat{H}/\hbar} | \mathbf{r}_k \rangle. \tag{3.10}$$

This can be calculated as

$$\begin{aligned} U(\mathbf{r}_{k+1}, \epsilon; \mathbf{r}_k, 0) &= \langle \mathbf{r}_{k+1} | \exp\left[-\frac{i\epsilon}{\hbar} \left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}}) \right) \right] | \mathbf{r}_k \rangle \\ &= \int d^3\mathbf{p}_k \langle \mathbf{r}_{k+1} | \mathbf{p}_k \rangle \langle \mathbf{p}_k | \exp\left[-\frac{i\epsilon}{\hbar} \left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}}) \right) \right] | \mathbf{r}_k \rangle. \end{aligned} \tag{3.11}$$

For small enough ϵ, one has

$$e^{-i\epsilon\widehat{H}/\hbar} \simeq I - \frac{i\epsilon}{\hbar}\left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}})\right), \tag{3.12}$$

and replacing

$$\begin{aligned} U(\mathbf{r}_{k+1},\epsilon;\mathbf{r}_k,0) &= \int d^3\mathbf{p}_k \langle \mathbf{r}_{k+1}|\mathbf{p}_k\rangle\langle\mathbf{p}_k| \exp\left[-\frac{i\epsilon}{\hbar}\left(\frac{\mathbf{p}_k^2}{2m} + V(\mathbf{r}_k)\right)\right]|\mathbf{r}_k\rangle \\ &= \int d^3\mathbf{p}_k \langle \mathbf{r}_{k+1}|\mathbf{p}_k\rangle e^{-i\epsilon H(\mathbf{p}_k,\mathbf{r}_k)/\hbar}\langle\mathbf{p}_k|\mathbf{r}_k\rangle \\ &= \int d^3\mathbf{p}_k \frac{e^{-i\mathbf{r}_{k+1}\cdot\mathbf{p}_k/\hbar}}{\sqrt{2\pi\hbar}} e^{-i\epsilon H(\mathbf{p}_k,\mathbf{r}_k)/\hbar}\frac{e^{i\mathbf{r}_k\cdot\mathbf{p}_k/\hbar}}{\sqrt{2\pi\hbar}} \\ &= \int \frac{d^3\mathbf{p}_k}{2\pi\hbar}\exp\left(-\frac{i\epsilon}{\hbar}\left[\frac{(\mathbf{r}_{k+1}-\mathbf{r}_k)}{\epsilon}\cdot\mathbf{p}_k + H(\mathbf{p}_k,\mathbf{r}_k)\right]\right). \end{aligned} \tag{3.13}$$

Finally, putting all factors together, one obtains for the probability amplitude the expression

$$\begin{aligned} U(\mathbf{r}_f,t_f;\mathbf{r}_i,t_i) &= \int \frac{d^3\mathbf{p}_0}{2\pi\hbar}\int\prod_{j=1}^{M-1}\left(\frac{d^3\mathbf{r}_j\, d^3\mathbf{p}_j}{2\pi\hbar}\right) \\ &\times \exp\left(-\frac{i\epsilon}{\hbar}\sum_{k=0}^{M-1}\left[\frac{(\mathbf{r}_{k+1}-\mathbf{r}_k)}{\epsilon}\cdot\mathbf{p}_k + H(\mathbf{p}_k,\mathbf{r}_k)\right]\right). \end{aligned} \tag{3.14}$$

In the limit of $M\to\infty$, $\epsilon\to 0$, one recognizes that the exponent is just the $i/\hbar$ times the integral of the classical Lagrangian of the particle

$$-\frac{i\epsilon}{\hbar}\sum_{k=0}^{M-1}\left[\frac{(\mathbf{r}_{k+1}-\mathbf{r}_k)}{\epsilon}\cdot\mathbf{p}_k + H(\mathbf{p}_k,\mathbf{r}_k)\right] \to \frac{i}{\hbar}\int_{t_i}^{t_f} dt\; L(\mathbf{r},\dot{\mathbf{r}}). \tag{3.15}$$

Denoting

$$\frac{d^3\mathbf{p}_0}{2\pi\hbar}\prod_{j=1}^{M-1}\left(\frac{d^3\mathbf{r}_j\, d^3\mathbf{p}_j}{2\pi\hbar}\right) \equiv [d\mathbf{r}][d\mathbf{p}], \tag{3.16}$$

one can write for the probability amplitude

$$U(\mathbf{r}_f,t_f;\mathbf{r}_i,t_i) = \int [d\mathbf{r}][d\mathbf{p}]\,\exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f} dt\; L(\mathbf{r},\dot{\mathbf{r}})\right]. \tag{3.17}$$

We note that one could integrate over the momenta and obtain the traditional Feynman path integral that involves only integrals over de coordinates. We decided to leave the integrals over the momenta variables because in the next sections, when discussing the path integral in terms of coherent states, we will arrive at expressions involving two coordinates that can formally be related to generalized coordinates and momenta.

The above derivation of the path integral representation of the partition function is not adequate when the Hamiltonian and number operators are given in the second quantization representation. Specifically, in the second quantization representation the *grand canonical potential operator*

$$\widehat{\Omega} \equiv \widehat{H} - \mu \widehat{N}, \tag{3.18}$$

that appears in the Boltzmann factor in Eq. (3.1) is given in terms of creation and annihilation operators $a^\dagger$ and a (or field operators $\psi^\dagger$ and ψ). In this case, coherent states provide an adequate framework to express the partition function in terms of *c-number* functions. Coherent states are eigenstates of the annihilation operator and a qualitative understanding of why they are useful is as follows. In the derivation of the path integral above, we have made repeated use of the completeness of the momentum eigenstates because in the exponent of the evolution operator one has the momentum operator. In order to use the same trick with the grand canonical potential operator in second quantization, which involves in general the operators in normal order (i.e. all annihilation operators appear to the right of all creation operators), one would need eigenstates of the second quantized operators. This is the subject of our next Sections.

3.2 Coherent states for bosons

For convenience we are going to use the occupation number representation. A generic many-particle state can be represented as

$$|\phi\rangle = \sum_{\{n_\alpha\}=0}^{\infty} \phi_{n_{\alpha_1}\cdots n_{\alpha_D}} |n_{\alpha_1}\cdots n_{\alpha_D}\rangle, \tag{3.19}$$

where the $\phi_{n_{\alpha_1}\cdots n_{\alpha_D}}$ are complex numbers and

$$|n_{\alpha_1}\cdots n_{\alpha_D}\rangle = \prod_{i=1}^{D} \frac{\left(a_{\alpha_i}^\dagger\right)^{n_{\alpha_i}}}{\sqrt{n_{\alpha_i}!}} |0\rangle. \tag{3.20}$$

Since we are not going to perform any change of basis, there should be no source of confusion if one simplifies the notation as

$$n_{\alpha_i} \to n_i \,, \tag{3.21}$$

so that, for example,

$$|\phi\rangle = \sum_{\{n\}=0}^{\infty} \phi_{n_1\cdots n_D} |n_1\cdots n_D\rangle, \tag{3.22}$$

and

$$|n_1 \cdots n_D\rangle = \prod_{i=1}^{D} \frac{\left(a_i^\dagger\right)^{n_i}}{\sqrt{n_i!}} |0\rangle. \tag{3.23}$$

We define a *coherent state* $|\phi\rangle$ as the eigenstate of the annihilation operators a_i

$$a_i|\phi\rangle = \phi_i|\phi\rangle, \tag{3.24}$$

where ϕ_i is the respective eigenvalue, in general a complex number. Before obtaining an explicit expression for the eigenstates we should notice the following. Using the generic notation for the commutation relation for boson and fermion operators, one sees that

$$0 = [a_k, a_j]_{-\zeta}|\phi\rangle = [\phi_k, \phi_j]_{-\zeta}|\phi\rangle, \tag{3.25}$$

which implies that

$$[\phi_k, \phi_j]_{-\zeta} = 0. \tag{3.26}$$

We see that if we were working with fermions, the "numbers" ϕ_i would anticommute, i.e. they would not be ordinary complex numbers and the concept of anticommuting c-numbers, known as *Grassmann numbers*, is required. Here we will concentrate on bosons, for which the eigenvalues ϕ_i are ordinary complex numbers.

Let us come back to Eq. (3.24). From the l.h.s. of this equation, using Eq. (3.22) one has

$$\begin{aligned} a_i|\phi\rangle &= \sum_{\{n\}=0}^{\infty} a_i\, \phi_{n_1\cdots n_D}\, |n_1 \cdots n_i \cdots n_D\rangle \\ &= \sum_{\{n\}=0}^{\infty} \phi_{n_1\cdots n_D} \sqrt{n_i}\, |n_1 \cdots (n_i - 1) \cdots n_D\rangle \\ &= \sum_{\{n\}=0}^{\infty} \phi_{n_1\cdots (n_i+1)\cdots n_D} \sqrt{n_i + 1}\, |n_1 \cdots n_i \cdots n_D\rangle. \end{aligned} \tag{3.27}$$

On the other hand, from the r.h.s. of Eq. (3.24), one has

$$\phi_i|\phi\rangle = \sum_{\{n\}=0}^{\infty} \phi_i\, \phi_{n_1\cdots n_D} |n_1 \cdots n_D\rangle. \tag{3.28}$$

From this and Eq. (3.27), one obtains the following recursive relation for the coefficients $\phi_{n_1\cdots n_D}$, for every n_i

$$\begin{aligned} \phi_{n_1\cdots (n_i+1)\cdots n_D} \sqrt{n_i + 1} &= \phi_i\, \phi_{n_1\cdots n_i\cdots n_D} \\ \phi_{n_1\cdots (n_i+1)\cdots n_D} &= \phi_i\, \frac{\phi_{n_1\cdots n_i\cdots n_D}}{\sqrt{n_i + 1}}. \end{aligned} \tag{3.29}$$

This can be solved fixing arbitrarily one of such coefficients. The simplest choice is

$$\phi_{n_1 \cdots n_D|_{\{n\}=0}} = 1, \tag{3.30}$$

so that

$$\phi_{n_1 \cdots n_D} = \frac{(\phi_1)^{n_1}}{\sqrt{n_1!}} \cdots \frac{(\phi_D)^{n_D}}{\sqrt{n_D!}} = \prod_{i=1}^{D} \frac{(\phi_i)^{n_i}}{\sqrt{n_i!}}. \tag{3.31}$$

In view of this result, the many-particle state in Eq. (3.22) can be written as

$$|\phi\rangle = \sum_{\{n\}=0}^{\infty} \prod_{i=1}^{D} \frac{(\phi_i)^{n_i}}{\sqrt{n_i!}} |n_1 \cdots n_D\rangle, \tag{3.32}$$

and, because of Eq. (3.23),

$$\begin{aligned} |\phi\rangle &= \sum_{\{n\}=0}^{\infty} \prod_{i=1}^{D} \frac{\left(\phi_i a_i^\dagger\right)^{n_i}}{n_i!} |0\rangle \\ &= \prod_{i=1}^{D} \sum_{n_i=0}^{\infty} \frac{\left(\phi_i a_i^\dagger\right)^{n_i}}{n_i!} |0\rangle \\ &= \prod_{i=1}^{D} \exp\left(\phi_i a_i^\dagger\right) |0\rangle. \end{aligned} \tag{3.33}$$

Since we are working with bosons,

$$[\phi_i a_i^\dagger, \phi_j a_j^\dagger]_- = \phi_i \, \phi_j \, [a_i^\dagger, a_j^\dagger]_- = 0, \tag{3.34}$$

the product of exponentials can be written as a single exponential as

$$|\phi\rangle = \exp\left(\sum_{i=1}^{D} \phi_i a_i^\dagger\right) |0\rangle. \tag{3.35}$$

This is the final general expression for the eigenstates of the annihilation operators. It is important to note that this result is valid for any complex numbers ϕ_i.

In order to obtain a path integral representation, we need a closure relation for the coherent states. Here we shall simply give the final expression and in Appendix C corroborate its correctness. Explicitly, the resolution of the identity for bosonic coherent states is

$$I = \frac{1}{\mathcal{N}} \int \prod_{i=1}^{D} d\phi_i^* d\phi_i \, \exp\left(-\sum_{j=1}^{D} \phi_j^* \phi_j\right) |\phi\rangle\langle\phi|, \tag{3.36}$$

where

$$\mathcal{N} = (2i\pi)^D \, . \tag{3.37}$$

We shall need also expressions for the internal product and for operators in the *coherent representation*. A general many-particle state can be written as

$$\begin{aligned} |g\rangle &= \sum_{\{n\}=0}^{\infty} g_{n_1\cdots n_D} |n_1 \cdots n_D\rangle \\ &= \sum_{\{n\}=0}^{\infty} g_{n_1\cdots n_D} \prod_{i=1}^{D} \frac{\left(a_i^\dagger\right)^{n_i}}{\sqrt{n_i!}} |0\rangle. \end{aligned} \tag{3.38}$$

If one defines for every state a function

$$g(x) \equiv \sum_{\{n\}=0}^{\infty} g_{n_1\cdots n_D} \prod_{i=1}^{D} \frac{(x)^{n_i}}{\sqrt{n_i!}}, \tag{3.39}$$

we have in the coherent representation the state $|g\rangle$ is given by

$$\langle \phi | g \rangle = \langle \phi | g(a^\dagger) | 0 \rangle = g(\phi^*) \langle \phi | 0 \rangle, \tag{3.40}$$

where we have used the eigenvalue equation Eq. (3.24). Now, because of the normalization choice in Eq. (3.30), we have that

$$\langle \phi | g \rangle = g(\phi^*) = \sum_{\{n\}=0}^{\infty} g_{n_1\cdots n_D} \prod_{i=1}^{D} \frac{(\phi_i^*)^{n_i}}{\sqrt{n_i!}}, \tag{3.41}$$

where the last equality follows from the definition in Eq. (3.39). This allows us to obtain immediately that the inner product of two general many-particle states $|f\rangle$ and $|g\rangle$ as

$$\begin{aligned} \langle f | g \rangle &= \frac{1}{(2i\pi)^D} \int \prod_{i=1}^{D} d\phi_i^* \, d\phi_i \, \exp\left(- \sum_{j=1}^{D} \phi_j^* \phi_j \right) \langle f | \phi \rangle \langle \phi | g \rangle \\ &= \frac{1}{(2i\pi)^D} \int \prod_{i=1}^{D} d\phi_i^* \, d\phi_i \, \exp\left(- \sum_{j=1}^{D} \phi_j^* \phi_j \right) [f(\phi^*)]^* \, g(\phi^*) \\ &= \frac{1}{(2i\pi)^D} \int \prod_{i=1}^{D} d\phi_i^* \, d\phi_i \, \exp\left(- \sum_{j=1}^{D} \phi_j^* \phi_j \right) f^*(\phi) g(\phi^*), \end{aligned} \tag{3.42}$$

where, of course,

$$f^*(x) \equiv \sum_{\{n\}=0}^{\infty} f^*_{n_1\cdots n_D} \prod_{i=1}^{D} \frac{(x)^{n_i}}{\sqrt{n_i!}}. \tag{3.43}$$

Let us now discuss the coherent-state representation of a general operator given in terms of creation and annihilation opertors $a^\dagger$ and a ,

$$\widehat{O} = O(a^\dagger, a). \tag{3.44}$$

This representation is most easily obtained when all the creation operators are on the left of the annihilation operators. Such a repositioning of the operators is always possible for any operator using the commutation rules. We will call such an ordering as *simple order*. As an example, for a one-dimensional Hilbert space we will define the specific function of operators already ordered by

$$O^{\odot}(a^{\dagger}, a) \equiv O^{\odot}_{00} + O^{\odot}_{10} a^{\dagger} + O^{\odot}_{01} a + O^{\odot}_{11} a^{\dagger} a. \tag{3.45}$$

Note that in essence the operator is the same

$$\widehat{O} = O^{\odot}(a^{\dagger}, a), \tag{3.46}$$

$O^{\odot}$ is just a specific function of $a^{\dagger}$ and a. In other words, although

$$\widehat{O}(a^{\dagger}, a) = \widehat{O}^{\odot}(a^{\dagger}, a), \tag{3.47}$$

in general

$$O(x, y) \neq O^{\odot}(x, y), \tag{3.48}$$

with x and y any type of variable.

For example, suppose one has an operator of the form

$$\widehat{K} = \sum_{i,j} K(i,j)\, a_i a_j^{\dagger}. \tag{3.49}$$

Assuming the following commutation relations, $[a_i, a_j^{\dagger}]_- = \delta_{ij}$, and $K(i,j) = K(j,i)$, one would have

$$\begin{aligned} \widehat{K} &= \widehat{K^{\odot}} = \sum_{i,j} K(i,j)\, a_i a_j^{\dagger} \\ &= \sum_{i,j} K(i,j) \left[\delta_{i,j} + a_j^{\dagger} a_i\right] = \sum_{i} K(i,i) + \sum_{i,j} K(i,j) a_i^{\dagger} a_j, \end{aligned} \tag{3.50}$$

and so

$$K^{\odot}_{00} = \sum_{i} K(i,i), \qquad K^{\odot}_{i0} = 0 = K^{\odot}_{0i}, \qquad K^{\odot}_{ij} = K(i,j). \tag{3.51}$$

Having introduced the notion of operators in simple order, one can write their coherent-state representation as

$$\langle \phi | \widehat{O} | \phi' \rangle = \langle \phi | O^{\odot}(a^{\dagger}, a) | \phi' \rangle = O^{\odot}(\phi^*, \phi') \langle \phi | \phi' \rangle. \tag{3.52}$$

Here we need the scalar product $\langle \phi | \phi' \rangle$

$$\langle \phi | \phi' \rangle = \sum_{\{n,n'\}=0}^{\infty} \prod_{i=1}^{D} \frac{(\phi_i^*)^{n_i}}{\sqrt{n_i!}} \prod_{j=1}^{D} \frac{\left(\phi_j'\right)^{n_j'}}{\sqrt{n_j'!}} \langle n_1 \cdots n_D | n_1' \cdots n_D' \rangle$$

$$= \sum_{\{n\}=0}^{\infty} \prod_{i=1}^{D} \frac{(\phi_i^*)^{n_i}}{\sqrt{n_i!}} \prod_{j=1}^{D} \frac{\left(\phi_j'\right)^{n_j}}{\sqrt{n_j!}} = \sum_{\{n\}=0}^{\infty} \prod_{i=1}^{D} \frac{(\phi_i^* \phi_i')^{n_i}}{n_i!}$$

$$= \prod_{i=1}^{D} \sum_{n_i=0}^{\infty} \frac{(\phi_i^* \phi_i')^{n_i}}{n_i!} = \exp\left(\sum_{i=1}^{D} \phi_i^* \phi_i'\right). \tag{3.53}$$

This leads to

$$\langle \phi | \widehat{O} | \phi' \rangle = O^{\odot}(\phi^*, \phi') \exp\left(\sum_{i=1}^{D} \phi_i^* \phi_i'\right). \tag{3.54}$$

Following similar steps, one can obtain a coherent-state representation of the trace of an operator

$$\begin{aligned}
\operatorname{Tr} \widehat{O} &= \sum_{\{n\}=0}^{\infty} \langle n_1 \cdots n_D | \widehat{O} | n_1 \cdots n_D \rangle \\
&= \frac{1}{(2i\pi)^D} \sum_{\{n\}=0}^{\infty} \langle n_1 \cdots n_D | \int \prod_{i=1}^{D} d\phi_i^* d\phi_i \exp\left(-\sum_{j=1}^{D} \phi_j^* \phi_j\right) |\phi\rangle \langle \phi | \widehat{O} | n_1 \cdots n_D \rangle \\
&= \frac{1}{(2i\pi)^D} \int \prod_{i=1}^{D} d\phi_i^* d\phi_i \exp\left(-\sum_{j=1}^{D} \phi_j^* \phi_j\right) \sum_{\{n\}=0}^{\infty} \langle \phi | \widehat{O} | n_1 \cdots n_D \rangle \langle n_1 \cdots n_D | \phi \rangle \\
&= \frac{1}{(2i\pi)^D} \int \prod_{i=1}^{D} d\phi_i^* d\phi_i \exp\left(-\sum_{j=1}^{D} \phi_j^* \phi_j\right) \langle \phi | \widehat{O} | \phi \rangle.
\end{aligned} \tag{3.55}$$

Using the operator in simple order, one obtains the final expression

$$\operatorname{Tr} \widehat{O} = \frac{1}{(2i\pi)^D} \int \prod_{i=1}^{D} d\phi_i^* d\phi_i \, O^{\odot}(\phi^*, \phi'). \tag{3.56}$$

Another case in which we can express an operator in the coherent representation is when the operator is *normal ordered*, i.e. all creation operators are put on the left of all annihilation operators, without using the commutation relations (in case of fermions, one must keep track of minus signs). The operation of normal ordering an operator $\widehat{O}$ is denoted by $: \widehat{O} :$, and the coherent-state matrix element of $: \widehat{O} :$ is given as (for bosons)

$$\langle \phi | : \widehat{O} : | \phi' \rangle = O(\phi^*, \phi') \, \exp\left(\sum_{i=1}^{D} \phi_i^* \phi_i'\right), \tag{3.57}$$

and its coherent-state trace is

$$\operatorname{Tr}(: \widehat{O} :) = \frac{1}{(2i\pi)^D} \int \prod_{i=1}^{D} d\phi_i^* d\phi_i \, O(\phi^*, \phi). \tag{3.58}$$

3.3 Grassmann algebras

When we discussed Eq. (3.26) we faced the need for *anticommuting numbers* when dealing with fermions. Grassmann Algebra is the mathematical framework universally used to address the anticommuting properties of the eigenvalues of the fermionic annnihilation operators as observed in Eq. (3.26). Here we will review the minimal material of Grassmann algebras necessary to build fermionic coherent states.

The *generators* of the Grassmann algebra, or *Grassmann numbers*(GN) are a set of objects $\{\xi_i\}$ with $i = 1, ..., n$ such that

$$[\xi_i, \xi_j]_+ = 0. \tag{3.59}$$

Note that, in particular

$$\xi_i^2 = 0\,. \tag{3.60}$$

We call a *basis* of a Grassmann algebra all the linearly independent products of the generators, i.e.

$$\{1, \xi_1, \cdots, \xi_n, \xi_1\xi_2, \cdots, \xi_1\xi_n, \xi_2\xi_3, \cdots, \xi_2\xi_n, \cdots, \xi_1\xi_2\xi_3, \cdots, \xi_1\xi_2\xi_n, \cdots, \xi_1 \cdots \xi_n\}. \tag{3.61}$$

The number of elements of the basis, or the *dimension,* is 2^n, since each generator has just two possibilities, or it appears once or it does not appear at all in the set above, because of the property in Eq. (3.60). An *element* of the algebra is any linear combination of the elements of the basis with complex coefficients, this elements can be labeled as functions of this generators $f(\xi)$. They are going to be used as the coherent state representation of a state $|f\rangle$. Note that a function of just one generator can only be linear

$$f(\xi) = f_0 + f_1\xi\,. \tag{3.62}$$

We have to define how these new variables are going to behave under the adjoint $(\xi_i)^\dagger$. As we are using them as numbers, we will need an analog to the complex conjugate and we will call it *conjugation operation* $(^*)$

$$(\xi_i)^\dagger = (\xi_i)^*. \tag{3.63}$$

Using the same symbol as the complex conjugate gives us a more friendly notation, but the two operations will be different by definition. No confusion should arise when $*$ is used because its apearance in both cases are excluyent. Both came from taking hermitic conjugate †, but in one case is over complex numbers and in the other one is over Grassmann numbers. To actually define the operation properly, let a GA

with an even number of generators $n = 2p$. We select p generators and through this operation we associate to each element only one element of the remaining p elements as

$$\xi_i^* \equiv (\xi_i)^* = \xi_{i+p}\,. \tag{3.64}$$

In order to avoid conflict when we use the symbol $*$ for both operations, we need the following auxiliary properties

$$(\xi_i^*)^* = \xi_i, \tag{3.65}$$

$$(\lambda\xi_i)^* = \lambda^*\,\xi_i^*\,, \tag{3.66}$$

where λ is an ordinary complex number. Now, since the adjoint of the product of noncommuting mathematical objects in general is given as

$$(\xi_i\xi_j)^\dagger = (\xi_j)^\dagger\,(\xi_i)^\dagger\,, \tag{3.67}$$

we need

$$(\xi_i\xi_j)^* = \xi_j^*\xi_i^*\,. \tag{3.68}$$

As an example for all these initial definitions, let's consider the simplest GA with conjugation operation, $n = 2$. The dimension of this GA is 2^2, with generators η and η^* that satisfy anticommutation relations according to Eq. (3.59),

$$[\eta\xi, \eta]_+ = 0, \qquad [\eta, \eta^*]_+ = 0, \qquad [\eta^*, \eta^*]_+ = 0. \tag{3.69}$$

A basis of the algebra is

$$\{1, \eta, \eta^*, \eta\eta^*\}. \tag{3.70}$$

The conjugated of $f(\eta^*)$ would be

$$\begin{aligned} [f(\eta^*)]^* &= (f_0 + f_1^*\eta)^* \\ &= f_0^* + f_1^*\eta \\ &= f^*(\eta), \end{aligned} \tag{3.71}$$

as in the Boson case.

We are not going to need a derivative with respect to GN's too much, but we are going to see a little of it just to get familiar with such an operation. Since there is no analog to an infinitesimal differential ($\Delta\xi \to 0$), one defines the *Grassmann derivative (GD)* as

$$\frac{\partial\lambda}{\partial\xi} \equiv 0 \qquad \text{and} \qquad \frac{\partial\xi}{\partial\xi} \equiv 1, \tag{3.72}$$

where λ is an ordinary complex number, and ξ is a GN. As GN are anticommuting variables, we need a rule on how to operate with a derivative on a product of two GN's, and the convention is

$$\frac{\partial}{\partial\xi}(\xi'\xi) = \frac{\partial}{\partial\xi}(-\xi\xi') = -\frac{\partial}{\partial\xi}(\xi\xi') = -\left(\frac{\partial}{\partial\xi}\xi\right)\xi' = -\xi'. \tag{3.73}$$

In contrast to derivatives, we are going to need integrals over GN's extensively. Even though there is no analog to the familiar sum motivating the Riemann integral, and neither can we work with integration limits, we do have three guiding principles that we can use to define integrals of GN in analogy to ordinary indefinite integrals. Let us suppose we are able to define coherent states $|\xi\rangle$ such that

$$a_i|\xi\rangle = \xi_i|\xi\rangle, \tag{3.74}$$

with a a closure relation in the form

$$I = \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \, |\xi\rangle \, k(\xi,\xi^*) \, \langle\xi|, \tag{3.75}$$

where k is a general function

$$k(\xi^*,\xi) \equiv k_0 + k_1\xi^* + k_2\xi + k_3\xi^*\xi. \tag{3.76}$$

We get the inner product in coherent representation using the closure relation as

$$\begin{aligned} \langle f|g\rangle &= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \langle f|\xi\rangle k(\xi^*,\xi)\langle\xi|g\rangle \\ &= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i f^*(\xi) k(\xi^*,\xi) g(\xi^*). \end{aligned} \tag{3.77}$$

It is clear that our choice in the definition of the integrals will affect the inner product, but we want to keep the scalar product representation independent. In Appendix D, we will make the case for explicitly choosing the following definition of an integral

$$\int d\xi\lambda = 0 \qquad \text{and} \qquad \int d\xi\xi = 1, \tag{3.78}$$

where λ is a complex number. This definition is not only for simplicity, it is also for convenience, as we shall see. Note that the definition above for the integral leads to results numerically identical to the corresponding derivatives. That means that any formula obtained for derivatives is valid for integrals as well. It is also customary to introduce a rule for the integration of products of GN's similar to the rule for the derivatives as

$$\int d\xi\, \xi'\xi = \int d\xi\, (-\xi\xi') = -\int d\xi\, \xi\xi' = -\left(\int d\xi\, \xi\right)\xi' = -\xi'. \tag{3.79}$$

3.4 Coherent states for fermions

In this Section we will obtain an explicit expression for $|\xi\rangle$. In order to do so, notice that we need twice as many generators for any possible state in the one-particle Hilbert space, in other words

$$p = D. \tag{3.80}$$

In the following, for simplicity of presentation will consider just for one generator ($D = 1$). The general form for a fermionic coherent state in this case is

$$|\xi\rangle = f(\xi)|0\rangle + g(\xi)|1\rangle, \tag{3.81}$$

with the defining condition

$$a|\xi\rangle = \xi|\xi\rangle. \tag{3.82}$$

As we don't have any criterion to determine whether the annihilation operators and its eigenvalues commute or anticommute,

$$[a, \xi]_{\mp} = 0, \tag{3.83}$$

we are going to proceed considering both possibilities. Recalling that in general one can have

$$f(\xi) = f_0 + f_1\xi, \qquad g(\xi) = g_0 + g_1\xi, \tag{3.84}$$

the l.h.s. of Eq. (3.82) can be written as

$$\begin{aligned} a|\xi\rangle &= a\left[f(\xi)|0\rangle + g(\xi)|1\rangle\right] = f(\pm\xi)a|0\rangle + g(\pm\xi)a|1\rangle \\ &= g(\pm\xi)|0\rangle = (g_0 \pm g_1\xi)\,|0\rangle, \end{aligned} \tag{3.85}$$

while its r.h.s. as

$$\xi|\xi\rangle = \xi\left[f(\xi)|0\rangle + g(\xi)|1\rangle\right] = f_0\xi|0\rangle + g_0\xi|1\rangle. \tag{3.86}$$

Therefore,

$$g_0 = 0, \qquad g_1 = \pm f_0. \tag{3.87}$$

On the other hand, we have

$$\langle 0|\xi\rangle = f(\xi)\langle 0|0\rangle + g(\xi)\langle 0|1\rangle = f(\xi). \tag{3.88}$$

Therefore, fixing the iterative constant $\langle 0|\xi\rangle$

$$\langle 0|\xi\rangle = 1 \qquad \Rightarrow \qquad f(\xi) = 1, \tag{3.89}$$

one then has

$$f_0 = 1, \qquad f_1 = 0, \qquad g_0 = 0, \qquad g_1 = \pm 1. \tag{3.90}$$

Replacing these results in Eq. (3.81), one finally has

$$|\xi\rangle \;\; = \;\; |0\rangle \pm \xi|1\rangle = (1 \pm \xi a^\dagger)|0\rangle = e^{\pm \xi a^\dagger}|0\rangle, \tag{3.91}$$

so that

$$[a, \xi]_\mp = 0 \qquad \Rightarrow \qquad |\xi\rangle = e^{\pm \xi a^\dagger}|0\rangle. \tag{3.92}$$

As said in the previous Section, the choice of definition of the Grassmann integrals determine the final expression for closure. Using the definitions given in Eq.(3.78) – see Appendix D, the closure is

$$I = \int d\xi^* d\xi e^{-\xi^* \xi} |\xi\rangle\langle\xi|. \tag{3.93}$$

Its generalization for many generators is

$$I = \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) |\xi\rangle\langle\xi|, \tag{3.94}$$

where, for this case, the coherent states are given by

$$|\xi\rangle = \prod_{i=1}^{D} \exp\left(\pm \xi_i a_i^\dagger\right)|0\rangle, \tag{3.95}$$

where the $\pm$ in the exponent depend on the choice for

$$[a_i, \xi_j]_\mp = 0, \tag{3.96}$$

as discussed above. Here we use the common choice

$$[a_i, \xi_j]_+ = 0. \tag{3.97}$$

In a vague common sense, the rational for such a choice is that, since we have two sets of different mathematical objects that anticommute separately (here, the a's and the ξ's), the most "natural" behavior seems to be that all of them anticommute among themselves. There is no profound physical or mathematical reason for such a choice and one could equally well pick the other option without any inconvenience. With this choice, the coherent state is given by

$$|\xi\rangle = \exp\left(-\sum_{i=1}^{D} \xi_i a_i^\dagger\right)|0\rangle, \tag{3.98}$$

and the corresponding bra by

$$\langle\xi| \;=\; \langle 0|\exp\left(-\sum_{i=1}^{D}\left(a_i^\dagger\right)^\dagger(\xi_i)^\dagger\right)=\langle 0|\exp\left(-\sum_{i=1}^{D}a_i\xi_i^*\right). \tag{3.99}$$

Now, to obtain a coherent-state representation of the inner product of $|f\rangle$ and $|g\rangle$ we use Eq. (3.94) so that

$$\begin{aligned}\langle f|g\rangle &= \int\prod_{i=1}^{D}d\xi_i^*d\xi_i\exp\left(-\sum_{j=1}^{D}\xi_j^*\xi_j\right)\langle f|\xi\rangle\langle\xi|g\rangle\\ &= \int\prod_{i=1}^{D}d\xi_i^*d\xi_i\exp\left(-\sum_{j=1}^{D}\xi_j^*\xi_j\right)f^*(\xi)g(\xi^*),\end{aligned} \tag{3.100}$$

where f and g are now functions of many generators

$$g(\xi^*) \;=\; \langle\xi|g\rangle=\langle\xi|\sum_{m_1,\ldots,m_D=0,1}g_{m_1,\cdots,m_D}|m_1\cdots m_D\rangle \tag{3.101}$$

$$\begin{aligned}&= \sum_{\{m\}=0,1}g_{m_1,\cdots,m_D}\langle\xi|\left(a_1^\dagger\right)^{m_1}\cdots\left(a_D^\dagger\right)^{m_D}|0\rangle\\ &= \sum_{\{m\}=0,1}g_{m_1,\ldots,m_D}\left(\xi_1^*\right)^{m_1}\cdots\left(\xi_D^*\right)^{m_D}=\sum_{\{m\}=0,1}g_{\{m\}}\prod_{i=1}^{D}\left(\xi_i^*\right)^{m_i},\end{aligned} \tag{3.102}$$

and similarly for $f^*(\xi)$,

$$\begin{aligned}f^*(\xi) &= [f(\xi^*)]^*=\left[\sum_{\{m\}=0,1}f_{m_1,\ldots,m_D}\left(\xi_1^*\right)^{m_1}\cdots\left(\xi_D^*\right)^{m_D}\right]^*\\ &= \sum_{\{m\}=0,1}f^*_{m_1,\cdots,m_D}\xi_D^{m_D}\cdots\xi_1^{m_1}=\sum_{\{m\}=0,1}f^*_{\{m\}}\prod_{i=D}^{1}\xi_i^{m_i}.\end{aligned} \tag{3.103}$$

Using these in the expression for the inner product above, one obtains

$$\begin{aligned}\langle f|g\rangle &= \int\prod_{i=1}^{D}d\xi_i^*d\xi_i\exp\left(-\sum_{j=1}^{D}\xi_j^*\xi_j\right)\sum_{\{m\}=0,1}\left(f^*_{\{m\}}\prod_{k=D}^{1}\xi_k^{m_k}\right)\\ &\times \sum_{\{n\}=0}^{1}\left(g_{\{n\}}\prod_{l=1}^{D}\left(\xi_l^*\right)^{n_l}\right)\\ &= \sum_{\{m,n\}=0,1}f^*_{\{m\}}g_{\{n\}}\int\prod_{i=2}^{D}d\xi_i^*d\xi_i\exp\left(-\sum_{j=2}^{D}\xi_j^*\xi_j\right)\prod_{k=D}^{2}\xi_k^{m_k}\\ &\times \int d\xi_1^*d\xi_1\exp\left(\xi_1\xi_1^*\right)\xi_1^{m_1}\left(\xi_1^*\right)^{n_1}\prod_{l=2}^{D}\left(\xi_l^*\right)^{n_l}\end{aligned}$$

$$= \sum_{\{m,n\}=0,1} f^*_{\{m\}} g_{\{n\}} \delta_{m_1 n_1} \int \prod_{i=3}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=3}^{D} \xi_j^* \xi_j\right) \prod_{k=D}^{3} \xi_k^{m_k} \tag{3.104}$$

$$\times \left(\int d\xi_2^* d\xi_2 \exp\left(\xi_2 \xi_2^*\right) \xi_2^{m_2} \left(\xi_2^*\right)^{n_2}\right) \prod_{l=3}^{D} \left(\xi_l^*\right)^{n_l}$$

$$= \sum_{\{m,n\}=0,1} f^*_{\{m\}} g_{\{n\}} \prod_{i=1}^{D} \delta_{m_i n_i} = \sum_{\{m\}=0,1} f^*_{m_1,\cdots,m_D} g_{m_1,\cdots,m_D} \,. \tag{3.105}$$

To make it clear, the coherent-state representation of the inner product of two many-fermion states gives the appropriated value

$$\langle f|g\rangle = \sum_{\{m\}=0,1} f^*_{m_1,\cdots,m_D} \, g_{m_1,\cdots,m_D} \,. \tag{3.106}$$

For the fermion coherent-state representation of a simple-ordered operator

$$\langle \xi|\widehat{O}|\xi'\rangle \;\; = \;\; \langle \xi|\widehat{O}^{\odot}(a^\dagger, a)|\xi'\rangle = O^{\odot}(\xi^*, \xi')\langle \xi|\xi'\rangle, \tag{3.107}$$

one needs to evaluate $\langle \xi|\xi'\rangle$. This is given as follows,

$$\langle \xi|\xi'\rangle \;\; = \;\; \langle 0| \prod_{i=1}^{D} \exp\left(-a_i \xi_i^*\right) \prod_{j=1}^{D} \exp\left(-\xi_j' a_j^\dagger\right)|0\rangle = \langle 0| \prod_{i=1}^{D} \exp\left(\xi_i^* a_i\right) \exp\left(-\xi_i' a_i^\dagger\right)|0\rangle$$

$$= \;\; \langle 0| \prod_{i=1}^{D} \left(1 + \xi_i^* a_i\right)\left(1 - \xi_i' a_i^\dagger\right)|0\rangle = \langle 0| \prod_{i=1}^{D} (1 - \xi_i' a_i^\dagger + \xi_i^* a_i + \xi_i^* a_i \xi_i' a_i^\dagger)|0\rangle$$

$$= \;\; \langle 0| \prod_{i=1}^{D} (1 + \xi_i^* \xi_i' a_i a_i^\dagger)|0\rangle = \langle 0| \prod_{i=1}^{D} [1 + \xi_i^* \xi_i' (1 - a_i^\dagger a_i)]|0\rangle$$

$$= \;\; \langle 0| \prod_{i=1}^{D} (1 + \xi_i^* \xi_i')|0\rangle = \exp\left(\sum_{i=1}^{D} \xi_i^* \xi_i'\right). \tag{3.108}$$

Therefore, the result for the fermion coherent-state representation of a simple-ordered operator is given by

$$\langle \xi|\widehat{O}|\xi'\rangle = O^{\odot}(\xi^*, \xi') \exp\left(\sum_{i=1}^{D} \xi_i^* \xi_i'\right). \tag{3.109}$$

Finally, we consider the coherent-state representation of trace of operators. First, let us consider the trace of an unordered operator

$$\mathrm{Tr}\, \widehat{O} \;\; = \;\; \sum_{\{n\}=0}^{\infty} \langle n_1 \cdots n_D|\widehat{O}|n_1 \cdots n_D\rangle$$

$$
\begin{aligned}
&= \sum_{\{n\}=0}^{\infty} \langle n_1 \cdots n_D| \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) |\xi\rangle\langle\xi|\widehat{O}|n_1 \cdots n_D\rangle \\
&= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) \sum_{\{n\}=0}^{\infty} \langle n_1 \cdots n_D|\xi\rangle\langle\xi|\widehat{O}|n_1 \cdots n_D\rangle \\
&= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) \sum_{\{n\}=0}^{\infty} \langle -\xi|\widehat{O}|n_1 \cdots n_D\rangle\langle n_1 \cdots n_D|\xi\rangle \\
&= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) \langle -\xi|\widehat{O}|\xi\rangle, \qquad (3.110)
\end{aligned}
$$

where the sign change in the bra $\langle -\xi|$ above comes from the exchange of the relative positions of $\langle n_1 \cdots n_D|\xi\rangle$ and $\langle\xi|\widehat{O}|n_1 \cdots n_D\rangle$ under the integral – this can be shown by writing each of such factors as in Eq. (3.84) and then regrouping them in reverse order. One can go a bit further in the evaluation of the above trace taking the operator in simple order, since then

$$
\begin{aligned}
\mathrm{Tr}\,\widehat{O} &= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) \langle -\xi|\widehat{O}^{\odot}(a^\dagger, a)|\xi\rangle \\
&= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) O^{\odot}(-\xi^*, \xi) \exp\left(-\sum_{i=1}^{D} \xi_i^* \xi_i\right) \\
&= \int \prod_{i=1}^{D} d\xi_i^* d\xi_i \exp\left(-2\sum_{j=1}^{D} \xi_j^* \xi_j\right) O^{\odot}(-\xi^*, \xi). \qquad (3.111)
\end{aligned}
$$

Now, making $\xi^* \to -\xi^*$, one obtains finally

$$
\mathrm{Tr}\,\widehat{O} = \int \prod_{i=1}^{D} d\xi_i d\xi_i^* \exp\left(2\sum_{j=1}^{D} \xi_j^* \xi_j\right) O^{\odot}(\xi^*, \xi). \qquad (3.112)
$$

For a normal ordered operator

$$
\langle\xi| :\widehat{O}: |\xi'\rangle = :O(\xi^*, \xi'): \exp\left(\sum_{i=1}^{D} \xi_i^* \xi_i'\right), \qquad (3.113)
$$

one has the result

$$
\mathrm{Tr}\,\left(:\widehat{O}:\right) = \int \prod_{i=1}^{D} d\xi_i d\xi_i^* \exp\left(2\sum_{j=1}^{D} \xi_j^* \xi_j\right) :O(\xi^*, \xi): . \qquad (3.114)
$$

Note that now it is important to indicate the normal ordering in $:O(\xi^*, \xi):$ since ξ^* and ξ anticommute and as such their relative positions in the function $O(\xi^*, \xi)$ matters – note that this was not necessary in the case of operators given in terms of boson operators, since ϕ^* and ϕ are complex numbers and therefore commute.

3.5 Path integral for bosons and fermions

In the present Section we make use of the formalism of coherent states developed above to obtain a path integral representation for the grand-canonical partition function of many-particle systems. The grand-canonical partition function was defined in Eq. (3.1) and can be written in terms of the grand-potential $\widehat{\Omega}$, Eq. (3.18), as

$$Z = \mathrm{Tr}\, e^{-\beta \widehat{\Omega}}. \tag{3.115}$$

Whenever possible we shall use a common notation for bosons and fermions. To this extent we denote by $|\xi\rangle$ a generic coherent state of bosons or fermions, i.e.

$$a_i|\xi\rangle = \xi_i|\xi\rangle, \qquad |\xi\rangle = \exp\left(\zeta \sum_{i=1}^{D} \xi_i a_i^\dagger\right)|0\rangle, \tag{3.116}$$

with $\zeta = 1$ for bosons and $\zeta = -1$ for fermions, $a_i^\dagger$ and a_i denote creation and annihilation operators that satisfy the generic commutation relations

$$[a_i, a_j^\dagger]_{-\zeta} = \delta_{ij}, \qquad [a_i^\dagger, a_j^\dagger]_{-\zeta} = 0 = [a_i, a_j]_{-\zeta}, \tag{3.117}$$

and the parameters ξ_i satisfy

$$[\xi_i, \xi_j]_{-\zeta} = 0. \tag{3.118}$$

The content of this last equation is that for bosons (and $\zeta = 1$), the ξ_i's are ordinary complex numbers (previously denoted as ϕ_i) so that they commute trivially. In addition, the closure relation is denoted as

$$I = \int \prod_{i=1}^{D} \left(\frac{d\xi_i^* d\xi_i}{\mathcal{N}}\right) \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) |\xi\rangle\langle\xi|, \tag{3.119}$$

with

$$\mathcal{N} \equiv \begin{cases} 2\pi i & \text{for bosons,} \\ 1 & \text{for fermions,} \end{cases}. \tag{3.120}$$

The coherent-state matrix elements of an operator $\widehat{O}$ is

$$\langle\xi|\widehat{O}|\xi'\rangle = O^{\odot}(\xi^*, \xi') \exp\left(\sum_{i=1}^{D} \xi_i^* \xi_i'\right), \tag{3.121}$$

and the trace of $\widehat{O}$ as

$$\mathrm{Tr}\, \widehat{O} = \int \prod_{i=1}^{D} \left(\frac{d\xi_i^* d\xi_i}{\mathcal{N}}\right) \exp\left(-\sum_{j=1}^{D} \xi_j^* \xi_j\right) \langle\zeta\xi|\widehat{O}|\xi\rangle, \tag{3.122}$$

or

$$\begin{aligned}\mathrm{Tr}\,\widehat{O} &= \int\prod_{i=1}^{D}\left(\frac{d\xi_i^* d\xi_i}{\mathcal{N}}\right)\exp\left(-\sum_{j=1}^{D}\xi_j^*\xi_j\right)O^{\odot}(\zeta\xi^*,\xi)\exp\left(\zeta\sum_{j=1}^{D}\xi_j^*\xi_j\right)\\ &= \int\prod_{i=1}^{D}\left(\frac{d\xi_i^* d\xi_i}{\mathcal{N}}\right)\exp\left((\zeta-1)\sum_{j=1}^{D}\xi_j^*\xi_j\right)O^{\odot}(\zeta\xi^*,\xi),\end{aligned}\tag{3.123}$$

when $\widehat{O}$ is put in simple order.

Having set the notation, one has that the coherent-state representation of the trace in Eq. (3.115) for both bosons and fermions can be written as

$$Z=\int\prod_{i=1}^{D}\left(\frac{d\xi_i^* d\xi_i}{\mathcal{N}}\right)\exp\left(-\sum_{j=1}^{D}\xi_j^*\xi_j\right)\langle\zeta\xi|e^{-\beta\widehat{\Omega}}|\xi\rangle.\tag{3.124}$$

Now, following the same strategy used in the derivation of the quantum-mechanical path integral, the interval $[0,\beta]$ is partitioned into M equal pieces as

$$\epsilon\equiv\frac{\beta}{M},\tag{3.125}$$

so that the matrix element $\langle\zeta\xi|e^{-\beta\widehat{\Omega}}|\xi\rangle$ appearing in the integral in Eq. (3.124) can be written as

$$\langle\zeta\xi|e^{-\beta\widehat{\Omega}}|\xi\rangle=\langle\zeta\xi|[e^{-\epsilon\widehat{\Omega}}]^M|\xi\rangle=\langle\zeta\xi|e^{-\epsilon\widehat{\Omega}}e^{-\epsilon\widehat{\Omega}}\cdots e^{-\epsilon\widehat{\Omega}}e^{-\epsilon\widehat{\Omega}}|\xi\rangle.\tag{3.126}$$

Next, we introduce the decomposition of the identity, Eq. (3.119), between any two consecutive exponentials so that

$$\begin{aligned}Z &= \int\prod_{i=1}^{D}\left(\frac{d\xi_i^* d\xi_i}{\mathcal{N}}\right)\exp\left(-\sum_{j=1}^{D}\xi_j^*\xi_j\right) &(3.127)\\ &\times \langle\zeta\xi|e^{-\epsilon\widehat{\Omega}}\int\prod_{i=1}^{D}\left(\frac{d\xi_{i,M-1}^* d\xi_{i,M-1}}{\mathcal{N}}\right)\exp\left(-\sum_{j=1}^{D}\xi_{j,M-1}^*\xi_{j,M-1}\right)|\xi_{M-1}\rangle\langle\xi_{M-1}|\\ &\times \cdots|\xi_2\rangle\langle\xi_2|\int\prod_{i=1}^{D}\left(\frac{d\xi_{i,1}^* d\xi_{i,1}}{\mathcal{N}}\right)\exp\left(-\sum_{j=1}^{D}\xi_{j,1}^*\xi_{j,1}\right)|\xi_1\rangle\langle\xi_1|e^{-\epsilon\widehat{\Omega}}|\xi\rangle\\ &= \int\prod_{i=1}^{D}\left(\frac{d\xi_i^* d\xi_i}{\mathcal{N}}\right)\int\prod_{i=1}^{D}\prod_{k=1}^{M-1}\left(\frac{d\xi_{i,k}^* d\xi_{i,k}}{\mathcal{N}}\right)\exp\left(-\sum_{j=1}^{D}\xi_j^*\xi_j\right)\\ &\times \exp\left(-\sum_{j=1}^{D}\sum_{l=1}^{M-1}\xi_{j,l}^*\xi_{j,l}\right)\langle\zeta\xi|e^{-\epsilon\widehat{\Omega}}|\xi_{M-1}\rangle\cdots\langle\xi_2|e^{-\epsilon\widehat{\Omega}}|\xi_1\rangle\langle\xi_1|e^{-\epsilon\widehat{\Omega}}|\xi\rangle. &(3.128)\end{aligned}$$

Here we have introduced the notation $\xi_{i,l}$ to indicate that for every insertion of the identity decomposition one needs a different dummy variable ξ_i, so that $l=1,\cdots,M-1$ because we have $M-1$ insertions. Defining

$$\xi_{i,0}\equiv\xi_i,\qquad \xi_{i,M}\equiv\zeta\xi_i,\tag{3.129}$$

one can rewrite Eq. (3.128) more succinctly as

$$Z = \int \prod_{i=1}^{D} \prod_{k=1}^{M} \left(\frac{d\xi_{i,k}^* d\xi_{i,k}}{\mathcal{N}} \right) \exp\left(- \sum_{j=1}^{D} \sum_{l=1}^{M} \xi_{j,l}^* \xi_{j,l} \right) \prod_{m=M}^{1} \langle \xi_m | e^{-\epsilon\, \widehat{\Omega}(a^\dagger, a)} | \xi_{m-1} \rangle. \quad (3.130)$$

Next, we have to evaluate the matrix elements $\langle \xi_m | e^{-\epsilon\, \widehat{\Omega}(a^\dagger, a)} | \xi_{m-1} \rangle$. We expand the exponent to first order in ϵ,

$$e^{-\epsilon\, \widehat{\Omega}(a^\dagger, a)} \simeq 1 - \epsilon\, \widehat{\Omega}(a^\dagger, a) = 1 - \epsilon\, \widehat{\Omega}^{\odot}(a^\dagger, a), \quad (3.131)$$

so that

$$\begin{aligned} \langle \xi_m | e^{-\epsilon\, \widehat{\Omega}(a^\dagger, a)} | \xi_{m-1} \rangle &\simeq \langle \xi_m | \left[1 - \epsilon\, \widehat{\Omega}^{\odot}(a^\dagger, a) \right] | \xi_{m-1} \rangle \\ &= \langle \xi_m | \xi_{m-1} \rangle \left[1 - \epsilon\, \Omega^{\odot}(\xi_m^*, \xi_{m-1}) \right] \\ &\simeq \langle \xi_m | \xi_{m-1} \rangle\, e^{-\epsilon\, \Omega^{\odot}(\xi_m^*, \xi_{m-1})} \\ &= \exp\left(\sum_{p=1}^{D} \xi_{p,\,m}^* \xi_{p,\,m-1} \right)\, e^{-\epsilon\, \Omega^{\odot}(\xi_m^*, \xi_{m-1})}. \end{aligned} \quad (3.132)$$

Using this result in Eq. (3.130), one obtains

$$\begin{aligned} Z &= \int \prod_{i=1}^{D} \prod_{k=1}^{M} \left(\frac{d\xi_{i,k}^* d\xi_{i,k}}{\mathcal{N}} \right) \exp\left(- \sum_{j=1}^{D} \sum_{l=1}^{M} \xi_{j,l}^* \xi_{j,l} \right) \\ &\times \prod_{m=M}^{1} \left[\exp\left(\sum_{p=1}^{D} \xi_{p,\,m}^* \xi_{p,\,m-1} \right) e^{-\epsilon\, \Omega^{\odot}(\xi_m^*, \xi_{m-1})} \right] \\ &= \int \prod_{k=0}^{M-1} \prod_{i=1}^{D} \left(\frac{d\xi_{i,k}^* d\xi_{i,k}}{\mathcal{N}} \right)\, e^{-S(\xi^*, \xi)}, \end{aligned} \quad (3.133)$$

where $S(\xi^*, \xi)$ is the result of combining the exponentials as

$$\begin{aligned} S(\xi^*, \xi) &= \sum_{k=1}^{M} \sum_{j=1}^{D} \xi_{j,k}^* \left(\xi_{j,k} - \xi_{j,k-1} \right) + \epsilon \sum_{k=1}^{M} \Omega^{\odot}(\xi_k^*, \xi_{k-1}) \\ &= \epsilon \sum_{k=1}^{M} \left[\sum_{j=1}^{D} \xi_{j,k}^* \frac{(\xi_{j,\,k} - \xi_{j,\,k-1})}{\epsilon} + \Omega^{\odot}(\xi_k^*, \xi_{k-1}) \right]. \end{aligned} \quad (3.134)$$

Now, if one imagines $M \to \infty$, then $\epsilon \to 0$, so that the index k in the exponential becomes a continuous variable τ,

$$\xi_{i,k} \to \xi_i(\tau), \quad (3.135)$$

and one recognizes in the same limit that

$$\frac{(\xi_{j,l}-\xi_{j,l-1})}{\epsilon}\rightarrow\frac{\partial\xi_j(\tau)}{\partial\tau}\qquad\text{and}\qquad\epsilon\sum_{k=1}^{M}f(\xi_{i,\,k})\rightarrow\int_0^\beta d\tau\,f(\xi_i(\tau)).\tag{3.136}$$

In addition, from (3.129) one has that the continuous variables $\xi_i(\tau)$ satisfy the "boundary condition"

$$\xi_i(\beta)=\zeta\xi_i(0).\tag{3.137}$$

Therefore, the partition function can be written as

$$Z=\int_{\xi(0)}^{\xi(\beta)}\mathcal{D}[\xi^*(\tau)\xi(\tau)]\;e^{-\mathcal{S}(\xi^*,\xi)},\tag{3.138}$$

where

$$\mathcal{S}(\xi^*,\xi)\equiv\int_0^\beta d\tau\;\left[\sum_{j=1}^{D}\xi_j^*(\tau)\frac{\partial\xi_j(\tau)}{\partial\tau}+\Omega^{\odot}(\xi^*(\tau),\xi(\tau))\right],\tag{3.139}$$

and we used the notation

$$\int\prod_{i=1}^{D}\prod_{k=1}^{M}\left(\frac{d\xi_{i,k}^*d\xi_{i,k}}{\mathcal{N}}\right)\rightarrow\int_{\xi(0)}^{\xi(\beta)}\mathcal{D}[\xi^*(\tau)\xi(\tau)],\tag{3.140}$$

This is the final result for the path integral representation for the grand-canonical partition function.

Sometimes it is useful to have an expression for $\mathcal{S}(\xi^*,\xi)$ that is symmetrical in the τ derivatives. This can be achieved averaging both expressions (see Appendix E)

$$\begin{aligned}S(\xi^*,\xi)\;&\equiv\;\epsilon\sum_{k=0}^{M-1}\left\{\frac{1}{2}\sum_{j=1}^{D}\left[\xi_{j,k'+1}^*\frac{(\xi_{j,k'+1}-\xi_{j,k'})}{\epsilon}-\frac{\left(\xi_{j,k+1}^*-\xi_{j,k}^*\right)}{\epsilon}\xi_{j,k}\right]\right.\\&+\;\left.\Omega^{\odot}(\xi_{k+1}^*,\xi_k)\right\}.\end{aligned}\tag{3.141}$$

In the "trajectory" notation

$$\begin{aligned}\mathcal{R}(\xi^*,\xi)\;&\equiv\;\int_0^\beta d\tau\left\{\frac{1}{2}\sum_{j=1}^{D}\left[\xi_j^*(\tau)\frac{\partial\xi_j(\tau)}{\partial\tau}-\left(\frac{\partial\xi_j^*(\tau)}{\partial\tau}\right)\xi_j(\tau)\right]\right.\\&+\;\left.\Omega^{\odot}(\xi^*(\tau),\xi(\tau))\right\}.\end{aligned}\tag{3.142}$$

$$=\;\int_0^\beta d\tau\left\{\sum_{j=1}^{D}\xi_j^*(\tau)\frac{\overleftrightarrow{\partial}}{\partial\tau}\xi_j+\Omega^{\odot}(\xi^*(\tau),\xi(\tau))\right\},\tag{3.143}$$

Finally, we note the formal analogy with the quantum mechanical path integral derived in Section 3.1. First, we note that if one defines in the quantum mechanical

path integral variables $\xi_i \sim p_i + i r_i$, and $\xi_i^* \sim p_i - i r_i$, the integration measure would simply be replaced by

$$\mathcal{D}[r_i\, p_i] \rightarrow \mathcal{D}[\xi_i^*\, \xi_i]. \tag{3.144}$$

Second, making $t \rightarrow -i\tau$, the exponent in Eq. (3.17) would be precisely of the form given above – with the exception that there is no finite limit on the "time" integral. This formal analogy means that the path integral for the partition function in statistical mechanics is equivalent to the quantum mechanical path integral for the probability amplitude in imaginary time τ – with the addition of the fields being periodic or antiperiodic in β.

One path integral one will need in Chapter 5 is the following

$$\begin{aligned} I(A, a^*, a) &= \int [d\xi^* d\xi]\; e^{-\xi^* A \xi + a^* \xi + \xi^* a} \\ &= \int \left[\prod_{i=1}^{N} d\xi_i^* d\xi_i\right] \exp\left[-\sum_{i=1}^{N}\sum_{j=1}^{N} \xi_i^* A_{ij} \xi_j + \sum_{i=1}^{N} (a_i^* \xi_i + \xi_i^* a_i)\right], \end{aligned} \tag{3.145}$$

where A is an $N \times N$ matrix and a and a^* are vectors of N components. Let us start with the following integral (b is an ordinary number)

$$\begin{aligned} I(b) &= \int d\xi^* d\xi\, e^{-b\xi^*\xi} \int d\xi^* d\xi\; (1 - b\xi^*\xi) = \int d\xi^* d\xi\; (1 + b\xi\xi^*) \\ &= b \int d\xi^* d\xi\, \xi\xi^* = b. \end{aligned} \tag{3.146}$$

Next, we consider the integral (A is an $N \times N$ matrix)

$$I(A) = \int \left[\prod_{i=1}^{N} d\xi_i^* d\xi_i\right] \exp\left(-\sum_{i=1}^{N}\sum_{j=1}^{N} \xi_i^* A_{ij} \xi_j\right). \tag{3.147}$$

Initially we prove that an integral over the set of Grassmann variables $\{\xi_i^*, \xi_i, i = 1, \cdots, N\}$ is invariant under unitary transformations. Let U be an $N \times N$ unitary matrix and define new Grassmann variables $\xi_i' = U_{ij}\, \xi_j$ (here and in the following we use the convention that there is a sum over repeated indices), then using the completely antisymmetric symbol in N-dimensions $\epsilon^{ij\cdots l}$ we can write

$$\begin{aligned} \prod_{i=1}^{N} \xi_i' &= \frac{1}{N!}\, \epsilon^{ij\cdots l}\, \xi_i' \xi_j' \cdots \xi_l' \\ &= \frac{1}{N!}\, \epsilon^{ij\cdots l}\, U_{ii'} \xi_{i'}\, U_{jj'} \xi_{j'} \cdots U_{ll'} \xi_{l'} \\ &= \frac{1}{N!}\, \epsilon^{ij\cdots l}\, U_{ii'}\, U_{jj'} \cdots U_{ll'}\, \epsilon^{i'j'\cdots l'} \prod_{i=1}^{N} \xi_i \\ &= (\det U) \prod_{i=1}^{N} \xi_i = \prod_{i=1}^{N} \xi_i, \end{aligned} \tag{3.148}$$

since U is unitary. Therefore, if we take U as being the unitary matrix that diagonalizes the matrix A, and λ_i are the eigenvalues of A, we obtain the result

$$\begin{aligned} I(A) &= \int \left[\prod_{i=1}^{N} d\xi_i^* d\xi_i\right] \exp\left(-\sum_{i=1}^{N}\sum_{j=1}^{N} \xi_i^* A_{ij} \xi_j\right) \\ &= \int \left[\prod_{i=1}^{N} d\xi_i^* d\xi_i\right] \exp\left(-\sum_{i=1}^{N} \lambda_i\, \xi_i^* \xi_i\right) \\ &= \prod_{i=1}^{N} \lambda_i = \det A. \end{aligned} \tag{3.149}$$

With this result we can now consider the integral $I(A, a^*, a)$. If one make the change of variables

$$\begin{aligned} \xi^* &= \xi^{*\prime} + a^* A^{-1}, \\ \xi &= \xi' + A^{-1} a, \end{aligned} \tag{3.150}$$

one has

$$\begin{aligned} -\xi^* A \xi + a^* \xi + \xi^* a &= -(\xi^{*\prime} + a^* A^{-1}) A (\xi' + A^{-1} a) \\ &+ a^*(\xi' + A^{-1} a) + (\xi^{*\prime} + a^* A^{-1}) a \\ &= -\xi^{*\prime} A \xi' - \xi^{*\prime} A A^{-1} a - a^* A^{-1} A \xi' - a^* A^{-1} A A^{-1} a \\ &+ a^* \xi' + a^* A^{-1} a + \xi^{*\prime} a + a^* A^{-1} a \\ &= -\xi^{*\prime} A \xi' + a^* A^{-1} a, \end{aligned} \tag{3.151}$$

and therefore

$$\begin{aligned} I(A, a^*, a) &= \int [d\xi^* d\xi]\; e^{\xi^* A \xi + a^* \xi + \xi^* a} \\ &= e^{a^* A^{-1} a} \int [d\xi^* d\xi]\; e^{\xi^* A \xi} \\ &= (\det A)\, e^{a^* A^{-1} a}. \end{aligned} \tag{3.152}$$

Another result we will need in Chapter 5 is related to the functional derivative of Grassmann functions. In analogy to the bosonic functional derivatives, one has that

$$\frac{\delta}{\delta \xi_i} \int [\prod_j d\xi_j'] f(\xi_j') = f[\xi_i]. \tag{3.153}$$

Capítulo 4

The Niterói Method

In the present Chapter we will review the Niterói method for obtaining the partition function of a many-fermion system without resorting to the path integral representation.

The aim is to evaluate the partition function

$$Z = \mathrm{Tr}\,(e^{-\beta\widehat{\Omega}}) \tag{4.1}$$

where $\widehat{\Omega}$ has been defined in Eq. (3.18), given by $\widehat{\Omega} \equiv \widehat{H} - \mu\widehat{N}$. As said above, the starting point is a high-temperature expansion of the exponential in Eq. (4.1) in the form

$$Z = \sum_{s=0}^{\infty} \frac{(-\beta)^s}{s!} \mathrm{Tr}\,(\widehat{\Omega})^s. \tag{4.2}$$

The first term $s = 0$ of the expansion is trivial. In essence, the method consists in calculating the remaining traces exclusively in the coherent-state representation. For a Hamiltonian that is quadratic in the creation and annihilation operators, as we shall see, the series can be summed and therefore the validity of the result obtained is not restricted to the high temperatures only.

4.1 Coherent-state representation of the trace of $(\widehat{\Omega})^s$

In order to grasp the essential steps to evaluate the traces of multiple products of $\widehat{\Omega}$ in Eq. (4.2), we start the discussion for $D = 1$. In this case, one has that the trace of an operator $\widehat{O}$ is given by Eq. (3.112), which translates for $D = 1$ to

$$\mathrm{Tr}\,\widehat{O} = \int d\xi d\xi^*\, e^{2\xi^*\xi}\, O^{\odot}(\xi^*, \xi). \tag{4.3}$$

We need the trace of the product of s operators in Eq. (4.2). But let us first consider the trace of the product of two operators using the expression for the trace of an unordered operator given in Eq. (3.110),

$$\mathrm{Tr}\,(\widehat{O}_1\widehat{O}_2) \;\; = \;\; \int d\xi^* d\xi\, e^{-\xi^*\xi}\, \langle -\xi|\widehat{O}\widehat{O}|\xi\rangle. \tag{4.4}$$

Next we insert between the two $\widehat{O}$ operators in this equation the decomposition of the identity given in Eq. (3.93)

$$I = \int d\xi^* d\xi \, e^{-\xi^* \xi} \, |\xi\rangle\langle\xi|, \tag{4.5}$$

so that one obtains,

$$\mathrm{Tr}\,(\widehat{O}_1\widehat{O}_2) = \int d\xi_1^* d\xi_1 d\xi_2 d\xi_2^* \, e^{-\xi_1^*\xi_1} \, e^{-\xi_2^*\xi_2} \, \langle -\xi_1|\widehat{O}_1|\xi_2\rangle \, \langle \xi_2|\widehat{O}_2|\xi_1\rangle. \tag{4.6}$$

Now, for each coherent-state matrix element above we use the $D = 1$ equivalent of Eq (3.109),

$$\langle\xi|\widehat{O}|\xi'\rangle = e^{\xi^*\xi'} \, O^{\odot}(\xi^*, \xi'), \tag{4.7}$$

which results in

$$\begin{aligned} \mathrm{Tr}\,(\widehat{O}_1\widehat{O}_2) &= \int d\xi_1^* d\xi_1 d\xi_2^* d\xi_2 \, e^{-\xi_1^*\xi_1} \, e^{-\xi_2^*\xi_2} \, e^{-\xi_1^*\xi_2} \, e^{\xi_2^*\xi_1} \, O_1^{\odot}(-\xi_1^*, \xi_2) \, O_2^{\odot}(\xi_2^*, \xi_1) \\ &= \int d\xi_1 d\xi_1^* d\xi_2^* d\xi_2 \, e^{\xi_1^*\xi_1} \, e^{-\xi_2^*\xi_2} \, e^{\xi_1^*\xi_2} \, e^{\xi_2^*\xi_1} \, O_1^{\odot}(\xi_1^*, \xi_2) \, O_2^{\odot}(\xi_2^*, \xi_1). \end{aligned} \tag{4.8}$$

Making the change of variables $\xi_1 \leftrightarrow \xi_2$ and rearranging the integration measure, one obtains the final result

$$\mathrm{Tr}\,(\widehat{O}_1\widehat{O}_2) = \int d\xi_1 d\xi_1^* d\xi_2 d\xi_2^* \, e^{\xi_1^*(\xi_1+\xi_2)} \, e^{\xi_2^*(\xi_2-\xi_1)} \, O_1^{\odot}(\xi_1^*, \xi_1) \, O_2^{\odot}(\xi_2^*, \xi_2). \tag{4.9}$$

It is not difficult to show that this result generalizes for the product of s operators to

$$\begin{aligned} \mathrm{Tr}\,(\widehat{O}_1 \cdots \widehat{O}_s) &= \int d\xi_1 d\xi_1^* \cdots d\xi_s d\xi_s^* \, e^{\xi_1^*(\xi_1+\xi_s)} \, e^{\xi_2^*(\xi_2-\xi_1)} \cdots e^{\xi_s^*(\xi_s-\xi_{s-1})} \\ &\times \; O_1^{\odot}(\xi_1^*, \xi_1) \, O_2^{\odot}(\xi_1^*, \xi_2) \cdots O_s^{\odot}(\xi_s^*, \xi_s) \, . \end{aligned} \tag{4.10}$$

Note that in the first exponential one has a positive sign on ξ_s. This is due to the antiperiodic boundary condition of the endpoint Grassmann number in the trace. The result coincides with the one given by Creutz in Ref. [34] – Eq. (13) of this reference.

Now, the result for a single-particle Hilbert space of arbitrary dimension D can be easily generalized from the result for $D = 1$ in Eq. (4.10). For that matter, one should notice that instead of only one ξ we will have D $\xi's$. Therefore, one can consider that each ξ in the integral in Eq. (4.10) is actually a vector with D components, so that $\xi_i = (\xi_{i,1}, \xi_{i,2}, \cdots, \xi_{i,D})$, for $i = 1, 2, \cdots, s$, and the products $\xi_1^*(\xi_1 + \xi_s)$ and $\xi_2^*(\xi_2 - \xi_1)$, $\cdots$ become

$$\xi_1^*(\xi_1 + \xi_s) = \sum_{l=1}^{D} \xi_{1,l}^*(\xi_{1,l} + \xi_{2,l}), \tag{4.11}$$

$$\xi_i^*(\xi_i - \xi_{i-1}) = \sum_{l=1}^{D} \xi_{i,l}^*(\xi_{i,l} - \xi_{i-1,l}), \tag{4.12}$$

With $i = 2, ..., s$. The product of the exponentials can then be rewritten as a single exponential with an exponent given by the sum

$$\sum_{l=1}^{D} \sum_{i=1}^{s} \xi_{i,l}^{*}(\xi_{i,l} - \xi_{i-1,l}), \tag{4.13}$$

with the boundary condition

$$\xi_{0,l} = -\xi_{s,l}. \tag{4.14}$$

With this, the final result for the trace of $(\widehat{\Omega})^s$ is simply

$$\begin{aligned} \mathrm{Tr}\,(\widehat{\Omega})^s &= \int \prod_{k=1}^{D} \prod_{i=1}^{s} d\xi_{i,k} d\xi_{i,k}^{*} \, \exp\left[\sum_{l=1}^{D} \sum_{i=1}^{s} \xi_{i,l}^{*}(\xi_{i,l} - \xi_{i-1,l})\right] \\ &\times \widehat{\Omega}^{\odot}(\xi_{1,1}^{*}, \cdots, \xi_{1,D}) \cdots \widehat{\Omega}^{\odot}(\xi_{s,1}^{*}, \cdots, \xi_{s,D}). \end{aligned} \tag{4.15}$$

This is the final expression for the trace of $(\Omega)^s$. In the next section we will obtain the expression for the matrix elements $\Omega^{\odot}(\xi^{*}, \cdots, \xi)$ in terms of the Grassmann numbers ξ^{*} and ξ.

4.2 Explicit expression for $\Omega^{\odot}(\xi^{*}, \xi)$

Evaluation of the multiple integral in Eq. (4.15) requires an explicit expression for $\Omega^{\odot}(\xi^{*}, \xi)$ in terms of the the Grassmann numbers ξ^{*} and ξ. This can be obtained as follows. Let us start again with the $D = 1$ case. When $\widehat{\Omega}(a^{\dagger}, a)$ is not already in normal order, it can be put in such order through

$$\widehat{\Omega}(a^{\dagger}, a) = \sum_{m=0,1} \sum_{n=0,1} \Omega_{m,n}^{\odot} \, (a^{\dagger})^m (a)^n, \tag{4.16}$$

where $\Omega_{m,n}^{\odot}$ can be obtained from the explicit representation of $\widehat{\Omega}(a^{\dagger}, a)$ – for an example, see Eqs. (3.49)-(3.51). Now, from Eq. (4.7)

$$\Omega^{\odot}(\xi^{*}, \xi) = e^{-\xi^{*}\xi} \, \langle \xi | \widehat{O} | \xi \rangle, \tag{4.17}$$

and inserting Eq. (4.16) in this one obtains

$$\begin{aligned} \Omega^{\odot}(\xi^{*}, \xi) &= e^{-\xi^{*}\xi} \sum_{m=0,1} \sum_{n=0,1} \Omega_{m,n}^{\odot} \, \langle \xi | (a^{\dagger})^m (a)^n | \xi \rangle \\ &= e^{-\xi^{*}\xi} \sum_{m=0,1} \sum_{n=0,1} \Omega_{m,n}^{\odot} \, (\xi^{*})^m \, (\xi)^n \, \langle \xi | \xi \rangle. \end{aligned} \tag{4.18}$$

Using the result given in Eq. (3.108), one has the final result

$$\Omega^{\odot}(\xi^{*}, \xi) = \sum_{m=0,1} \sum_{n=0,1} \Omega_{m,n}^{\odot} \, (\xi^{*})^m \, (\xi)^n. \tag{4.19}$$

This can now be extended to a D-dimensional space. First, Eq. (4.16) becomes

$$\widehat{\Omega}(a^\dagger, a) = \sum_{\{m\}=0,1} \sum_{\{n\}=0,1} \Omega^{\odot}_{m_1,\cdots,m_D;n_1,\cdots,n_D} \, (a_D^\dagger)^{m_D} \cdots (a_1^\dagger)^{m_1} (a_1)^{n_1} \cdots (a_D)^{n_D}. \tag{4.20}$$

Therefore, $\widehat{\Omega}^{\odot}(\xi_1^*, \cdots, \xi_D^*, \xi_1, \cdots, \xi_D)$ is given by

$$\begin{aligned} \widehat{\Omega}^{\odot}(\xi_1^*, \cdots, \xi_D^*, \xi_1, \cdots, \xi_D) &= \sum_{\{m\}=0,1} \sum_{\{n\}=0,1} \Omega^{\odot}_{m_1,\cdots,m_D;n_1,\cdots,n_D} \\ &\times \; (\xi_D^*)^{m_D} \cdots (\xi_1^*)^{m_1} (\xi_1)^{n_1} \cdots (\xi_D)^{n_D}. \end{aligned} \tag{4.21}$$

4.3 Evaluation of the Grassmann integrals in $\mathrm{Tr}(\Omega)^s$

The multidimensional Grassmann integral in Eq. (4.15), with the $\Omega^{\odot}_{m_1,\cdots,m_D;n_1,\cdots,n_D}$ given by Eq. (4.21), is not trivial when $D > 1$. However, it can be done more easily by condensing the notation. Specifically, instead of using the two sets of indices $\{k = 1, \cdots D\}$ and $\{i = 1, \cdots, s\}$, Eq. (4.15) can be simplified by using a single set of indices, $\{I = 1, \cdots, sD\}$, for each Grassmann number.

Let us consider first the example of $D = 2$. This corresponds to a system with two degrees of freedom, e.g. $k = 1 = \uparrow$ and $k = 2 = \downarrow$. For this case, we have that the exponent in the integral is given by

$$\sum_{l=1}^{D} \sum_{i=1}^{s} \xi^*_{i,l}(\xi_{i,l} - \xi_{i-1,l}) = \sum_{i=1}^{s} \xi^*_{i,\uparrow}(\xi_{i,\uparrow} - \xi_{i-1,\uparrow}) + \sum_{i=1}^{s} \xi^*_{i,\downarrow}(\xi_{i,\downarrow} - \xi_{i-1,\downarrow}). \tag{4.22}$$

The sum over $\uparrow$ terms can be organized as follows:

$$\begin{aligned} \sum_{i=1}^{s} \xi^*_{i,\uparrow}(\xi_{i,\uparrow} - \xi_{i-1,\uparrow}) = &+ \xi^*_{1,\uparrow}\,\xi_{1,\uparrow} + 0 + \cdots + 0 + \xi^*_{1,\uparrow}\,\xi_{s,\uparrow} \\ &- \xi^*_{2,\uparrow}\,\xi_{1,\uparrow} + \xi^*_{2,\uparrow}\,\xi_{2,\uparrow} + 0 + \cdots + 0 \qquad (4.23) \\ &+ 0 + 0 + \cdots - \xi^*_{s,\uparrow}\,\xi_{s-1,\uparrow} + \xi^*_{s,\uparrow}\xi_{s,\uparrow} \qquad (4.24) \\ = &\sum_{i=1}^{s} \xi^*_{i,\uparrow}\,(A^{\uparrow\uparrow})_{i,j}\,\xi_{j,\uparrow} \equiv \sum_{i=1}^{s} \eta^*_i\,(A^{\uparrow\uparrow})_{i,j}\,\eta_j, \qquad (4.25) \end{aligned}$$

where we have changed the notation $\xi_{i,\uparrow} \to \eta_i$, and the matrix $A^{\uparrow\uparrow}$ is, by inspection

of the sum above, given by

$$A^{\uparrow\uparrow} = \left.\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 1 \\ -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}\right\} s \text{ elements} \tag{4.26}$$

Note that we are using the transpose of the matrices used by Charret et al. in Ref. [9]. It is clear that the matrix corresponding to the sum over $\downarrow$ terms, $A^{\downarrow\downarrow}$, is precisely the same as $A^{\uparrow\uparrow}$, and the sum over $\uparrow$ terms is organized as follows:

$$\sum_{i=1}^{s} \xi^*_{i,\downarrow}(\xi_{i,\downarrow} - \xi_{i-1,\downarrow}) = \sum_{i=1}^{s} \xi^*_{i,\downarrow}\ (A^{\downarrow\downarrow})_{i,j}\ \xi_{j,\downarrow} \equiv \sum_{i=s+1}^{2s} \eta^*_i\ (A^{\uparrow\uparrow})_{i,j}\ \eta_j. \tag{4.27}$$

Moreover, the matrices $A^{\uparrow\downarrow}$ and $A^{\downarrow\uparrow}$ are null.

Therefore, if one considers a matrix of the form

$$A = \begin{pmatrix} A^{\uparrow\uparrow} & 0 \\ 0 & A^{\downarrow\downarrow} \end{pmatrix} \tag{4.28}$$

one can write Eq. (4.15) as

$$\mathrm{Tr}\,(\widehat{\Omega})^s = \int \prod_{I=1}^{N} d\eta_I d\eta^*_I \exp\left(\sum_{J=1}^{N}\sum_{K=1}^{N} \eta^*_J\, A_{JK}\, \eta_K\right) \Omega^{\odot}(\eta^*_1, \eta_1) \cdots \Omega^{\odot}(\eta^*_N, \eta_N). \tag{4.29}$$

This integral requires further elaboration. Because the matrix A is block diagonal, the integral factorizes in a product of 2 multidimensional integrals of dimension s. The integrand contains the exponential factor and products of Grassmann numbers coming from the product of s operators $\Omega^{\odot}(\xi^*_1, \xi^*_2, \xi_1, \xi_2)$. Therefore, in general, each of the s-dimensional integrals is a moment of a Grassmann Gaussian integral of the form

$$M(L,K) = \int \prod_{i=1}^{s} d\eta_i d\eta^*_i\ \exp\left(\sum_{J=1}^{s}\sum_{K=1}^{s} \eta^*_J\, A^{\sigma\sigma}_{JK}\, \eta_K\right)\ \eta^*_{l_1}\, \eta_{k_1}\ \cdots\ \eta^*_{l_m}\, \eta_{k_m}, \tag{4.30}$$

where $L = l_1, \cdots, l_m$ and $K = k_1, \cdots, k_m$, with $m \leq s$. We also assume that the product of η^* and η are ordered as $l_1 < l_2 < \cdots < l_m$ and $k_1 < k_2 < \cdots < k_m$.

Obtention of an explicit solution of an integral like Eq (4.30) is quite involved but it is possible. In a very detailed and clear derivation, Charret, Corrêa Silva, Souza, O. Rojas Santos, Thomaz, and Carneiro in Ref. [9] obtained the explicit expression

$$M(L,K) = (-1)^{l_1+\cdots+l_m}(-1)^{k_1+\cdots+k_m}\, A(L,K), \tag{4.31}$$

where $A(L,K)$ is a co-factor of the matrix $A^{\sigma\sigma}$ with respect to the rows $l_1,\cdots,l_m$ and the columns $k_1,\cdots,k_m$ – the determinant of $A^{\sigma\sigma}$ with the rows $l_1,\cdots,l_m$ and the columns $k_1,\cdots,k_m$ removed.

For a system with D degrees of freedom, the dimension of the matrix A is $N = sD$ and its the structure remains block-diagonal, where each matrix on the diagonal is equal to the matrices $A^{\uparrow\uparrow}$ and $A^{\downarrow\downarrow}$ – instead of the numbers 1 and 0, one actually have the $N \times N$ identity and null matrices. In addition, the integrals necessary to evaluate the trace of $(\widehat{\Omega})^s$, Eq. (4.29), have as solutions Eqs. (4.30) and (4.31), the only difference as compared to the $D = 2$ case, is that being that now there are D of such integrals.

Despite of the closed form of the result of the multidimensional Grassmann integral, explicit evaluation of the remaining determinants is still a formidable task. Fortunately, Charret, Corrêa Silva, Souza, Rojas Santos and Thomaz [13] were able to diagonalize the $A^{\sigma\sigma}$ through a similarity transformation, exploiting the block-structure of these matrices. This was a tremendous achievement, in that it opens the possibility for explicit evaluation of traces of products of an arbitrary number of normal-ordered fermionic operators without resorting to large scale computer evaluations.

This completes the review on the Niterói method. As already commented, the highlight of the method is its ability of calculating the partition function of a many-fermion system at finite temperature and chemical potential in closed form in the high temperature limit, i.e. in principle each term of the series expansion in β, Eq. (4.2), is known explicitly. Of course, the evaluation of each term becomes complicated for high powers β^s and therefore it will be useful for temperatures sufficiently high such that the series can be truncated at some low value of s. On the other hand, when the operator $\widehat{\Omega}$ in the Boltzmann factor, Eq. (4.1), is quadratic in the field operators, one can re-sum the series expansion in β and so the validity of the result *is not* restricted to high temperatures.

One might think that quadratic $\widehat{\Omega}$'s represent essentially noninteracting particles, since interaction terms involve at least four field operators. However, this is not the case, since many approximate, nonperturbative methods in many-body physics have as starting point an ansatz for $\widehat{\Omega}$ that is quadratic in the field operators and corrections to the ansatz are then calculated perturbatively. Examples include Hartree-Fock and BCS-type of methods, optimized perturbation theory, etc. Another important example is the use of the Hubbard-Stratonovich [8] transformation that, with the introduction of auxiliary bosonic fields, allows to express a four-fermion interaction into a quadratic Hamiltonian. Therefore, once one calculates the trace over the fermionic fields, there remains a trace over bosonic fields that

can be calculated perturbatively or numerically. Moreover, one *ab initio* method of approaching many-body problems is through Monte Carlo simulations on a Euclidean space-time lattice. However, such methods loose accuracy for large values of the chemical potential because of the non-positivity of the Euclidean action, commented in the Introduction. The Niterói method, on the other hand, can in principle evade this problem when used in connection with some approximation scheme.

In the next Chapter we will discuss some simple applications of the Niterói method. In addition, we will indicate further, novel applications of the method to many systems of modern interest.

Capítulo 5

Applications to simple problems and possible extensions

In the present Chapter we present applications of the Niterói method to simple problems. Initially, in the next Section, we consider the trivial, but illustrative case of the free Fermi gas. Next, in Section 5.2 we consider mean field type of approximations to the interacting non-relativistic Fermi gas. Here the aim is to reobtain the well known results of the traditional Hartree-Fock and BCS approximations [1] [2]. Here we make use of the Bogoliubov-Valatin [36] canonical transformation to bring the Hamiltonian to a diagonal form such that the Niterói method can be applied directly and trivially. In Section 5.3 we discuss how to obtain the well known results of perturbation theory on the top of the mean field approximation. All these results are not new and actually can be obtained with other methods. It should be understood that the aim here is to show that the method is reliable and should be useful in other contexts. With this in mind, in Section 5.4 we propose to use the Niterói method in connection with the Hubbard-Stratonovich [8] transformation to implement high order optimized perturbation theory [14]-[17] to improve on the mean field approximation. And finally, we discuss the application of the method to the lattice formulation of field theories.

5.1 Non-interacting non-relativistic Fermi gas

Here we consider the problem of calculating the grand-canonical partition function of the nonrelativistic Fermi gas. We shall initially consider the traditional calculation of direct evaluation by means of the second quantization formalism. Then we will reobtain the result using the Niterói method just discussed above.

The Hamiltonian for a system of noninteracting nonrelativistic fermions is given

in terms of field operators $\psi_\sigma(\mathbf{x})$ and $\psi^\dagger_\sigma(\mathbf{x})$ as

$$\widehat{H} = \sum_\sigma \int d^3\mathbf{x}\, \psi^\dagger_\sigma(\mathbf{x}) \left(-\frac{1}{2m}\boldsymbol{\nabla}^2_x\right) \psi_\sigma(\mathbf{x}), \tag{5.1}$$

where $\sigma = \downarrow, \uparrow$. Here and elsewhere we use $\hbar = 1$. The field operators satisfy the usual anticommutation relations

$$\begin{aligned} &\{\psi_\sigma(\mathbf{x}), \psi^\dagger_{\sigma'}(\mathbf{x}')\} = \delta_{\sigma'\sigma}\, \delta(\mathbf{x}' - \mathbf{x}), \\ &\{\psi^\dagger_\sigma(\mathbf{x}), \psi^\dagger_{\sigma'}(\mathbf{x}')\} = 0, \qquad \{\psi_\sigma(\mathbf{x}), \psi_{\sigma'}(\mathbf{x}')\} = 0. \end{aligned} \tag{5.2}$$

It is convenient to work in momentum space, so we perform a Fourier decomposition of the fields in a large volume V of the space

$$\psi_\sigma(\mathbf{x}) = \frac{1}{V^{1/2}} \sum_{\mathbf{k}} a_\sigma(\mathbf{k})\, e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{5.3}$$

$$\psi^\dagger_\sigma(\mathbf{x}) = \frac{1}{V^{1/2}} \sum_{\mathbf{k}} a^\dagger_\sigma(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{5.4}$$

Using Eq. (5.2), one can easily shown that $a_\sigma(\mathbf{k})$ and $a^\dagger_\sigma(\mathbf{k})$ satisfy the anticommutation relations

$$\begin{aligned} &\{a_\sigma(\mathbf{k}), a^\dagger_{\sigma'}(\mathbf{k}')\} = \delta_{\sigma'\sigma}\, \delta(\mathbf{k}' - \mathbf{k}), \\ &\{a^\dagger_\sigma(\mathbf{k}), a^\dagger_{\sigma'}(\mathbf{k}')\} = 0, \qquad \{a_\sigma(\mathbf{x}), a_{\sigma'}(\mathbf{k}')\} = 0. \end{aligned} \tag{5.5}$$

Replacing Eqs. (5.4) in the Hamiltonian, one obtains

$$\widehat{H} = \sum_\sigma \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2m}\, \hat{n}_\sigma(\mathbf{k}), \tag{5.6}$$

where

$$\hat{n}_\sigma(\mathbf{k}) = a^\dagger_\sigma(\mathbf{k})\, a_\sigma(\mathbf{k}). \tag{5.7}$$

The number operator $\widehat{N}$,

$$\widehat{N} = \sum_\sigma \int d^3\mathbf{x}\, \psi^\dagger_\sigma(\mathbf{x})\, \psi_\sigma(\mathbf{x}), \tag{5.8}$$

in momentum space is given by

$$\widehat{N} = \sum_\sigma \sum_{\mathbf{k}} \hat{n}_\sigma(\mathbf{k}). \tag{5.9}$$

Given $\widehat{H}$ and $\widehat{N}$, the operator $\widehat{\Omega}$ in momentum space can be written as

$$\widehat{\Omega} = \sum_\sigma \widehat{\Omega}_\sigma = \sum_{\mathbf{k}} \widehat{\Omega}_\sigma(\mathbf{k}) = \sum_\sigma \sum_{\mathbf{k}} \Omega_\sigma(\mathbf{k})\, \hat{n}_\sigma(\mathbf{k}), \tag{5.10}$$

where, for later convenience, we have defined the quantities

$$\widehat{\Omega}_\sigma = \sum_{\mathbf{k}} \widehat{\Omega}_\sigma(\mathbf{k}), \quad \widehat{\Omega}_\sigma(\mathbf{k}) = \Omega_\sigma(\mathbf{k})\, \hat{n}_\sigma(\mathbf{k}), \quad \Omega_\sigma(\mathbf{k}) = \frac{\mathbf{k^2}}{2m} - \mu_\sigma. \tag{5.11}$$

The dependence on σ in μ_σ allows the possibility for different numbers of particles with spin $\uparrow$ and $\downarrow$ in the system. The grand canonical partition function is given by

$$Z \;=\; \mathrm{Tr}\; e^{-\beta\widehat{\Omega}} = \mathrm{Tr}\; e^{-\beta\sum_\sigma \widehat{\Omega}_\sigma} = \mathrm{Tr}\; e^{-\beta(\widehat{\Omega}_\uparrow + \widehat{\Omega}_\downarrow)}. \tag{5.12}$$

Since $[\widehat{\Omega}_\uparrow, \widehat{\Omega}_\downarrow] = 0$, the partition function is given by the product

$$Z = \mathrm{Tr}_\uparrow(e^{-\beta\widehat{\Omega}_\uparrow})\, \mathrm{Tr}_\downarrow(e^{-\beta\widehat{\Omega}_\downarrow}). \tag{5.13}$$

This can be easily shown using as basis the eigenstates $\{|n_\sigma(\mathbf{k})\rangle\}$ of the operator $\hat{n}_\sigma(\mathbf{k})$

$$\hat{n}_\sigma(\mathbf{k})|n_\sigma(\mathbf{k})\rangle = n_\sigma(\mathbf{k})|n_\sigma(\mathbf{k})\rangle, \quad \text{with} \quad n_\sigma(\mathbf{k}) = 0, 1. \tag{5.14}$$

Moreover, using this same basis, one can also show that

$$\mathrm{Tr}_\uparrow\; e^{-\beta\widehat{\Omega}_\uparrow} = \mathrm{Tr}_\uparrow e^{-\beta\sum_{\mathbf{k}} \Omega_\uparrow(\mathbf{k})\widehat{n}_\uparrow(\mathbf{k})} = \prod_{\mathbf{k}} \mathrm{Tr}_\uparrow \left[e^{-\beta\Omega_\uparrow(\mathbf{k})\widehat{n}_\uparrow(\mathbf{k})}\right], \tag{5.15}$$

and a similar expression for $\mathrm{Tr}_\downarrow\; e^{-\beta\widehat{\Omega}_\downarrow}$.

One can calculate the traces above directly using the basis of Eq. (5.14) as

$$\mathrm{Tr}_\uparrow\; e^{-\beta\widehat{\Omega}_\uparrow} = \prod_{\mathbf{k}} \mathrm{Tr}_\uparrow \left[e^{-\beta\Omega_\uparrow(\mathbf{k})\widehat{n}_\uparrow(\mathbf{k})}\right] = \prod_{\mathbf{k}} e^{-\beta\Omega_\uparrow(\mathbf{k})n_\uparrow(\mathbf{k})}, \tag{5.16}$$

and so, because $n_\uparrow(\mathbf{k}) = 0, 1$ and $n_\downarrow(\mathbf{k}) = 0, 1$, we obtain

$$\begin{aligned} Z \;&=\; \left(\prod_{\mathbf{k}_1} e^{-\beta\,\Omega_\uparrow(\mathbf{k}_1)n_\uparrow(\mathbf{k})}\right)\left(\prod_{\mathbf{k}_2} e^{-\beta\,\Omega_\downarrow(\mathbf{k}_2)n_\downarrow(\mathbf{k})}\right) \\ &=\; \prod_{\mathbf{k}_1}\left(1 + e^{-\beta\,\Omega_\uparrow(\mathbf{k}_1)}\right)\prod_{\mathbf{k}_2}\left(1 + e^{-\beta\,\Omega_\downarrow(\mathbf{k}_2)}\right). \end{aligned} \tag{5.17}$$

This is the final result for the grand-canonical partition function for a polarized (i.e. different number of particles with spin $\uparrow$ and $\downarrow$) noninteracting, nonrelativistic Fermi gas. When $\mu_\uparrow = \mu_\downarrow = \mu$, we have have $\Omega_\uparrow(\mathbf{k}) = \Omega_\downarrow(\mathbf{k}) = \mathbf{k}^2/2m - \mu$ and obtain the well-known result for the partition function of a free Fermi gas

$$Z = \left\{\prod_{\mathbf{k}}\left[1 + e^{-\beta\,(\mathbf{k}^2/2m - \mu)}\right]\right\}^2. \tag{5.18}$$

Next, we reobtain the above results using the Niterói method. We start from the general result of Eq. (Z-prod-k) and expand the exponential in powers of β

$$\begin{aligned}
\mathrm{Tr}_\uparrow\, e^{-\beta\widehat{\Omega}_\uparrow} &= \prod_{\mathbf{k}} \mathrm{Tr}_\uparrow \left[e^{-\beta\Omega_\uparrow(\mathbf{k})\widehat{n}_\uparrow(\mathbf{k})}\right] = \prod_{\mathbf{k}} \mathrm{Tr}_\uparrow \sum_{s=0}^{\infty} \frac{[-\beta\Omega_\uparrow(\mathbf{k})]^s}{s!}\, [\widehat{n}_\uparrow(\mathbf{k})]^s \\
&= \prod_{\mathbf{k}} \sum_{s=0}^{\infty} \frac{[-\beta\Omega_\uparrow(\mathbf{k})]^s}{s!}\, \mathrm{Tr}_\uparrow\, [\widehat{n}_\uparrow(\mathbf{k})]^s \\
&= \prod_{\mathbf{k}} \left\{ \mathrm{Tr}_\uparrow(1) + \sum_{s=1}^{\infty} \frac{[-\beta\Omega_\uparrow(\mathbf{k})]^s}{s!}\, \mathrm{Tr}_\uparrow\, [\widehat{n}_\uparrow(\mathbf{k})]^s \right\}. \qquad (5.19)
\end{aligned}$$

The trace of 1 is simply

$$\mathrm{Tr}_\uparrow(1) = \int d\eta d\eta^* \exp\left(2\eta^*\eta\right) = 2. \qquad (5.20)$$

The trace of $[\widehat{n}_\uparrow(\mathbf{k})]^s$ is to be calculated using Eq. (5.21). We note that since the trace is calculated for $\mathbf{k}$ held fixed, we can simply ignore $\mathbf{k}$ in the Grassmann numbers when applying Eq. (5.21). Specifically,

$$\begin{aligned}
\mathrm{Tr}\, [\widehat{n}_\uparrow]^s &= \int \prod_{I=1}^{s} d\eta_I d\eta_I^* \exp\left(\sum_{J=1}^{s}\sum_{K=1}^{s} \eta_J^*\, A_{JK}^{\uparrow\uparrow}\, \eta_K\right) n_\uparrow^{\odot}(\eta_1^*,\eta_1)\, \cdots\, n_\uparrow^{\odot}(\eta_s^*,\eta_s) \\
&= \int \prod_{I=1}^{s} d\eta_I d\eta_I^* \exp\left(\sum_{J=1}^{s}\sum_{K=1}^{s} \eta_J^*\, A_{JK}^{\uparrow\uparrow}\, \eta_K\right) \eta_1^*\,\eta_1\, \cdots\, \eta_s^*\,\eta_s, \qquad (5.21)
\end{aligned}$$

where we have used the fact that $n_\uparrow^{\odot}(\eta^*,\eta) = \eta^*\,\eta$. The value of the integral is given by Eq. (5.22), that for the present case is given by

$$M(,K) = (-1)^{1+\cdots+s}(-1)^{1+\cdots+1}\, A(L,K). \qquad (5.22)$$

Removing the first s lines and s first columns from the matrix $A^{\uparrow\uparrow}$, one obtains that the determinant of the remaining matrix is simply 1, and so

$$\begin{aligned}
Tr_\uparrow\, e^{-\beta\widehat{\Omega}_\uparrow(\mathbf{k})} &= 2 + \sum_{s=1}^{\infty} \frac{[-\beta\Omega_\uparrow(\mathbf{k})]^s}{s!} \\
&= 1 + e^{-\beta\,\Omega_\uparrow(\mathbf{k})}. \qquad (5.23)
\end{aligned}$$

Therefore, one obtains precisely the same value for the partition function as calculated directly.

Note that for a quadratic $\widehat{\Omega}$ one can obtain the trace of $e^{-\beta\Omega}$ directly from

$$\mathrm{Tr}\,\widehat{O} = \int d\xi d\xi^*\, e^{2\xi^*\xi}\, O^{\odot}(\xi^*,\xi). \qquad (5.24)$$

This will be clear in the discussions of the next Section.

5.2 Interacting nonrelativistic Fermions, canonical transformations

In this Section we will discuss the application of the Niterói method to an interacting many-fermion system. However, our aim here is not to use the high temperature expansion for the entire interacting Hamiltonian. Rather, our aim is to use the method in conjunction with some nonperturbative approximation schemes. In particular, here we will use canonical transformations to obtain the traditional mean-field approximations and to improve on such mean-field approximations within the Niterói method. We remark that we *are not* going to obtain new results, rather we will show how to obtain known results within the Niterói method and indicate future directions for obtaining new results. The point of showing this is that in some circumstances when dealing with many-fermion systems, e.g. in a lattice formulation of relativistic field theory, as commented earlier, the traditional Monte Carlo method cannot be applied because of the Euclidean action is not real and positive. Therefore, having an approximation scheme that does not suffer from such a problem is welcomed.

Initially we will start reobtaining the traditional finite-temperature Bardeen-Cooper-Schrieffer (BCS) gap equation [35] for a many-fermion system. This will be obtained employing a Bogoliubov-Valatin canonical transformation [36]. The quadratic part of the resulting Hamiltonian can then be diagonalized and used to obtain the grand canonical partition function. Certainly there is nothing new here, however, this provides a stating point for us to discuss possible ways on how to improve on this in the context of the Niterói method. Notation and the Bogoliubov-Valatin transformation we are going to use here is heavily based on Section 37 of the book of Fetter and Walecka [2].

When considering interactions, the most general, nonrelativistic Hamiltonian for a system of fermions interacting through a local two-body potential $\widehat{V}$ can be written in terms of the field operators $\psi_\sigma(\mathbf{x})$ and $\psi^\dagger_\sigma(\mathbf{x})$ as

$$\begin{aligned}
\widehat{H} &= \widehat{H}_0 + V \\
&= \sum_\sigma \int d^3\mathbf{x}\, \psi^\dagger_\sigma(\mathbf{x}) \left(-\frac{1}{2m}\boldsymbol{\nabla}^2_x\right) \psi_\sigma(\mathbf{x}) \\
&+ \frac{1}{2}\int d^3\mathbf{x} d^3\mathbf{y}\, \psi^\dagger_{\sigma_1}(\mathbf{x})\psi^\dagger_{\sigma_2}(\mathbf{y})\, V_{\sigma_1\sigma_2,\sigma_3\sigma_4}(\mathbf{x}-\mathbf{y})\, \psi_{\sigma_4}(\mathbf{y})\psi_{\sigma_3}(\mathbf{x}), \qquad (5.25)
\end{aligned}$$

where $V_{\sigma_1\sigma_2,\sigma_3,\sigma_4}(\mathbf{x}-\mathbf{y}) = V_{\sigma_3\sigma_4,\sigma_1\sigma_2}(\mathbf{y}-\mathbf{x})$ for identical particles. For the purposes of simplifying the notation and explaining the main ideas, we will take an interaction of the form [38]

$$V_{\sigma_1\sigma_2,\sigma_3\sigma_4}(\mathbf{x}-\mathbf{y}) = \delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4}\,\delta_{\sigma_1\uparrow}\,\delta_{\sigma_2\downarrow}\,V(\mathbf{x}-\mathbf{y}). \qquad (5.26)$$

As in the noninteracting case, we perform a Fourier transformation and obtain for the grand canonical operator $\widehat{\Omega}$ the following expression

$$\begin{aligned}\widehat{\Omega} &= \sum_{\sigma}\sum_{\mathbf{k}}\left(\frac{\mathbf{k}^2}{2m}-\mu_\sigma\right)\hat{n}_\sigma(\mathbf{k}) \\ &+ \frac{1}{2}\sum_{\sigma_1\sigma_2}\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}\langle\mathbf{k}_1\mathbf{k}_2|V|\mathbf{k}_3\mathbf{k}_4\rangle\, a^\dagger_\uparrow(\mathbf{k}_1)\, a^\dagger_\downarrow(\mathbf{k}_2)\, a_\downarrow(\mathbf{k}_2)\, a_\uparrow(\mathbf{k}'), \qquad (5.27)\end{aligned}$$

where

$$\langle\mathbf{k}_1\mathbf{k}_2|V|\mathbf{k}_3\mathbf{k}_4\rangle = \frac{1}{V^2}\int d^3\mathbf{x}d^3\mathbf{y}\, e^{-i(\mathbf{k}_1\cdot\mathbf{x}+\mathbf{k}_2\cdot\mathbf{y})}V(\mathbf{x}-\mathbf{y})\, e^{-i(\mathbf{k}_3\cdot\mathbf{x}+\mathbf{k}_4\cdot\mathbf{y})}. \qquad (5.28)$$

Next, we make a canonical transformation on this Hamiltonian by introducing new creation and annihilation operators as [2] [37]

$$\begin{aligned}b_1(\mathbf{k}) &= u(k)\, a_\uparrow(\mathbf{k}) - v(k)\, a^\dagger_\downarrow(-\mathbf{k}), \\ b_2(\mathbf{k}) &= u(k)\, a_\downarrow(-\mathbf{k}) + v(k)\, a^\dagger_\downarrow(\mathbf{k}), \qquad (5.29)\end{aligned}$$

where $u(k)$ and $v(k)$ are c-number functions to be determined, such that

$$\begin{aligned}\{b_1(\mathbf{k}), b_1^\dagger(\mathbf{k}')\} &= \delta(\mathbf{k}'-\mathbf{k}), \\ \{b_2(\mathbf{k}), b_2^\dagger(\mathbf{k}')\} &= \delta(\mathbf{k}'-\mathbf{k}), \qquad (5.30)\end{aligned}$$

and all other anticommutators are zero. This leads to the condition that

$$u^2(k)+v^2(k)=1. \qquad (5.31)$$

This condition is not sufficient to determine u and v and more input is needed. This will be provided by the imposition that part of the resulting Hamiltonian should be diagonal, which results in addition into a *gap equation*.

The canonical transformation proceeds in replacing the original operators $a_\sigma(\mathbf{k})$ and $a^\dagger_\sigma(\mathbf{k})$ in favor of the $b_1(\mathbf{k})$, $b_1^\dagger(\mathbf{k})$, b_2 and $b_2^\dagger$ in the Hamiltonian, and then arranging them in normal ordering (i.e. putting the resulting Hamiltonian in simple order). The idea behind this procedure is that such a transformed Hamiltonian can be brought to a diagonal form, plus an interaction term that should be small. The meaning of small is in the sense that the main features of the original Hamiltonian are captured by the diagonal part of the new Hamiltonian. There are different ways to implement this and as mentioned by Fetter and Walecka [2] the easiest way is to use Wick's theorem. We will not review this here, simply quote the final result (we use $\mu_\uparrow = \mu_\downarrow$)

$$\begin{aligned}\widehat{\Omega} &= U + \sum_{\mathbf{k}} E(k)\,[b_1^\dagger(\mathbf{k})b_1(\mathbf{k}) + b_2^\dagger(\mathbf{k})b_2(\mathbf{k})] + :\widehat{V}(b): \\ &+ \sum_{\mathbf{k}} F(k)\,[b_2^\dagger(\mathbf{k})b_2^\dagger(\mathbf{k}) + b_1(\mathbf{k})b_2(\mathbf{k})], \qquad (5.32)\end{aligned}$$

where U is a constant (not relevant for our purposes here), and

$$E(k) = [u^2(k) - v^2(k)]\varepsilon(k) + 2u(k)v(k)\Delta(k), \tag{5.33}$$

$$F(k) = 2u(k)v(k)\varepsilon(k) - [u^2(k) - v^2(k)]\Delta(k), \tag{5.34}$$

with

$$\varepsilon(k) = \frac{\mathbf{k}^2}{2m} - \mu + \sum_{\mathbf{k}\mathbf{k}'} \langle \mathbf{k}\mathbf{k}'|\bar{V}|\mathbf{k}\mathbf{k}'\rangle v^2(k') \left[1 - 2f(\mathbf{k}')\right],$$

$$\Delta(k) = -\frac{1}{2}\sum_{\mathbf{k}'} \langle \mathbf{k} - \mathbf{k}|V|\mathbf{k}' - \mathbf{k}'\rangle \, u(k')v(k') \, \left[1 - 2f(\mathbf{k}')\right], \tag{5.35}$$

where $\langle \mathbf{k}\mathbf{k}'|\bar{V}|\mathbf{k}\mathbf{k}'\rangle = \langle \mathbf{k}\mathbf{k}'|V|\mathbf{k}\mathbf{k}'\rangle - \langle \mathbf{k}\mathbf{k}'|V|\mathbf{k}'\mathbf{k}\rangle + \langle \mathbf{k}-\mathbf{k}'|V|\mathbf{k}-\mathbf{k}'\rangle$ gives the Hartree-Fock mean field contribution to the energy, and $f(k)$ is the thermal average of $b^\dagger b$,

$$f(k) = \langle b_i^\dagger(\mathbf{k}) b_i(\mathbf{k})\rangle = \mathrm{Tr}\, \left[b_i^\dagger(\mathbf{k}) b_i(\mathbf{k})\, e^{-\beta\widehat{\Omega}}\right], \qquad i = 1, 2. \tag{5.36}$$

In addition, $:\widehat{V}(b):$ is obtained from the original $\widehat{V}$ in Eq. (5.25) by replacing the $a_\sigma^\dagger$ and a_σ with

$$a_\uparrow^\dagger(\mathbf{k}) = u(k)\, b_1(\mathbf{k}) + v(k)\, b_2^\dagger(-\mathbf{k}),$$

$$a_\downarrow(\mathbf{k}) = u(k)\, b_2(\mathbf{k}) - v(k)\, b_1^\dagger(-\mathbf{k}), \tag{5.37}$$

and then normal ordering the resulting expression.

The idea now is to diagonalize $\widehat{\Omega}$, neglecting $:\widehat{V}(b):$ on the assumption that the main effect of the interaction has been captured by the diagonal part, as discussed above. This is achieved by demanding that the *anomalous Bogoliubov term* be equal to zero, i.e.

$$F(k) = 0 \rightarrow [u^2(k) - v^2(k)]\, \Delta(k) = 2u(k)v(k)\varepsilon(k). \tag{5.38}$$

Note that this equation has to be solved under the constraint of Eq. (5.31). As shown explicitly in Fetter and Walecka [2], this leads to

$$E(k) = \left[\varepsilon^2(k) + \Delta^2(k)\right]^{1/2}, \tag{5.39}$$

$$u(k)v(k) = \frac{\Delta(k)}{2E(k)}, \quad u^2(k) = \frac{1}{2}\left[1 + \frac{\varepsilon(k)}{E(k)}\right],$$

$$v^2(k) = \frac{1}{2}\left[1 - \frac{\varepsilon(k)}{E(k)}\right], \tag{5.40}$$

and $\Delta(k)$ satisfies the gap equation

$$\Delta(k) = -\frac{1}{2}\sum_{\mathbf{k}'} \langle \mathbf{k} - \mathbf{k}'|V|\mathbf{k}' - \mathbf{k}'\rangle \frac{\Delta(k')}{E(k')} \left[1 - 2f(k')\right]. \tag{5.41}$$

All thermodynamic properties of the system can then be obtained from the partition function calculated with the quadratic grand potential operator $\widehat{\Omega}$, which can be calculated analytically, given by

$$Z = \left[\prod_{\mathbf{k}} \left(1 + e^{-\beta E(k)}\right)\right]^2 . \tag{5.42}$$

Eq. (5.41) always admits a trivial solution, i.e. $\Delta(k) = 0$. In this case one would have then the familiar Hartree-Fock approximation, which still requires a self-consistent solution, since the thermal average $f(k)$ appears in in $\varepsilon(k)$, see Eq. (5.35).

The central question now is how to include the effects of the neglected term, $:\widehat{V}(b):$, the normal ordered potential. Of course, in case these effects are small, but not entirely negligible, perturbation theory would be the natural approach ro pursue. In the next section we discuss this issue.

5.3 Perturbation on the mean field

Let us start reobtaining the traditional perturbative improvement on the mean field result. We rewrite the $\widehat{\Omega}$ of Eq. (5.32) (without the irrelevant constant U and with the anomalous Bogoliubov term already made zero) as

$$\widehat{\Omega} = \widehat{\Omega}_0 + \delta \ :\widehat{V}:, \tag{5.43}$$

where

$$\widehat{\Omega}_0 = \sum_{\mathbf{k}} E(k) \left[b_1^\dagger(\mathbf{k}) b_1(\mathbf{k}) + b_2^\dagger(\mathbf{k}) b_2(\mathbf{k})\right], \tag{5.44}$$

and where $:\widehat{V}:$ contains all possible normal ordered products of two creation operators $b_1^\dagger$ and $b_2^\dagger$, and two annihilation operators b_1 and b_2 . The parameter δ is just for bookkeeping purposes, it will be taken $\delta = 1$ at the end. The partition function is then

$$Z = \mathrm{Tr}\, e^{-\beta(\widehat{\Omega}_0 + \delta :\widehat{V}:)}. \tag{5.45}$$

The idea is to expand the exponent in powers of δ. Since $\widehat{\Omega}_0$ and $:\widehat{V}:$ do not commute, the expansion is not straightforward. However, it is well known how such an expansion can be made, by going to the "interaction representation, as explained in Refs. [1][2]. Specifically, the expansion is (see Section 24 of Fetter and Walecka, Ref. [2])

$$Z \ = \ \mathrm{Tr}\, e^{-\beta(\widehat{\Omega}_0 + \delta :\widehat{V}:)}$$

$$
\begin{aligned}
&= \mathrm{Tr}\, e^{-\beta\widehat{\Omega}_0}\left[1+\sum_{n=1}^{\infty}\frac{(-\beta\delta)^n}{n!}\int_0^{\beta}d\lambda_1\int_0^{\lambda_1}d\lambda_2\cdots\int_0^{\lambda_{n-1}}d\lambda_n\right.\\
&\times\ \left.\widehat{V}(\lambda_1)\,\widehat{V}(\lambda_2)\cdots\widehat{V}(\lambda_n)\right]\\
&= \mathrm{Tr}\left[1+\sum_{n=1}^{\infty}\frac{(-\beta\delta)^n}{n!}\int_0^{\beta}d\lambda_1\int_0^{\lambda_1}d\lambda_2\cdots\int_0^{\lambda_{n-1}}d\lambda_n\right.\\
&\times\ \left.\widehat{V}(\lambda_1)\,\widehat{V}(\lambda_2)\cdots\widehat{V}(\lambda_n)\right]e^{-\beta\widehat{\Omega}_0}\\
&\equiv \mathrm{Tr}\, P_\lambda\, e^{-\beta\delta\widehat{V}(\lambda)}\,e^{-\beta\widehat{\Omega}_0} = \mathrm{Tr}\,\widehat{\mathcal{V}}\,e^{-\beta\widehat{\Omega}_0},
\end{aligned}
\tag{5.46}
$$

where P_λ denotes *path ordering in* λ, the ordered chain of integrals in $\lambda_1,\cdots,\lambda_n$, and

$$
\widehat{V}(\lambda) = e^{\lambda\widehat{\Omega}_0}\ :\widehat{V}:\ e^{-\lambda\widehat{\Omega}_0}. \tag{5.47}
$$

We want to use the coherent-state representation of the trace. First, let us simplify notation writing

$$
\widehat{\Omega}_0 = \sum_{\mathbf{k}} E(k)\,[b_1^\dagger(\mathbf{k})b_1(\mathbf{k}) + b_2^\dagger(\mathbf{k})b_2(\mathbf{k})] \equiv \sum_i E_i\, b_i^\dagger b_i, \tag{5.48}
$$

where we have condensed the indices $\mathbf{k}$ and 1 and 2 into i. Next, we use Eq. (4.9) to write the trace of the product of the two operators $\widehat{\mathcal{V}}$ and $\widehat{U}\equiv e^{-\beta\widehat{\Omega}_0}$ as

$$
\begin{aligned}
\mathrm{Tr}\,(\widehat{\mathcal{V}}\,e^{-\beta\widehat{\Omega}_0}) &= \int d\xi d\xi^* d\xi' d\xi'^*\, e^{\xi^*(\xi+\xi')}\, e^{\xi'^*(\xi'-\xi)}\,\mathcal{V}^{\odot}(\xi^*,\xi)\,U^{\odot}(\xi',\xi')\\
&= \int d\xi d\xi^*\, e^{\xi^*\xi}\,\mathcal{V}^{\odot}(\xi^*,\xi)\\
&\times \int d\xi' d\xi'^*\, e^{\xi'^*(\xi'-\xi)+\xi^*\xi'}\,U^{\odot}(\xi'^*,\xi'),
\end{aligned}
\tag{5.49}
$$

where it should be clear here that $\xi,\xi',\cdots$ refer to sets $\{\xi_i,\xi_i',\cdots\}$, where the index i stands for $\mathbf{k}$ and 1 and 2, and products like $\xi'^*(\xi'-\xi)$ mean $\sum_i \xi'^*_i(\xi_i'-\xi_i)$. Let us add *source terms* into the first integral above as

$$
\begin{aligned}
\mathrm{Tr}\,(\widehat{\mathcal{V}}\,e^{-\beta\widehat{\Omega}_0}) &= \int d\xi d\xi^*\, e^{\xi^*\xi}\,\mathcal{V}^{\odot}(\xi^*,\xi)\, e^{\bar{J}\xi+\xi^*J}\\
&\times \int d\xi' d\xi'^*\, e^{\xi'^*(\xi'-\xi)+\xi^*\xi'}\,U^{\odot}(\xi'^*,\xi'),
\end{aligned}
\tag{5.50}
$$

where J_i and $\bar{J}_i$ are Grassmann numbers. Next, one uses the common trick of writing

$$\mathcal{V}^{\odot}(\xi^*,\xi)\, e^{(\bar{J}_i\xi_i+\xi_i^* J_i)} = \mathcal{V}^{\odot}\left(\frac{\delta}{\delta J_i},\frac{\delta}{\delta \bar{J}_i}\right) e^{(\bar{J}_i\xi_i+\xi_i^* J_i)}, \tag{5.51}$$

where $\delta/\delta J_i$ and $\delta/\delta\bar{J}_i$ are Grassmann functional derivatives – see Eq. (3.153). Then, the expression for the trace can be written as

$$\begin{aligned}\mathrm{Tr}\,(\widehat{\mathcal{V}}\, e^{-\beta\widehat{\Omega}_0}) &= \mathcal{V}^{\odot}\left(\frac{\delta}{\delta J_i},\frac{\delta}{\delta \bar{J}_i}\right)\int d\xi d\xi^*\, e^{\xi^*\xi}\, e^{\bar{J}_i\xi_i+\xi_i^* J_i} \\ &\times \int d\xi' d\xi'^*\, e^{\xi'^*(\xi'-\xi)+\xi^*\xi'}\, U^{\odot}(\xi'^*,\xi'). \end{aligned}\tag{5.52}$$

The remaining integrals can be integrated analytically. First, let us perform the integral over ξ' and ξ'^*. The ordered form of the operator $\widehat{U} = e^{-\beta\widehat{\Omega}_0}$ can be obtained as [34]

$$\begin{aligned} e^{-\beta\widehat{\Omega}_0} &= e^{-\beta\sum_i E_i b_i^\dagger b_i} = \prod_i e^{-\beta E_i b_i^\dagger b_i} \\ &= \prod_i \left[1+\left(e^{-\beta E_i}-1\right) b_i^\dagger b_i\right] = \prod_i :\, e^{(e^{-\beta E_i}-1) b_i^\dagger b_i}\, : \\ &= :\exp\left[\sum_i \left(e^{-\beta E_i}-1\right) b_i^\dagger b_i\right]:, \end{aligned}\tag{5.53}$$

and $U^{\odot}(\xi^*,\xi)$ is given by

$$U^{\odot}(\xi^*,\xi) = \exp\left[\sum_i \left(e^{-\beta E_i}-1\right)\xi_i^*\xi_i\right]. \tag{5.54}$$

Therefore, from Eq. (3.152), one has

$$\begin{aligned}\int d\xi' d\xi'^*\, e^{\xi'^*(\xi'-\xi)+\xi^*\xi'}\, U^{\odot}(\xi'^*,\xi') &= \int d\xi' d\xi'^*\, e^{\xi'^* D^{-1}\xi'+\xi^{*\prime}(-\xi)+\xi\xi^{*\prime}} \\ &= -\frac{1}{\mathrm{Det}\, D}\, e^{\xi^* D\xi}, \end{aligned}\tag{5.55}$$

where D is the diagonal matrix

$$D_{ij} = e^{\beta E_i}\,\delta_{ij}. \tag{5.56}$$

Inserting this result into the integral over ξ and ξ^* and performing the integral, one obtains

$$\begin{aligned} -\frac{1}{\mathrm{Det}\, D}\int d\xi d\xi^*\, e^{\xi^*\xi}\, e^{\bar{J}_i\xi_i+\xi_i^* J_i}\, e^{\xi^* D\xi} &= -\frac{1}{\mathrm{Det}\, D}\int d\xi d\xi^*\, e^{\xi^*(1+D)\xi+\bar{J}_i\xi_i+\xi_i^* J_i} \\ &= \frac{\mathrm{Det}\,(1+D)}{\mathrm{Det}\, D}\, e^{-\bar{J}\,(1+D)^{-1}J}. \end{aligned}\tag{5.57}$$

With this, we arrived at the well known result for the perturbative expansion of the partition function

$$\frac{Z}{Z_0} = \mathcal{V}^{\odot}\left(\frac{\delta}{\delta J_i}, \frac{\delta}{\delta \bar{J}_i}\right) e^{-\sum_{i,j} \bar{J}_i (1+D)^{-1}_{i,j} J_i}. \tag{5.58}$$

Plain perturbation theory would be simply to calculate physical quantities using the partition function in Eq. (5.58) with $D = e^{\beta E_i}$ where E_i the energy calculated as in the previous section. A better perturbation theory corresponds to recalculate the energy in a self-consistent way from the perturbed partition function, Eq. (5.58) – i.e. D is to be determined from the partition function defined in terms of the unknown D. Of course, in any practical sense, one would be able to do so by restricting the expansion in Eq. (5.46) to lowest orders in δ.

5.4 Optimized perturbation theory

At this point it should be clear that one does not need the Niterói method to do perturbation theory on a mean field approximation, since Eq. (5.58) is known from other techniques. But, having shown how to derive the traditional perturbative series, we will make use part of the material above to motivate a method that might be more useful for practical results. The method we propose makes interchangeable use of the path integral method and the direct calculation of the trace by the Niterói method.

The basic idea of optimized perturbation theory in one of its simplest forms – known as the optimized linear δ expansion – is the following [14]-[17]. Suppose the Hamiltonian of the system is of the generic form

$$\widehat{H} = \widehat{K} + \widehat{V} \tag{5.59}$$

where $\widehat{K}$ is quadratic in the field operators and $\widehat{V}$ contains more than two field operators. Then, one adds and subtracts a a term for the Hamiltonian in the form

$$\widehat{H} = \left(\widehat{K} + \widehat{O}(p_1, p_2, \cdots)\right) + \delta\, \left(\widehat{V} - \widehat{O}(p_1, p_s, \cdots)\right), \tag{5.60}$$

where $\widehat{O}(p_1, p_2, \cdots)$ is given in terms of field operators, $p_1, p_2, \cdots$ are functions of the coordinates in general, and δ is a dimensionless parameter that is introduced for bookkeeping purposes and is to be taken equal to 1 at the end of calculation. The idea is to choose $\widehat{O}$ judiciously so that the theory with $\left(\widehat{K} + \widehat{O}\right)$ is exactly soluble, and corrections to this solution are calculated in perturbation theory in δ. If one would be able to calculate in all orders of δ, we of course would have obtained the exact solution and the result would be independent of $p_1, p_2, \cdots$. Since we are going

to truncate the expansion in some power of δ, the results do depend on $p_1, p_2, \cdots$. In order to minimize the sensitivity of the results on μ, we use the *principle of minimal sensitivity* (PMS) [14], in that one requires that a physical quantity $Q(p_1, p_2, \cdots)$ satisfy

$$\frac{\delta Q(p_1, p_s, \cdots)}{\delta p_i} = 0. \tag{5.61}$$

This physical quantity can be the grand canonical potential,

$$e^{-\beta\,\Xi} = Z \rightarrow \Xi = -\beta^{-1}\,\ln Z. \tag{5.62}$$

In order to explain the approach we propose in the perspective of the Fermi gases in the unitarity limit discussed in the Introduction, we use for $\widehat{\Omega}$ the following expression [38]

$$\widehat{\Omega} = \sum_{\sigma} \int d^3\mathbf{x}\, \psi^{\dagger}_{\sigma}(\mathbf{x})\, K(\mathbf{x})\, \psi_{\sigma}(\mathbf{x}) - g \int d^3\mathbf{x}\, \psi^{\dagger}_{\uparrow}(\mathbf{x}) \psi^{\dagger}_{\downarrow}(\mathbf{x})\, \psi_{\downarrow}(\mathbf{x}) \psi_{\uparrow}(\mathbf{x}), \tag{5.63}$$

where

$$K_{\sigma}(\mathbf{x}) = -\frac{1}{2m}\boldsymbol{\nabla}^2_x - \mu_{\sigma}, \tag{5.64}$$

and g is the coupling strength – the minus sign is used for later convenience. The idea behind of the Hubbard-Stratonovich is to "linearize" the interaction term through the introduction of auxiliary fields. This is done making use of the identity

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\phi\, e^{-\phi^2/2 - a\,\phi} = e^{a^2/2}. \tag{5.65}$$

In the present case, a would stand for the pairs of field operators $\psi^{\dagger}_{\uparrow}(x)\psi_{\uparrow}(x)$, $\psi^{\dagger}_{\downarrow}(x)\psi_{\downarrow}(x)$, $\psi^{\dagger}_{\uparrow}(x)\psi^{\dagger}_{\downarrow}(x)$ and $\psi_{\uparrow}(x)\psi_{\downarrow}(x)$. For each of these pairings, one would introduce one auxiliary field $\phi(x)$. There is, however, one slight complication because we cannot use directly the formula of Eq. (5.65) with the $\widehat{\Omega}$ given in Eq. (5.63), because the kinetic and the interaction terms of this operator do not commute. One way to proceed is to change to the interaction representation as done in Section 5.3 that effectively factorizes the exponential into two exponentials in which one of them is path ordered. For our purposes here however, for clarity of presentation the easiest way to proceed is like Hubbard proceeded in Ref. [8], namely he used the ordering label technique of Feynman [39]. This is simply a simplification on the notation, the final result is not different from the traditional path-ordering used above – in Appendix F we have reviewed this technique. To further simplify the discussion and for better exposition, we will perform the Hubbard-Stratonovich transformation using only the "diagonal" pairings, i.e. we will linearize the interaction using only the $\psi^{\dagger}_{\uparrow}(x)\psi_{\uparrow}(x)$ and $\psi^{\dagger}_{\downarrow}(x)\psi_{\downarrow}(x)$ pairs. In addition, we will take $\mu_{\uparrow} = \mu_{\downarrow} = \mu$. This will

simplify our discussion because we will need only one auxiliary field. In this case, the partition function can be written as

$$\begin{aligned} Z &= \mathrm{Tr}\, e^{-\beta\widehat{\Omega}} \\ &= \mathrm{Tr}\, \exp\int_0^\beta ds \left[\sum_\sigma \int d\mathbf{x}\, \psi^\dagger_\sigma(\mathbf{x},s)\, K(\mathbf{x},s)\, \psi_\sigma(\mathbf{x},s)\right. \\ &- \left. g\int d\mathbf{x}\, \psi^\dagger_\uparrow(\mathbf{x},s)\psi_\uparrow(\mathbf{x},s)\psi^\dagger_\downarrow(\mathbf{x},s)\psi_\downarrow(\mathbf{x},s)\right], \end{aligned} \tag{5.66}$$

where now the kinetic and potential terms in the exponential can be taken as commuting – the integral over s is due to Feynman ordering technique, see Appendix F. Now we introduce an auxiliary field φ through the Hubbard-Stratonovich transformation as

$$\begin{aligned} Z &= \int [\mathcal{D}\varphi(\mathbf{x},s)]\, \exp\left[-\frac{1}{2}\int_0^\beta \int d\mathbf{x}\, \varphi^2(\mathbf{x},s)\right] \\ &\times \mathrm{Tr}\, \exp\int_0^\beta ds \int d\mathbf{x} \left\{\sum_\sigma \psi^\dagger_\sigma(\mathbf{x},s)\, K(\mathbf{x},s)\, \psi_\sigma(\mathbf{x},s)\right. \\ &+ \left. g^{1/2}\, \varphi(\mathbf{x},s)\left[\psi^\dagger_\uparrow(\mathbf{x},s)\psi_\uparrow(\mathbf{x},s) + \psi^\dagger_\downarrow(\mathbf{x},s)\psi_\downarrow(\mathbf{x},s)\right]\right\}. \end{aligned} \tag{5.67}$$

At this point, since the exponential in the trace is diagonal in the Fermi fields, the trace can be evaluated exactly. The result of the trace would be the square of the determinant of the matrix $K + g^{1/2}\varphi$ and what remains is an integral over the auxiliary field φ. Had we used $\mu_\uparrow \neq \mu_\downarrow$, one would have obtained the product of two determinants. It is here where the sign problem enters, since it is not guaranteed that the product of the determinants is positive. Our aim is not to proceed this route, we want to implement a mean field approximation and to use optimized perturbation theory on the top of the mean field, as explained in the Introduction. Why one would give up the possibility of obtaining an exact result in favor of an approximate scheme? First, as said previously, it is important to understand how corrections affect the zeroth-order mean field results. Second, the exact solution can be very involved due to the sign problem and also requires intensive use of Monte Carlo methods. It is hoped that through an expansion in a modified interaction one can capture most of the physics relevant to the problem and that a milder or even no sign problem arises – of course this we will only know with explicit calculations.

We implement the step indicated in Eq. (5.60) as follows. Let us define a c-number mean field $\varphi_0(\mathbf{x})$ so that

$$\begin{aligned} \psi^\dagger_\uparrow(\mathbf{x})\psi_\uparrow(\mathbf{x})\psi^\dagger_\downarrow(\mathbf{x})\psi_\downarrow(\mathbf{x}) &= -\varphi_0^2(\mathbf{x}) + \varphi_0(\mathbf{x})\, \psi^\dagger_\uparrow(\mathbf{x})\psi_\uparrow(\mathbf{x}) + \varphi_0(\mathbf{x})\, \psi^\dagger_\downarrow(\mathbf{x})\psi_\downarrow(\mathbf{x}) \\ &+ \Big[\psi^\dagger_\uparrow(\mathbf{x})\psi_\uparrow(\mathbf{x}) - \varphi_0(\mathbf{x})\Big]\Big[\psi^\dagger_\downarrow(\mathbf{x})\psi_\downarrow(\mathbf{x}) - \varphi_0(\mathbf{x})\Big]. \end{aligned} \tag{5.68}$$

Note that this is an identity. Now we replace this into the expression for Z in the following way, already using the Hubbard-Stratonovich transformation of the four-field term

$$\begin{aligned} Z(\varphi_0) &= e^{-\beta\, g \int d\mathbf{x}\, \varphi_0^2(\mathbf{x})} \int [\mathcal{D}\varphi(\mathbf{x},s)]\, e^{-\frac{1}{2}\int_0^\beta ds \int d\mathbf{x}\, \varphi^2(\mathbf{x},s)} \\ &\times \mathrm{Tr}\, e^{-\int_0^\beta ds \int d\mathbf{x}\, \mathcal{K}_0(\mathbf{x},s,\varphi_0)}\; e^{\delta \int_0^\beta ds \int d\mathbf{x}\, \mathcal{V}(\mathbf{x},s,\varphi_0)}, \end{aligned} \tag{5.69}$$

where

$$\mathcal{K}_0(\mathbf{x},s,\varphi_0) = \sum_\sigma \psi_\sigma^\dagger(\mathbf{x},s)\; [K(\mathbf{x},s) - g\,\varphi_0(\mathbf{x})]\; \psi_\sigma(\mathbf{x},s), \tag{5.70}$$

and

$$\begin{aligned} \mathcal{V}(\mathbf{x},s,\varphi_0) &= g^{1/2}\Big[\sigma(\mathbf{x},s) - g^{1/2}\,\varphi_0(\mathbf{x})\Big]\Big[\psi_\uparrow^\dagger(\mathbf{x},s)\psi_\uparrow(\mathbf{x},s) + \psi_\downarrow^\dagger(\mathbf{x},s)\psi_\downarrow(\mathbf{x},s)\Big] \\ &+ g\,\varphi_0^2(\mathbf{x}). \end{aligned} \tag{5.71}$$

Up to here, there have been no approximations and all expressions are exact. The implementation of the optimized perturbation theory proceeds in the following way. One expands the second exponential in the trace in Eq. (5.69) up some order of δ, perform the trace using the Niterói method, then perform the path integral over φ, and finally use the principle of minimal sensitivity to determine φ_0. Since both exponentials commute due to the Feynman ordering notation, and and since both exponentials are quadratic, the trace should be easily evaluated.

One could think that it would be easier to evaluate the complete trace and then expand the resulting determinant in powers of δ. Obviously this can be done in some cases, but the Niterói method is of general applicability and would not require the expansion of a complicated determinant.

Let us examine the $\mathcal{O}(\delta^0)$ approximation to the partition function. In this case, one would have simply

$$\begin{aligned} Z_0(\varphi_0) &\equiv e^{-\beta\, g \int d\mathbf{x}\, \varphi_0^2(\mathbf{x})} \int [\mathcal{D}\varphi(\mathbf{x},s)]\, e^{-\frac{1}{2}\int_0^\beta ds \int d\mathbf{x}\, \varphi^2(\mathbf{x},s)} \\ &\times \mathrm{Tr}\, e^{-\int_0^\beta ds \int d\mathbf{x}\, \mathcal{K}_0(\mathbf{x},s,\varphi_0)} \end{aligned} \tag{5.72}$$

Since the trace does not depend upon φ, the functional integral gives simply 1. Also, the Feynman ordering becomes is trivial, and one would get for $Z_0(\varphi_0)$

$$Z_0(\varphi_0) \equiv e^{-\beta\, g \int d\mathbf{x}\, \varphi_0^2(\mathbf{x})}\; \mathrm{Tr}\, e^{-\beta \int d\mathbf{x}\, \mathcal{K}(\mathbf{x},\varphi_0)} \tag{5.73}$$

The mean field φ_0 is determined from the grand canonical potential

$$\begin{aligned} \Xi(\phi_0) &= -\beta^{-1} \ln Z_0(\varphi_0) \\ &= g \int d\mathbf{x}\, \varphi_0^2(\mathbf{x}) - \beta^{-1} \ln \mathrm{Tr}\, e^{-\beta \int d\mathbf{x}\, \mathcal{K}(\mathbf{x},\varphi_0)}, \end{aligned} \tag{5.74}$$

from the PMS condition of Eq. (5.61)

$$\frac{\delta\,\Xi(\varphi_0)}{\delta\varphi_0(\mathbf{x})} = 0. \tag{5.75}$$

Applying this to the result in Eq. (5.74), one obtains

$$2\,g\,\varphi_0(\mathbf{x}) - \frac{\beta^{-1}}{Z_0(\phi_0)}\,\beta g\,\mathrm{Tr}\,e^{-\beta\int d\mathbf{x}\,\mathcal{K}(\mathbf{x},\varphi_0)}\,\sum_\sigma \psi^\dagger_\sigma(\mathbf{x})\psi^\dagger_\sigma(\mathbf{x}) = 0. \tag{5.76}$$

That is, the mean field is determined by the gap equation

$$\varphi_0(\mathbf{x}) = \langle\psi^\dagger_\uparrow(\mathbf{x})\psi_\uparrow(\mathbf{x})\rangle_{\varphi_0} = \langle\psi^\dagger_\downarrow(\mathbf{x})\psi_\downarrow(\mathbf{x})\rangle_{\varphi_0}. \tag{5.77}$$

This is a self-consistent equation for φ_0.

The result is reassuring, in that it is the traditional mean field (Hartree) result and it has been obtained in an elegant and relatively easy way. As explained, corrections to this mean field solution are obtained by expanding in powers of δ the complete partition function. We will not proceed to evaluate such corrections, since the aim here was to set up the approach and an explicit evaluation of high order corrections would require an specific model. In addition, for higher order corrections, the functional integral over φ and Feynman ordering are not trivial as for the $\mathcal{O}(\delta^0)$. The evaluation of the functional integral most likely will require a Monte Carlo method when working at high orders in δ – an interesting question is to see whether the sign problem is as severe as in the exact evaluation. Moreover, the point-like interaction used here requires renormalization and further elaboration is need to obtain numerical results. All this would extrapolate the scope of the present dissertation and therefore we leave these issues for future work.

We finalize this Chapter mentioning that pairings of the type $\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x)$ and $\psi_\uparrow(x)\psi_\downarrow(x)$ can be incorporated by introducing extra mean fields and extra Hubbard-Stratonivich auxiliary fields. Although straightforward, the algebra is a little heavier and more gap equations through the PMS condition would arise. Proceeding as above, the traditional BCS solution would follow form the $\mathcal{O}(\delta^0)$ result. Corrections would then be calculated in the same way as explained above.

Capítulo 6

Conclusions and perspectives

The primary aim of the present dissertation was to present a review on the use of coherent states in the evaluation of the quantum grand canonical partition function of spin-1/2 fermions at finite temperature. There main motivation for studying such systems is due to the recent experimental developments in the area of fermionic atoms. These developments have created great excitement in the Physics community in view of the possibility of exploring and manipulating matter composed of particles with no classical analogue. Contrary to bosons, fermions cannot be described in terms of the dynamical dynamical variables like position and momentum, they require new dynamical variables that are not familiar to the human experience, like Grassmann variables. In addition, fermionic systems at the unitarity limit – when the scattering length characterizing the interaction strength is much larger than the inter-particle spacing – are encountered in different fields of physics, like in nuclear physics, astro-particle physics and condensed matter physics. In view of this, this is a fascinating subject and it is important to develop mathematical methods to study such systems in different contexts.

The fundamental quantity in the mathematical treatment of many-body systems at finite temperature is the grand canonical partition function. It can very seldom be calculated in closed form and approximation schemes and numerical methods have been developed to study this quantity. In particular, there is great activity in the field of Monte Carlo simulations of the path integral representation of the partition function. Path integral formulations of fermion fields involve the use of anti-commuting Grassmann variables but tricks need to be employed for their numerical evaluation, since Grassmann numbers cannot be generated directly in a computer. Problems arise in implementing many of such tricks, like the sign problem, which arises when one formally integrates over such variables and re-express the result in terms of path integrals over auxiliary fields.

In the present dissertation we have concentrated on an alternative to the path

integral formulation of the grand canonical partition function, namely the Niterói Method. This method is based on the direct evaluation of the trace over Grassmann variables using a high temperature expansion of the Boltzmann factor in the partition function. The method makes use of the coherent-state representation of the trace, and each term of the expansion is evaluated exactly exploiting the anti-commuting nature of the Grassmann numbers. A good part of the present dissertation has concentrated on the review of this novel method, the main results are collected in Chapter 4. This was done after a brief discussion on the second quantization formalism for many-particle systems and the Feynman path integral in Chapter 2, and a short review in Chapter 3 on the use of coherent states for calculating traces over fermionic variables and have also discussed the path integral representation of the partition function using coherent states.

In addition to reviewing the Niterói method, we indicated further developments beyond the high temperature expansion of the Boltzmann factor. In particular we make the case for using the method in the context of improving mean field type of approximations through the combined use of the Hubbard-Stratonovich transformation and the ideas of optimized perturbation theory. Our approach starts from a mean field type of approximation and then corrections are implemented making use of an expansion in powers of a modified interaction, where the effects of the mean field have been subtracted from the original interaction. In Chapter 5, initially we have shown that known mean field type of approximations can be obtained trivially within the Niteói method, and have also shown that one can reproduce standard formulas for perturbative corrections to the mean field approximations within the same method. Since perturbative corrections to mean field approximations become very involved when higher order corrections are needed, we have proposed an alternative so that high order corrections can be calculated in the context of an optimized perturbation theory, in that terms are added and subtracted from the original Hamiltonian and re-arranged in way that a remaining interaction can be expanded perturbatively. The results are optimized in the sense that parameters introduced via the new terms in the Hamiltonian are fixed through a principle of minimal sensitivity, i.e. they are fixed by requiring that the grand canonical potential is stationary with respect to variations in these parameters.

As perspectives, we envisage application of the proposed method in different fields. One immediate application is in the field of atomic fermionic gases, in which a contemporary goal is to go beyond the framework of mean field physics to access manifestations of strong interactions and correlations. Work in this direction has been started. We also believe that our proposed method can be extended to strong coupling lattice QCD. The strong coupling expansion of the QCD action resembles

in many respects the high temperature expansion and as such the Niterói method should be of direct applicability. Work in this direction is underway.

Apêndice A

Two-body operators - Change of representation

Let a two body operator, see (2.37), such that every $\widehat{O}_{ij}$ is diagonal in the basis $\{|\alpha_{k_1}\cdots\alpha_{k_N})\}$

$$\widehat{O}_{ij}|\alpha_{k_1}\cdots\alpha_{k_N}) = O_{k_ik_j}|\alpha_{k_1}\cdots\alpha_{k_N}), \tag{A.1}$$

and as we are going to consider identical particles again, all the $\widehat{O}_{ij}$ are equal, but acting specifically in its respective i,j-subspace.

On a general element of the symmetric basis

$$\begin{aligned}
\widehat{O}|\alpha_{k_1}\cdots\alpha_{k_N}\} &= \sum_{i,j=1(i\neq j)}^{N}\widehat{O}_{ij}\frac{1}{\sqrt{N!}}\sum_P \varsigma^P|\alpha_{Pk_1}\rangle\otimes\cdots\otimes|\alpha_{Pk_N}\rangle \\
&= \frac{1}{\sqrt{N!}}\sum_P \varsigma^P\sum_{(i\neq j)}^{N}\widehat{O}_{ij}|\alpha_{Pk_1}\rangle\otimes\cdots\otimes|\alpha_{Pk_N}\rangle \\
&= \frac{1}{\sqrt{N!}}\sum_P \varsigma^P\sum_{(i\neq j)}^{N}O_{Pk_iPk_j}|\alpha_{Pk_1}\rangle\otimes\cdots\otimes|\alpha_{Pk_N}\rangle \\
&= \frac{1}{\sqrt{N!}}\sum_P \varsigma^P\sum_{l,m=1}^{D}\left(n_{\alpha_l}n_{\alpha_m}-\delta_{lm}n_l\right)O_{lm}|\alpha_{Pk_1}\rangle\otimes\cdots\otimes|\alpha_{Pk_N}\rangle \\
&= \frac{1}{\sqrt{N!}}\sum_P \varsigma^P\sum_{l,m=1}^{D}\left(\widehat{n}_{\alpha_l}\widehat{n}_{\alpha_m}-\delta_{lm}\widehat{n}_{\alpha_l}\right)O_{lm}|\alpha_{Pk_1}\rangle\otimes\cdots\otimes|\alpha_{Pk_N}\rangle \\
&= \sum_{l,m=1}^{D}O_{lm}\left(\widehat{n}_{\alpha_l}\widehat{n}_{\alpha_m}-\delta_{lm}\widehat{n}_{\alpha_l}\right)|\alpha_{k_1}\cdots\alpha_{k_N}\}.
\end{aligned} \tag{A.2}$$

By linear independence

$$\begin{aligned}
\widehat{O} &= \sum_{l,m=1}^{D}O_{lm}\left(a^\dagger_{\alpha_l}a_{\alpha_l}a^\dagger_{\alpha_m}a_{\alpha_m}-\delta_{lm}a^\dagger_{\alpha_l}a_{\alpha_l}\right) \\
&= \sum_{l,m=1}^{D}O_{lm}a^\dagger_{\alpha_l}\left(a_{\alpha_l}a^\dagger_{\alpha_m}-\delta_{lm}\right)a_{\alpha_m} \\
&= \sum_{l,m=1}^{D}O_{lm}a^\dagger_{\alpha_l}\left(\varsigma a^\dagger_{\alpha_m}a_{\alpha_l}\right)a_{\alpha_m} \\
&= \sum_{l,m=1}^{D}O_{lm}a^\dagger_{\alpha_l}a^\dagger_{\alpha_m}a_{\alpha_m}a_{\alpha_l}.
\end{aligned} \tag{A.3}$$

Now to the M'-dimensional basis $\{|\lambda_i\rangle\}$

$$\begin{aligned}
\widehat{O} &= \sum_{l,m,p,q=1}^{D} (\alpha_p\alpha_q|\widehat{O}_{ij}|\alpha_l\alpha_m) a^\dagger_{\alpha_p} a^\dagger_{\alpha_q} a_{\alpha_m} a_{\alpha_l} \\
&= \sum_{l,m,p,q=1}^{D} (\alpha_p\alpha_q| \left(\sum_{r,s=1}^{D'} |\lambda_r\lambda_s)(\lambda_r\lambda_s| \right) \widehat{O}_{ij} \\
&\qquad\qquad \times \left(\sum_{t,u=1}^{D'} |\lambda_t\lambda_u)(\lambda_t\lambda_u| \right) |\alpha_l\alpha_m) a^\dagger_{\alpha_p} a^\dagger_{\alpha_q} a_{\alpha_m} a_{\alpha_l} \\
&= \sum_{r,s,t,u=1}^{D'} (\lambda_r\lambda_s|\widehat{O}_{ij}|\lambda_t\lambda_u) \sum_{p,q=1}^{D} (\alpha_p\alpha_q|\lambda_r\lambda_s) a^\dagger_{\alpha_p} a^\dagger_{\alpha_q} \sum_{l,m=1}^{D} (\lambda_t\lambda_u|\alpha_l\alpha_m) a_{\alpha_m} a_{\alpha_l} \\
&= \sum_{r,s,t,u=1}^{D'} (\lambda_r\lambda_s|\widehat{O}_{ij}|\lambda_t\lambda_u) a^\dagger_{\alpha_r} a^\dagger_{\alpha_s} a_{\alpha_u} a_{\alpha_t} \,. \qquad \text{(A.4)}
\end{aligned}$$

Apêndice B

Evaluation of $U(\mathbf{r}_{n+1}, \epsilon; \mathbf{r}_n, 0)$

In the present Appendix we evaluate explicitly the matrix element $U(\mathbf{r}_{n+1}, \epsilon; \mathbf{r}_n, 0)$ that we used in Sectiion 3.1.

Let us start from

$$U(\mathbf{r}_{n+1}, \epsilon; \mathbf{r}_n, 0) = \langle \mathbf{r}_{n+1}| \exp\left[-\frac{i\epsilon}{\hbar}\left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}})\right)\right] |\mathbf{r}_n\rangle \quad \text{(B.1)}$$

$$= \int \frac{d^3p_n}{(2\pi\hbar)^{3/2}} \langle \mathbf{r}_{n+1}|\mathbf{p}_n\rangle\langle \mathbf{p}_n| \exp\left[-\frac{i\epsilon}{\hbar}\left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}})\right)\right] |\mathbf{r}_n\rangle. \quad \text{(B.2)}$$

We expand the exponential as

$$e^{-i\epsilon\widehat{H}/\hbar} = \sum_{j=0}^{\infty} \frac{1}{j!}\left(-\frac{i\epsilon}{\hbar}\right)^j \left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}})\right)^j \quad \text{(B.3)}$$

$$= I - \frac{i\epsilon}{\hbar}\left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}})\right)$$

$$- \frac{\epsilon^2}{2\hbar^2}\left(\frac{\widehat{\mathbf{p}}^4}{4m^2} + \frac{\widehat{\mathbf{p}}^2}{2m}V(\widehat{\mathbf{r}}) + V(\widehat{\mathbf{r}})\frac{\widehat{\mathbf{p}}^2}{2m} + V^2(\widehat{\mathbf{r}})\right) + \cdots. \quad \text{(B.4)}$$

Next, we order the operators in a symmetric way

$$\left(e^{-i\epsilon\widehat{H}/\hbar}\right)^{(Ord)} = \sum_{j=0}^{\infty} \frac{1}{j!}\left(-\frac{i\epsilon}{\hbar}\right)^j \sum_{k=0}^{j} \frac{j!}{k!(j-k)!}\left(\frac{\widehat{\mathbf{p}}^2}{2m}\right)^{j-k} [V(\widehat{\mathbf{r}})]^k \quad \text{(B.5)}$$

$$= I - \frac{i\epsilon}{\hbar}\left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(\widehat{\mathbf{r}})\right)$$

$$- \frac{\epsilon^2}{2\hbar^2}\left(\frac{\widehat{\mathbf{p}}^4}{4m^2} + 2\frac{\widehat{\mathbf{p}}^2}{2m}V(\widehat{\mathbf{r}}) + V^2(\widehat{\mathbf{r}})\right) + \cdots. \quad \text{(B.6)}$$

Therefore, one has that

$$e^{-i\epsilon\widehat{H}/\hbar} = \left(e^{-i\epsilon\widehat{H}/\hbar}\right)^{(Ord)} + O(\epsilon^2). \quad \text{(B.7)}$$

and neglecting terms of $O(\epsilon^2)$, one obtains

$$U(\mathbf{r}_{n+1},\epsilon;\mathbf{r}_n,0) \simeq \int \frac{d^3p_n}{(2\pi\hbar)^{3/2}}\langle \mathbf{r}_{n+1}|\mathbf{p}_n\rangle\langle \mathbf{p}_n|e^{-i\epsilon\widehat{H}^{(Ord)}/\hbar}|\mathbf{r}_n\rangle \tag{B.8}$$

$$\simeq \int \frac{d^3p_n}{(2\pi\hbar)^{3/2}}\frac{e^{i\mathbf{r}_{n+1}\cdot\mathbf{p}_n/\hbar}}{(2\pi\hbar)^{3/2}}\left[e^{-i\epsilon H^{(Ord)}(\mathbf{p}_n,\mathbf{r}_n)/\hbar}\right], \tag{B.9}$$

where

$$\left(e^{-i\epsilon H(\mathbf{p}_n,\mathbf{r}_n)/\hbar}\right)^{(Ord)} = e^{-i\epsilon H(\mathbf{p}_n,\mathbf{r}_n)/\hbar}. \tag{B.10}$$

Then, finally

$$U(\mathbf{r}_{n+1},\epsilon;\mathbf{r}_n,0) \simeq \int \frac{d^3p_n}{(2\pi\hbar)^3}\exp\left[\frac{i\mathbf{r}_{n+1}\cdot\mathbf{p}_n}{\hbar} - \frac{i\epsilon}{\hbar}\left(\frac{\mathbf{p}_n^2}{2m}+V(\mathbf{r}_n)\right)\right]. \tag{B.11}$$

Apêndice C

Closure for bosonic coherent states

In the present Appendix we show the correctness of Eq. (3.36). We start from the expression given in the main text,

$$\begin{aligned} 1 &= \frac{1}{\mathcal{N}} \int \prod_{i=1}^{D} d\phi_i^* \, d\phi_i \, \exp\left(- \sum_{j=1}^{D} \phi_j^* \phi_j \right) |\phi\rangle\langle\phi| \\ &= \frac{1}{\mathcal{N}} \int \prod_{i=1}^{D} d\phi_i^* \, d\phi_i \, \exp\left(- \sum_{j=1}^{D} \phi_j^* \phi_j \right) \\ &\times \sum_{\{n\}=0}^{\infty} \prod_{i=1}^{D} \frac{(\phi_i)^{n_i}}{\sqrt{n_i!}} |n_1 \cdots n_D\rangle \sum_{\{n'\}=0}^{\infty} \prod_{j=1}^{D} \frac{\left(\phi_j^*\right)^{n'_j}}{\sqrt{n'_j!}} \langle n'_1 \cdots n'_D|. \end{aligned} \tag{C.1}$$

Making the change of variables

$$\phi = \sqrt{\rho}\, e^{i\theta}, \tag{C.2}$$

with ρ and θ real, one has

$$\rho = \phi^* \phi, \qquad e^{2i\theta} = \frac{\phi}{\phi^*} \Rightarrow \theta = -\frac{i}{2} \ln\left(\frac{\phi}{\phi^*} \right). \tag{C.3}$$

To obtain the the Jacobian (J) of the transformation, we note that

$$\frac{\partial \rho}{\partial \phi} = \phi^*, \qquad \frac{\partial \rho}{\partial \phi^*} = \phi, \tag{C.4}$$

$$\frac{\partial \theta}{\partial \phi} = -\frac{i}{2} \frac{\frac{1}{\phi^*}}{\frac{\phi}{\phi^*}} = -\frac{i}{2} \frac{1}{\phi}, \qquad \frac{\partial \theta}{\partial \phi^*} = -\frac{i}{2} \frac{\left(-\frac{\phi}{(\phi^*)^2} \right)}{\frac{\phi}{\phi^*}} = \frac{i}{2} \frac{1}{\phi^*}, \tag{C.5}$$

and then

$$J = \phi^* \left(\frac{i}{2} \frac{1}{\phi^*} \right) - \left(-\frac{i}{2} \frac{1}{\phi} \right) \phi = i. \tag{C.6}$$

In terms of the new variables, one obtains

$$1 = \frac{i^D}{\mathcal{N}} \int \prod_{i=1}^{D} d\rho_i \, d\theta_i \, \exp\left(- \sum_{j=1}^{D} \rho_j \right)$$

$$
\begin{aligned}
\times \quad & \sum_{\{n\}=0}^{\infty} \prod_{k=1}^{D} \frac{\left(\sqrt{\rho_k}\, e^{i\theta_k}\right)^{n_k}}{\sqrt{n_k!}} |n_1 \cdots n_D\rangle \sum_{\{n'\}=0}^{\infty} \prod_{j=1}^{D} \frac{\left(\sqrt{\rho_j}\, e^{-i\theta_j}\right)^{n'_j}}{\sqrt{n'_j!}} \langle n'_1 \cdots n'_D| \\
= \quad & \frac{i^D}{\mathcal{N}} \int \prod_{i=1}^{D} d\rho_i\, d\theta_i\, \exp\left(-\sum_{j=1}^{D} \rho_j\right) \sum_{\{n,n'\}=0}^{\infty} \prod_{j=1}^{D} \frac{\sqrt{\rho_j}^{\,n_j+n'_j}\, e^{i\theta_j\left(n_j-n'_j\right)}}{\sqrt{n_j! n'_j!}} \\
\times \quad & |n_1 \cdots n_D\rangle\langle n'_1 \cdots n'_D|. \qquad \text{(C.7)}
\end{aligned}
$$

Using the results

$$
\int_0^{2\pi} d\theta\, e^{i(n-n')\theta} = 2\pi\delta_{n,n'}, \qquad \int_0^{\infty} d\rho\, e^{-\rho}\rho^n = n!, \qquad \text{(C.8)}
$$

we get

$$
\begin{aligned}
1 \quad = \quad & \frac{(2\pi i)^D}{\mathcal{N}} \int \prod_{i=1}^{D} d\rho_i \exp\left(-\sum_{j=1}^{D} \rho_j\right) \sum_{\{n\}=0}^{\infty} \prod_{j=1}^{D} \frac{\rho_j^{n_j}}{n_j!} |n_1 \cdots n_D\rangle\langle n_1 \cdots n_D| \qquad \text{(C.9)} \\
= \quad & \frac{(2i\pi)^D}{\mathcal{N}} \sum_{\{n\}=0}^{\infty} |n_1 \cdots n_D\rangle\langle n_1 \cdots n_D| = \frac{(2i\pi)^D}{\mathcal{N}}. \qquad \text{(C.10)}
\end{aligned}
$$

Therefore, with $\mathcal{N} = (2\pi i)^D$ given in Eq. (3.37), one has proven the completeness relation.

Apêndice D

Numerical values of the fundamental Grassmann integrals

For simplicity the following argumentation will be for one generator only. We know that the l.h.s. of (3.77) is

$$\langle f|g\rangle = f_0^* g_0 + f_1^* g_1, \tag{D.1}$$

but the r.h.s. needs some work before, lets define it as

$$\begin{aligned}(f,g) &\equiv \int d\eta^* d\eta\, f^*(\eta) k(\eta^*,\eta) g(\eta^*) \\ &= \int d\eta^* d\eta (f_0^* + f_1^*\eta)(k_0 + k_1\eta^* + k_2\eta + k_3\eta^*\eta) g(\eta^*) \\ &= \int d\eta^* d\eta (f_0^* k_0 + f_0^* k_1 \eta^* + f_0^* k_2 \eta \\ &\qquad + f_0^* k_3 \eta^*\eta + f_1^* k_0 \eta + f_1^* k_1 \eta\eta^*) g(\eta^*). \end{aligned} \tag{D.2}$$

Because of we are working with anticommuting variables we are going to impose, analogously to the derivative, that any variable has to be next to the integral before to operate

$$\begin{aligned}(f,g) &= \int d\eta^* d\eta (f_0^* k_0 + f_0^* k_1 \eta^* + f_0^* k_2 \eta - f_0^* k_3 \eta\eta^* + f_1^* k_0 \eta + f_1^* k_1 \eta\eta^*) g(\eta^*) \\ &= \int d\eta^* (f_0^* k_0 I_0 + f_0^* k_1 I_0 \eta^* + f_0^* k_2 I_1 \\ &\qquad - f_0^* k_3 I_1 \eta^* + f_1^* k_0 I_1 + f_1^* k_1 I_1 \eta^*) g(\eta^*), \end{aligned} \tag{D.3}$$

where we have defined

$$I_0(\eta) \equiv \int d\eta \qquad \text{and} \qquad I_1(\eta) \equiv \int d\eta\, \eta, \tag{D.4}$$

and beign functions of one generator the I's are of the form

$$I(\eta) = a + b\eta. \tag{D.5}$$

Continuing

$$\begin{aligned}(f,g) &= \int d\eta^*[(f_0^*k_0I_0 + f_0^*k_2I_1 + f_1^*k_0I_1) \\ &\quad +(f_0^*k_1I_0 - f_0^*k_3I_1 + f_1^*k_1I_1)\eta^*](g_0 + g_1\eta^*) \\ &= \int d\eta^*[(f_0^*k_0I_0 + f_0^*k_2I_1 + f_1^*k_0I_1)g_0 + (f_0^*k_0I_0 + f_0^*k_2I_1 + f_1^*k_0I_1)g_1\eta^* \\ &\quad +(f_0^*k_1I_0 - f_0^*k_3I_1 + f_1^*k_1I_1)g_0\eta^*] \\ &= \int d\eta^*\{[f_0^*k_0I_0(\eta) + f_0^*k_2I_1(\eta) + f_1^*k_0I_1(\eta)]g_0 \\ &\quad +\eta^*[f_0^*k_0I_0(-\eta) + f_0^*k_2I_1(-\eta) + f_1^*k_0I_1(-\eta)]g_1 \\ &\quad +\eta^*[f_0^*k_1I_0(-\eta) - f_0^*k_3I_1(-\eta) + f_1^*k_1I_1(-\eta)]g_0\} \\ &= I_0(\eta^*)[f_0^*k_0I_0(\eta) + f_0^*k_2I_1(\eta) + f_1^*k_0I_1(\eta)]g_0 \\ &\quad +I_1(\eta^*)[f_0^*k_0I_0(-\eta) + f_0^*k_2I_1(-\eta) + f_1^*k_0I_1(-\eta)]g_1 \\ &\quad +I_1(\eta^*)[f_0^*k_1I_0(-\eta) - f_0^*k_3I_1(-\eta) + f_1^*k_1I_1(-\eta)]g_0, \end{aligned} \tag{D.6}$$

for simplicity

$$I_0' \equiv I_0(\eta^*) \qquad \text{and} \qquad I_1' \equiv I_1(\eta^*), \tag{D.7}$$

replacing

$$\begin{aligned}(f,g) &= f_0^*g_0\left[k_0I_0'I_0(\eta) + k_2I_0'I_1(\eta) + k_1I_1'I_0(-\eta) - k_3I_1'I_1(-\eta)\right] \\ &\quad +f_1^*g_0\left[k_0I_0'I_1(\eta) + k_1I_1'I_1(-\eta)\right] + f_0^*g_1\left[k_0I_1'I_0(-\eta) + k_2I_1'I_1(-\eta)\right] \\ &\quad +f_1^*g_1\left[k_0I_1'I_1(-\eta)\right]. \end{aligned} \tag{D.8}$$

If we equate this to Eq. (D.1) we get four equations

$$k_0I_0'I_0(\eta) + k_2I_0'I_1(\eta) + k_1I_1'I_0(-\eta) - k_3I_1'I_1(-\eta) = 1, \tag{D.9}$$

$$k_0I_0'I_1(\eta) + k_1I_1'I_1(-\eta) = 0, \tag{D.10}$$

$$k_0I_1'I_0(-\eta) + k_2I_1'I_1(-\eta) = 0, \tag{D.11}$$

$$k_0I_1'I_1(-\eta) = 1. \tag{D.12}$$

From the last one

$$k_0 \neq 0 \tag{D.13}$$

and

$$I_1', I_1 \in C - \{0\} \qquad \Rightarrow \qquad I_1' = I_1. \tag{D.14}$$

Rewriting the four equations considering those two last conditions

$$k_0I_0'I_0(\eta) + k_2I_0'I_1 + k_1I_1I_0(-\eta) - k_3I_1^2 = 1, \tag{D.15}$$

$$k_0I_0'I_1 + k_1I_1^2 = 0, \tag{D.16}$$

$$k_0I_1I_0(-\eta) + k_2I_1^2 = 0, \tag{D.17}$$

$$k_0I_1'I_1 = 1. \tag{D.18}$$

From the third one and because of $k_0 \neq 0$

$$I_0 \in C \qquad \Rightarrow \qquad I_0' = I_0, \tag{D.19}$$

so

$$\begin{aligned} I_0(k_0 I_0 + k_2 I_1) + k_1 I_1 I_0 - k_3 I_1^2 &= 1, & \text{(D.20)} \\ (k_0 I_0 + k_1 I_1) I_1 &= 0, & \text{(D.21)} \\ I_1(k_0 I_0 + k_2 I_1) &= 0, & \text{(D.22)} \\ k_0 I_1^2 &= 1. & \text{(D.23)} \end{aligned}$$

As $I_1 \neq 0$ and using the third equation in the first one

$$\begin{aligned} I_1(k_2 I_0 - k_3 I_1) &= 1, & \text{(D.24)} \\ (k_0 I_0 + k_1 I_1) &= 0, & \text{(D.25)} \\ (k_0 I_0 + k_2 I_1) &= 0, & \text{(D.26)} \\ k_0 I_1^2 &= 1 & \text{(D.27)} \end{aligned}$$

we find

$$\begin{aligned} k_0 &= \frac{1}{I_1^2}, & \text{(D.28)} \\ k_1 &= k_2 = -\frac{I_0}{I_1^3}, & \text{(D.29)} \\ k_3 &= -\frac{1}{I_1^2}\left(1 + \frac{I_0^2}{I_1^2}\right). & \text{(D.30)} \end{aligned}$$

So far we have found strong similarities beetwen all the Boson and Fermion equations, our third reason is related to this. We are going to fix these new parameters in order to keep this symmetry. From the previous section we know the form of the inner product of two functions in the Boson coherent representation (3.42), that tell us to do

$$\begin{aligned} k_0 &\equiv 1, & \text{(D.31)} \\ k_1 &= k_2 \equiv 0, & \text{(D.32)} \\ k_3 &\equiv -1. & \text{(D.33)} \end{aligned}$$

With those we find the original function k

$$\begin{aligned} k(\eta^*, \eta) &= 1 - \eta^* \eta \\ &= e^{-\eta^* \eta}; & \text{(D.34)} \end{aligned}$$

the inner product

$$\langle f|g\rangle = \int d\eta^* d\eta f^*(\eta) e^{-\eta^*\eta} g(\eta^*); \tag{D.35}$$

and then, the closure

$$\begin{aligned} I &= \int d\eta^* d\eta \, |\eta\rangle e^{-\eta^*\eta} \langle\eta| \\ &= \int d\eta^* d\eta e^{-\eta^*\eta} |\eta\rangle\langle\eta|, \end{aligned} \tag{D.36}$$

it is worth notice that it doesn't have any normalization factor. Now the integrals are almost fixed

$$I_0 = 0, \tag{D.37}$$

$$I_1 = \pm 1. \tag{D.38}$$

We are going to choose

$$I_0 = \int d\xi 1 = 0 \qquad \text{and} \qquad I_1 \equiv \int d\xi \xi = 1, \tag{D.39}$$

not only for simplicity, but in order to have the same numerical values than of the derivatives too.

Apêndice E

Symmetrical term for the exponential in the partition function

In Section 3.5, Path Integral for bosons and fermions, we mentioned that one can arrive at two choices for the calculation of the partition function in the ordering of the Grassmann variables, the second choice is

$$\langle \xi_{m+1}|e^{-\epsilon\Omega(a^\dagger,a)}|\xi_m\rangle \qquad \text{with } m=0,\cdots,M-1. \tag{E.1}$$

We are going to follow the exact same steps. After we introduce the $M-1$ identities (3.119)

$$Z=\int\prod_{i=1}^{D}\prod_{k=0}^{M-1}\left(\frac{d\xi_{i,k}^{*}d\xi_{i,k}}{\mathcal{N}}\right)\exp\left(-\sum_{l=0}^{M-1}\sum_{j=1}^{D}\xi_{j,l}^{*}\xi_{j,l}\right)\prod_{m=M-1}^{0}\langle\xi_{m+1}|e^{-\epsilon\Omega(a^\dagger,a)}|\xi_m\rangle, \tag{E.2}$$

we simple order it, and use (3.121)

$$\begin{aligned} Z &= \int\prod_{k=0}^{M-1}\prod_{i=1}^{D}\left(\frac{d\xi_{i,k}^{*}d\xi_{i,k}}{\mathcal{N}}\right)\exp\left(-\sum_{l=0}^{M-1}\sum_{j=1}^{D}\xi_{j,l}^{*}\xi_{j,l}\right) \\ &\qquad \prod_{m=M-1}^{0}\left[\exp\left(\sum_{p=1}^{D}\xi_{p,m+1}^{*}\xi_{p,m}\right)e^{-\epsilon\Omega^{\odot}(\xi_{m+1}^{*},\xi_m)}\right]. \end{aligned} \tag{E.3}$$

Putting together the exponentials, the argument would be

$$\begin{aligned} &\sum_{l=0}^{M-1}\left(\sum_{j=1}^{D}\left(\xi_{j,l+1}^{*}-\xi_{j,l}^{*}\right)\xi_{j,l}-\epsilon\Omega^{\odot}(\xi_{l+1}^{*},\xi_l)\right) \\ &= -\epsilon\sum_{l=0}^{M-1}\left[-\sum_{j=1}^{D}\frac{\left(\xi_{j,l+1}^{*}-\xi_{j,l}^{*}\right)}{\epsilon}\xi_{j,l}+\Omega^{\odot}(\xi_{l+1}^{*},\xi_l)\right]. \end{aligned} \tag{E.4}$$

Replacing it in the partition

$$Z=\int\prod_{k=0}^{M-1}\prod_{i=1}^{D}\left(\frac{d\xi_{i,k}^{*}d\xi_{i,k}}{\mathcal{N}}\right)e^{-R(\xi^{*},\xi)}, \tag{E.5}$$

with

$$R(\xi^*,\xi) \equiv \epsilon \sum_{k=0}^{M-1} \left[-\sum_{j=1}^{D} \frac{\left(\xi^*_{j,k+1} - \xi^*_{j,k}\right)}{\epsilon} \xi_{j,k} + \Omega^{\odot}(\xi^*_{k+1}, \xi_k) \right]. \tag{E.6}$$

Taking the limit $M \to \infty$

$$\lim_{M\to\infty} Z = \int_{\xi(0)}^{\xi(\beta)} \mathcal{D}[\xi^*(\tau)\xi(\tau)] \rceil^{-\mathcal{R}(\xi^*,\xi)}, \tag{E.7}$$

where

$$\int_{\xi(0)}^{\xi(\beta)} \mathcal{D}[\xi^*(\tau)\xi(\tau)] \equiv \lim_{\mathcal{M}\to\infty} \int \prod_{\|=\prime}^{\mathcal{M}-\infty} \prod_{\rangle=\infty}^{\mathcal{D}} \left(\frac{\lceil \xi^*_{\rangle,\|} \lceil \xi_{\rangle,\|}}{\mathcal{N}} \right), \tag{E.8}$$

and

$$\mathcal{R}(\xi^*,\xi) \equiv \int_{\prime}^{\beta} \lceil \tau \left[-\sum_{|=\infty}^{\mathcal{D}} \left(\frac{\partial \xi^*_{|}(\tau)}{\partial \tau} \right) \xi_{|}(\tau) + \otimes^{\odot}(\xi^*(\tau), \xi(\tau)) \right]. \tag{E.9}$$

In which

$$\lim_{M\to\infty} \left(\epsilon \sum_{l=0}^{M-1} \right) \to \int_0^{\beta} d\tau, \tag{E.10}$$

and

$$\lim_{\epsilon\to 0} \frac{\left(\xi^*_{j,l} - \xi^*_{j,l-1}\right)}{\epsilon} \to \frac{\partial \xi^*_j(\tau)}{\partial \tau}. \tag{E.11}$$

Apêndice F

The Feynman ordering label technique

In the present Appendix we will explain Feynman's ordering label technique that we used in Section 5.4. As remarked there, this technique provides a simplification on the notation, the final result is not different from the traditional path-ordering we used in section 5.3. The issue is in some sense trivial, but nevertheless we believe it is instructive to have an Appendix to to clarify the notation. We shall follow the original exposition of Feynman in Ref. [39].

The problem of ordering two operators $\hat{A}$ and $\hat{B}$ appears because their algebra is noncommutative in general, that is $\hat{A}\hat{B} \neq \hat{A}\hat{B}$. The rules of ordinary algebra and analysis for ordinary numbers are not directly applicable. For a single operator $\hat{\alpha}$, there is no problem in defining a function of $\hat{\alpha}$, like through its power series

$$\begin{aligned} \hat{A} = e^{\hat{\alpha}} &\equiv 1 + \hat{\alpha} + \frac{1}{2}\,\hat{\alpha}\hat{\alpha} + \frac{1}{3!}\,\hat{\alpha}\hat{\alpha}\hat{\alpha} + \cdots \\ &= 1 + \hat{\alpha} + \frac{1}{2}\,(\hat{\alpha})^2 + \frac{1}{3!}\,(\hat{\alpha})^3 + \cdots . \end{aligned} \tag{F.1}$$

In these cases the rules of ordinary algebra and analysis apply as for ordinary numbers. The situation complicates when functions of another operator $\hat{\beta}$, with $\hat{\alpha}\hat{\beta} \neq \hat{\beta}\hat{\alpha}$, are considered. Suppose $\hat{B} = \exp\hat{\beta}$, then in general $\hat{B}\hat{A} \neq \hat{A}\hat{B}$, i.e.

$$\hat{B}\hat{A} = e^{\hat{\beta}}\, e^{\hat{\alpha}} \neq e^{\hat{\beta}+\hat{\alpha}} \quad \text{for} \quad \hat{\alpha}\hat{\beta} \neq \hat{\beta}\hat{\alpha}. \tag{F.2}$$

Let us suppose that $\hat{\beta}$ small and expand the exponential to first order in $\hat{\beta}$. The zeroth order in $\hat{\beta}$ is of course $\exp\hat{\alpha}$, but the first order is neither $(\exp\hat{\alpha})\hat{\beta}$ nor $\hat{\beta}(\exp\hat{\alpha})$.

Feynman devised a method to indicate the order in which operators are to operate so as to free them of their noncommutative aspects. Feynman proposed to attach an index to the operator with the convention that the operator with higher index operates later. For example, both $\hat{B}_1\hat{A}_0$ and $\hat{A}_0\hat{B}_1$ mean $\hat{B}\hat{A}$, i.e. the order of the indexed operators can be commuted freely as $\hat{A}_0$ and $\hat{B}_1$ were ordinary numbers.

Thus, if $\hat{A} = \exp\hat{\alpha}$ and $\hat{B} = \exp\hat{\beta}$, one can safely write

$$\hat{B}\hat{A} = e^{\hat{\alpha}_0+\hat{\beta}_1}, \tag{F.3}$$

since there is only one way to interpret the exponential, namely

$$e^{\hat{\alpha}_0+\hat{\beta}_1} = 1 + \hat{\alpha}_0 + \hat{\beta}_1 + \frac{1}{2}\left(\hat{\alpha}_0 + \hat{\beta}_1\right)^2 + \cdots \tag{F.4}$$

$$= 1 + \hat{\alpha}_0 + \hat{\beta}_1 + \frac{1}{2}\left(\hat{\alpha}_0^2 + 2\hat{\alpha}_0\hat{\beta}_1 + \hat{\beta}_1^2\right) \tag{F.5}$$

$$= 1 + \hat{\alpha} + \hat{\beta} + \frac{1}{2}\left(\hat{\alpha}^2 + 2\hat{\alpha}\hat{\beta} + \hat{\beta}^2\right) + \cdots. \tag{F.6}$$

This is the correct answer, since

$$e^{\hat{\alpha}}\, e^{\hat{\beta}} = \left(1 + \hat{\alpha} + \frac{1}{2}\,\hat{\alpha}^2 + \cdots\right)\left(1 + \hat{\beta} + \frac{1}{2}\,\hat{\beta}^2 + \cdots\right) \tag{F.7}$$

$$= 1 + \hat{\beta} + \frac{1}{2}\,\hat{\beta}^2 + \hat{\alpha} + \hat{\alpha}\hat{\beta} + \frac{1}{2}\,\hat{\alpha}^2 + \cdots \tag{F.8}$$

$$= 1 + \hat{\alpha} + \hat{\beta} + \frac{1}{2}\left(\hat{\alpha}^2 + 2\hat{\alpha}\hat{\beta} + \hat{\beta}^2\right) + \cdots. \tag{F.9}$$

Let us write the exponential of the sum $\hat{\alpha} + \hat{\beta}$ as

$$\begin{aligned}\exp(\hat{\alpha}+\hat{\beta}) &= \lim_{n\to\infty}\left[\exp\frac{1}{n}(\hat{\alpha}+\hat{\beta})\right]^n \\ &= \lim_{n\to\infty}\left[1+\frac{1}{n}(\hat{\alpha}+\hat{\beta})\right]^n \\ &= \lim_{n\to\infty}\underbrace{\left[1+\frac{1}{n}(\hat{\alpha}+\hat{\beta})\right]\left[1+\frac{1}{n}(\hat{\alpha}+\hat{\beta})\right]\cdots\left[1+\frac{1}{n}(\hat{\alpha}+\hat{\beta})\right]}_{n\text{ times}}.\end{aligned} \tag{F.10}$$

In each factor $1+1/n\,(\hat{\alpha}+\hat{\beta})$ we replace $\hat{\alpha}+\hat{\beta}$ by $\hat{\alpha}_i+\hat{\beta}_i$, with $1 \le i \le n$, and write

$$\begin{aligned}\exp(\hat{\alpha}+\hat{\beta}) &= \lim_{n\to\infty}\left[1+\frac{1}{n}(\hat{\alpha}_n+\hat{\beta}_n)\right]\left[1+\frac{1}{n}(\hat{\alpha}_{n-1}+\hat{\beta}_{n-1})\right]\cdots\left[1+\frac{1}{n}(\hat{\alpha}_1+\hat{\beta}_1)\right] \\ &= \lim_{n\to\infty}\left[1+\frac{1}{n}(\hat{\alpha}_n+\hat{\beta}_n)+\frac{1}{n}(\hat{\alpha}_{n-1}+\beta_{n-1})+\cdots+\frac{1}{n}(\hat{\alpha}_1+\hat{\beta}_1)\right] \\ &= \lim_{n\to\infty}\exp\left[\frac{1}{n}\sum_{i=1}^{n}(\hat{\alpha}_i+\hat{\beta}_i)\right].\end{aligned} \tag{F.11}$$

In the limit of $n \to \infty$, the discrete index becomes continuous $i/n \to s, 0 \leq s \leq 1$, with $1/n \to ds$, $\hat{\alpha}_i \to \hat{\alpha}(s)$, $\hat{\beta}_i \to \hat{\beta}(s)$, and

$$\exp(\hat{\alpha} + \hat{\beta}) = \exp \int_0^1 ds \, [\hat{\alpha}(s) + \hat{\beta}(s)]. \tag{F.12}$$

As Feynman remarked, it is evident that this expression is correct: calling $\hat{\alpha}(s) + \hat{\beta}(s) = \gamma(s)$, with γ a definite operator operating at order s, one has that

$$\exp\left[\int_0^1 ds \, \hat{\gamma}(s)\right] = \exp\left[\int_0^1 ds \, \hat{\gamma}\right], \tag{F.13}$$

since γ does not need to have the s dependence, it commutes with itself the integral, and therefore

$$\int_0^1 ds \, \hat{\gamma}(s) = \gamma \int_0^1 ds = \gamma. \tag{F.14}$$

The expression in Eq. (F.12) at itself is trivial, but its nontrivial feature is that the r.h.s. can be manipulated as $\hat{\alpha}(s)$ and $\hat{\beta}(s)$ were ordinary functions of s, since the order of operations will always be automatically specified by the index. For example, in particular

$$\begin{aligned} \exp(\hat{\alpha} + \hat{\beta}) &= \exp \int_0^1 ds \, [\hat{\alpha}(s) + \hat{\beta}(s)] \\ &= \exp\left[\int_0^1 ds_1 \, \hat{\alpha}(s_1) + \int_0^1 ds_2 \, \hat{\beta}(s_2)\right] \\ &= \left[\exp \int_0^1 ds_1 \, \hat{\alpha}(s_1)\right] \left[\int_0^1 ds_2 \, \hat{\beta}(s_2)\right]. \end{aligned} \tag{F.15}$$

Let us check this for the lowest nontrivial order. The l.h.s. of this expression gives

$$\exp(\hat{\alpha} + \hat{\beta}) = 1 + \hat{\alpha} + \hat{\beta} + \frac{1}{2}\left(\hat{\alpha}^2 + \hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha} + \hat{\beta}^2\right) + \cdots. \tag{F.16}$$

The ordering issue here is with respect to the term $(\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha})/2$. Let us see how this ordering appears with the integrals on the r.h.s. of Eq. (F.15). The ordering comes from the product of integrals $\int_0^1 ds_1 \, \hat{\alpha}(s_1) \int_0^1 ds_2 \, \hat{\beta}(s_2)$, which can be written as

$$\begin{aligned} \int_0^1 ds_1 \, \hat{\alpha}(s_1) \int_0^1 ds_2 \, \hat{\beta}(s_2) &= \int_0^1 ds_1 \, \hat{\alpha}(s_1) \int_0^{s_1} ds_2 \, \hat{\beta}(s_2) \\ &+ \int_0^1 ds_1 \, \hat{\alpha}(s_1) \int_{s_1}^{s_1} ds_2 \, \hat{\beta}(s_2). \end{aligned} \tag{F.17}$$

In the first integral on the r.h.s. one has $s_1 > s_2$, so that $\hat{\alpha}(s_1)\hat{\beta}(s_2) = \hat{\alpha}\hat{\beta}$ and the value of the integral is

$$\int_0^1 ds_1 \, \hat{\alpha}(s_1) \int_0^{s_1} ds_2 \, \hat{\beta}(s_2) = \hat{\alpha}\hat{\beta} \int_0^1 ds_1 \int_0^{s_1} ds_2$$

$$= \hat{\alpha}\hat{\beta}\int_0^1 ds_1 s_1$$

$$= \frac{1}{2}\hat{\alpha}\hat{\beta}. \tag{F.18}$$

In the second integral, one has $s_2 > s_1$, then $\hat{\alpha}(s_1)\hat{\beta}(s_2) = \hat{\beta}\hat{\alpha}$, and the value of the integral is

$$\begin{aligned}\int_0^1 ds_1\,\hat{\alpha}(s_1)\int_{s_1}^0 ds_2\,\hat{\beta}(s_2) &= \hat{\beta}\hat{\alpha}\int_0^1 ds_1\int_{s_1}^1 ds_2 \\ &= \hat{\beta}\hat{\alpha}\int_0^1 ds_1(1-s_1) \\ &= \hat{\alpha}\hat{\beta}\left(1-\frac{1}{2}\right) \\ &= \frac{1}{2}\hat{\alpha}\hat{\beta}. \end{aligned} \tag{F.19}$$

A case of interest to the present dissertation is when we want to expand $\exp(\hat{\alpha}+\hat{\beta})$ for $\hat{\beta}$ small. Let us consider the expansion to first order in $\hat{\beta}$,

$$\begin{aligned}\exp(\hat{\alpha}+\hat{\beta}) &= \left[\exp\int_0^1 ds_1\,\hat{\alpha}(s_1)\right]\left[\int_0^1 ds_2\,\hat{\beta}(s_2)\right] \\ &\approx \left[\exp\int_0^1 ds_1\,\hat{\alpha}(s_1)\right]\left(1+\int_0^1 ds_2\,\hat{\beta}(s_2)\right) \\ &= \exp\int_0^1 ds_1\,\hat{\alpha}(s_1) + \left[\exp\int_0^1 ds_1\,\hat{\alpha}(s_1)\right]\int_0^1 ds_2\,\hat{\beta}(s_2). \end{aligned} \tag{F.20}$$

The first term is trivial and gives $\exp\hat{\alpha}$. In the second term, we break the integral over s_1 as

$$\left[\exp\int_0^1 ds_1\,\hat{\alpha}(s_1)\right] = \left[\exp\int_{s_2}^1 ds_1\,\hat{\alpha}(s_1)\right]\left[\exp\int_0^{s_2} ds_1\,\hat{\alpha}(s_1)\right]. \tag{F.21}$$

So, we have to consider the ordering of

$$\left[\exp\int_{s_2}^1 ds_1\,\hat{\alpha}(s_1)\right]\left[\exp\int_0^{s_2} ds_1\,\hat{\alpha}(s_1)\right]\hat{\beta}(s_2). \tag{F.22}$$

The $\hat{\alpha}(s_1)$ in the first factor acts after $\hat{\beta}(s_2)$ and is for all effects independent of s_1, but $\hat{\alpha}(s_1)$ in the second term is to act before $\hat{\beta}(s_2)$. So, if we write $\hat{\beta}(s_2)$ between both terms and imply the usual convention, the $\hat{\alpha}(s_1)$'s become independent of s_1 in the range from 0 to s_2 and one may perform the integrals

$$\begin{aligned}\left[\exp\int_0^1 ds_1\,\hat{\alpha}(s_1)\right]\int_0^1 ds_2\,\hat{\beta}(s_2) &= [\exp\hat{\alpha}]\int_0^1 ds\,[\exp(-s)\hat{\alpha}]\;\hat{\beta}\,[\exp s\hat{\alpha}] \\ &= e^{\hat{\alpha}}\int_0^1 ds\,e^{-s\alpha}\,\hat{\beta}\,e^{s\hat{\alpha}}. \end{aligned} \tag{F.23}$$

That is, we have obtained the result

$$e^{\hat{\alpha}+\hat{\beta}} = e^{\hat{\alpha}} \left[1 + \int_0^1 ds\, e^{-s\alpha}\, \hat{\beta}\, e^{s\hat{\alpha}} + \cdots \right], \tag{F.24}$$

which coincides with Eq. (5.46) to first order.

It is important to note that in a practical calculation, an expression like $\int_0^1 ds\, \hat{\alpha}(s)$ standing alone is obviously equal to α, but it is far from trivial when multiplied by factors involving $\int_0^1 ds\, \hat{\beta}(s)$. This means one must consider the complete expression as a functional of $\hat{\alpha}(s)$, $\hat{\beta}(s)$, etc.

One last remark: if one has

$$\exp[-\lambda(\hat{\alpha}+\hat{\beta})], \tag{F.25}$$

where λ is an ordinary number, Feynman's formula is

$$\begin{aligned} \exp[-\lambda(\hat{\alpha}+\hat{\beta})] &= \exp \int_0^\lambda ds\, [\hat{\alpha}(s) + \hat{\beta}(s)] \\ &= \left[\exp \int_0^\lambda ds_1\, \hat{\alpha}(s_1) \right] \left[\int_0^\lambda ds_2\, \hat{\beta}(s_2) \right], \end{aligned} \tag{F.26}$$

as can be easily checked.

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