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Path integral theory of interacting fermionic many-body systems: towards a semiclassical approximation

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Introduction

Among the many unfortunate statements in Physics, one can mention Erwin Schrödinger's take on experiments involving only one of a given kind of particle [1]:

"This is the obvious way of registering the fact, that we never experiment with just one electron or atom or (small) molecule. In thought-experiments we sometimes assume that we do ; this invariably entails ridiculous consequences [...] In the first place it is fair to state that we are not experimenting with single particles, any more than we can raise Ichthyosauria in the zoo."

Seventy years later, both manipulating and measuring individual particles without destroying their quantum state has indeed been made possible. However, the point here is certainly not to dwell on a mistake made by a great mind, but to emphasize just how big of an achievement this is. Sharing a Nobel prize awarded in 2012, S. Haroche and D. Wineland have accomplished this impressive feat with individual photons [2] (1990) and individual ions [3] (1987) respectively. This achievement is the culmination of numerous technologies and techniques, developed and perfected over the 20^{th} century. These include the development of laser cooling, a technique that somehow paradoxically cools atoms by exposing them to the beam of a laser, which resulted in a Nobel prize in 1997. Atoms cooled in this way can reach temperatures lower than 0.1 nK [4], which is within what is called the ultracold regime. Trapping individual atoms has opened the way to many applications in research and industry. The first that comes in mind is obviously Quantum Computing, but we can also mention quantum clocks, and the study of quantum effects at the fundamental scale (*i.e.* a single particle or a handful of particles).

In parallel, the improvement of cooling and trapping techniques has allowed scientists to create lattices of traps made from electromagnetic waves and containing ultracold atoms. Those lattices, usually called optical lattices, have a very wide range of use in condensed matter physics, since they can simulate systems very close from particles in the periodic potential of a crystalline structure [5]. Studying these lattices also allow for testing many-body models such as the Bethe ansatz [6], the spin chains [7] or the Fermi-Hubbard model [8, 9] to name a few. Increased possibilities in the control and the measurement of particles have made possible the realization of devices known as quantum simulators: devices that can run experiments on a handful of particles at the quantum scale, but that can be programmed in order to prepare systems in a specific state. They allow for studying the very complicated laws of many-body systems in a precise and reproducible way, pushing the boundaries of our knowledge on the rich topic, both in open questions and in applications, that is condensed physics.

Unrelated to what was exposed above, the second half of the 20th century also saw the appearance of Feynman's path integral, born in the pages of Feynman's thesis in 1942 [10]. The path integral was built on the goal to obtain a Lagrangian formulation of quantum mechanics, as opposed to the Hamiltonian formulation developed by Schrödinger and Heisenberg among others. This Lagrangian formulation made use of the concept of action, which plays a central role in classical mechanics, being the trajectory-dependent quantity minimized by the real trajectory followed by a classical system. Feynman's work showed that this idea of minimization could be recovered for classical systems as a special case of a quantum rule. This is Feynman's path integral: if one wants to know the probability for a system to go from a given state to another in a given time, one "simply" computes a phase factor for each path relating the two states in the required time and adds them together. The probability, represented in quantum mechanics by a quantity called the propagator, is then high or low depending on if the phase factors interfere constructively or destructively [11]. In the classical limit, one essentially recovers that the classical paths of the system are the only ones contributing to this sum. If we consider a very simple system, e.g. a single classical particle, the probability of transition between two given states is then 1 if the two states are related by the classical path, and 0 otherwise. If we instead consider a system of many classical particles described by a probability density, it is now all the classical paths starting from a point where the probability of finding a particle is non-zero that contribute. In both cases, one only has to consider paths given by the classical laws of motion.

The probability given by the path integral is exact as long as all paths relating the two states are taken into account, let them be classical or non-classical. In the simple case of a ball rolling horizontally, one would have to consider paths were the ball teleports one or several times, to include effects of quantum tunneling. Computing the propagator for a given system via Feynman's path integral is in general not a simple task. One of the main complexity factors is the fact that there often exists an infinite number of paths relating two states. For this reason, approximation strategies to the path integral have been developed. One of such approximations was obtained by Martin C. Gutzwiller in the late 1960s [12], about fifteen years after Feynman had submitted his doctoral thesis. This approximate propagator, known as the van Vleck-Gutzwiller propagator, is computed from classical trajectories only, but still takes into account the quantum interference phenomenon¹. It is at the root of many practical applications of the path integral. In particular, the van Vleck-Gutzwiller propagator is a very interesting tool to study quantum chaos [13], a lively field of modern research in quantum physics. We can also cite Gutzwiller's trace formula which expresses the energy spectrum of a single-particle quantum system using its periodic trajectories. The extension of semiclassical techniques to many-body systems is still a work in progress [13]. Among successful generalizations, we can mention the application of Gutzwiller's trace formula to many-bosons systems [14].

A useful tool when considering the propagator of a many-body system is the coherent state representation [15]. Coherent states are the most classical quantum states, in the sense that they minimize the uncertainty of physical observables inherent to quantum mechanics. They describe, for instance, the state of a laser beam. They have been used several times in the literature to obtain the propagator of a many-body system [13–16]. Although referred to as "the most classical states", they can be used to express any quantum state of the system [17], and are thus very general. However, coherent states for fermions require the introduction of anti-commuting numbers and this makes the fermionic coherent states nonphysical. If used, these anti-commuting numbers need to be eliminated one way or another in order to obtain quantities that are physical. Because of that, other representations are sometimes used for fermions [18, 19].

The goal of this master thesis is to express the dynamics of many interacting fermions on a lattice via a purely bosonic propagator. In order to do so, we first need to involve bosons, and so we relate the fermionic system to a system where the fermions interact with each other by boson exchange. Such systems are called mixed systems since they contains both bosons and fermions. Both fermions and bosons will be described by coherent states. Similar case have already been treated in the literature. In particular, the spin-boson model describes a field with a non-zero spin interacting with a bosonic reservoir [20]. The propagator of a generic fermionic system has also been treated semiclassically without the use of a bosonic field [18, 19], but in a representation other than the coherent state representation. Once the relation between the fermionic system and the mixed system has been established, we attempt to eliminate the fermions from the propagator of the mixed system, resulting in a propagator that contains only bosonic degrees of freedom and the initial and final fermionic state. The motivation for this goal is twofold. On the one hand, it is a way of dealing with the anti-commuting numbers relative to fermionic coherent states. On the other hand, many results have already been obtained for bosonic many-body systems [16]. Semiclassical treatments of many-fermions systems however are less documented. Re-expressing the dynamics of the fermions through the bosons mediating their interaction could then be a gateway to a semiclassical theory for fermions, benefiting from the existing literature on semiclassical bosonic theories. The present work aims to add to the existing literature by investigating a way to express generic interacting fermionic systems in coherent state representation through the dynamics of a bosonic field, working towards a general method for expressing the dynamics of the fermions through bosonic degrees of freedom. A semiclassical approximation could then be applied on the resulting bosonic propagator.

The first chapter of this work reviews the general framework of many-body systems of indistinguishable particles. In particular, the concepts of creation/annihilation operators, Fock space and (anti-)symmetrized states are exposed. The last part of chapter 1 is dedicated to the exposition of the system under consideration, namely fermions on a lattice interacting via bosons. In the second chapter, we briefly remind the reader of the fundamentals of Lagrangian mechanics before discussing Feynman's path integral and its link to the Hamiltonian formulation of quantum mechanics. Chapter 3 then introduces mathematically the concept of coherent states, some of their properties along with useful formulae in the context of coherent state path integrals. An introductory example of such a path integral for a simple mixed system is then presented. Chapter 4 begins with the detailed exposition of the proposed method for re-expressing the dynamics of the fermionic system using bosons. It then continues with the first step of this method, which is to compute the elimination of the bosonic degrees of freedom from the mixed propagator to obtain a fermionic propagator. We then verify that this elimination yields the dynamics of the interacting fermionic system we wish to describe. In chapter 5, we carry out the elimination of the fermionic degrees of freedom and discuss prospects for application of semiclassical approximations to the resulting propagator.

¹It does not, however, recover quantum tunneling effect.

Chapter 1

Theoretical Description of Many-body Systems

This chapter reviews the theoretical description of many-body quantum systems. The *N*-particle Hilbert space is constructed and states that are symmetrized appropriately for describing systems with indistinguishable particles are introduced. The Fock space is then presented and constructed using those states. In this context, operators that modify the number of particles in a state, the creation and annihilation operators are introduced. These operators allow for a convenient representation of many-body operators, and this representation is exposed. The last part of this chapter describes the system of interest of this work, using the concept of product states. The Hamiltonian representing the system is written out in second quantization form, and such form will be used for operators in upcoming chapters.

1.1 Many-Body Hilbert space, Fock space and second quantization

N-Particles Hilbert Space

Let \mathcal{H}_1 denote the space of square-integrable functions, *i.e.* the Hilbert space containing the single-particle wave functions. We can describe N indistinguishable particles by N single-particle wave functions. The Hilbert space of the N-particle wave functions is given by

$$\mathcal{H}_N = \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_1 \tag{1.1.1}$$

If the set $\{ |\phi_0\rangle, |\phi_1\rangle, \dots \} \equiv \{ |\phi_k\rangle \}_{k \in \mathbb{N}}$ is an orthonormal basis of the single-particle Hilbert space \mathcal{H}_1 , then a basis of \mathcal{H}_N is given by

$$\mathcal{B}_N \equiv \{ |\phi_{k_1}\phi_{k_2}\cdots\phi_{k_N}\rangle \}_{k_1,\dots,k_N \in \mathbb{N}}$$
(1.1.2)

Here, $|\phi_{k_1}\phi_{k_2}\cdots\phi_{k_N}\rangle$ is a shorthand for $|\phi_{k_1}\rangle\otimes\cdots\otimes|\phi_{k_N}\rangle$, the tensor product of N single-particle basis states which represents a N-particles state. Note that nothing *a priori* forbids two labels k_i and k_j from having the same value if the system contains only bosonic particles. These N-particles basis states are orthogonal to each other:

$$\left\langle \phi_{k_1}\phi_{k_2}\cdots\phi_{k_N} \middle| \phi_{k'_1}\phi_{k'_2}\cdots\phi_{k'_N} \right\rangle = \delta_{k_1k'_1}\delta_{k_2k'_2}\cdots\delta_{k_Nk'_N} \tag{1.1.3}$$

One-body operators acting in \mathcal{H}_N are constructed by considering their action in \mathcal{H}_1 on each particle of the system. Formally, if the action of the operator \hat{A} expressed in the single-particle basis $\{|\phi_k\rangle\}_{k\in\mathbb{N}}$ of \mathcal{H}_1 is given by

$$A = \sum_{k,k' \in \mathbb{N}} \langle \phi_k | A | \phi_{k'} \rangle | \phi_k \rangle \langle \phi_{k'} | = \sum_{k,k' \in \mathbb{N}} A_{kk'} | \phi_k \rangle \langle \phi_{k'} |$$
(1.1.4)

then the action of its extension to the N-particle state is defined as follows:

$$\hat{A} |\phi_{k_1}\phi_{k_2}\cdots\phi_{k_N}\rangle = A |\phi_1\rangle\otimes\cdots\otimes|\phi_N\rangle + |\phi_1\rangle\otimes A |\phi_2\rangle\otimes\cdots\otimes|\phi_N\rangle + \cdots$$
(1.1.5)

where $A |\phi_k\rangle$ is obtained by replacing A with (1.1.4). The general expression of A extended to the N-particle Hilbert space \mathcal{H}_N , denoted \hat{A} , is given by

$$\hat{A} = \sum_{n=1}^{N} \sum_{k_1, k_1' \in \mathbb{N}} \cdots \sum_{k_N, k_N' \in \mathbb{N}} \delta_{k_1 k_1'} \cdots \delta_{k_{n-1} k_{n-1}'} A_{k_n k_n'} \delta_{k_{n+1} k_{n+1}'} \cdots \delta_{k_N k_N'} \left| \phi_{k_1} \phi_{k_2} \cdots \phi_{k_N} \right\rangle \left\langle \phi_{k_1'} \phi_{k_2'} \cdots \phi_{k_N'} \right| \quad (1.1.6)$$

Similar extensions can be done for two, three, and n-body operators with n > 3. Representing generic operators in \mathcal{H}_N is however quite cumbersome. We also note that the states in \mathcal{H}_N are restricted to a fixed number of particles N, which is not appropriate to describe a system where particles can be created or destroyed. This concern will be addressed shortly. Moreover, the way we represented wave functions of \mathcal{H}_N is not very suited for the case of indistinguishable particles, since each particle has a label represented by its position in the vector $|\phi_{k_1}\phi_{k_2}\cdots\phi_{k_N}\rangle$. The state of the system then contains information about which particle is in which state, and this information is irrelevant. Indeed, the particles are indistinguishable, meaning that it makes no physical sense to know the state of a specific particle. The only sensible question is how many particles there is in each state, without arbitrarily labelling the particles. Such concerns are addressed by considering only a specific kind of N-body states, namely states that are totally symmetric or anti-symmetric.

Symmetrized and anti-symmetrized states

In order to define states that make physical sense for systems of indistinguishable particles, namely symmetrized and anti-symmetrized states, we must first state for which transformation they are symmetrical or anti-symmetrical. This transformation is given by the transposition operator. It acts in \mathcal{H}_N by permuting the states¹ of two components of the global state vector $|\phi_{k_1}\phi_{k_2}\cdots\phi_{k_N}\rangle$:

$$\hat{\Pi}_{ij} | \cdots \phi_{k_i} \cdots \phi_{k_j} \cdots \rangle = | \cdots \phi_{k_j} \cdots \phi_{k_i} \cdots \rangle$$
(1.1.7)

A state $|\Psi_+\rangle$ of \mathcal{H}_N is said to be totally symmetric if for all pairs of $i, j \in \{1, \ldots, N\}$, we have

$$\hat{\Pi}_{ij} |\Psi_+\rangle = |\Psi_+\rangle \tag{1.1.8}$$

Conversely, a state $|\Psi_{-}\rangle$ is said to be totally anti-symmetric if for all pairs of $i, j \in \{1, \ldots, N\}, i \neq j$, we have

$$\hat{\Pi}_{ij} |\Psi_{-}\rangle = -|\Psi_{-}\rangle \tag{1.1.9}$$

The Hilbert space of symmetric (resp. anti-symmetric) N-particles states is naturally denoted \mathcal{H}_N^+ (resp. \mathcal{H}_N^-). An important assumption in the description of many-body quantum systems is the symmetrization postulate. It postulates that many-body systems with indistinguishable particles are always described by a symmetrized state in the bosonic case, and by an anti-symmetrized states in the fermionic case. The requirement for states of Nindistinguishable particles to belong either to \mathcal{H}_N^+ or to \mathcal{H}_N^- can be understood intuitively by considering the following reasoning: since the particles are indistinguishable, it should not matter which particle is in which state. Therefore, permuting particles should have no impact on probabilities and physical observables. In particular, let $|\Phi\rangle$ be the state of the system and $|\Psi\rangle$ be another possible state. If the system has a probability $P = |\langle \Psi | \Phi \rangle|^2$ of being measured in state $|\Psi\rangle$, then two permuting particles should leave this probability unchanged. Quantitatively, this means that we must have

$$|\langle \Psi | \Phi \rangle|^{2} = \left| \left\langle \Psi \left| \hat{\Pi}_{ij} \right| \Phi \right\rangle \right|^{2} \qquad \forall i, j \in \{1, \dots, N\}$$
(1.1.10)

The only two options that preserve this equality are $\hat{\Pi}_{ij} |\Phi\rangle = |\Phi\rangle$ and $\hat{\Pi}_{ij} |\Phi\rangle = -|\Phi\rangle$ for all $i, j \in \{1, \ldots, N\}$. This reasoning makes no assumption on the particular state the system is in, and thus each possible state of the system must be either symmetrized or anti-symmetrized.

The process of constructing those states is straightforward but will only be touched briefly as the introduction of (anti-)symmetrized states mainly serve the purpose of constructing the Fock space in a following section. The interested reader will find more details about the symmetrization postulate and symmetrized states in any standard many-body quantum mechanics textbook, e.g. in [17]. Taking the simple case of N = 2, let $\{|\phi_{k_1}\phi_{k_2}\rangle\}_{k_1,k_2\in\mathbb{N}}$ be a basis of the two-particle Hilbert space \mathcal{H}_2 . The basis

$$\mathcal{B}_{2}^{+} \equiv \{ |\phi_{k_{1}}\phi_{k_{2}}\rangle_{+} \}_{k_{1} \le k_{2} \in \mathbb{N}}$$
(1.1.11)

is a basis of the space of symmetrized (bosonic) states \mathcal{H}_2^+ . The condition on k_1 , k_2 prevents \mathcal{B}_2^+ from containing the same states twice. The basis states have the following simple expression:

$$|\phi_{k_1}\phi_{k_2}\rangle_+ = C^+_{k_1,k_2} \left(|\phi_{k_1}\phi_{k_2}\rangle + |\phi_{k_2}\phi_{k_1}\rangle\right) \tag{1.1.12}$$

It is easy to verify that such states are indeed symmetric by permutation of the two particles. The prefactor C_{k_1,k_2}^+ equals $1/\sqrt{2}$ if k_1 is not equal to k_2 , meaning that the two states in the two-body state are different, and 1/2

 $^{^{1}}$ It is worth emphasizing that only labels are exchanged. There are no changes in the state of the system if we do not take into account which particle is considered as the first, the second, etc.

if they are the same. Symmetric states defined in that way are normalized if the 2-particles states $|\phi_{k_1}\phi_{k_2}\rangle$ are normalized, which we assume. We now turn to the case of fermions. A basis of the anti-symmetrized two-particle space \mathcal{H}_2^- is given by

$$\mathcal{B}_{2}^{-} \equiv \{ |\phi_{k_{1}}\phi_{k_{2}}\rangle_{-} \}_{k_{1} < k_{2} \in \mathbb{N}}$$
(1.1.13)

where

$$|\phi_{k_1}\phi_{k_2}\rangle_{-} = \frac{1}{\sqrt{2}} \left(|\phi_{k_1}\phi_{k_2}\rangle - |\phi_{k_2}\phi_{k_1}\rangle \right)$$
(1.1.14)

Again it is easy to verify that such a state is normalized and is antisymmetric by exchange of the two particles. Note that fermions differ from bosons in that k_1 is restricted to values strictly less than k_2 . This is easily understood by considering the state

$$\left|\phi_{k}\phi_{k}\right\rangle_{-} = \frac{1}{\sqrt{2}}\left(\left|\phi_{k}\phi_{k}\right\rangle - \left|\phi_{k}\phi_{k}\right\rangle\right) = 0 \tag{1.1.15}$$

Thus, anti-symmetrized states are zero if they contain any state more than once. This observation is of great importance as it implements the Pauli exclusion principle, stating that the same state cannot be occupied by two fermions. The exclusion principle is fundamental in the stability of matter and many other observed phenomena. It is therefore welcome that this principle is recovered by our description of many-body systems.

Symmetrized and anti-symmetrized states are generalized to N > 2 using all permutations of the N particles:

$$|\phi_{k_1} \cdots \phi_{k_N}\rangle_{\pm} = \frac{1}{\sqrt{N! \prod_{k \in \mathbb{N}} n_k!}} \sum_{\pi \in S_N} (\pm 1)^{\pi} |\phi_{k_{\pi(1)}} \cdots \phi_{k_{\pi(N)}}\rangle$$
(1.1.16)

where S_N denotes the set of all permutations of numbers $\{1, \ldots, N\}$, and $(-1)^{\pi}$ is a shorthand for the sign of the permutation π . The product in the prefactor is responsible for implementing the normalization in the case where some states appear multiple times, generalizing what was discussed for N = 2. The number n_k represents the number of occurrences of ϕ_k in $\{\phi_{k_1}, \ldots, \phi_{k_N}\}$ and is called the occupation number of state $|\phi_k\rangle$. We of course have $\sum_{k \in \mathbb{N}} n_k = N$. Occupation numbers allow for a more sensible representation of (anti-)symmetrized N-body states, namely the occupation number representation. For instance, let a state $|\phi_{k_1}\phi_{k_2}\cdots\phi_{k_N}\rangle_+$ be the symmetrized state containing one particle in state $|\phi_{k_1}\rangle$, one particle in state $|\phi_{k_2}\rangle$ etc. It can then be written as

$$\phi_{k_1}\phi_{k_2}\cdots\phi_{k_N}\rangle_+ \equiv |n_0n_1\cdots n_k\cdots\rangle_+ \tag{1.1.17}$$

For instance, the two-particles symmetrized state $|\phi_0\phi_2\rangle_+$ would be represented as $|1, 0, 1, 0, \ldots\rangle_+$ in occupation number representation. Using the notation $|\cdots\rangle_-$ for anti-symmetrized states, the symmetrization postulate is implemented in occupation number representation by requiring

$$\hat{\Pi}_{ij} | n_0 n_1 \cdots n_k \cdots \rangle_{\pm} = \pm | n_0 n_1 \cdots n_k \cdots \rangle_{\pm}$$
(1.1.18)

for any $i, j \neq i$. In the case of fermionic states, the occupation number cannot take any value other than 0 or 1. This is a direct consequence of the generalization of (1.1.15) to numbers of particles greater than 2. We mention that states considered in further developments will either belong to \mathcal{H}_N^+ or \mathcal{H}_N^- , since states that are not totally symmetric or anti-symmetric are not relevant for describing systems of many indistinguishable particles such as the system we are interested in.

The Fock Space

When considering a particle number that can vary, it cannot suffice to consider only one Hilbert space $\mathcal{H}_{\mathcal{N}}$ containing N-particles states. Instead, Hilbert spaces with all possible number of particles must be considered. A realization of this concept is the Fock Space, constructed as the direct sum of n-particles Hilbert spaces for all values of n:

$$\mathcal{F} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots \oplus \mathcal{H}_n \oplus \dots = \bigoplus_{n \in \mathbb{N}} \mathcal{H}_n$$
(1.1.19)

The Fock space contains the basis states of each \mathcal{H}_n as given in (1.1.2), for all number of particles n. As previously stated, state vectors that are either symmetrized or anti-symmetrized are the only relevant vectors to describe systems of N indistinguishable particles. Thus, we are only interested in Fock spaces restricted to such states:

$$\mathcal{F}^+ = \bigoplus_{n \in \mathbb{N}} \mathcal{H}_n^+ \tag{1.1.20}$$

for bosons, and

$$\mathcal{F}^{-} = \bigoplus_{n \in \mathbb{N}} \mathcal{H}_{n}^{-} \tag{1.1.21}$$

for fermions. Inheriting the notation for symmetrized and anti-symmetrized states, fermionic Fock states will be denoted $|\cdots\rangle_{-}$, and bosonic states $|\cdots\rangle_{+}$ when a distinction is required. Because it is constructed as a direct sum, a basis of the Fock space is given by the union of the basis of each *n*-particles Hilbert space. Any Fock state $|f\rangle$ can thus be expanded as a sum over all number of particles of those basis states:

$$|f\rangle_{\pm} = \sum_{n=0}^{\infty} \sum_{k_1,\dots,k_n} B_{k_1,\dots,k_n} |\phi_{k_1}\cdots\phi_{k_n}\rangle_{\pm}$$
(1.1.22)

Equivalently, a generic Fock state can be expanded in occupation number representation as:

$$|f\rangle_{\pm} = \sum_{n_0,\dots,n_k,\dots}^{\infty} C_{n_0,\dots,n_k,\dots} |n_0\cdots n_k\cdots\rangle_{\pm}$$
(1.1.23)

Creation and annihilation operators

Working in a space where particle number can vary allows for the introduction of operators that add or remove particles from the system. Such operators are called creation and annihilation operators respectively. As will be seen shortly, these operators behave quite differently for fermions and bosons. This difference has led to the introduction of a convention to distinguish between the two. The symbol \hat{b}_k^{\dagger} (resp. \hat{c}_k^{\dagger}) will denote the creation operator for a bosonic (resp. fermionic) particle in the state $|\phi_k\rangle$, and \hat{b}_k (resp. \hat{c}_k) will denote the annihilation operator for a bosonic (resp. fermionic) particle in the same state. In the case where no knowledge on the particle's family is required, creation and annihilation operators will be denoted \hat{a}_k^{\dagger} and \hat{a}_k respectively.

The first difference between bosonic and fermionic creation and annihilation operators is that the former satisfy to a commutation relation, while the latter satisfy to an anti-commutation relation. We have, for bosons:

$$[\hat{b}_{k}, \hat{b}_{k'}^{\dagger}] \equiv \hat{b}_{k} \hat{b}_{k'}^{\dagger} - \hat{b}_{k'}^{\dagger} \hat{b}_{k} = \delta_{kk'}$$
(1.1.24)

$$[\hat{b}_{k}^{\dagger}, \hat{b}_{k'}^{\dagger}] = [\hat{b}_{k}, \hat{b}_{k'}] = 0, \qquad (1.1.25)$$

and for fermions,

$$\{\hat{c}_k, \hat{c}_{k'}^{\dagger}\} \equiv \hat{c}_k \hat{c}_{k'}^{\dagger} + \hat{c}_{k'}^{\dagger} \hat{c}_k = \delta_{kk'}$$
(1.1.26)

$$\{\hat{c}_{k}^{\dagger}, \hat{c}_{k'}^{\dagger}\} = \{\hat{c}_{k}, \hat{c}_{k'}\} = 0 \tag{1.1.27}$$

The action of bosonic creation and annihilation operators on a bosonic Fock state are defined in the following way:

$$\hat{b}_{k}^{\dagger} |n_{0}n_{1}\cdots n_{k}\cdots\rangle_{+} = \sqrt{n_{k}+1} |n_{0}n_{1}\cdots n_{k}+1\cdots\rangle_{+}$$
$$\hat{b}_{k} |n_{0}n_{1}\cdots n_{k}\cdots\rangle_{+} = \sqrt{n_{k}} |n_{0}n_{1}\cdots n_{k}-1\cdots\rangle_{+}$$
(1.1.28)

Their fermionic counterpart is

$$\hat{c}_{k}^{\dagger} |n_{0}n_{1}\cdots n_{k}\cdots\rangle_{-} = (-1)^{s}\sqrt{1-n_{k}} |n_{0}n_{1}\cdots n_{k}+1\cdots\rangle_{-}$$
$$\hat{c}_{k} |n_{0}n_{1}\cdots n_{k}\cdots\rangle_{-} = (-1)^{s}\sqrt{n_{k}} |n_{0}n_{1}\cdots n_{k}-1\cdots\rangle_{-}, \qquad (1.1.29)$$

with $s = \sum_{i=0}^{k-1} n_k$. For details on these formulae, see e.g. [17]. The action of these operators is defined in such a way as to simplify the writing of operators in second quantization. Note that some of the coefficients that appear after the action of a creation/annihilation operator have a fairly instinctive form. First, applying the annihilation operator with label k on a state containing no particle in the state $|\phi_k\rangle$ should yield a null vector, and the coefficient $\sqrt{n_k}$ deals precisely with this case. Second, the coefficient $\sqrt{1-n_k}$ in equation (1.1.29) is 0 when a fermion in state $|\phi_k\rangle$ already exists, taking care of implementing the Pauli principle.

Operators in second quantization

Recall, as mentioned in (1.1.4), that an arbitrary one-body operator has the following development in \mathcal{H}_1 :

$$A = \sum_{k,k'} A_{kk'} \left| \phi_k \right\rangle \left\langle \phi_{k'} \right|, \qquad (1.1.30)$$

Because of how we defined creation and annihilation operators, it can be shown [17] that we can write it in second quantization as:

$$\hat{A} = \sum_{k,k'} A_{kk'} \hat{a}_k^{\dagger} \hat{a}_{k'}$$
(1.1.31)

where \hat{A} now belongs to the Fock space \mathcal{F} . Operators written in this way have a very simple interpretation: the action of the operator $\hat{a}_k^{\dagger} \hat{a}_k$ on a state is to destroy a particle in state $|\phi_{k'}\rangle$ and create a particle in state $|\phi_k\rangle$. The operator \hat{A} is obtained by taking each pair of one-particles states labels, k and k' and coupling the corresponding states, *i.e.* allowing for a transition between them, with a coupling constant $A_{kk'}$. Two-body operators can be considered in a similar fashion. Let B be a two-body operator acting in the space \mathcal{H}_2 . As previously stated, a basis of this space is given by the tensor products states $|\phi_{k_1}\phi_{k_2}\rangle$. Expressed in this basis, the two-body operator B takes the form

$$B = \sum_{k_1 k_2 k_1' k_2'} B_{k_1 k_2 k_1' k_2'} \left| \phi_{k_1} \phi_{k_2} \right\rangle \left\langle \phi_{k_1'} \phi_{k_2'} \right|$$
(1.1.32)

In second quantization, it can be shown that we have

$$\hat{B} = \frac{1}{2} \sum_{k_1 k_2 k_1' k_2'} B_{k_1 k_2 k_1' k_2'} \hat{a}_{k_1}^{\dagger} \hat{a}_{k_2}^{\dagger} \hat{a}_{k_2'} \hat{a}_{k_1'}$$
(1.1.33)

A notion that occasionally allows for simplification is the notion of a diagonalized operator. A one body operator is said to be diagonal in a given basis $\{|\phi_k\rangle\}_{k\in\mathbb{N}}$ if it can be expressed in this basis as

$$O = \sum_{k \in \mathbb{N}} \langle \phi_k | O | \phi_k \rangle | \phi_k \rangle \langle \phi_k |$$

=
$$\sum_{k \in \mathbb{N}} O_k | \phi_k \rangle \langle \phi_k |$$
 (1.1.34)

The physical interpretation of such operator is the following: assuming that the basis states are orthogonal to each other, the action of O cannot cause transitions between basis states. It acts on each basis state by multiplying it by a constant O_k . In second quantization, a diagonalized operator reads

$$\hat{O} = \sum_{k} O_k \hat{a}_k^{\dagger} \hat{a}_k \tag{1.1.35}$$

Using the relations (1.1.28) and (1.1.29), we observe that the operator $\hat{a}_k^{\dagger} \hat{a}_k$ simply counts the amount of particles in state $|\phi_k\rangle$. In the bosonic case, for example, we find:

$$\hat{b}_{k}^{\dagger}\hat{b}_{k}\left|n_{0}n_{1}\cdots n_{k}\cdots\right\rangle_{+} = \sqrt{n_{k}}\,\hat{b}_{k}^{\dagger}\left|n_{0}n_{1}\cdots n_{k}-1\cdots\right\rangle_{+}$$
$$= n_{k}\left|n_{0}n_{1}\cdots n_{k}\cdots\right\rangle_{+}$$
(1.1.36)

We thus give it the name of number operator for state $|\phi_k\rangle$, and denote it \hat{n}_k . Using the number operator, we can write a diagonalized one-body operator in Fock space as:

$$\hat{O} = \sum_{k} O_k \hat{n}_k \tag{1.1.37}$$

and it appears clearly that it acts on Fock states in the same way as it acts on the single-body state $|\phi_k\rangle$ but as many times as there is particles in state $|\phi_k\rangle$ in the Fock state. Operators up to N-body can be constructed as well, but the present work will not consider more than two-body interactions, and the corresponding operators.

1.2 Mixed many-body system with multiple sites

The aim of this work is to re-express the dynamics of a system of interacting fermions through the bosons that mediate interactions. For instance, the dynamics of a system of fermionic ions would be expressed using the photons that carry the electromagnetic interaction between them. In order to do so, we postulate a mixed system that will then be compared to the purely fermionic system. The specific system considered in this work is a periodic lattice of potential wells, also referred to as sites, containing fermionic particles, as shown in figure 1.1. The particles can interact with each other by boson exchange. For trapped fermions, an experimental realization of this type of system is given in [21], with ultracold fermionic atoms trapped in lattices formed of interfering laser beams, called optical lattices. The particles trapped in the lattice can experience a one-body interaction with the potential and a particle-particle interaction. The latter is modeled by a two-body interaction. Higher order interactions might occur but are expected to be significantly less likely than two-body interactions, and are thus neglected. Note that taking those interactions into account only adds to the computational complexity of the proposed method, and do not *a priori* bring any fundamental complication.



Figure 1.1: Schematic view of the system of interest. Fermionic particles, e.g. ⁶Li, are trapped in a 2-dimensional lattice of potential wells. Particles interact with the potential as well as with other particles. Reference: Jpagett, 2020. CC BY-SA 4.0

In order to simplify the description of the system, we make the approximation that the fermionic particles are well localized inside the sites, which is a common approach in the treatment of atoms on a lattice. One can more formally think about this step as expanding the state of the fermions in Wannier functions [8], which are a set of orthogonal and maximally localized functions particularly suited for describing particles in periodic potential wells. This allows for eliminating every spatial degree of freedom from the system except for a discrete index corresponding to the site containing the particle. We also make the assumption that only one energy level is available for the fermions. The state of a fermion is then described by the ket $|k, \sigma\rangle$ with k the site index of the fermion and σ its spin state. To each site is associated a state $|\psi_k\rangle$ representing the fermions in this site. Those states are for now generic Fock states. A representation more suited to our needs will be introduced in chapter 3.

What matters at the time being is to understand how the multiple sites of the system are handled. They are implemented using what is called product states. Product states are in some way an analog to the process of constructing the N-particle Hilbert space \mathcal{H}_N from the single-particle space \mathcal{H}_1 . The product state representing the system is the tensor product of each state representing individual sites. If the state of site 1 is $|\psi_1\rangle$, the state of site 2 is $|\psi_2\rangle$ etc, then a system with L sites is represented by the product state

$$|\psi\rangle = |\psi_1\rangle \otimes \dots \otimes |\psi_L\rangle \tag{1.2.1}$$

As already stated, only one energy level is considered for the fermions, and thus the only degree of freedom considered aside from the site is the spin of the fermion. Creation and annihilation operators acting only on a specific site are introduced in the following way: the annihilation operator associated with site k and spin σ , for example, is denoted $\hat{c}_{k,\sigma}$. It is defined as a tensor product of fermionic identity operators $\hat{\mathbb{1}}_F$ everywhere except at the k^{th} place where the annihilation operator for a fermion in spin state $|\sigma\rangle$ is inserted:

$$\hat{c}_{k,\sigma} = \hat{\mathbb{1}}_F \otimes \cdots \otimes \hat{c}_\sigma \otimes \hat{\mathbb{1}}_F \otimes \cdots \otimes \hat{\mathbb{1}}_F \tag{1.2.2}$$

Defined in this way, the operator $\hat{c}_{k,\sigma}$ only acts on the k^{th} site and leaves the others unchanged. The same construction is done for creation operators.

Now that the fermionic part of the system has been considered, we are left with the bosonic part. The bosons considered are not restricted to specific sites, and thus there is no requirement for a product state approach. A single state ϕ will represent the bosonic field. The total state of the system is simply the tensor product of the fermionic product state $|\psi\rangle$ and the state of the bosonic field $|\phi\rangle$:

$$|\Psi\rangle = |\psi\rangle \otimes |\phi\rangle \equiv |\psi\phi\rangle \tag{1.2.3}$$

We now move on to writing the Hamiltonian describing our system. The form taken by this Hamiltonian will be quite generic. It is similar to other lattice-many body models such as the Bose-Hubbard model [22] or the Fermi-Bose-Hubbard model [9, 21] but with two main differences. First, our Hamiltonian will need to belong to a mixed boson-fermion Hilbert space. Second, two-body interactions are in our case replaced by an interaction term between the fermions and the bosonic field. Let L/2 be the number of sites available in the lattice. The one-body fermionic Hamiltonian can be written in the following diagonalized form:

$$\hat{H}_F = \sum_{k=1}^{L/2} \sum_{\sigma=\uparrow\downarrow} E_{F,k\sigma} \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma}$$
(1.2.4)

with $E_{F,k\sigma}$ the energy associated to a fermion in site k with spin σ . Following [16], we simplify the notation by introducing an index μ for each pair of indices $k\sigma$. Since two spin states are available for each of the L/2 sites, the indices μ can take L different values and the Hamiltonian \hat{H}_F is written in the shorter form

$$\hat{H}_{F} = \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu}$$
(1.2.5)

In this way, spin states are treated as generalized sites. Figure 1.2 illustrates how such sites can be defined from spin states.



Figure 1.2: A way of converting the spin state of the particles into a degree of freedom analog to the site index. The spin is taken into account in the coupling constant between this new set of sites containing "spin up" and "spin down" sites. Adapted from T. Engl, 2015 [16].

Since \hat{H}_F belongs to the fermionic Fock space, it needs to be extended to the total (mixed) Hilbert space. The corresponding Hamiltonian in the total Hilbert space is $\hat{H}_F \otimes \hat{\mathbb{1}}_B$ with $\hat{\mathbb{1}}_B$ the bosonic identity operator. It will often be written as \hat{H}_F , by abusive notation. Assuming that there exist N distinct bosonic modes², the Hamiltonian for the energy associated to the bosonic modes is written as:

$$\hat{H}_B = \sum_{n=1}^{N} E_{B,n} \hat{b}_n^{\dagger} \hat{b}_n \tag{1.2.6}$$

Notice that \hat{H}_B is also assumed to be diagonalized. This is only possible because it lives in a different space than \hat{H}_F , and thus it is possible to find a basis of each space that makes these operators diagonal. Similarly to the case of \hat{H}_F , the abusive notation \hat{H}_B will be used for the total bosonic Hamiltonian $\hat{\mathbb{1}}_F \otimes \hat{H}_B$. So far, our Hamiltonian lacks an interaction between the fermions and the bosonic field, and so the term

$$\hat{H}_{int} = \sum_{\mu=1}^{L} \sum_{\nu=1}^{L} \sum_{n=1}^{N} C_{\mu\nu n} \hat{c}^{\dagger}_{\mu} \hat{c}_{\nu} (\hat{b}^{\dagger}_{n} + \hat{b}_{n})$$
(1.2.7)

is introduced to implement them, where μ and ν are again generalized site indices. This term allows two fermions to interact: first, a fermion emits a boson n and transitions from state $|\phi_{\nu}\rangle$ to state $|\phi_{\mu}\rangle$. The boson can then be absorbed by another fermion and cause it to change state as well, effectively representing an interaction between the two fermions. The coefficients $C_{\mu\nu n}$ are responsible for implementing coupling between different sites, including spin interactions. Note that unlike the one-body terms \hat{H}_F and \hat{H}_B , this interactions term changes the number of bosons in the system. The number of fermions, on the other hand, remains fixed as assumed.

The total Hamiltonian is simply the sum of each individual term. It reads:

$$\hat{H} = \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}^{\dagger}_{\mu} \hat{c}_{\mu} + \sum_{n=1}^{N} E_{B,n} \hat{b}^{\dagger}_{n} \hat{b}_{n} + \sum_{\mu=1}^{L} \sum_{\nu=1}^{L} \sum_{n=1}^{N} C_{\mu\nu n} \hat{c}^{\dagger}_{\mu} \hat{c}_{\nu} (\hat{b}^{\dagger}_{n} + \hat{b}_{n})$$
(1.2.8)

Now that the Hamiltonian describing the system has been established, Feynman's path integral theory will be introduced, with the aim to apply it to the Hamiltonian (1.2.8).

 $^{^{2}}$ The term "mode" will often be used for the bosons, replacing "state". Although both could be used, the former is preferred, since the bosonic part of the system of interest is the electromagnetic field.

Chapter 2

The Path Integral Formalism and Semiclassical Approximation

In 1942, R. Feynman submitted his doctoral thesis titled "The Principle of Least Action in quantum mechanics". Following earlier developments by Paul Dirac on a Lagrangian formulation $[10]^1$ of quantum mechanics, Feynman developed a new way of describing the dynamics of a quantum system based on the Lagrangian formalism of classical mechanics, whereas quantum mechanics had been predominantly based on the Hamiltonian formalism. Further developing his method eventually led him to formulate the path-integral formalism. This new formalism, being based on a Lagrangian rather than on an Hamiltonian, notably obeyed the symmetries required to allow for the unification of quantum mechanics and special relativity. The resulting theory is called Quantum Field Theory and is still to this day the dominant theory in the study of fundamental quantum processes. Another important feature of this formulation is that it allows for great insights on the semiclassical limit of a system [16], *i.e.* the limit where the action of the system (see section 2.1 for a refresher) is large compared to the fundamental quantum of action \hbar . Semiclassical approximations are of great interest for studies on quantum chaos [13, 14, 23]. In this chapter, the Lagrangian formalism of classical mechanics is briefly reviewed. Then, the Principle of Least Action, which is of fundamental importance in classical mechanics, is stated. The bridge with quantum mechanics and Feynman's work is made through the double slit experiment. The path integral formalism is then presented in two different ways, and applied to the case of a bosonic system. An emphasis is made on the quantum propagator, which is of great importance for several theoretical developments in the fields of condensed matter physics and quantum chaos [12, 14, 16, 23, 24]. The chapter ends with a discussion on the classical limit to the path integral, its relation to the Least Action principle and perspectives on the study of many-body quantum systems using the path integral formalism.

2.1 Principle of least action in classical mechanics

When searching for the equation of motion of a mechanical system, or in other words the path followed by a system, the Principle of Least Action seem to underlie many important results in a wide range of areas. It can be used to derive Newton's second law of motion, the classical theory of electrodynamics, as well as Einstein's equation in general relativity [25], among others.

Let us first clarify the notion of a path. We call "path" the trajectory followed by the system in a given space as a function of time. For instance, the trajectory of a ball falling free through the air is described by the evolution in time of its three coordinates x, y and z. We can summarize this problem as the determination of the vector $\vec{r}(t) = (x, y, z)$ representing the position of the ball. Another example would be the path of a simple pendulum, *i.e.* a mass suspended to a support by a weightless and inextensible string in a plane. In this case, determining the motion of the pendulum is equivalent to knowing the evolution of the polar coordinate $\theta(t)$ of the pendulum. Note that one could also think of using two spatial coordinates, named for instance x and y. However, since each point of the trajectory lies on a circle, there is a redundancy² as one can deduce the value of y from the value of x. In such cases where two variables are not independent, the formalism presented below requires that only one variable is kept.

¹The book by L. Brown contains a reproduction of the article by P. Dirac. The original article was published in Physikalische Zeitschrift der Sowjetunion, Band 3, Heft 1 (1933), pp. 64–72.

²To be more specific, the vertical coordinates is redundant when the angle of the pendulum do not excess $\pi/2$ in any of the two directions.

Generalized coordinates and the Lagrangian

There is no requirement to restrict the choice of coordinates for the system to spatial coordinates. Instead, it is only required from the set of coordinates that they be independent of each other, and that they entirely characterize the state of the system, *i.e.* that they cover every degree of freedom of the system. Such coordinates are called generalized coordinates. More formally, we denote by \mathbf{q} the generalized coordinates characterizing the system we are interested into. For instance, the generalized coordinates of the free-falling ball are $\mathbf{q}(t) = \{x(t), y(t), z(t)\}$. Even though in this case, they represent a spatial vector, it is not generally the case, which justifies that the notation \mathbf{q} is favoured over \vec{q} . Note also that the time dependency of the generalized coordinates \mathbf{q} is often implicit. In the discussions that follow, functions $f(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)$ will often be shortened to $f(\mathbf{q}, \dot{\mathbf{q}}, t)$ for readability concerns.

Using these generalized coordinates and the generalized velocities $\dot{\mathbf{q}}(t)$, where the dot denotes the derivative with respect to time, one can express the Lagrangian of the system, which is simply given by its kinetic energy T minus its potential energy V:

$$\mathcal{L} = T - V \tag{2.1.1}$$

where \mathcal{L} , T and V are functionals: they are functions of time, but also of the generalized coordinates $\mathbf{q}(t) = \{q_1(t), \ldots, q_N(t)\}$, the generalized velocities $\dot{\mathbf{q}}(t) = \{\dot{q}_1(t), \ldots, \dot{q}_N(t)\}$, which are themselves functions. Let us now show how to use the Lagrangian to determine the path of the system, which in this example will be a free-falling ball. Assume that the free-falling ball is subjected to gravity only. Denoting the mass of the ball by m and using z as the vertical axis, the Lagrangian of the falling ball reads

$$\mathcal{L}_{ball}\left(\mathbf{q}, \dot{\mathbf{q}}, t\right) = \frac{1}{2}m\left(\dot{x}^{2}(t) + \dot{y}^{2}(t) + \dot{z}^{2}(t)\right) - mgz$$
(2.1.2)

The equations of motion of the system can be obtained from its Lagrangian \mathcal{L} using the Euler-Lagrange equations:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) = \frac{\partial \mathcal{L}}{\partial q_i} \tag{2.1.3}$$

This equation, central in Lagrangian mechanics, is of great importance in many areas of physics including classical field theory, optics, and quantum field theory, and is a direct consequence of the Principle of Least Action. A noteworthy application of Lagrangian mechanics is Noether's theorem, proven in 1915 by mathematician Emmy Noether. It states that to each continuous symmetry of a Lagrangian corresponds a conservation law. For instance, the invariance of the Lagrangian of a system by time translation yields the conservation of the total energy of the system. This theorem is extensively used in Quantum Field Theory to derive conserved quantities for a given Lagrangian. Note that Noether's theorem also extends to symmetries that leave the Lagrangian invariant up to the time derivative of an arbitrary function, as adding such a term do not modify the equations of motion. However, this discussion is out of the scope of this introduction.

Back to the dynamics of the free-falling ball, we can find the equation of motion for say, z(t), by applying the Euler-Lagrange equation (2.1.3). We obtain

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}_{ball}}{\partial \dot{z}} \right) = \frac{\partial \mathcal{L}_{ball}}{\partial z} \quad \Leftrightarrow \quad \ddot{z} = g \tag{2.1.4}$$

which is exactly the result obtained using Newton's second law of motion. In the same way, we find $\ddot{x} = \ddot{y} = 0$, the expected result as there is no force acting in the x or y direction for a free-falling ball.

The Principle of Least Action

Before exposing the Principle of Least Action, we must first define the action of a system. Using the Lagrangian defined above, we define the action of a system by

$$S = \int_{t_i}^{t_f} \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, t) \, dt \tag{2.1.5}$$

The action takes a value for each path of the system, given by its position $\mathbf{q}(t)$ and velocities $\dot{\mathbf{q}}(t)$ between time t_i and t_f . It can thus have different values for different paths. The Principle of Least Action states that the real trajectory followed by the system, in other words the solution to the equations of motion for the system, is a stationary point of the action functional. More formally, if $\bar{\mathbf{q}}(t)$ is a real trajectory of the system, then the quantity

$$S = \int_{t_i}^{t_f} \mathcal{L}(\bar{\mathbf{q}}, \dot{\bar{\mathbf{q}}}, t) \, dt \tag{2.1.6}$$

is stationary with respect to small changes in $\bar{\mathbf{q}}$. This is more often expressed as a variational problem : consider a path $\bar{\mathbf{q}}(t)$. It is a real trajectory of the system if an infinitesimally small perturbation $\epsilon(t)$ around the trajectory leaves the action invariant :

$$\delta S = \int_{t_i}^{t_f} \delta \mathcal{L}(\bar{\mathbf{q}}, \dot{\bar{\mathbf{q}}}, t) = \int_{t_i}^{t_f} \left[\mathcal{L}(\bar{\mathbf{q}} + \epsilon, \dot{\bar{\mathbf{q}}} + \dot{\epsilon}, t) - \mathcal{L}(\bar{\mathbf{q}}, \dot{\bar{\mathbf{q}}}, t) \right] dt = 0$$
(2.1.7)

From this equation, the Euler-Lagrange equations can be derived, as well as Newton's equation of motion and Hamilton's equations, which are another important formulation of classical mechanics. In the quantum mechanical world, this equation can be used in a certain framework to obtain the dynamics of all quantum fields. Those fields describe the physics of every known particle and all known fundamental interactions except for gravitation. Their study has yielded theories such as Quantum Electrodynamics, which is often referred to as the "most precisely tested theory of physics". The generality of this principle is still a mystery today, and it is a very important object from a philosophical point of view [26]. In any case, it is safe to say that the Least Action Principle is one of the most important principles of modern physics.

To conclude this section, we mention that there is in fact no requirement for the action to be minimal for the principle to apply. It suffice for the action to be stationary. The name "Stationary-Action Principle" is thus more appropriate. However, the name "Principle of Least Action" was used by Feynman in its thesis and subsequent development of what is called the Path integral formulation of quantum mechanics [11], which is the subject of the remaining sections of chapter 2. Path integrals have many applications in theoretical physics. The most notable of them probably being the path-integral formulation of quantum field theory, which is one of the most influential theories in modern physics and the closest we currently have from a theory of everything. It might, then, be reasonable to assume that Feynman had a role to play in the use of the slightly misleading appellation of "Least Action Principle".

2.2 The double slit experiment

The classical Principle of Least Action cannot be applied as it stands to quantum mechanics as will be seen shortly. It was Dirac's work, continued and completed by Feynman, that provided an equivalent of the principle (2.1.7) for quantum mechanics. A famous experiment that highlights the inadequacy of the Least Action Principle for quantum mechanics is the double slit experiment. We will also come back to this experiment for insights on the path integral formalism.

The double slit experiment (see figure 2.1 and 2.2) was first performed with visible light. A beam of photons reaches an opaque screen with two holes in it. Photons pass through either of the two holes and are then stopped by a screen. Information about where they are stopped is collected. Putting together data for large enough numbers of photon reveals a periodic succession of areas that collected few photons and areas that collected many. These results can be explained by the wave-like behaviour of light. The two waves associated with photons passing through one slit or the other can then interfere constructively or destructively as illustrated in figure 2.1, producing the observed interference pattern that appear on the detecting screen in figure 2.2.

With the arrival of quantum mechanics, massive particles like electrons or protons were assumed to exhibit a wave-like behaviour as well. The double slit experiment provided a fairly straightforward way of testing this assumption and results similar to those obtained with light were indeed observed in 1961 with electrons [27, 28], thus confirming the relevance of the quantum view of particles. More recent works have extended double-slit experiments to molecules [29, 30], yielding once again results in accordance with the wave-like behaviour of matter predicted by quantum mechanics. For electrons, protons, and matter in general, the interference occurs between the wave functions associated to particles passing by either slit. These wave functions represent the probability of presence of matter particles at a given point in space. Depending on the phase difference between waves, this interference can again be destructive or constructive. A destructive interference at a given point means a low amplitude of the wave function at that point, and thus a low probability of finding particles. Constructive interference, on the other hand, corresponds to high probability of finding particles. Since even a single particle is described by a wave-function in quantum mechanics, a particle can interfere with itself. As a consequence, the same interference pattern should be observed even when particles are fired one by one, a particle being emitted only after the previous one has hit the screen. This was observed in 1976 [31], again with electrons.

The above discussion has a fundamental consequence on the notion of the path of the system in quantum mechanics. Let us first consider what the result of the double experiment would be if particles behaved classically. In that case, particles found at a certain point x either came from the first slit or the second. The probability of finding a particle at point x is then given by the probability that the particle reached x after going through the first slit plus the probability that it reached x coming from the second slit. One could measure those probabilities experimentally by firing the beam with one slit closed and the other opened, and counting the amount of particles



Figure 2.1: Diffraction of light by two slits at a fixed time. By virtue of the superposition principle, the wave amplitude at each point is the sum of the amplitudes of each individual wave. The black lines represent the wavefronts, *i.e.* the points in space where the amplitude of the wave is maximal. Constructive interference occur where the two waves are in phase, *i.e.* that they are either both maximal or both minimal at that point. Destructive interference occurs where one wave is minimal when the other is maximal, meaning that the resulting amplitude is zero. This image belongs to the public domain.



Figure 2.2: Schematic view of the double slit experiment. In this particular instance, a beam of particles comes from the left. Classically, particles would go through either of the slits and reach the screen. Quantum mechanically though, individual particles can have a component of their wave function go through each slit. The components can interfere constructively or destructively, creating interference patterns on the detecting screen. Reference: Johannes Kalliauer, 2017. CC BY-SA 4.0.

that have reached x. Then, one could swap which slit is closed and which is opened and repeat the experiment. The sum of the two probabilities would then yields the correct probability for classical particles to reach point x on the detecting screen. Quantum mechanically though, it was just mentioned that the wave function describing the particles produced interference because of the slits, resulting in an interference pattern on the detecting screens. These results cannot be resembled by an argument similar to the classical case. In other words, we cannot express the quantum probability of finding a particle at point x as a sum of two independent probabilities. This is shown in figure 2.3, where the probabilities computed by closing slits in the quantum case are compared to the real probability distribution observed in experiments. What emerges from this discussion is that the notion of the "path taken by the particles" makes no sense. Even in the simple case of the double slit experiment, the two possible paths for the particles interact with each other and can't be seen as independent. There is thus no "path taken by the particles". Instead, each path needs to be taken into account in order to obtain the correct probability [11].



Figure 2.3: Probability P of finding particles at the position x on a 1-dimensional slice of the screen when (a) both slits are opened, (b)(c) only one slit is opened. The sum of the probability distributions b and c is given in (d). If the paths associated to taking either slit were independent, curves a and d would be equal. Diagram taken from Feynman's textbook on path integrals [11], p.4.

2.3 Feynman's path integral

In the previous section, it was concluded that the concept of the "path taken by the particle" made no sense, because paths are not independent from one another and thus cannot be separated into distinct trajectories. As a consequence, the classical Principle of Least Action cannot be applied. Indeed, even if a trajectory of a quantum system was to minimize (2.1.6), it would be absurd to call it the "trajectory of the system".

Since the question of the path followed by the system is not a sensible one, we must content ourselves with describing the evolution of the system using another quantity, namely the amplitude of probability of going from an initial state $|\psi_i\rangle$ to a final state $|\psi_f\rangle$ [11]. Note that in the particular case of the double slit experiment, the initial state was fixed. We now search for a way of describing this probability using the concept of paths. Recall that in section 2.2, the interference patterns for the wave function of the particles were associated with a phase difference between the waves coming from either of the slits. For instance, if the two waves are out of phase from a factor π at a point, they interfere destructively and the probability to find a particle at that point is zero. This idea will now be formalized as we summarize the core idea of Feynman's path integral.

Lagrangian path integral formulation

Starting from the observation that probabilities are related to phase differences, the natural way of computing probabilities in the simple case of the double slit experiment is the following: given a point in space, sum the phase factors associated to the two paths "the particle went through the first slit and reached the point" and "the particle went through the second slit and reached the point". Obtaining the value of the phase factor for a given path was one of the achievements of Feynman's thesis [10]. Expressed as a functional of the taken path $\psi(t)$, it has the expression [11]:

$$\Phi[\psi(t)] = C \, \exp\left(\frac{i}{\hbar}S[\psi(t)]\right) \tag{2.3.1}$$

with C a normalization constant that will not be of any importance in the present discussion and that will be omitted from now on. $S[\psi(t)]$ is the action of the path $\psi(t)$ as defined in (2.1.6). The probability amplitude to find the particle at a point x on the screen, called the propagation amplitude to x, is then given by

$$K(x) = \Phi_1(x) + \Phi_2(x) \tag{2.3.2}$$

with $\Phi_1(x)$, $\Phi_2(x)$ the phase factors for the path that passes through the first and the second slit respectively. The probability is then computed as it is standard in quantum mechanics by the square of the amplitude:

$$P(x) = |K(x)|^2 = |\Phi_1(x) + \Phi_2(x)|^2$$
(2.3.3)

This expression is notably different from the sum of the individual probabilities $|\Phi_i(x)|^2$ to reach the point x if slits other than the i^{th} were obstructed. If we now consider a system more complex than the double slit experiment, some additional comments are required. First, the initial state of the system is not restricted to a particle fired by a source anymore. It must therefore be included in the expression for the amplitude. In general, we write the propagation amplitude from a state $|\psi_a\rangle$ to a state $|\psi_b\rangle$ as $K(\psi_a, \psi_b)$. Second, there can be any number of paths



Figure 2.4: Three paths relating the initial state q_4 at time t_0 to the final state q_3 at time t_{10} . Time is discretized, and the state of the system at each discrete time is represented by a generalized coordinate **q**. The set of all paths relating the initial and final states is obtained by considering each combination of one coordinate q_i per time t_m . The path integral thus consider paths with discontinuities corresponding to quantum tunneling effects such as the green and blue paths, which would not exist in a classical description of the system.

between two arbitrary states of the system, especially when non-classical paths are considered. See for instance figure 2.4. Third, time is now considered as a variable as well. The general way of writing the amplitude between two states $|\psi_i\rangle$ at the time t_i and $|\psi_f\rangle$ at time t_f is given by:

$$K(\psi_f, t_f; \psi_i, t_i) = \sum_{\psi \in P} \Phi[\psi(t)] = \sum_{\psi \in P} \exp\left(\frac{i}{\hbar} S[\psi(t)]\right)$$
(2.3.4)

with P the set of all paths $\psi(t)$ such that $\psi(t_i) = \psi_i$ and $\psi(t_f) = \psi_f$. It might not be obvious that this last expression generalizes the classical Principle of Least Action (2.1.7), but it will be shown in section 2.4 that it is indeed the case.

The complexity of evaluating this expression lies both in the fact that there can be infinitely many paths relating the two states considered, and in finding ways of expressing every such paths. One way was developed by Feynman in order to make the computation of (2.3.4) more practical [10, 11]. If the state of the system can be described by a set of generalized coordinates \mathbf{q} , then the set of paths relating the two states can be constructed by discretizing the time interval $[t_i, t_f]$ into M time steps t_0, t_1, \ldots, t_M with $t_0 \equiv t_i$ and $t_M \equiv t_f$. All the possible paths are then characterized by letting the state of the system at each time t_j take any possible value $\mathbf{q}(t_j) \equiv \mathbf{q}_j$ as shown in figure 2.4. If \mathbf{q} is a continuous parameter as in most real cases, the process of summing over every discretized path amounts to computing an integral over all values of \mathbf{q} for each time step, giving the path integral its name. This idea of discretizing space and time to represent paths will be used in more detail in the discussion that follow, where the path integral from the Hamiltonian formalism is presented.

Hamiltonian path integral formulation

We shall now introduce the propagator starting from the Hamiltonian formalism. We do so for two main reasons. First, this new formulation makes use of the Schrödinger equation, which the reader is probably familiar with. Obtaining formulae from several ways allows for testing the consistency of our knowledge. The second reason is simply that we mainly work with Hamiltonians. A proof of the equivalence of the two methods will not be presented in general, but it will be shown for an illustrative example in section 3.3. See e.g. [17] for a general proof.

We begin by considering a generic quantum system described at time t by a state vector $|\psi(t)\rangle$, and the operator that takes the state of the system at time t_i to the state of the system at time t_f :

$$\hat{K}(t_f; t_i) |\psi(t_i)\rangle = |\psi(t_f)\rangle \tag{2.3.5}$$

This operator is called the propagator of the system. The name will be justified shortly, after the general expression for the propagator has been obtained. The state of the system satisfies to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}(t)\left|\psi(t)\right\rangle \tag{2.3.6}$$

with $\hat{H}(t)$ the Hamiltonian representing the energy of the system. Following [16] we substitute the state $\hat{K}(t_0, t) |\psi(t_0)\rangle$ for $|\psi(t)\rangle$ in equation (2.3.6). By projecting the equation on $\langle \psi(t_0) |$, we obtain for \hat{K} :

$$i\hbar\frac{\partial}{\partial t}\hat{K}(t;t_0) = \hat{H}(t)\hat{K}(t;t_0)$$
(2.3.7)

with the initial value condition

$$\hat{K}(t_0; t_0) = \hat{\mathbb{1}}$$
 (2.3.8)

The solution to this equation is

$$\hat{K}(t,t_0) = \hat{T} \exp\left(-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') \, dt'\right)$$
(2.3.9)

with \hat{T} the time ordering operator. The operator \hat{T} sorts the product of operators right to it in chronological order such that every operator in the product is evaluated at a time larger than its neighbour to the right. Without time ordering, the propagator $\hat{K}(t, t_0)$ would contain terms with Hamiltonian operators in the wrong chronological order, which does not make physical sense. Evaluating time-ordered expressions is not an easy task in general, although some results such as Wick's theorem exist to handle them. Fortunately for us however, the system we are interested in is described by the time-independent Hamiltonian mentioned in equation (1.2.8). The expression for the propagator between times t_0 and t, equation (2.3.9), thus simplifies to

$$\hat{K}(t,t_0) = \exp\left(-\frac{i}{\hbar}(t-t_0)\hat{H}\right)$$
(2.3.10)

Let's now consider matrix elements of the propagator. Let $|\psi_i\rangle$ and $|\psi_f\rangle$ be two possible states for the system. The probability of measuring the system in state $|\psi_f\rangle$ at time t_f if it was in state $|\psi(t_i)\rangle \equiv |\psi_i\rangle$ at t_i is given by

$$\left|\left\langle\psi_{f}\left|\psi(t_{f})\right\rangle\right|^{2} = \left|\left\langle\psi_{f}\left|\hat{K}(t_{f};t_{i})\left|\psi(t_{i})\right\rangle\right|^{2} = \left|\left\langle\psi_{f}\left|\hat{K}(t_{f};t_{i})\left|\psi_{i}\right\rangle\right|^{2} = \left|K(\psi_{f},t_{f};\psi_{i},t_{i})\right|^{2}$$
(2.3.11)

This object is exactly the same as that described in equations (2.3.3) and (2.3.4) since it also gives the probability of transition from state $|\psi_i\rangle$ at time t_i to state $|\psi_f\rangle$ at time t_f . The two formulations differ by the way they express the propagation amplitude³ $K(\psi_f, t_f; \psi_i, t_i)$: equation (2.3.4) for the original Feynman's formulation and the matrix elements of the operator defined in equation (2.3.9) for the Hamiltonian formulation.

We now work towards expressing the propagation amplitude as a path integral. First, we use the fact that \hat{H} commutes with itself in order to split the exponential into M exponentials. A reader not familiar with the process of splitting exponentials of commuting quantities other than numbers can consult appendix D where a general proof for this property is presented. In the case of out propagator, it yields

$$\exp\left(-\frac{i}{\hbar}(t_f - t_i)\hat{H}\right) = \exp\left(-\frac{i}{\hbar}\sum_{m=1}^M \Delta t\,\hat{H}\right) = \prod_{m=1}^M \exp\left(-\frac{i}{\hbar}\Delta t\,\hat{H}\right)$$
(2.3.12)

with $\Delta t = \frac{t_f - t_i}{M}$. Physically, it means that for time-independent Hamiltonians, applying the propagator once for a time $t_f - t_i$ is the same as applying it M times for a time $\frac{t_f - t_i}{M}$. As we are interested in physical quantities such as probabilities rather than operators, we now consider the propagation amplitude $K(\psi_f, t_f; \psi_i, t_i)$. The step we're about to perform is arguably the most important, as it will shed light on the link between the current development and the notion of paths. Starting from equation (2.3.12), we have for the propagation amplitude:

$$K(\psi_f, t_f; \psi_i, t_i) = \left\langle \psi_f \left| \prod_{m=1}^M \exp\left(-\frac{i}{\hbar} \Delta t \, \hat{H}\right) \right| \psi_i \right\rangle$$
(2.3.13)

We then insert a closure relation between each of the M terms of the product. To keep the discussion general, we consider generic closure relations of the form

$$\int d\psi_i |\psi_i\rangle \langle \psi_i| = \hat{\mathbb{1}}, \qquad (2.3.14)$$

where ψ_i is a generic notation for a set of degrees of freedom that entirely characterize the state of the system. It can include the position of the particles, their energy states, etc. If the degree of freedom is discrete, e.g. in

 $^{^{3}}$ Note that the name "propagator" is sometimes used for the propagation amplitude by misuse of language. If a difference has to be made, the propagator will represent the operator whereas the propagation amplitude will represent matrix elements of this operator.

the case of a spin, the integral is replaced by a sum over each possible discrete value. In both cases, these closure relations run over all possible value of the degrees of freedom describing the system. Introducing the convenient notations $|\psi_i\rangle \equiv |\psi_0\rangle$ and $|\psi_f\rangle \equiv |\psi_M\rangle$, the propagation amplitude reads

$$K(\psi_M, t_M; \psi_0, t_0) = \int d\psi_{M-1} \cdots \int d\psi_1 \left\langle \psi_M \left| \exp\left(-\frac{i}{\hbar} \Delta t \,\hat{H}\right) \right| \psi_{M-1} \right\rangle \times \cdots \times \left\langle \psi_1 \left| \exp\left(-\frac{i}{\hbar} \Delta t \,\hat{H}\right) \right| \psi_0 \right\rangle$$
$$= \prod_{m=1}^{M-1} \left[\int d\psi_m \right] \prod_{m=1}^M \left[\left\langle \psi_m \left| \exp\left(-\frac{i}{\hbar} \Delta t \,\hat{H}\right) \right| \psi_{m-1} \right\rangle \right]$$
(2.3.15)

The integral $\prod_{m=1}^{M-1} \left[\int d\psi_m \right]$ is recognized as running over all possible paths between the initial and final states in the discrete-time configuration space of the system, in a similar way as shown in figure 2.4. In the limit where $M \to \infty$, the time axis becomes continuous and the expression (2.3.15) effectively computes a sum over all possible paths between the two points $|\psi_0\rangle$ and $|\psi_M\rangle$.

This result can be illustrated by recalling the double slit experiment. Imagine that instead of an opaque screen with two slits, an opaque screen with a number N of slits was introduced between the source and the detecting screen. The probability of detecting a particle at position x on the detecting screen is computed following Feynman's idea, by considering a path for each possible slit. Now, imagine that the number of slits on the opaque screen increases and becomes infinite, in a manner such that the slits form a continuum on the screen. Paths can now be characterized by a continuous parameter x_1 and the sum over paths can be done by an integral over x_1 . This corresponds to the introduction of a closure relation over the parameter x_1 . Now suppose that instead of just one opaque screen with a continuum of slits, several such screens were placed between the source and the detecting screen. These multiple screens are then seen as multiple closure relations as in (2.3.15). The particles can pass through any of the slits of the first screen, any of the slits of the second screen, etc. Between each screen, the particles needs to be propagated. Each passage from a screen to another or from the source to the first screen is represented by a factor $\langle \psi_m | \exp\left(-(i/\hbar)\Delta t \hat{H}\right) | \psi_{m-1} \rangle$ called an elementary propagator. In the limit where M goes to infinity, this infinite product of terms represent the evolution of the free particle in space.

2.4 The semiclassical approximation and stationary-phase approximation

The aim of this section is to provide the reader with an outlook on the applications of this work's goal. The propagator as presented is in many practical cases difficult to compute, and one has to rely on approximations. Semiclassical approximation are a class of approximations to the propagator that attempt to describe a given quantum system using only classical quantities, such as classical paths. By expressing a system of many fermions using only the bosons that carry interactions, one can hope to leverage the many approximations to the propagator that exist in the literature and that have not yet been generalized to generic many-fermions systems [16]. We will first attempt to summarize important results of semiclassical approximations to many-body system. The stationary-phase approximation will then presented. Since this approximation is not yet applied in this work, a first-time reader may only read the qualitative description and safely skip the mathematical developments. This semiclassical approximation is the key ingredient for deriving the van Vleck-Gutzwiller propagator from Feynman's path integral, and has a wide range of applications [13, 14, 16, 18], making it a promising tool in the pursuit of this work's goal.

Brief summary of semiclassical results

An early derivation of an approximation to the quantum-mechanical amplitude using only a classical trajectory was written by J. H. van Vleck back in 1928 [32]. The resulting formula already included an exponential factor containing the classical action divided by the quantum of action \hbar , as in (2.3.4), allowing for discussions when the action was significantly greater than \hbar . This case will be referred to as the semiclassical limit and will be discussed in the context of the stationary phase approximation. The next commonly recognized milestone in semiclassical approximations to the propagator was set more than forty years later by M. C. Gutzwiller in a series of four papers [12, 33–35], based on Feynman's path integral which had since appeared. The result obtained was similar to van Vleck's formula, and was in fact recognized as a refinement to the latter (by Gutzwiller among others [36]). It is therefore called the van Vleck-Gutzwiller propagator and is written down below. We also mention that van Vleck's formula can be used as a starting point to derive Gutzwiller's [24]. The main addition made by Gutzwiller to van Vleck's formula is to take into account several classical trajectories instead of just one, allowing for effects such as interference between trajectories that are necessary for an accurate description of some quantum phenomena. We would now like to write down the van Vleck-Gutzwiller propagator, because of its fundamental importance for many other results [23, 24, 36, 37] but also because it represents an example of the stationary phase approximation to be discussed shortly. Neither a proof nor a detailed discussion of its application will be presented here. We redirect the interested reader to the textbook written by Gutzwiller himself [36]. For a single particle in position representation, the van Vleck-Gutzwiller propagator in d spatial dimensions reads [13]

$$K(\mathbf{r}_f, t_f; \mathbf{r}_i, t_i) = \sum_{\mathbf{r} \in P} \frac{1}{(2i\pi\hbar)^{d/2}} \sqrt{\left|\frac{\partial^2 S_{\mathbf{r}}}{\partial \mathbf{r}_i \partial \mathbf{r}_f}\right|} \exp\left(\frac{i}{\hbar} S_{\mathbf{r}} - i\frac{\pi}{2}\nu_{\mathbf{r}}\right)$$
(2.4.1)

with $S_{\mathbf{r}}$ the action for path \mathbf{r} as defined in (2.1.6) and P the set of classical paths defined on $[t_i, t_f]$ such that $\mathbf{r}(t_i) = \mathbf{r}_i$ and $\mathbf{r}(t_f) = \mathbf{r}_f$. The indices $\nu_{\mathbf{r}}$ are an addition from Gutzwiller to the van Vleck propagator [12], and are referred to as Maslov indices [13]. Here, we will simply say that these indices take into account some topological characteristic of the paths $\mathbf{r}(t)$.

This result however was derived for single-particle dynamics. Additional work had to be done to extend it to the many-body domain and this area of research is still relatively new. It is nonetheless a very rich field as can be seen from the review article by K. Richter [13]. In this review, the many-body van Vleck-Gutzwiller propagator is obtained in the case of bosons. Examples of its application such as the study of coherent backscattering [38] or the spectral properties of many-body systems [14] are also presented. The fermionic case is less well covered from a literature point of view. Worth mentioning is the example of spin-chains, which are systems of many interacting spins. Such systems have immediate applications in quantum information. One of the few theoretical tools available for studying them was obtained in [39] using the Truncated Wigner Approach, an approach that can be in most cases obtained from the many-body van Vleck-Gutzwiller propagator [13]. As was stated in the introduction, the more abundant body of literature available in the bosonic case provides an important motivation for re-expressing a fermionic propagator in terms of bosonic degrees of freedom.

An interested reader who would have consulted the provided references for this section would immediately notice that the term "quantum chaos" appears a lot. Aside from the fact that many-body systems are intrinsically chaotic, this can be explained by the fact that the van Vleck-Gutzwiller propagator allows for computing the dynamics of integrable and chaotic systems regardless [13] and is thus a very useful tool for studying quantum chaos. It was in fact successfully applied to many single-particle chaotic systems, a list of which can be found in [16] or in F. Hakee's textbook on quantum chaos [23]. The link between the semiclassical approximation to the propagator and quantum chaos, along with the abundant literature on the latter provides yet another motivation for the development of semiclassical approaches to many-body fermionic systems.

Stationary phase approximation

The van Vleck-Gutzwiller propagator is essentially obtained from Feynman's path integral formulation of the propagator by assuming that the action of the system is much larger than the fundamental action quantum \hbar . As a consequence, only a subset of all possible paths will contribute significantly to the phase, which allows for more practical computations. Looking back at (2.3.4), we see that for actions that are large as compared to \hbar , the argument of the exponential in the phase of a given path $\psi(t)$ of the system,

$$\Phi[\psi(t)] = \exp\left(\frac{i}{\hbar}S[\psi(t)]\right), \qquad (2.4.2)$$

is then very large, causing very fast oscillation of the imaginary exponential for small variations in the path. The probability amplitude contributions of neighbouring paths are then very unlikely to interfere in a constructive way since they have very different phase contributions. Therefore, large contributions to the probability amplitude are only expected from regions where changes in paths make only little change to the action, with a maximum effect where the action S is stationary with respect to small changes in paths. As the action gets larger and larger, large oscillations will occur for smaller and smaller variations, to the point where paths leaving the action stationary are the only one left to contribute. Paths that leave the action stationary are immediately recognized as the classical paths introduced in the context of the classical Principle of Least Action in section 2.1. One can then hope to compute the dynamics of a quantum system with an action large enough using only classical paths. The resulting approximation is thus a semiclassical one according to our definition.

The limit where the action becomes large as compared to \hbar is called the semiclassical limit as it corresponds to systems that move further and further away from the quantum domain (e.g. with large masses, number of particles, times etc). We note that because the paths to be considered in this case are the classical ones, the phase-integral (2.3.4) in the classical limit recovers the classical Principle of Least Action. As a result, this principle is sometimes



Figure 2.5: (a) Oscillating exponential for $s(x) = x^2$ and $\lambda = 1$ (b) The value of the integral $I(x) = \int_{-\infty}^{x} \exp(i\lambda s(x))$ for $\lambda = 1$ and (c) I(x) for $\lambda = 10$. We see that the bigger the λ , the less values of x other than x = 0 contribute to the integral. Note that these examples are far several orders of magnitude smaller than what is expected from values of the action in the classical limit. They are thus only illustrative.

referred to as "quantum Principle of Least Action" even though considerations on minimizing the action are not part of it aside from the classical limit.

The computation of quantities such as (2.3.4) in the case of very fast oscillation of the imaginary exponentials can be done using what is called the stationary phase approximation. Since this approximation will only be used qualitatively in future discussions, the mathematical considerations presented below may be skipped without affecting the reader's understanding of upcoming calculations. It is however a fundamental approximation in the context of our goal, and a brief overview of the mathematical aspects of it is presented below. For a comprehensive treatment, see e.g. [17] or [36]. Suppose that we have to evaluate an integral of the form

$$I = \int_{-\infty}^{+\infty} dx f(x) \exp\left(i\lambda s(x)\right)$$
(2.4.3)

When λ is large as compared to 1, the imaginary exponential oscillates very fast for small variations of s(x). In that case, the only significant contributions to the integral come from regions where s is stationary with respect to x. This is illustrated in figure 2.5. In order to compute an integral of this form, denote by x_j the set of stationary points of the function s(x). Around those points, the function s(x) does not vary to first order. The integral can then be approximated as a sum of contributions, with one term for each stationary point:

$$I \approx \sum_{x_j} \int_{x_j - \epsilon}^{x_j + \epsilon} dx f(x_j) \exp\left(i\lambda \left(s(x_j) + \frac{1}{2} \frac{\partial^2 s(x)}{\partial x^2}\Big|_{x = x_j} x_j^2\right)\right)$$
(2.4.4)

with ϵ a parameter that becomes smaller the bigger λ gets. The value of this integral is found to be [16]:

$$I \approx \sum_{x_j} f(x_j) \sqrt{\frac{2i\pi}{\lambda \left|\frac{\partial^2 s(x)}{\partial x^2}\right|}} \exp\left(i\lambda s(x_j)\right)$$
(2.4.5)

In the case of a multivariate function $s(\mathbf{x})$, the quantity $\left|\frac{\partial^2 s(x)}{\partial x^2}\right|$ becomes the determinant of the Hessian matrix $\left(\frac{\partial^2 s(\mathbf{x})}{\partial x_i \partial x_j}\right)_{ij}$. This determinant is the one that occur in the van Vleck-Gutzwiller propagator (2.4.1).

Results involving stationary phase approximations are common in the description of many-body systems as discussed in the summary of semiclassical results presented in the beginning of the current section. In particular, semiclassical approximations to bosonic systems have received considerable attention [13, 14, 38, 40]. By re-expressing a fermionic system as a set of bosonic degrees of freedom, one could hope to exploit established results in new situations. Working towards this goal, the next chapter sees the introduction of the coherent state representation for states of Fock space. Using this representation, the next chapter will describe the path-integral theory of a mixed system, which will then be applied to the system under consideration in chapters 4 and 5.

Chapter 3

Path Integral in Terms of Coherent States

When considering the path integral theory of a many-body system, two options are usually considered for representing the state of the system. The first one is the position $|\mathbf{r}\rangle$ and momentum $|\mathbf{p}\rangle$ representation of quantum mechanics. The second representation for many-body path integrals, commonly used in the context of many-body systems, is the coherent-state representation [9, 14, 16]. Coherent states are Fock states constructed in a way such that they are right eigenstates of the annihilation operator. They are thus a natural choice for dealing with Hamiltonians and operators expressed in second quantization. They can be obtained both for bosons and fermions. They form an (overcomplete) basis of the Fock space, meaning that any Fock state can be expanded in terms of coherent states. Bosonic coherent states also have interesting properties that have led to them being called the "most classical" quantum states [41]. This chapter introduces the concept of coherent states for bosons and derive their general form in terms of Fock states. In order to obtain coherent states for fermions, a special kind of number is then introduced. Those numbers are called Grassmann numbers and have the property of being anti-commutative. Other properties of Grassmann numbers as well as those of functions of Grassmann numbers are derived. Fermionic coherent states are then constructed. The chapter is concluded with the formulation of the coherent state path integral and its illustrative application to a very simple case of a mixed system.

3.1 Bosonic coherent states

Driven by the fact that our Hamiltonians are expressed in second quantization, we wish to construct right eigenstates of the annihilation operator in Fock space. Operators expressed in second quantization then act on such states in a trivial way. in this section we expose the details of their construction in the bosonic case. As it turns out, such states are particularly appropriate to describe certain type of bosonic many-body systems such as photons in a laser beam [42, 43]. They can also be used to express any symmetrized state of the Fock space, as will be seen when we will discuss closure relations over coherent states. It is worth emphasising that we wish the coherent states to be eigenstates of all annihilation operators $\{\hat{a}_k\}_k$. We search for those eigenstates among the symmetrized Fock states introduced in chapter 1. A Fock states containing only one particle number, for instance the three-particles state $|1, 2, 0, \ldots\rangle$, is manifestly not eigenstate of all annihilation operators. Indeed, the action of \hat{a}_0 on this state gives the state $|0, 2, 0, \ldots\rangle$ which is not a multiple of the initial state. We can however consider a superposition of Fock states spanning all particle numbers, as will be done below.

Let's first quickly note that unlike bosonic annihilation operators, bosonic creation operators cannot have such eigenstates in general. Indeed, consider a Fock state in occupation number notation as written in (1.1.23):

$$|f\rangle_{+} = \sum_{n_0,\dots,n_k,\dots}^{\infty} C_{n_0\dots n_k\dots} |n_0 \cdots n_k \cdots \rangle_{+}$$
(3.1.1)

where the $C_{n_0...n_k,...}$ are simply complex coefficients. This vector necessarily has a component with a minimal number of particles: either it has a non-zero coefficient in front of a vector containing 0 particles, or it has all zero coefficient up to a certain number of particles. Let n denote the number of particles corresponding to that minimal component. The action of any creation operator will raise n by one, and thus the resulting vector cannot be a multiple of the initial one. This means that the eigenvalue equation

$$\hat{b}_{k}^{\dagger} \left| f \right\rangle_{+} = \lambda_{k} \left| f \right\rangle_{+} \tag{3.1.2}$$

cannot be satisfied for all bosonic creation operator. And thus, the equivalent of coherent states does not exist for bosonic creation operators.

There is nothing that forbids a bosonic Fock state containing states with all particle numbers from being eigenvectors of the annihilation operators in general. By action of an annihilation operator labeled k on a state, each N-particle component becomes either a N - 1-particles state or a null vector depending on if it contained more than 0 particle in state $|\phi_k\rangle$. But as the sum runs from 0 to infinity, the N + 1-particles component can replace the N-particles component if the coefficients $C_{n_0...n_k,...}$ are chosen in the right way.

Coefficients of the expansion of a bosonic coherent state in Fock space

As a convention, we assume that a state denoted by α , β or γ will always be a bosonic coherent state. If the reader was to forgot these conventions, they can be found again in appendix A. In order to find the general form of the coefficients in (3.1.1) for bosonic coherent states, we express the eigenvalue equation for bosonic coherent states:

$$\hat{b}_k |\alpha\rangle = \alpha^k |\alpha\rangle, \quad k = 0, 1, \dots$$
(3.1.3)

with $|\alpha\rangle$ a bosonic coherent state and α^k a complex number. Note that the upper index on α^k is a label relating it to an annihilation operator, not to be confused with powers of eigenvalues which will be denoted using parenthesis. This convention and other conventions that could cause confusion are summarized, again in appendix A. We will now calculate the value of each coefficient $C_{n_0...n_k...}$, using the eigenvalue equation as a condition. Plugging expression (3.1.1) in the bosonic eigenvalue equation (3.1.3), we find

$$\sum_{n_0,\dots,n_k,\dots}^{\infty} C_{n_0\dots n_k\dots} \hat{b}_k |n_0 n_1 \cdots n_k \cdots \rangle = \alpha^k \sum_{n_0,\dots,n_k,\dots}^{\infty} C_{n_0\dots n_k\dots} |n_0 n_1 \cdots n_k \cdots \rangle,$$

$$\Leftrightarrow \sum_{n_0,\dots,n_k,\dots}^{\infty} C_{n_0\dots n_k\dots} \sqrt{n_k} |n_0 n_1 \cdots n_k - 1 \cdots \rangle = \alpha^k \sum_{n_0,\dots,n_k,\dots}^{\infty} C_{n_0\dots n_k\dots} |n_0 n_1 \cdots n_k \cdots \rangle$$
(3.1.4)

where equation (1.1.28) has been used in passing from the first line to the second line. The orthogonality of Fock states implies that the coefficient in front of each component must match in order for the equality to be satisfied, and thus

$$C_{n_0...n_k...}\sqrt{n_k} = \alpha^k C_{n_0...n_k-1...}$$
(3.1.5)

This equation can be used as a recursive formula to compute the coefficients in front of each component of a bosonic coherent state. Following [17], we arbitrarily set to 1 the coefficient in front of the 0-particle component, $|0\cdots 0\cdots\rangle \equiv |0\rangle$. We have:

$$\begin{cases} C_{0\dots 0\dots} = 1\\ C_{1,0,\dots 0\dots} = \alpha^0 C_{0\dots 0\dots}\\ C_{n,0,\dots 0\dots} \sqrt{n} = \alpha^0 C_{n-1,\dots,0,\dots} \end{cases}$$
(3.1.6)

Combining the three equations above, we find:

$$C_{n,0,\dots,0\dots} = \frac{(\alpha^0)^n}{\sqrt{n!}}$$
(3.1.7)

Applying the same reasoning to every k, we finally obtain

$$C_{n_0,n_1,\dots n_k\dots} = \frac{(\alpha^0)^{n_0}}{\sqrt{n_0!}} \frac{(\alpha^1)^{n_1}}{\sqrt{n_1!}} \cdots \frac{(\alpha^k)^{n_k}}{\sqrt{n_k!}} \cdots$$
(3.1.8)

It is now possible to find a very condensed notation for coherent states. Starting from the 0-particle state $|0\rangle$, every Fock state can be obtained by the application of the appropriate creation operators. Applying the same reasoning used to obtain the coefficients $C_{n_0,n_1,\ldots,n_k,\ldots}$, we have, with equation (1.1.28):

$$\begin{cases} \hat{b}_0^{\dagger} |0\rangle = |1, 0 \cdots 0 \cdots \rangle \\ \hat{b}_0^{\dagger} |n-1, 0 \cdots 0 \cdots \rangle = \sqrt{n} |n, 0 \cdots 0 \cdots \rangle \end{cases}$$
(3.1.9)

meaning that

$$|n, 0\cdots 0\cdots\rangle = \frac{(\hat{b}_0^{\dagger})^n}{\sqrt{n!}} |0\rangle$$
(3.1.10)

Applying this idea to all k yields

$$|n_0, n_1 \cdots n_k \cdots \rangle = \frac{(\hat{b}_0^{\dagger})^{n_0}}{\sqrt{n_0!}} \frac{(\hat{b}_0^{\dagger})^{n_1}}{\sqrt{n_1!}} \cdots \frac{(\hat{b}_k^{\dagger})^{n_k}}{\sqrt{n_k!}} \cdots |0\rangle$$
(3.1.11)

Combining results (3.1.8) and (3.1.11), we can write our eigenstate of the bosonic annihilation operators as

$$\begin{aligned} |\alpha\rangle &= \left(\sum_{n_0,\dots,n_k,\dots}^{\infty} \frac{\left(\alpha^0 \hat{b}_0^{\dagger}\right)^{n_0}}{n_0!} \frac{\left(\alpha^1 \hat{b}_1^{\dagger}\right)^{n_1}}{n_1!} \cdots \frac{\left(\alpha^k \hat{b}_k^{\dagger}\right)^{n_k}}{n_k!} \cdots\right) |0\rangle \\ &= \left(\sum_{n_0}^{\infty} \frac{\left(\alpha^0 \hat{b}_0^{\dagger}\right)^{n_0}}{n_0!}\right) \cdots \left(\sum_{n_k}^{\infty} \frac{\left(\alpha^k \hat{b}_k^{\dagger}\right)^{n_k}}{n_k!}\right) |0\rangle \\ &= \exp\left(\alpha^0 \hat{b}_0^{\dagger}\right) \cdots \exp\left(\alpha^k \hat{b}_k^{\dagger}\right) |0\rangle \end{aligned}$$
(3.1.12)

Noting that two bosonic creation operators always commute, we can merge the exponentials, and we finally have

$$|\alpha\rangle = \exp\left(\sum_{k} \alpha^{k} \hat{b}_{k}^{\dagger}\right)|0\rangle \tag{3.1.13}$$

Recall that the only property we required of coherent state was that they be eigenstates of the annihilation operator. We found that to any set of eigenvalues $\{\alpha^k\}_k$, there corresponds a vector $|\alpha\rangle$ made of a combination of Fock states such that $|\alpha\rangle$ is an eigenvector of each bosonic annihilation operator \hat{b}_k with the eigenvalue α^k .

Properties of bosonic coherent states

It is worthwhile to review some of the basic properties of bosonic coherent states. First, they are trivially left eigenstates of the creation operator b_k^{\dagger} with eigenvalue α^{*k} :

$$\hat{b}_{k} |\alpha\rangle = \alpha^{k} |\alpha\rangle$$

$$\Leftrightarrow \left(\hat{b}_{k} |\alpha\rangle\right)^{\dagger} = \left(\alpha^{k} |\alpha\rangle\right)^{\dagger}$$

$$\Leftrightarrow \left\langle\alpha\right| \hat{b}_{k}^{\dagger} = \left\langle\alpha\right| \alpha^{*k}$$
(3.1.14)

We can also compute the overlap of two coherent states. Let $|\beta\rangle$ be another bosonic coherent state:

$$|\beta\rangle = \sum_{n'_0,\dots,n'_k,\dots}^{\infty} C'_{n'_0\dots n'_k\dots} |n'_0 \cdots n'_k \cdots\rangle$$
(3.1.15)

Using the orthogonality of Fock states (1.1.3) and the expression of the coefficient of the coherent state expansion in Fock states (3.1.8), the overlap of two bosonic coherent states can be computed:

$$\langle \alpha \,|\, \beta \rangle = \sum_{n_0,\dots,n_k,\dots}^{\infty} \sum_{n'_0,\dots,n'_k,\dots}^{\infty} C^*_{n_0\dots n_k\dots} C'_{n'_0\dots n'_k\dots} \langle n_0 n_1 \cdots n_k \cdots \,|\, n'_0 n'_1 \cdots n'_k \cdots \rangle$$

$$= \sum_{n_0,\dots,n_k,\dots}^{\infty} \sum_{n'_0,\dots,n'_k,\dots}^{\infty} C^*_{n_0\dots n_k\dots} C'_{n'_0\dots n'_k\dots} \delta_{n_0 n'_0} \cdots \delta_{n_k n'_k} \cdots$$

$$= \sum_{n_0,\dots,n_k,\dots}^{\infty} C^*_{n_0\dots n_k\dots} C'_{n_0\dots n_k\dots}$$

$$= \sum_{n_0,\dots,n_k,\dots}^{\infty} \frac{(\alpha^{*0})^{n_0}}{\sqrt{n_0!}} \frac{(\alpha^{*1})^{n_1}}{\sqrt{n_1!}} \cdots \frac{(\alpha^{*k})^{n_k}}{\sqrt{n_k!}} \cdots \frac{(\beta^0)^{n_0}}{\sqrt{n_0!}} \frac{(\beta^1)^{n_1}}{\sqrt{n_1!}} \cdots \frac{(\beta^k)^{n_k}}{\sqrt{n_k!}} \cdots$$

$$(3.1.16)$$

Separating the sums and recognizing the power series of the exponential, we obtain

$$\langle \alpha \,|\, \beta \rangle = \exp\left(\sum_{k} \alpha^{*k} \beta^{k}\right)$$
(3.1.17)

Bosonic closure relation

Coherent states form a complete set of the Fock space, meaning that any state of Fock space can be expanded in terms of coherent states. A way to prove this fact is by showing that a closure relation over the Fock space can be expressed out of coherent states. However, the proof requires mathematical background that will not be useful outside of this specific case. Furthermore, the emphasis of the present work is on coherent states, and Fock states are merely used as a step for defining the former. The closure relation will thus only be proven in the case of coherent states. A general proof can be found, e.g. in [17]. The closure relation reads

$$\prod_{k} \left[\int_{-\infty}^{+\infty} \int_{-\infty}^{\infty} \frac{d\Re(\alpha^{k})d\Im(\alpha^{k})}{\pi} e^{-|\alpha^{k}|^{2}} \right] |\alpha\rangle \langle \alpha| = \hat{\mathbb{1}}$$
(3.1.18)

However, we will often write it as

$$\prod_{k} \left[\int \frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] |\alpha\rangle \langle \alpha| = \hat{\mathbb{1}}, \qquad (3.1.19)$$

keeping in mind that its rigorous definition of the measure and limits for the integration are given by (3.1.18). A way to prove this relation is to verify that the left hand side is indeed equivalent to the identity operator when inserted between two arbitrary coherent states. We thus proceed accordingly. Let $|\beta\rangle$, $|\gamma\rangle$ be two arbitrary coherent states, and β_k , γ_k the eigenvalues associated to the corresponding state for the operator \hat{b}_k . Let α^k be the eigenvalues associated to the vector $|\alpha\rangle$ for the operator \hat{b}_k . We have

$$\langle \beta | \prod_{k} \left[\int \frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] |\alpha\rangle \langle \alpha | \gamma\rangle$$

$$= \prod_{k} \left[\int \frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] \exp\left(\sum_{k} \beta^{*k} \alpha^{k}\right) \exp\left(\sum_{k} \alpha^{*k} \gamma^{k}\right)$$

$$= \prod_{k} \left[\int \frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] \exp\left(\sum_{k} \left[\beta^{*k} \alpha^{k} + \alpha^{*k} \gamma^{k}\right] \right)$$

$$(3.1.20)$$

Note that the exponentials coming from closure relations will always be written in the e^{\dots} form in order to easily distinguish them from other exponentials. This integral is quite easy to compute by hand. However, this type of integral is quite frequent when it comes to path-integral in coherent state representation, and a formula has been developed. It is presented and proven in appendix B.1. It reads as follows:

$$\int \prod_{n=1}^{N} \left[\frac{d\alpha^{*n} d\alpha^n}{2i\pi} e^{-a_n |\alpha^n|} \right] \exp\left(\sum_{n=1}^{N} b_n \alpha^{*n} + c_n \alpha^n\right) = \frac{1}{\prod_{n=1}^{N} a_n} \exp\left(\sum_{n=1}^{N} \frac{b_n c_n}{a_n}\right)$$
(3.1.21)

Putting $a_k = 1$, $b_k = \beta_k$, $c_k = \beta_k^*$ for each k, we have

$$\prod_{k} \left[\int \frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] \exp\left(\sum_{k} \left[\beta^{*k} \alpha^{k} + \alpha^{*k} \gamma^{k} \right] \right) = \prod_{k} \exp\left(\beta^{*k} \gamma^{k} \right) = \exp\left(\sum_{k} \beta^{*k} \gamma^{k} \right) = \langle \beta | \gamma \rangle \quad (3.1.22)$$

We thus have shown that coherent states form a complete basis with respect to coherent states. Incidentally, assuming that this statement is true for the whole Fock space (for a proof, see e.g. [17]). More precisely, they form an overcomplete set over Fock space. This is because the overlap between two different coherent states is given by (3.1.17) and is thus never 0. meaning that two coherent states cannot be orthogonal.

In a more physical sense, bosonic coherent states correspond to what can be called the "most classical" manybody states. This designation is justified by the fact that they exhibit the minimal amount of uncertainty on the position and momentum of the particles that they describe [41], which can be thought of as minimizing the quantum behaviour of the system. In a quantum field framework, the coherent states are those that minimize the quantum fluctuation of the field [43], making them in some sense the quantum states of the field that are the closest from a classical field. An example of coherent state in everyday life is given by the state of photons in the beam of a laser.

3.2 Fermionic coherent states

We can also construct right eigenstates of the fermionic annihilation operator, in the same way as what was developed for bosonic coherent states. Although their properties are rather similar, there are some slight differences between bosonic and fermionic coherent states. The first one is that unlike bosonic creation operators, fermionic creation operators can have right eigenstates. This is a consequence of the fact that the occupation number for any fermionic state is either 0 or 1. Because of this property, there is a symmetry between a fermion in a state and the absence of a fermion in a state (referred to as a hole). If $|\xi\rangle$ is a right eigenstate of the fermionic annihilation operator, than the ket $|\bar{\xi}\rangle$ obtained by replacing every fermion with a hole and every hole with a fermion in $|\xi\rangle$ is a right eigenstate of the fermionic creation operator. Note that this previous property was mentioned for the sake of completeness. Right eigenstates of the fermionic creation operator will not be considered here, and we will content ourselves with right eigenstates of the annihilation operator.

The second difference between the bosonic and the fermionic case, which has more consequences in the context of this work, lies in the nature of the eigenvalues associated to fermionic coherent states. Start from the eigenvalue equation for fermionic coherent states:

$$\hat{c}_k \left| \xi \right\rangle = \xi^k \left| \xi \right\rangle \tag{3.2.1}$$

with $|\xi\rangle$ a fermionic coherent state. Using the anti-commutation property (1.1.27), we find for the eigenvalues:

$$\hat{c}_{k}\hat{c}_{k'}|\xi\rangle = -\hat{c}_{k'}\hat{c}_{k}|\xi\rangle$$

$$\Leftrightarrow \xi^{k}\xi^{k'}|\xi\rangle = -\xi^{k'}\xi^{k}|\xi\rangle \qquad (3.2.2)$$

This means that the eigenvalues of fermionic coherent states are not simply complex numbers, but rather anticommuting numbers. Such numbers are called Grassmann numbers. Their properties will be discussed in more details shortly. These properties will then be used to show how fermionic coherent states replicate properties of the bosonic ones. It must be said that because of the requirement to extend the Fock space beyond complex numbers, fermionic coherent states do not represent physical states. For instance, some physical observables, e.g. the average number of particles, do not make sense for a fermionic coherent state [17]. Instead, fermionic coherent state will be seen as a mathematical tool that embodies the inherent anti-symmetry of fermions. A more comprehensive treatment of fermionic coherent states can be found e.g. in [44]. The reason why they are still useful is because like the bosonic coherent states, they can be used to express any fermionic Fock state, which are physical. This is shown by the existence of a fermionic coherent state closure relation over Fock space, which will be discussed after Grassmann numbers have been introduced.

Generalities on Grassmann algebras

Formally, a Grassmann algebra is defined by a set of generators $\{z_k\}_k$ that anti-commute:

$$z_k z_l = -z_l z_k, \quad \forall k, l \tag{3.2.3}$$

In particular, we have

$$z_k^2 = 0$$
 (3.2.4)

Aside from anti-commutativity, Grassmann generators act like ordinary numbers. The product of Grassmann generators has the usual distributivity property with respect to the sum:

$$z_j(z_k + z_l) = z_j z_k + z_j z_l (3.2.5)$$

and both operations are associative.

We also mention that a Grassmann algebra can be complex, meaning that each Grassmann generator has an associated complex conjugate defined by

$$(z_k)^* = z_k^* (z_k^*)^* = z_k$$
(3.2.6)

The set of generators is then $\{z_k, z_k^*\}_k$. The complex conjugates of a generator is a distinct generator, and we still have:

$$z_k z_k^* = -z_k^* z_k (3.2.7)$$

A complex algebra is mandatory in order to replicate the bosonic coherent states properties, and from now on Grassmann algebras will be assumed to be complex. We will now review some properties Grassmann algebras and their generators.

Properties of Grassmann generators

Let $\{z_k, z_k^*\}_k$ be a set of Grassmann generators. A basis of the Grassmann algebra is given by all the distinct products that can be made from the generators. For example, consider only one generator z and its complex conjugate, a basis of the corresponding algebra is $\{1, z, z^*, zz^*\}$. Any linear combination (with ordinary numbers as coefficient) of these generators is a Grassmann number. Two Grassmann numbers do not anti-commute in general, but neither do they commute: let $a = a_0 + a_1 z$ and $b = b_0 + b_1 z^*$ be two linear combinations of the four generators $\{1, z, z^*, zz^*\}$. We have

$$ab = (a_0 + a_1 z)(b_0 + b_1 z^*)$$

= $a_0 b_0 + a_0 b_1 z^* + a_1 b_0 z + a_1 b_1 z z^*$
= $a_0 b_0 + a_0 b_1 z^* + a_1 b_0 z + a_1 b_1 z^* z + 2a_1 b_1 z z^*$
= $(b_0 + b_1 z^*)(a_0 + a_1 z) + 2a_1 b_1 z z^* \neq \pm ba$ (3.2.8)

However, if we restrict ourselves to linear combinations of individual Grassmann generators (excluding independent terms and pairs of Grassmann generators), the anti-commutativity property can be recovered: let $c = c_1 z + c_2 z^*$, $d = d_1 z + d_2 z^*$. We have:

$$cd = (c_1 z + c_2 z^*)(d_1 z + d_2 z^*) = c_1 d_2 z z^* + c_2 d_1 z^* z = -dc$$
(3.2.9)

These two properties generalize to a set with more that one generator z and its conjugate. It is also useful to notice that pairs of Grassmann generators commute with any combination of generators. Consider a product of Grassmann generators $\mathcal{Z} = z_{k_1} \cdots z_{k_l}$. For any i, j, we have:

$$z_i z_j \mathcal{Z} = (-1)^l z_i \mathcal{Z} z_j = (-1)^{2l} \mathcal{Z} z_i z_j = \mathcal{Z} z_i z_j$$
(3.2.10)

If any of the two i, j is in $\{k_1, \ldots, k_l\}$, then both sides of the equation are 0 and the commutativity property is still satisfied. This result is easily generalized from pairs to terms containing any even power of Grassmann generators.

A corollary of this result is that any function of Grassmann pairs commute with any expression containing Grassmann generators:

$$a(z_i z_j) \mathcal{Z} = \mathcal{Z} a(z_i z_j), \tag{3.2.11}$$

for $Z = z_{k_1} \cdots z_{k_l}$. This can be shown easily by writing out the power series of the considered function and applying the result above to each term of the series.

Functions of Grassmann generators

Consider a generic function a(z). Its power series reads:

$$a(z) = a(0) + a'(0)z + \frac{a''(0)}{2!}z^2 + \cdots$$
(3.2.12)

However, equation (3.2.4) implies that z^2 and higher powers of z are actually 0, meaning that a(z) has the simple expression in z:

$$a(z) = a(0) + a'(0)z \tag{3.2.13}$$

which will be more conveniently written as

$$a(z) = a_0 + a_1 z \tag{3.2.14}$$

The application of this reasoning to an exponential function of Grassmann generators is very straightforward and yields:

$$e^{z} = 1 + z + \frac{z^{2}}{2} + \dots = 1 + z$$
 (3.2.15)

If we instead consider a product of Grassmann generators, we find

$$e^{z_1 \cdots z_k} = 1 + z_1 \cdots z_k + \frac{(z_1 \cdots z_k)^2}{2} + \cdots$$
 (3.2.16)

The quantity $(z_1 \cdots z_k)^2$ is still found to be 0 by permuting, say, the z_1 variable k-1 times to obtain

$$(z_1 \cdots z_k)^2 = (-1)^{k-1} z_1^2 (z_2 \cdots z_k)^2 = 0$$
(3.2.17)

by (3.2.4). Thus, the power series of the exponential of a product of Grassmann generators still stops at order 1:

$$e^{z_1 \cdots z_k} = 1 + z_1 \cdots z_k \tag{3.2.18}$$

In the context of path integrals, many expressions involve exponentials of Grassmann generators. We expose below the general formulae that allow to treat such exponentials. First, consider an exponential of pairs of Grassmann generators. As shown in (3.2.10), pairs of Grassmann generators commute with other such pairs. They also commute with sums of pairs since they commute with each term of the sum individually. We thus have

$$\exp\left(\sum_{k} C_{k} z_{k}^{*} z_{k}\right) = \prod_{k} \exp(C_{k} z_{k}^{*} z_{k}) = \prod_{k} (1 + C_{k} z_{k}^{*} z_{k})$$
(3.2.19)

for any sets of Grassmann generators $\{z_k\}_k$ and $\{z_k\}_k$ and any complex number C_k . The reader who is not familiar with exponentials of commuting quantities can consult appendix D for a refresher. Another recurrent expression in upcoming chapters is the exponential of a double sum of Grassmann pairs. In the case where there is no constant in front of the pair, the following equation is verified:

$$\exp\left(\sum_{k,l} z_k z_l\right) = 1 + \sum_{k,l} z_k z_l \tag{3.2.20}$$

This can be shown by re-expressing the sum in the exponential:

$$\sum_{k,l} z_k z_l = \left(\sum_k z_k\right) \left(\sum_l z_l\right)$$
(3.2.21)

As mentioned in (3.2.9), a sum of Grassmann generators exhibits the same properties as a generator. Thus, we can write this sum as xy for $x = (\sum_k z_k)$ and $y = (\sum_l z_l)$ two Grassmann numbers that follow equation (3.2.9). We thus have

$$\exp\left(\sum_{k,l} z_k z_l\right) = \exp\left(xy\right) = 1 + xy \tag{3.2.22}$$

where the development of an exponential of a product of Grassmann generators (3.2.18) was used. This proves equation (3.2.20). Note however that this result do not apply if coefficients depending on both k and l are assigned to each member of the sum.

Integration over Grassmann generators

As will be seen in chapter 2, in order to compute the evolution operator of a system using the path-integral formalism, one needs to be able to integrate over Grassmann generators. Integration over Grassmann generators can be defined with the two following properties:

$$\int dz_k \, 1 = 0$$

$$\int dz_k \, z_k = 1 \tag{3.2.23}$$

We draw the attention of the reader to the fact that the first property applies to any expression that is a constant with respect to the integrated generator. These properties also imply that

$$\int dz_k \, z'_k = \delta_{kk'},\tag{3.2.24}$$

which is used extensively when computing Grassmann integrals.

It should be noted that Grassmann integration has no analogous with the Riemann sum or other definitions of integration over fields like \mathbb{R} or \mathbb{C} [17]. The differential dz_k is a mere notation and does not represent a Grassmann generator nor a Grassmann number. In particular, it does not make sense to write

$$\int dz_k \, z_k = -\int z_k \, dz_k \tag{3.2.25}$$

Instead, $\int dz_k$ is seen only as an operator defined by the properties (3.2.23). Putting these definitions to work, we now compute the equivalent of a scalar product for Grassmann integrals. This development can be seen as a motivation for the way Grassmann integrals are defined, and as an example of the application of these definitions. The results themselves will not be of particular use in the upcoming chapters, and thus the reader is free to skip to the construction of fermionic coherent states. Let $f(z^*)$, $g(z^*)$ be two functions expressed in the form of (3.2.14). Writing their scalar product in bra-ket notation, we have

$$\langle g | f \rangle = \int dz^* \int dz \, e^{-z^* z} g^*(z) f(z^*)$$
 (3.2.26)

with z, z^* two Grassmann generators. The exponential factor will soon be identified as the normalization factor for the closure relation on Grassmann generators, but for now we simply acknowledge it. Substituting in the power series (3.2.14) for the functions and (3.2.18) for the exponential, we obtain

$$\langle g | f \rangle = \int dz^* \int dz \, (1 - z^* z) (g_0^* + g_1^* z) (f_0 + f_1 z^*)$$

= $\int dz^* \int dz \, (g_0^* f_0 + g_0^* f_1 z^* + g_1^* f_0 z + g_1^* z f_1 z^* - z^* z g_0^* f_0)$
= $\int dz^* \int dz \, (g_1^* z f_1 z^* - z^* z g_0^* f_0)$ (3.2.27)

The second equality is obtained by identifying terms with duplicate Grassmann variables and setting them to 0 by virtue of (3.2.4). The third equality makes use of equation (3.2.23) to eliminate terms that do not contain both z and z^* , since such terms will run into the case $\int dz 1$ which is 0.

It is now necessary to proceed with caution. In the definition of the integral, the operator $\int dz$ is applied to z directly from the left in order to yield 1. We thus need to bring z in front of the second term, multiplying it by a factor -1. As a reminder, the f_i 's and g_i 's are simply complex number and commute with both complex and Grassmann variables. Doing the required commutation, the last line reads

$$\int dz^* \int dz \left(zz^* g_1^* f_1 + zz^* g_0^* f_0 \right) = \int dz^* \left(z^* g_1^* f_1 + z^* g_0^* f_0 \right) = g_1^* f_1 + g_0^* f_0$$
(3.2.28)

which indeed resemble the usual scalar product of the Hilbert space of complex-valued functions. In fact, it can be shown that the space of Grassmann variable-valued functions has the structure of a Hilbert space [17], which is a required property for spaces describing quantum systems. These properties will now be applied to fermionic states defined by the eigenvalue equation (3.2.1). It will be shown that they exhibit most of the properties of bosonic coherent states.

Construction of fermionic coherent states

Complementing the convention for bosonic coherent states, we assume that a state denoted by ζ , χ or ξ will always be a fermionic coherent state. At the beginning of this section, section 3.2, it was shown that the eigenvalues of a fermionic annihilation operator must be anti-commuting numbers rather than complex numbers. An algebra of anti-commuting numbers, called a Grassmann algebra, was then introduced. The link between such numbers and coherent states is done as follows: a Grassmann generator ξ^k is associated with each annihilation operator \hat{c}_k as its eigenvalue for the fermionic coherent state $|\xi\rangle$, and the conjugate Grassmann generator ξ^{*k} is associated with the corresponding creation operator \hat{c}_k^{\dagger} . Again, the use of an upper index indicates that these variables are eigenvalues associated to coherent states and is not to be confused with powers of the eigenvalues. We verify that such eigenvalues are indeed in accordance with the fermionic anti-commutation relation (1.1.27):

$$\hat{c}_{k}\hat{c}_{k'}|\xi\rangle = \xi^{k}\xi^{k'}|\xi\rangle = -\xi^{k'}\xi^{k}|\xi\rangle = -\hat{c}_{k'}\hat{c}_{k}|\xi\rangle$$
(3.2.29)

In order to replicate the properties of bosonic coherent states, we must also impose an anti-commutation relation between Grassmann generators and creation/annihilation operators [17]:

$$\{\xi^{k}, \hat{c}_{k'}\} = \{\xi^{*k}, \hat{c}_{k'}\} = 0 \quad \forall k, k' \{\xi^{k}, \hat{c}_{k'}^{\dagger}\} = \{\xi^{*k}, \hat{c}_{k'}^{\dagger}\} = 0 \quad \forall k, k'$$
(3.2.30)

We repeat the fact that associating Grassmann numbers to operators in Fock space requires to expand the coefficient space to include Grassmann numbers. Consequently, the fermionic coherent states are no longer physical

states, which raises concerns about the relevance of their introduction. However, it will be seen that these states form an overcomplete set over the fermionic Fock space, meaning that any fermionic Fock state can be expressed by a combination of fermionic coherent states.

We will now construct states in a way analogous to the bosonic state and show that they are indeed eigenstates of the annihilation operators. Mirroring equation (3.1.13), we write a state as:

$$\left|\xi\right\rangle = \exp\left(\sum_{k} \hat{c}_{k}^{\dagger} \xi^{k}\right) \left|0\right\rangle, \qquad (3.2.31)$$

with $\{\xi^k\}_k$ the set of Grassmann generators associated with the annihilation operators $\{\hat{c}_k\}_k$. Using the anticommutation rule (3.2.30), we notice that all the quantities $\hat{c}_k^{\dagger}\xi^k$, $\hat{c}_l^{\dagger}\xi^l$, ... actually commute with each other. Indeed, fermionic creation operators associated with different k's anti-commute, and thus

$$\hat{c}_{k}^{\dagger}\xi^{k}\hat{c}_{l}^{\dagger}\xi^{l} = (-1)^{4}\hat{c}_{l}^{\dagger}\xi^{l}\hat{c}_{k}^{\dagger}\xi^{k} = \hat{c}_{l}^{\dagger}\xi^{l}\hat{c}_{k}^{\dagger}\xi^{k}$$
(3.2.32)

This result will prove very useful later in this section, where simplifying functions containing pairs of Grassmann variables is required.

Knowing that the quantities $\hat{c}_k^{\dagger} \xi^k$ commute with each other, we are left with the exponential of a sum of commuting variables, and we can decompose it as in (3.2.19) as a product of exponentials. We can then make use of the property of exponentials of Grassmann variables, equation (3.2.18), to develop the exponentials into first order polynomials in ξ^k :

$$|\xi\rangle = \exp\left(\sum_{k} \hat{c}_{k}^{\dagger} \xi^{k}\right) |0\rangle = \prod_{k} \exp\left(\hat{c}_{k}^{\dagger} \xi^{k}\right) |0\rangle = \prod_{k} \left(1 + \hat{c}_{k}^{\dagger} \xi^{k}\right) |0\rangle$$
(3.2.33)

We can now verify that it satisfies to the eigenvalue equation by computing the quantity $\hat{c}_k |\xi\rangle$. We have:

$$\hat{c}_{k} |\xi\rangle = \hat{c}_{k} \prod_{k'} \left(1 + \hat{c}_{k'}^{\dagger} \xi^{k'} \right) |0\rangle$$

$$= \prod_{k' \neq k} \left[\left(1 + \hat{c}_{k'}^{\dagger} \xi^{k'} \right) \right] \hat{c}_{k} \left(1 + \hat{c}_{k}^{\dagger} \xi^{k} \right) |0\rangle$$

$$= \prod_{k' \neq k} \left[\left(1 + \hat{c}_{k'}^{\dagger} \xi^{k'} \right) \right] \left(\hat{c}_{k} + \hat{c}_{k} \hat{c}_{k}^{\dagger} \xi^{k} \right) |0\rangle$$
(3.2.34)

where the commutation relation (3.2.32) was used to bring the factor relative to k at the end of the product. The quantity $(\hat{c}_k + \hat{c}_k \hat{c}_k^{\dagger} \xi^k) |0\rangle$ can be further analyzed using the anti-commutation relations (1.1.26). Combined with the fact that $\hat{c}_k |0\rangle = 0$, they yield:

$$\begin{pmatrix} \hat{c}_k + \hat{c}_k \hat{c}_k^{\dagger} \xi^k \end{pmatrix} |0\rangle = (1 - \hat{c}_k^{\dagger} \hat{c}_k) \xi^k |0\rangle$$

$$= \xi^k \left(1 - \hat{c}_k^{\dagger} \hat{c}_k \right) |0\rangle$$

$$= \xi^k |0\rangle$$

$$= \xi^k \left(1 + \hat{c}_k^{\dagger} \xi^k \right) |0\rangle$$

$$(3.2.35)$$

In order to find the last equality, we freely add a $\hat{c}_k^{\dagger} \xi^k$ term as its product with ξ^k gives 0. Inserting this result back and using again commutation relation (3.2.32), we finally obtain

$$\hat{c}_{k}\left|\xi\right\rangle = \prod_{k'} \left(1 + \hat{c}_{k'}^{\dagger} \xi^{k'}\right) \xi^{k} \left(1 + \hat{c}_{k}^{\dagger} \xi^{k}\right) \left|0\right\rangle = \xi^{k} \left|\xi\right\rangle$$

$$(3.2.36)$$

A formula similar to (3.1.17) is also recovered by this definition of fermionic coherent states. First, taking the hermitian conjugate of equation (3.2.33), We have:

$$\langle \xi | = \langle 0 | \prod_{k} \left(1 + \xi^{*k} \hat{c}_k \right)$$
(3.2.37)

The overlap of fermionic coherent states is also analogous to the bosonic case, equation (3.1.17). Remembering that $\hat{c}_k |0\rangle = 0$ and $\langle 0| \hat{c}_k^{\dagger} = 0$, we can compute

$$\begin{split} \langle \xi | \chi \rangle &= \langle 0 | \prod_{k} (1 + \xi^{*k} \hat{c}_{k}) (1 + \hat{c}_{k}^{\dagger} \chi^{k}) | 0 \rangle \\ &= \langle 0 | \prod_{k} (1 + \xi^{*k} \hat{c}_{k} + \hat{c}_{k}^{\dagger} \chi^{k} + \xi^{*k} \hat{c}_{k} \hat{c}_{k}^{\dagger} \chi^{k}) | 0 \rangle \\ &= \langle 0 | \prod_{k} (1 + \xi^{*k} \hat{c}_{k} \hat{c}_{k}^{\dagger} \chi^{k}) | 0 \rangle \\ &= \langle 0 | \prod_{k} (1 + \hat{c}_{k} \xi^{*k} \chi^{k} \hat{c}_{k}^{\dagger}) | 0 \rangle \\ &= \prod_{k} (1 + \xi^{*k} \chi^{k}) \\ &= \exp\left(\sum_{k} \xi^{*k} \chi^{k}\right) \end{split}$$
(3.2.38)

where the fact that $\hat{c}_k^{\dagger} |0\rangle = |0 \cdots 1 \cdots \rangle$ and the normalization of Fock states were used in obtaining the 5th equality. The last fermionic equivalent of bosonic results we are interested in is the analog to the closure relation (3.1.19). We will show that the following expression:

$$\prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \right] |\xi\rangle \langle\xi|$$
(3.2.39)

is indeed a closure relation over the Fock space restricted to coherent states. Again, it can be shown that the same expression is a closure relation over the whole fermionic Fock space, but this property won't be used for upcoming developments. For a proof of the closure over the whole Fock space, see e.g. [17].

Our proof will make use of several of the most important results developed in this section, and will thus constitute a good summary of properties of fermionic coherent states. To prove that the expression above is a closure relation, it suffice to show that

$$\langle \zeta | \prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \right] |\xi\rangle \,\langle \xi | \chi\rangle = \langle \zeta | \chi\rangle \,, \tag{3.2.40}$$

for two arbitrary coherent states $|\zeta\rangle$ and $|\chi\rangle$. First, we apply the formula (3.2.38) for the overlap of coherent states:

$$\langle \zeta | \prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k} \xi^{k}} \right] |\xi\rangle \,\langle \xi | \chi\rangle = \prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k} \xi^{k}} \right] \exp\left(\sum_{k} \zeta^{*k} \xi^{k}\right) \exp\left(\sum_{k} \xi^{*k} \chi^{k}\right)$$
(3.2.41)

We then make use of the property (3.2.19) for exponentials of sums of Grassmann pairs, and of the commutation relation (3.2.11):

$$\prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \right] \exp\left(\sum_{k} \zeta^{*k}\xi^{k}\right) \exp\left(\sum_{k} \xi^{*k}\chi^{k}\right) \\
= \prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \right] \prod_{k} \left[\exp\left(\zeta^{*k}\xi^{k}\right) \right] \prod_{k} \left[\exp\left(\xi^{*k}\chi^{k}\right) \right] \\
= \prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \exp\left(\zeta^{*k}\xi^{k}\right) \exp\left(\xi^{*k}\chi^{k}\right) \right]$$
(3.2.42)

Each exponential now contain a single Grassmann product and can be developed according to equation (3.2.18). Developing the resulting products gives

$$\prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} \left(1 - \xi^{*k} \xi^{k} \right) (1 + \zeta^{*k} \xi^{k}) (1 + \xi^{*k} \chi^{k}) \right] = \prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} \left(1 - \xi^{*k} \xi^{k} + \zeta^{*k} \xi^{k} + \xi^{*k} \chi^{k} + \zeta^{*k} \xi^{k} \xi^{k} \xi^{k} \chi^{k} \right) \right]$$
(3.2.43)
where the terms containing duplicates of the same Grassmann generator have already been eliminated. Applying the integration rules (3.2.23), each term that do not contain both ξ^k and ξ^{*k} is 0 and we are left with

$$\prod_{k} \left[(1 + \chi^{*k} \xi^k) \right] = \exp\left(\sum_{k} \chi^{*k} \xi^k\right) = \langle \chi | \xi \rangle$$
(3.2.44)

This proves that fermionic coherent states verify the following closure relation:

$$\prod_{k} \left[\int d\xi^{*k} \int d\xi^{k} \, e^{-\xi^{*k} \xi^{k}} \right] |\xi\rangle \, \langle\xi| = \hat{\mathbb{1}}$$
(3.2.45)

Two useful formulae

We will conclude this section with two formulae of great use for upcoming computations in chapters 4 and 5. First-time readers may safely skip those formulae and come back to them later when they are referenced. Note that an algebraic proof for these formulae has not been obtained yet. Numeric tools developed in the context of this work were used, and are presented in appendix C. The first formulae states the following. Let \mathbf{A} , \mathbf{B} be two square matrices of order L. We have:

$$\prod_{k}^{L} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \right] \exp\left(\sum_{k,l}^{L} \mathbf{A}_{kl} \zeta^{*k} \xi^{l}\right) \exp\left(\sum_{k,l}^{L} \mathbf{B}_{kl} \xi^{*k} \chi^{l}\right) = \exp\left(\sum_{k,l}^{L} (\mathbf{A}\mathbf{B})_{kl} \zeta^{*k} \chi^{l}\right)$$
(3.2.46)

with (AB) representing the usual matrix product between matrices **A** and **B**. Note that this result extends to integrals of the form

$$\prod_{k=1}^{L} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \right] \exp\left(\sum_{k}^{L} \mathbf{A}_{k} \zeta^{*k} \xi^{k}\right) \exp\left(\sum_{k,l}^{L} \mathbf{B}_{kl} \xi^{*k} \chi^{l}\right)$$
(3.2.47)

by defining the diagonal matrix $\mathbf{A} = \text{diag}(A_1, A_2, \dots, A_L)$ and applying formula (3.2.46). The second formula applies in cases such as those that arise when considering two-body Hamiltonians. Let \mathbf{A} , \mathbf{B} be two square matrices of order L, \mathbf{D} a diagonal matrix of order L and ζ^k , ξ^k and χ^k be three Grassmann generators for $k \in \{1, \dots, L\}$. We have

$$\prod_{k=1}^{L} \left[\int d\xi^{*k} \int d\xi^{k} e^{-\xi^{*k}\xi^{k}} \right] \exp\left(\sum_{k=1}^{L} \mathbf{D}_{k}\zeta^{*k}\xi^{k}\right) \exp\left(\sum_{k,l,m,n=1}^{L} \mathbf{A}_{kl}\mathbf{B}_{mn}\xi^{*k}\xi^{*l}\chi^{m}\chi^{n}\right) \exp\left(\sum_{k=1}^{L}\xi^{*k}\chi^{k}\right) \\ = \exp\left(\sum_{k=1}^{L} \mathbf{D}_{k}\zeta^{*k}\chi^{k}\right) \exp\left(\sum_{k,l,m,n=1}^{L} (\mathbf{D}\mathbf{A}\mathbf{D})_{kl}\mathbf{B}_{mn}\zeta^{*k}\zeta^{*l}\chi^{m}\chi^{n}\right)$$
(3.2.48)

3.3 Path integral theory by means of coherent states

The path integral will now be applied to a simple case, namely a mixed Hamiltonian with no interaction between the fermions and the bosons. Despite being of very little practical interest, this case will prove useful as an introductory example to the use of coherent states in path integrals. Carrying out the calculations will show techniques that will be used in a very similar manner in upcoming chapters. Furthermore, the propagator computed in the case where there is no interaction gives the propagator of the free fermionic and bosonic field, which we should recover in upcoming calculations when considering vanishing interactions. We also introduce in this section the shorthand notations adopted in this work. These notations can be found at any time in appendix A. We first write out the path-integral theory for the mixed system in coherent state representation. In order to carry out the calculation of this propagator, two results have to be mentioned, namely the Baker-Campbell-Hausdorff formula and the effect of exponentials of creation/annihilation operators on coherent states. The total propagator is then computed and discussed. In the last part of this section, we show the equivalence of the path integral in the Hamiltonian formulation and in Feynman's Lagrangian formulation (2.3.4) which was mentioned in chapter 2, in the particular case of our non-interacting system. The general proof can be found e.g. in [17].

Path integral theory of the mixed Hamiltonian

We consider a mixed system with L fermionic states and N bosonic states. Its Hamiltonian expressed in second quantization reads

$$\hat{H} = \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu} + \sum_{n=1}^{N} E_{B,n} \hat{b}_{n}^{\dagger} \hat{b}_{n} = \hat{H}_{F} + \hat{H}_{B}$$
(3.3.1)

with \hat{H}_F and \hat{H}_B the fermionic and bosonic parts of the Hamiltonian \hat{H} respectively. Since we work with operators in second quantization, the coherent state representation described in sections 3.1 and 3.2 is a natural choice to represent the state of the system. With the results from these sections in mind, we can proceed to the computation of the path integral.

We begin by mentioning that since we consider no interaction between the fermions and bosons, one expects the bosonic and fermionic parts of the system to yield distinct propagators. The probability of transition from a mixed state $|\zeta\rangle \otimes |\alpha\rangle \equiv |\zeta\alpha\rangle$ to another mixed state $|\chi\rangle \otimes |\beta\rangle \equiv |\chi\beta\rangle$ is then trivially given by the product of the two independent probabilities of observing the transition from $|\zeta\rangle$ to $|\chi\rangle$ and the transition from $|\alpha\rangle$ to $|\beta\rangle$, which we will verify using the path integral formalism.

Let $|\zeta_i \alpha_i \rangle$, $|\zeta_f \alpha_f \rangle$ be two states of our mixed system. We wish to compute the probability for the system to be in state $|\zeta_f \alpha_f \rangle$ at time t_f if it was in state $|\zeta_i \alpha_i \rangle$ at time t_i . We thus want to compute the probability amplitude $K(\zeta_f \alpha_f, t_f; \zeta_i \alpha_i, t_i)$. Following what was done in chapter 2, we start from equation (2.3.15). Replacing the generic closure relations by the closure relation on both bosonic and fermionic coherent states (3.1.19) yields

$$K(\zeta_M \alpha_M, t_M; \zeta_0 \alpha_0, t_0) = \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^N \frac{d\alpha_m^{n*} d\alpha_m^n}{2i\pi} e^{-|\alpha_m^n|^2} \int \prod_{\mu=1}^L d\zeta_m^{\mu*} d\zeta_m^{\mu} e^{-\zeta_m^{\mu} \zeta_m^{\mu}} \right] \\ \times \prod_{m=1}^M \left[\left\langle \zeta_m \alpha_m \left| \exp\left(-\frac{i}{\hbar} \Delta t \, \hat{H}\right) \right| \zeta_{m-1} \alpha_{m-1} \right\rangle \right]$$
(3.3.2)

with $\Delta t = \frac{t_f - t_i}{M}$. Again, the notations $|\zeta_i \alpha_i\rangle \equiv |\zeta_0 \alpha_0\rangle$ and $|\zeta_f \alpha_f\rangle \equiv |\zeta_M \alpha_M\rangle$ have been used. A way to compute this propagator is by separating the bosonic and the fermionic part of the Hamiltonian. We first note that even if the total Hamiltonian \hat{H} commutes with itself, there is no reason for the terms composing \hat{H} to commute with each other in general. Although it is the case here since \hat{H}_F and \hat{H}_B belong to different spaces, it will not be the case in upcoming chapters when we consider interaction Hamiltonians containing both bosons and fermions. In such cases, the exponential of the total Hamiltonian cannot simply be split into a product of two or more exponentials, and a more general formula has to be used.

Baker-Campbell-Hausdorff formula

The Baker-Campbell-Hausdorff (BCH) formula gives the relation between the exponential of a sum of two non-commuting quantities and the product of the exponentials of the two quantities [45]. In our case, it reads:

$$\exp\left(-\frac{i}{\hbar}\Delta t\,\hat{H}_F\right)\exp\left(-\frac{i}{\hbar}\Delta t\,\hat{H}_B\right) = \exp\left(-\frac{i}{\hbar}\Delta t\,\left(\hat{H}_F + \hat{H}_B\right) - \frac{1}{2\hbar^2}\Delta t^2\,\left[\hat{H}_F,\hat{H}_B\right] + \cdots\right)$$
(3.3.3)

Where '...' denotes terms of higher order in Δt involving more commutators. If we take the limit $M \to \infty$, Δt becomes an infinitesimal quantity denoted δt , and the terms involving commutators can be neglected, yielding the simple result

$$\exp(-\frac{i}{\hbar}\delta t\,\hat{H}_F)\exp(-\frac{i}{\hbar}\delta t\,\hat{H}_B) = \exp\left(-\frac{i}{\hbar}\delta t\,\left(\hat{H}_F + \hat{H}_B\right)\right)$$
(3.3.4)

Even though this formula is not required in this simple case, its exposition is motivated by the fact that it will prove useful later on, when we need to split an Hamiltonian with a mixed term. It is also part of the standard toolbox of path integrals and is required in many cases, for instance when extending the path integral formulation to Hamiltonians that are not time-independent. Indeed, such Hamiltonians do not commute with themselves if they are evaluated at two different times, and the BCH formula is required to obtain the form (2.3.15).

Equipped with the BCH formula, we can begin the calculation of the propagator. Taking the limit for $M \to \infty$, we first compute the elementary propagator $\left\langle \zeta_m \alpha_m \right| \exp\left(-\frac{i}{\hbar} \delta t \hat{H}\right) \left| \zeta_{m-1} \alpha_{m-1} \right\rangle$ which represents the amplitude of propagation from state $|\alpha_{m-1}\rangle$ to the infinitesimally close state $|\alpha_m\rangle$. In the limit where M goes to infinity, the

BCH formula (3.3.4) can be applied to split the exponential into two parts, here a bosonic and a fermionic part. Closure relations can then be inserted, yielding:

$$\left\langle \zeta_{m}\alpha_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1}\alpha_{m-1} \right\rangle = \left\langle \zeta_{m}\alpha_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{F}\right) \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{B}\right) \right| \zeta_{m-1}\alpha_{m-1} \right\rangle$$

$$= \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*}d\beta_{m}^{n}}{2i\pi} e^{-|\beta_{m}^{n}|^{2}} \right] \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{\mu*}d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \left\langle \zeta_{m}\alpha_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{F}\right) \right| \xi_{m}\beta_{m} \right\rangle$$

$$\times \left\langle \xi_{m}\beta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{B}\right) \right| \zeta_{m-1}\alpha_{m-1} \right\rangle$$
(3.3.5)

We now encounter another obstacle calling for the exposition of another (and final) theoretical discussion. Indeed, although previous sections considered the action of creation and annihilation operators on coherent states, we have not yet considered the action of exponential of these operators. This action can be easily computed in the limit where M goes to infinity, as will be seen shortly.

Exponentials of creation and annihilation operators

Recall that coherent states are defined as eigenstates of the annihilation operator and thus, left eigenstates of the creation operator. The eigenvalues are labeled in the following way:

$$\hat{b}_n |\alpha\rangle = \alpha^n |\alpha\rangle$$
 and $\hat{c}_\mu |\zeta\rangle = \zeta^\mu |\zeta\rangle$ (3.3.6)

In the context of path integrals, one needs to compute the action of the exponential of the Hamiltonian on states, and so we compute it in coherent states representation. Let $|\alpha\rangle$, $|\beta\rangle$ be two bosonic coherent state. Most of these formulae rely on the fact that the argument of the exponential is infinitesimal, as is the case in the context of path integrals. We first consider the exponential of the one-body bosonic Hamiltonian \hat{H}_B , which is the same as the one appearing in the general system under consideration described by the Hamiltonian (1.2.8). Starting slow, we consider the simple case of a system with a single bosonic mode accessible. Using the power series of the exponential, we have

$$\left\langle \alpha \left| \exp\left(-\frac{i}{\hbar}\delta t \, E\hat{b}^{\dagger}\hat{b}\right) \right| \beta \right\rangle = \left\langle \alpha \left| \sum_{j=0}^{\infty} \frac{1}{j!} \left(-\frac{i}{\hbar}\delta t \, E\hat{b}^{\dagger}\hat{b}\right)^{j} \right| \beta \right\rangle$$
(3.3.7)

Since δt is infinitesimal, the exponential power series stops at order 1 in δt and we have

$$\left\langle \alpha \left| \left(\hat{1} - \frac{i}{\hbar} \delta t \, E \hat{b}^{\dagger} \hat{b} \right) \right| \beta \right\rangle = \left(1 - \frac{i}{\hbar} \delta t \, E \alpha^{*} \beta \right) \langle \alpha \left| \beta \right\rangle$$
$$= \exp\left(-\frac{i}{\hbar} \delta t \, E \alpha^{*} \beta \right) \langle \alpha \left| \beta \right\rangle$$
(3.3.8)

We can now make the calculation for N bosonic modes. Denoting by \hat{H}_B the bosonic part of the Hamiltonian (3.3.1), we have:

$$\left\langle \alpha \left| \exp\left(-\frac{i}{\hbar}\delta t \,\hat{H}_B\right) \right| \beta \right\rangle = \left\langle \alpha \left| \left(1 - \frac{i}{\hbar}\delta t \,\sum_{n=1}^N E_n \hat{b}_n^{\dagger} \hat{b}_n\right) \right| \beta \right\rangle$$
$$= \left(1 - \frac{i}{\hbar}\delta t \,\sum_{n=1}^N E_n \alpha_n^* \beta_n\right) \langle \alpha \left| \beta \right\rangle$$
$$= \exp\left(-\frac{i}{\hbar}\delta t \,\sum_{n=1}^N E_n \alpha_n^* \beta_n\right) \langle \alpha \left| \beta \right\rangle$$
$$= \exp\left(-\frac{i}{\hbar}\delta t \,H_B(\alpha^*, \beta)\right) \langle \alpha \left| \beta \right\rangle$$
(3.3.9)

where $H_B(\alpha^*, \beta)$ represents the one-body Hamiltonian where creation operators have been replaced by the corresponding left eigenvalue for $|\alpha\rangle$, and the annihilation operators by the corresponding right eigenvalues for $|\beta\rangle$. For the fermionic part of the Hamiltonian, let $|\zeta\rangle$ and $|\xi\rangle$ be two fermionic coherent states. We have

$$\left\langle \zeta \left| \exp\left(-\frac{i}{\hbar}\delta t \, \hat{H}_F\right) \right| \xi \right\rangle = \left\langle \zeta \left| \exp\left(-\frac{i}{\hbar}\delta t \, \sum_{\mu=1}^L E_{F,\mu} \hat{c}^{\dagger}_{\mu} \hat{c}_{\mu}\right) \right| \xi \right\rangle \tag{3.3.10}$$

Since the creation and annihilation pairs in the exponential are relative to distinct sites, they commute and we can use property (3.2.19) to split the exponential into a product of exponentials:

$$\left\langle \zeta \left| \exp\left(-\frac{i}{\hbar}\delta t \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu}\right) \right| \xi \right\rangle = \left\langle \zeta \left| \prod_{\mu=1}^{L} \left(1 - \frac{i}{\hbar}\delta t E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu}\right) \right| \xi \right\rangle$$
(3.3.11)

This quantity can easily be computed using the appropriate anti-commutation relations. For L = 2, we have

$$\left\langle \zeta \left| \prod_{\mu=1}^{2} \left(1 - \frac{i}{\hbar} \delta t \, E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu} \right) \right| \xi \right\rangle = \left\langle \zeta \left| \left(1 - \frac{i}{\hbar} \delta t \, E_{F,1} \hat{c}_{1}^{\dagger} \hat{c}_{1} \right) \left(1 - \frac{i}{\hbar} \delta t \, E_{F,2} \hat{c}_{2}^{\dagger} \hat{c}_{2} \right) \right| \xi \right\rangle$$
$$= \left\langle \zeta \left| \left(1 - \frac{i}{\hbar} \delta t \, E_{F,1} \zeta^{*1} \hat{c}_{1} \right) \left(1 - \frac{i}{\hbar} \delta t \, E_{F,2} \hat{c}_{2}^{\dagger} \xi^{2} \right) \right| \xi \right\rangle$$
(3.3.12)

Recalling that creation and annihilation operators relative to distinct states anti-commute by virtue of (1.1.27) and that Grassmann generators anti-commute with other generators and with each creation/annihilation operator, we conclude that since they anti-commute twice, the two pairs $\zeta^{*1}\hat{c}_1$ and $\hat{c}_2^{\dagger}\xi^2$ commute and we have

$$\left\langle \zeta \left| \left(1 - \frac{i}{\hbar} \delta t \, E_{F,1} \zeta^{*1} \hat{c}_1 \right) \left(1 - \frac{i}{\hbar} \delta t \, E_{F,2} \hat{c}_2^{\dagger} \xi^2 \right) \right| \xi \right\rangle = \left\langle \zeta \left| \left(1 - \frac{i}{\hbar} \delta t \, E_{F,2} \hat{c}_2^{\dagger} \xi^2 \right) \left(1 - \frac{i}{\hbar} \delta t \, E_{F,1} \zeta^{*1} \hat{c}_1 \right) \right| \xi \right\rangle$$
$$= \left\langle \zeta \left| \left(1 - \frac{i}{\hbar} \delta t \, E_{F,2} \zeta^{*2} \xi^2 \right) \left(1 - \frac{i}{\hbar} \delta t \, E_{F,1} \zeta^{*1} \xi^1 \right) \right| \xi \right\rangle$$
$$= \exp\left(-\frac{i}{\hbar} \delta t \, \sum_{\mu=1}^2 E_{F,\mu} \zeta^{*\mu} \xi^{\mu} \right) \left\langle \zeta \right| \xi \right\rangle$$
(3.3.13)

This result is easily generalized for any L by applying the same commutation step until each operator has acted on an eigenstate. We finally have

$$\left\langle \zeta \left| \exp\left(-\frac{i}{\hbar}\delta t \,\hat{H}_F\right) \right| \xi \right\rangle = \exp\left(-\frac{i}{\hbar}\delta t \,\sum_{\mu=1}^{L} E_{F,\mu}\zeta^{*\mu}\xi^{\mu}\right) \left\langle \zeta \left| \xi \right\rangle \right.$$
$$\left. = \exp\left(-\frac{i}{\hbar}\delta t \,H_F(\zeta^*,\xi)\right) \left\langle \zeta \left| \xi \right\rangle \right.$$
(3.3.14)

with $H_F(\zeta^*,\xi)$ the Hamiltonian \hat{H}_F where creation and annihilation operators have been replaced with the corresponding left eigenvalues for state $|\zeta\rangle$ and right eigenvalues for state $|\xi\rangle$.

Computation of the total propagator

We can at last resume to the computation of the propagator (3.3.2). In order to do so, we first go back to the elementary propagator (3.3.5) and let each operator act on the vector to its left or right using the properties we just showed:

$$\left\langle \zeta_{m}\alpha_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1}\alpha_{m-1} \right\rangle$$

$$= \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*}d\beta_{m}^{n}}{2i\pi} e^{-|\beta_{m}^{n}|^{2}} \right] \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{\mu*}d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \exp\left(-\frac{i}{\hbar}\delta t\,H_{F}(\zeta_{m}^{*},\xi_{m})\right)$$

$$\times \exp\left(-\frac{i}{\hbar}\delta t\,H_{B}(\beta_{m}^{*},\alpha_{m-1})\right) \left\langle \zeta_{m}\alpha_{m} \left| \xi_{m}\beta_{m} \right\rangle \left\langle \xi_{m}\beta_{m} \left| \zeta_{m-1}\alpha_{m-1} \right\rangle \right.$$

$$(3.3.15)$$

We now wish to compute the integrals over β_m and ξ_m . We begin with the latter. Putting aside the bosonic part of the elementary propagator, we are left with

$$I_{F}(\zeta_{m}^{*},\zeta_{m-1}) = \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{\mu*} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \exp\left(-\frac{i}{\hbar} \delta t \, H_{F}(\zeta_{m}^{*},\xi_{m})\right) \left\langle \zeta_{m} \,|\,\xi_{m}\right\rangle \left\langle \xi_{m} \,|\,\zeta_{m-1}\right\rangle \\ = \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{\mu*} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \exp\left(-\frac{i}{\hbar} \delta t \, \sum_{\mu=1}^{L} E_{F,\mu} \zeta_{m}^{*\mu} \xi_{m}^{\mu}\right) \exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu} \xi_{m}^{\mu}\right) \exp\left(\sum_{\mu=1}^{L} \xi_{m}^{*\mu} \zeta_{m-1}^{\mu}\right) \\ = \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{\mu*} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu} \xi_{m}^{\mu}} \right] \exp\left(\sum_{\mu=1}^{L} \left(1 - \frac{i}{\hbar} \delta t \, E_{F,\mu}\right) \zeta_{m}^{*\mu} \xi_{m}^{\mu}\right) \exp\left(\sum_{\mu=1}^{L} \xi_{m}^{*\mu} \zeta_{m-1}^{\mu}\right)$$
(3.3.17)

This integral is easily computed using formula (3.2.46). Identifying the matrices from the formula, \mathbf{B} is the identity matrix, and \mathbf{A} is the matrix

$$\mathbf{A} = \operatorname{diag}\left(1 - \frac{i}{\hbar}\delta t \, E_{F,1}, \dots, 1 - \frac{i}{\hbar}\delta t \, E_{F,L}\right) = \mathbb{1} - \frac{i}{\hbar}\delta t \operatorname{diag}(E_{F,1}, \dots, E_{F,L}) \tag{3.3.18}$$

The integral is thus equal to

$$I_{F}(\zeta_{m}^{*},\zeta_{m-1}) = \exp\left(\sum_{\mu=1}^{L} \mathbf{A}_{\mu}\zeta_{m}^{*\mu}\zeta_{m-1}^{\mu}\right) = \exp\left(-\frac{i}{\hbar}\delta t \, H_{F}(\zeta_{m},\zeta_{m-1})\right) \exp\left(\sum_{\mu=1}^{L}\zeta_{m}^{*\mu}\zeta_{m-1}^{\mu}\right)$$
(3.3.19)

We now turn to the integral on the bosonic variable β_m . Omitting the fermionic part, we have to compute

$$I_{B}(\alpha_{m}^{*},\alpha_{m-1}) = \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*}d\beta_{m}^{n}}{2i\pi} e^{-|\beta_{m}^{n}|^{2}} \right] \exp\left(-\frac{i}{\hbar}\delta t H_{B}(\beta_{m}^{*},\alpha_{m-1})\right) \langle \alpha_{m} | \beta_{m} \rangle \langle \beta_{m} | \alpha_{m-1} \rangle$$

$$= \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*}d\beta_{m}^{n}}{2i\pi} e^{-|\beta_{m}^{n}|^{2}} \right] \exp\left(-\frac{i}{\hbar}\delta t \sum_{n=1}^{N} E_{B,n}\beta_{m}^{*n}\alpha_{m-1}^{n}\right) \exp\left(\sum_{n=1}^{N} \alpha_{m}^{*n}\beta_{m}^{n}\right) \exp\left(\sum_{n=1}^{N} \beta_{m}^{*n}\alpha_{m-1}^{n}\right)$$

$$= \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*}d\beta_{m}^{n}}{2i\pi} e^{-|\beta_{m}^{n}|^{2}} \right] \exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar}\delta t E_{B,n}\right)\beta_{m}^{*n}\alpha_{m-1}^{n}\right) \exp\left(\sum_{n=1}^{N} \alpha_{m}^{*n}\beta_{m}^{n}\right)$$
(3.3.20)

This time, the integration variables are complex rather than Grassmannian, and we use formula (3.1.21). Identifying the coefficients in front of $|\beta_m^n|^2$, β_m^{n*} and β_m^n , we find

$$\begin{cases} a_n = 1\\ b_n = \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m-1}^n\\ c_n = \alpha_m^{*n} \end{cases}$$
(3.3.21)

and thus we have

$$I_B(\alpha_m^*, \alpha_{m-1}) = \exp\left(\sum_{n=1}^N \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_m^{*n} \alpha_{m-1}^n\right)$$
$$= \exp\left(-\frac{i}{\hbar} \delta t \, H_B(\alpha_m^*, \alpha_{m-1})\right) \exp\left(\sum_{n=1}^N \alpha_m^{*n} \alpha_{m-1}^n\right)$$
(3.3.22)

The elementary propagator (3.3.5) now reads

$$\left\langle \zeta_m \alpha_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}\right) \right| \zeta_{m-1} \alpha_{m-1} \right\rangle = \exp\left(-\frac{i}{\hbar} \delta t \left[H_F(\zeta_m^*, \zeta_{m-1}) + H_B(\alpha_m^*, \alpha_{m-1})\right]\right) \\ \times \exp\left(\sum_{\mu=1}^L \zeta_m^{*\mu} \zeta_{m-1}^{\mu}\right) \exp\left(\sum_{n=1}^N \alpha_m^{*n} \alpha_{m-1}^n\right)$$
(3.3.23)

As was already mentioned, the Hamiltonian under consideration represents a system with decoupled bosonic and fermionic parts, and we expected the transition probabilities relative to the bosonic and fermionic part of the system to be independent from one another. Writing the whole propagator, we see that indeed,

$$K(\zeta_{M}\alpha_{M}, t_{M}; \zeta_{0}\alpha_{0}, t_{0}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^{N} \frac{d\alpha_{m}^{n*} d\alpha_{m}^{n}}{2i\pi} e^{-|\alpha_{m}^{n}|^{2}} \int \prod_{\mu=1}^{L} d\zeta_{m}^{\mu*} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu}} \zeta_{m}^{\mu} \right] \\ \times \prod_{m=1}^{M} \left[\exp\left(-\frac{i}{\hbar} \delta t \left[H_{F}(\zeta_{m}^{*}, \zeta_{m-1}) + H_{B}(\alpha_{m}^{*}, \alpha_{m-1}) \right] \right) \\ \times \exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu}\right) \exp\left(\sum_{n=1}^{N} \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \right]$$
(3.3.24)

can be written as two separate propagators. Using the BCH formula (3.3.4) to rearrange the exponentials, we find

$$K(\zeta_{M}\alpha_{M}, t_{M}; \zeta_{0}\alpha_{0}, t_{0}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} d\zeta_{m}^{\mu*} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu}\zeta_{m}^{\mu}} \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu}\zeta_{m-1}^{\mu} - \frac{i}{\hbar} \delta t \, H_{F}(\zeta_{m}^{*}, \zeta_{m-1}) \right) \right] \\ \times \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^{N} \frac{d\alpha_{m}^{n*} d\alpha_{m}^{n}}{2i\pi} e^{-|\alpha_{m}^{n}|^{2}} \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{n=1}^{N} \alpha_{m}^{*n} \alpha_{m-1}^{n} - \frac{i}{\hbar} \delta t \, H_{B}(\alpha_{m}^{*}, \alpha_{m-1}) \right) \right] \\ \equiv K^{F}(\zeta_{M}, t_{M}; \zeta_{0}, t_{0}) K^{B}(\alpha_{M}, t_{M}; \alpha_{0}, t_{0})$$
(3.3.25)

We can thus compute the propagator by computing two propagators separately. Let us begin with the bosonic propagator. We proceed by recurrence. We have, for the approximation to the propagator with M = 1 (which will be referred to as the 1st approximation to the propagator):

$$K_1^B(\alpha_1, t_1; \alpha_0, t_0) = \exp\left(\sum_{n=1}^N \alpha_1^{*n} \alpha_0^n - \frac{i}{\hbar} \delta t \, H_B(\alpha_1^*, \alpha_0)\right)$$
(3.3.26)

where following the usual convention, α_1 is the final state of the bosonic field and α_0 its initial state. If we now consider the case M = 2, we immediately see that it can be written using the 1st approximation to the propagator:

$$K_{2}^{B}(\alpha_{2}, t_{2}; \alpha_{0}, t_{0}) = \int \prod_{n=1}^{N} \left[\frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \right] \exp\left(\sum_{n=1}^{N} \alpha_{2}^{*n} \alpha_{1}^{n} - \frac{i}{\hbar} \delta t \, H_{B}(\alpha_{2}^{*}, \alpha_{1})\right) \exp\left(\sum_{n=1}^{N} \alpha_{1}^{*n} \alpha_{0}^{n} - \frac{i}{\hbar} \delta t \, H_{B}(\alpha_{1}^{*}, \alpha_{0})\right)$$
$$= \int \prod_{n=1}^{N} \left[\frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \right] \exp\left(\sum_{n=1}^{N} \alpha_{2}^{*n} \alpha_{1}^{n} - \frac{i}{\hbar} \delta t \, H_{B}(\alpha_{2}^{*}, \alpha_{1})\right) K_{1}^{B}(\alpha^{1}, t_{1}; \alpha_{0}, t_{0}) \qquad (3.3.27)$$

Applying this reasoning m-1 times, we find the recursive formula for the m^{th} approximation to the propagator:

$$K_m^B(\alpha_m, t_m; \alpha_0, t_0) = \int \prod_{n=1}^N \left[\frac{d\alpha_{m-1}^{n*} d\alpha_{m-1}^n}{2i\pi} e^{-|\alpha_{m-1}^n|^2} \right] \exp\left(\sum_{n=1}^N \alpha_m^{*n} \alpha_{m-1}^n - \frac{i}{\hbar} \delta t \, H_B(\alpha_m^*, \alpha_{m-1})\right) \times K_{m-1}^B(\alpha_{m-1}, t_{m-1}; \alpha_0, t_0)$$
(3.3.28)

and this recurrence formula for K_m^B will be used shortly. We must first compute our base case, which we choose to be M = 2. Once again, we rely on formula (3.1.21) to compute the integrals in (3.3.27) and identify the coefficients in front of $|\alpha_1^n|^2$, α_1^{*n} and α_1^n to be:

$$\begin{cases} a_n = 1\\ b_n = \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_0^n\\ c_n = \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_2^{*n} \end{cases}$$
(3.3.29)

where the expression for $H_B(\alpha_m^*, \alpha_{m-1})$ has been used. We thus have proven that

$$K_2^B(\alpha_2, t_2; \alpha_0, t_0) = \exp\left(\sum_{n=1}^N \left(1 - \frac{i}{\hbar} E_{B,n}\right)^2 \alpha_2^{*n} \alpha_0^n\right)$$
(3.3.30)

Giving it a little bit of thought, we can convince ourselves that the recurrence pattern is simply

$$K_m^B(\alpha_m, t_m; \alpha_0, t_0) = \exp\left(\sum_{n=1}^N \left(1 - \frac{i}{\hbar} E_{B,n}\right)^m \alpha_m^{*n} \alpha_0^n\right)$$
(3.3.31)

To show it, we assume that the above formula is valid for m-1 and compute K_m^B using (3.3.28):

$$K_{m}^{B}(\alpha_{m}, t_{m}; \alpha_{0}, t_{0}) = \int \prod_{n=1}^{N} \left[\frac{d\alpha_{m-1}^{n*} d\alpha_{m-1}^{n}}{2i\pi} e^{-|\alpha_{m-1}^{n}|^{2}} \right] \exp\left(\sum_{n=1}^{N} \alpha_{m}^{*n} \alpha_{m-1}^{n} - \frac{i}{\hbar} \delta t \, H_{B}(\alpha_{m}^{*}, \alpha_{m-1})\right) \\ \times \exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} E_{B,n}\right)^{m} \alpha_{m-1}^{*n} \alpha_{0}^{n}\right)$$
(3.3.32)

In order to apply formula (3.1.21), we identify

$$\begin{cases} a_n = 1\\ b_n = \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right)^{m-1} \alpha_0^n\\ c_n = \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_m^{*n} \end{cases}$$
(3.3.33)

and thus we finally find

$$K_m^B(\alpha_m, t_m; \alpha_0, t_0) = \exp\left(\sum_{n=1}^N \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right)^m \alpha_m^{*n} \alpha_0^n\right)$$
(3.3.34)

which proves equation (3.3.31). The propagator of the bosonic part of the system is given by K_M^B where M goes to infinity. In that case, using the fact that $\delta t = \frac{t_m - t_0}{M}$ is infinitesimal, the factor in front of $\alpha_M^{*n} \alpha_0^n$ is recognized as the definition of the exponential. Going back to the notation $|\alpha_f\rangle$ and $|\alpha_i\rangle$ for the initial and final states, we have

$$K^B(\alpha_f, t_f; \alpha_i, t_i) = \exp\left(\sum_{n=1}^N e^{-\frac{i}{\hbar}E_{B,n}(t_f - t_i)} \alpha_f^{*n} \alpha_i^n\right)$$
(3.3.35)

A similar result can be obtained for the fermionic part of the system using formula (3.2.46) in the particular case of diagonal matrices. The calculations are somewhat simpler than in the bosonic case since each integral amounts to the multiplication of two diagonal matrices. The final result is

$$K^{F}(\zeta_{f}, t_{f}; \zeta_{i}, t_{i}) = \exp\left(\sum_{\mu=1}^{L} e^{-\frac{i}{\hbar}E_{F,\mu}(t_{f}-t_{i})} \zeta_{f}^{*\mu} \zeta_{i}^{\mu}\right)$$
$$= \prod_{\mu=1}^{L} \left(1 - e^{-\frac{i}{\hbar}E_{F,\mu}(t_{f}-t_{i})} \zeta_{f}^{*\mu} \zeta_{i}^{\mu}\right)$$
(3.3.36)

where the last equality follows from the fact that $\zeta_f^{*\mu}$ and ζ_i^{μ} are Grassmann generators. Those two propagators correspond to the propagators of the free bosonic and fermionic field respectively. They will occasionally be useful to check the consistency of results obtained in the context of an interacting system. We indeed expect those results to yield the free field solution in the limit of vanishing interactions. Now that the reader has been exposed to some of the computation techniques that will be used in practical examples, we propose to conclude the chapter with a discussion on the link between the Hamiltonian and Lagrangian formulation of the path integral.

Equivalence between the Hamiltonian and Lagrangian formulation

In order to show that the propagator in (3.3.2) is equivalent to Feynman's original definition given in (2.3.4), elementary concepts from Hamiltonian mechanics will be used. Only the bare minimum will be exposed. For a review, see e.g. [46] or any other textbook on classical mechanics. A reader who has followed the discussion so far already knows the quantum Hamiltonian operator, representing the energy of the quantum system. The quantum Hamiltonian of a system is obtained from the classical Hamiltonian by replacing variables such as the position \mathbf{r} by an operator, $\hat{\mathbf{r}}$ in the case of the position. The classical Hamiltonian is itself obtained from the Lagrangian via the transformation

$$\mathcal{H}(\mathbf{p}, \mathbf{q}, t) = \mathbf{p}\dot{\mathbf{q}} - \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, t)$$
(3.3.37)

with \mathbf{q} the generalized coordinates of the system introduced in the review of Lagrangian mechanics (section 2.1), and \mathbf{p} the generalized momenta associated to \mathbf{q} . Those momenta replace the generalized velocities $\dot{\mathbf{q}}$ in the context of Hamiltonian mechanics. They are defined as

$$\mathbf{p} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} \tag{3.3.38}$$

For completeness, we mention that the equations of motion for the system are obtained from the Hamiltonian using

$$\begin{cases} \dot{\mathbf{q}} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} \\ \dot{\mathbf{p}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} \end{cases}$$
(3.3.39)

What we need to take away from this short summary is the transformation (3.3.37). Indeed, going from (3.3.2) to an expression for the propagator similar to (2.3.4) requires the ability to transform the Hamiltonian into a Lagrangian. We shall see that this transformation allows us to make the transition between the Hamiltonian propagator and Feynman's original formulation.

Looking back to the equation for the propagator (3.3.2), we can replace the elementary propagator by the result obtained in (3.3.5):

$$K(\zeta_{M}\alpha_{M}, t_{M}; \zeta_{0}\alpha_{0}, t_{0}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^{N} \left[\frac{d\alpha_{m}^{n*} d\alpha_{m}^{n}}{2i\pi} e^{-|\alpha_{m}^{n}|^{2}} \right] \int \prod_{\mu=1}^{L} \left[d\zeta_{m}^{\mu*} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu} \zeta_{m}^{\mu}} \right] \right] \\ \times \prod_{m=1}^{M} \left[\exp\left(-\frac{i}{\hbar} \delta t \left[H_{F}(\zeta_{m}, \zeta_{m-1}) + H_{B}(\alpha_{m}^{*}, \alpha_{m-1}) \right] \right) \exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu} \right) \exp\left(\sum_{n=1}^{N} \alpha_{m}^{*n} \alpha_{m-1}^{n} \right) \right]$$
(3.3.40)

We first note that in the limit where M goes to infinity, the integrals run over all possible paths for the variables α^{*n} , α^n , $\zeta^{*\mu}$ and ζ^{μ} . We therefore use the notation

$$\prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} d\zeta_m^{\mu*} d\zeta_m^{\mu} \int \prod_{n=1}^{N} \frac{d\alpha_m^{n*} d\alpha_m^n}{2i\pi} \right] \to \int_{\zeta_0 \alpha_0}^{\zeta_M \alpha_M} D\left[\alpha(t), \zeta(t)\right]$$
(3.3.41)

with $\alpha(t)$ being a symbolic notation representing the paths taken by all the variables α^{*n} , α^n , and similarly for $\zeta(t)$. This notation is the coherent state equivalent to the notation used by Feynman for generalized coordinates in the context of path integrals [11]. The sum of the bosonic and the fermionic Hamiltonians is recognized as being the total Hamiltonian that we naturally denote $H(\zeta_m^*, \alpha_m^*, \zeta_{m-1}, \alpha_{m-1})$. We then assemble the exponentials from the elementary propagator with those from the closure relations. For m = M, the exponentials from the closure are missing and we therefore add them artificially, multiplying the overall expression by a factor $\prod_{n=1}^{N} e^{|\alpha_M^n|^2} \prod_{\mu=1}^{L} e^{\zeta_M^* \zeta_M^\mu}$. We have, for the overall exponential:

$$\begin{split} &\prod_{m=1}^{M-1} \left[\exp\left(-\sum_{n=1}^{N} |\alpha_m^n|^2\right) \exp\left(-\sum_{\mu=1}^{L} \zeta_m^{*\mu} \zeta_m^{\mu}\right) \right] \prod_{m=1}^{M} \left[\exp\left(-\frac{i}{\hbar} \delta t \, H(\zeta_m^*, \alpha_m^*, \zeta_{m-1}, \alpha_{m-1})\right) \right] \\ &\times \exp\left(\sum_{\mu=1}^{L} \zeta_m^{*\mu} \zeta_{m-1}^{\mu}\right) \exp\left(\sum_{n=1}^{N} \alpha_m^{*n} \alpha_{m-1}^{n}\right) \right] \\ &= \exp\left(\sum_{n=1}^{N} |\alpha_M^n|^2\right) \exp\left(\sum_{\mu=1}^{L} \zeta_M^{*\mu} \zeta_M^{\mu}\right) \prod_{m=1}^{M} \left[\exp\left(-\sum_{n=1}^{N} \alpha_m^{*n} \left(\alpha_m^n - \alpha_{m-1}^n\right) - \sum_{\mu=1}^{L} \zeta_m^{*\mu} \left(\zeta_m^\mu - \zeta_{m-1}^\mu\right) \right) \right] \\ &\times \exp\left(-\frac{i}{\hbar} \delta t \, H(\zeta_m^*, \alpha_m^*, \zeta_{m-1}, \alpha_{m-1})\right) \right] \\ &= \exp\left(\sum_{n=1}^{N} |\alpha_M^n|^2\right) \exp\left(\sum_{\mu=1}^{L} \zeta_M^{*\mu} \zeta_M^{\mu}\right) \\ &\times \prod_{m=1}^{M} \left[\exp\left(\frac{i}{\hbar} \delta t \, \left(i\hbar \sum_{n=1}^{N} \alpha_m^{*n} \left(\frac{\alpha_m^n - \alpha_{m-1}^n}{\delta t}\right) + i\hbar \sum_{\mu=1}^{L} \zeta_m^{*\mu} \left(\frac{\zeta_m^\mu - \zeta_{m-1}^\mu}{\delta t}\right) - H(\zeta_m^*, \alpha_m^*, \zeta_{m-1}, \alpha_{m-1}) \right) \right) \right] \end{aligned}$$
(3.3.42)

In the limit where M goes to infinity, we follow [17] and identify the quantities $\frac{\alpha_m^n - \alpha_{m-1}^n}{\delta t}$ and $\frac{\zeta_m^\mu - \zeta_{m-1}^\mu}{\delta t}$ to derivatives. The quantity inside the exponential then reads

$$\frac{i}{\hbar}\delta t \left(i\hbar \sum_{n=1}^{N} \alpha_m^{*n} \frac{\partial \alpha^n}{\partial t}\Big|_{\alpha^n = \alpha_m^n} + i\hbar \sum_{\mu=1}^{L} \zeta_m^{*\mu} \frac{\partial \zeta^\mu}{\partial t}\Big|_{\zeta^\mu = \zeta_m^\mu} - H(\zeta_m^*, \alpha_m^*, \zeta_{m-1}, \alpha_{m-1})\right)$$
(3.3.43)

The next step will require to accept that $\sqrt{i\hbar\alpha_m^{*n}}$ can be seen as the conjugate momentum to $\sqrt{i\hbar\alpha_m^n}$ for all n (which is shown in appendix D for the interested reader), and that the same is true for ζ_m^{μ} . The equation above is then recognized as the transformation (3.3.37), yielding the time-independent Lagrangian of the system at time step m. Using this transformation and the notation (3.3.41), equation (3.3.40) can then be re-written as

$$K(\zeta_{M}\alpha_{M}, t_{M}; \zeta_{0}\alpha_{0}, t_{0}) = C \int_{\zeta_{i}\alpha_{i}}^{\zeta_{f}\alpha_{f}} D\left[\alpha(t), \zeta(t)\right] \lim_{M \to \infty} \prod_{m=1}^{M} \exp\left(\frac{i}{\hbar} \delta t \mathcal{L}\left(\zeta_{m}, \frac{\partial \zeta}{\partial t}\Big|_{\zeta=\zeta_{m}}, \alpha_{m}^{n}, \frac{\partial \alpha^{n}}{\partial t}\Big|_{\alpha^{n}=\alpha_{m}^{n}}\right)\right)$$
$$= C \int_{\zeta_{i}\alpha_{i}}^{\zeta_{f}\alpha_{f}} D\left[\alpha(t), \zeta(t)\right] \lim_{M \to \infty} \exp\left(\frac{i}{\hbar} \sum_{m=1}^{M} \delta t \mathcal{L}\left(\zeta_{m}, \frac{\partial \zeta}{\partial t}\Big|_{\zeta=\zeta_{m}}, \alpha_{m}^{n}, \frac{\partial \alpha^{n}}{\partial t}\Big|_{\alpha^{n}=\alpha_{m}^{n}}\right)\right)$$
(3.3.44)

with C the normalization constant

$$C = \exp\left(\sum_{n=1}^{N} |\alpha_M^n|^2\right) \exp\left(\sum_{\mu=1}^{L} \zeta_M^{*\mu} \zeta_M^{\mu}\right)$$
(3.3.45)

Note that both this constant and the propagator contain Grassmann variables. As a consequence, this propagator is not yet physical in the sense that it does not represent a transition probability between physical fermionic states. In order to make it physical, one would have to eliminate those Grassmann variables one way or another. This will be discussed in chapters 4 and 5 where the actual calculations begin. For now, we will content ourselves with showing that we recover Feynman's initial formulation for the path integral from the Hamiltonian formalism. Using again the fact that M goes to infinity, the quantity inside of the exponential is recognized as an integral and we finally have

$$K(\zeta_M \alpha_M, t_M; \zeta_0 \alpha_0, t_0) = C \int_{\zeta_i \alpha_i}^{\zeta_f \alpha_f} D\left[\alpha(t), \zeta(t)\right] \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} dt \,\mathcal{L}\left(\zeta(t), \dot{\zeta(t)}, \alpha(t), \dot{\alpha(t)}\right)\right)$$
(3.3.46)

which is indeed analogous to the formulation (2.3.4), since the integral runs over all paths relating the states $|\zeta_0 \alpha_0\rangle$ and $|\zeta_M \alpha_M\rangle$. This demonstration can be done for a generic system in coherent state representation provided that the Hamiltonian is bounded from below [17], *i.e.* that the action of the Hamiltonian on coherent states do not produce negative constants that can be arbitrarily large.

Now that useful techniques in the treatment of mixed system path integrals have been exposed, we will tackle the more practical case of the mixed system presented in section 1.2. The long-term goal is now to eliminate the fermions from the propagator in order to obtain a purely bosonic propagator on which some semiclassical techniques can hopefully be applied. Working towards this goal, chapter 4 will be devoted to show that the postulated mixed system is relevant in the sense that the elimination of bosonic degrees of freedom from it yields a system of interacting fermions, as we want to describe. The elimination of the fermionic degrees of freedom from this mixed system will then be performed in chapter 5.

Chapter 4

From a Mixed to a Fermionic Propagator

With this chapter begin the actual computations towards achieving our goal, which we will repeat here. We wish to express the dynamics of an interacting fermionic system with the bosons that mediate their interactions in order to find a semiclassical expression for the propagator of an interacting fermionic system using existing bosonic results. In this chapter, we compute what is the result of the elimination of the bosons from the mixed propagator. The path integral formulation of our mixed Hamiltonian is first obtained. Then, the elimination of bosonic degrees of freedom is carried out over the whole propagator. A last calculation is done to verify that the obtained propagator corresponds to the dynamics of an interacting fermionic system. We conclude the chapter with a discussion on the obtained result, and in particular on the treatment of the initial state and final state of the bosonic field. For the sake of simplicity, a bosonic field with a single mode will be considered in this chapter.

Description of the method

Since this is the first chapter where our method is applied in a concrete way, we find that it is a good time to explain it in more detail. The core idea of the method is to use the mixed system as an intermediate step to establish the correspondence between the dynamics of an interacting fermionic system and those of a bosonic system. In each case, the dynamics of the system are expressed using Feynman's path integral formalism. As was seen in the last section of chapter 3, the propagator of the mixed system contains an infinite number of bosonic and fermionic closure relations: one for each infinitesimal time steps. Using techniques such as recurrence, one can compute those closure relations, thus eliminating all the degrees of freedom from the propagator except for the initial and final state. In this way, one can eliminate, for instance, the fermionic degrees of freedom from the mixed propagator without the use of any approximation or additional integrals. The obtained propagator is thus exact.

The first step of the method is to find the mixed system corresponding to the fermionic system we wish to describe, which is represented by the mixed Hamiltonian (1.2.8). We thus have to make the hypothesis that the fermions we study interact with a bosonic field, or else bosons would be independent from the fermions and would therefore be unable to contain any information about the dynamics of the fermions. An example of fermions interacting via bosons is given by the case for charged fermionic particles that interact electromagnetically. In order to verify the correspondence between the mixed system and the fermionic system, we eliminate the bosons from the mixed propagator and compare it to the purely fermionic propagator of an interacting fermionic system and check if they contain similar dynamics for the fermions. This is done here, in chapter 4. Once this correspondence has been established, the next step is to eliminate the fermions from the mixed propagator and study the resulting bosonic propagator. This is done in chapter 5. The final step, which could be treated in a future work, is to find the general correspondence between an interacting fermionic system and a bosonic system without having to express an intermediate mixed system, if such correspondence exist. This is schematically exposed in figure 4.1.



Figure 4.1: Schematic view of the method proposed in this work to express the dynamics of interacting fermions through the dynamics of the bosons mediating their interactions. Red arrows correspond to the integration of degrees of freedom in the propagator. We first need to verify that the proposed mixed Hamiltonian yields the correct fermionic dynamics when bosonic degrees of freedom are integrated over. We can then go from the fermionic system to the mixt system and integrate the bosonic degrees of freedom.

4.1 Path-integral formulation

We wish to write the path-integral theory of a system described by the mixed Hamiltonian

$$\hat{H} = \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu} + E_B \hat{b}^{\dagger} \hat{b} + \sum_{\mu,\nu=1}^{L} C_{\mu\nu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\nu} (\hat{b}^{\dagger} + \hat{b})$$

= $\hat{H}_F + \hat{H}_B + \hat{H}_{int}$ (4.1.1)

As a reminder, \hat{H}_F is a purely fermionic term corresponding to the interaction between the fermions and the optical trap. The Hamiltonian \hat{H}_B is a purely bosonic term corresponding to the interaction of the bosonic field with the optical trap. The term \hat{H}_{int} contains the interaction between the fermions and the bosonic field, allowing fermions to interact with each other via bosons. We now write the propagator $K(\zeta_f \alpha_f, t_f; \zeta_i \alpha_i, t_i)$ between the two states of the mixed system $|\zeta_i \alpha_i\rangle$ at time t_i and $|\zeta_f \alpha_f\rangle$ at time t_f . We remind the reader that the square of this propagator gives the probability to find the system in state $|\zeta_f \alpha_f\rangle$ at time t_f if it was in state $|\zeta_i \alpha_i\rangle$ at time t_i . Using the Hamiltonian above, the propagator reads:

$$K(\zeta_{f}\alpha_{f}, t_{f}; \zeta_{i}\alpha_{i}, t_{i}) = \left\langle \zeta_{f}\alpha_{f} \middle| \hat{K}(t_{f}; t_{i}) \middle| \zeta_{i}\alpha_{i} \right\rangle$$
$$= \left\langle \zeta_{f}\alpha_{f} \middle| \hat{T}\exp\left(-\frac{i}{\hbar}\int_{t_{i}}^{t_{f}}\hat{H}(t)dt\right) \middle| \zeta_{i}\alpha_{i} \right\rangle$$
$$= \left\langle \zeta_{f}\alpha_{f} \middle| \exp\left(-\frac{i}{\hbar}(t_{f} - t_{i})\hat{H}\right) \middle| \zeta_{i}\alpha_{i} \right\rangle$$
(4.1.2)

The last equality follows from the fact that the considered Hamiltonian is time-independent. Following the method exposed in chapter 2 and 3, we divide the time interval $[t_i, t_f]$ in M sub-intervals of width $\Delta t = (t_f - t_i)/M$. Using the fact that \hat{H} commutes with itself, we separate the exponential into M time steps to obtain

$$K(\zeta_f \alpha_f, t_f; \zeta_i \alpha_i, t_i) = \left\langle \zeta_f \alpha_f \left| \prod_{m=1}^M \left[\exp\left(-\frac{i}{\hbar} \Delta t \, \hat{H} \right) \right] \right| \zeta_i \alpha_i \right\rangle$$
(4.1.3)

Inserting M-1 fermionic closure relation and using the notation $|\zeta_f \alpha_f \rangle \rightarrow |\zeta_M \alpha_M \rangle$ and $|\zeta_i \alpha_i \rangle \rightarrow |\zeta_0 \alpha_0 \rangle$, we finally obtain the path-integral formulation of the propagator for the mixed Hamiltonian:

$$K(\zeta_M \alpha_M, t_M; \zeta_0 \alpha_0, t_0) = \langle \alpha_M | \int \prod_{m=1}^{M-1} \left[\prod_{\mu=1}^L d\zeta_m^{*\mu} d\zeta_m^{\mu} e^{-\zeta_m^{*\mu} \zeta_m^{\mu}} \right] \prod_{m=1}^M \left[\left\langle \zeta_m \left| \exp\left(-\frac{i}{\hbar} \Delta t \, \hat{H}\right) \right| \zeta_{m-1} \right\rangle \right] |\alpha_0\rangle \quad (4.1.4)$$

Unlike the similar development in chapter 3, we did not insert the bosonic closure relations yet. They will instead be inserted into the elementary propagator $\langle \zeta_m | \exp\left(-\frac{i}{\hbar}\Delta t \hat{H}\right) | \zeta_{m-1} \rangle$, along with other closure relations, which yields a strictly equivalent result. In the limit where $M \to \infty$, Δt becomes an infinitesimal quantity denoted δt and we can separate the exponential of the total Hamiltonian into a bosonic, fermionic and mixed exponential using the BCH formula (3.3.4). Inserting three bosonic and one fermionic closure relations, we have

$$\left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1} \right\rangle = \left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{F}\right) \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{B}\right) \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{int}\right) \right| \zeta_{m-1} \right\rangle$$

$$= \int \frac{d\beta_{3,m}^{*}d\beta_{3,m}}{2i\pi} \int \frac{d\beta_{2,m}^{*}d\beta_{2,m}}{2i\pi} \int \frac{d\beta_{1,m}^{*}d\beta_{1,m}}{2i\pi} e^{-(|\beta_{3,m}|^{2}+|\beta_{2,m}|^{2}+|\beta_{1,m}|^{2})}$$

$$\times \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu}d\xi_{m}^{\mu}e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{F}\right) \right| \xi_{m} \right\rangle$$

$$\times \left\langle \beta_{3,m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{B}\right) \right| \beta_{2,m} \right\rangle \left\langle \beta_{2,m}\xi_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}_{int}\right) \right| \beta_{1,m}\zeta_{m-1} \right\rangle$$

$$\times |\beta_{3,m}\rangle \left\langle \beta_{1,m} |$$

$$(4.1.5)$$

Let $\int d\left[\beta_{3,m},\beta_{2,m},\beta_{1,m},\xi_m\right]$ denote the integrals from the four closure relations. The action of the creation and annihilation operators in the Hamiltonians yield

$$\left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \left| \zeta_{m-1} \right\rangle = \int d\left[\beta_{3,m},\beta_{2,m},\beta_{1,m},\xi_{m}\right] e^{-\left(|\beta_{3,m}|^{2}+|\beta_{2,m}|^{2}+|\beta_{1,m}|^{2}\right)} \prod_{\mu=1}^{L} \left[e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \right. \\ \left. \times \left\langle \zeta_{m} \left| \xi_{m} \right\rangle \left\langle \beta_{3,m} \left| \beta_{2,m} \right\rangle \left\langle \beta_{2,m} \left| \beta_{1,m} \right\rangle \left\langle \xi_{m} \left| \zeta_{m-1} \right\rangle \exp\left(-\frac{i}{\hbar}\delta t\,H_{F}\left(\zeta_{m}^{*},\xi_{m}\right)\right) \right. \right. \\ \left. \times \exp\left(-\frac{i}{\hbar}\delta t\,H_{B}\left(\beta_{3,m}^{*},\beta_{2,m}\right)\right) \exp\left(-\frac{i}{\hbar}\delta t\,H_{int}\left(\xi_{m}^{*},\beta_{2,m}^{*},\zeta_{m-1},\beta_{1,m}\right)\right) \right. \\ \left. \times \left. \left| \beta_{3,m} \right\rangle \left\langle \beta_{1,m} \right| \right. \right.$$

$$\left. \left. \left(4.1.6 \right) \right] \right\}$$

with the notations

$$\begin{cases} H_F\left(\zeta_m^*, \xi_m\right) = \sum_{\mu=1}^L E_{F,\mu} \zeta_m^{*\mu} \xi_m^{\mu} \\ H_B\left(\beta_{3,m}^*, \beta_{2,m}\right) = E_B \beta_{3,m}^* \beta_{2,m} \\ H_{int}\left(\xi_m^*, \beta_{2,m}^*, \zeta_{m-1}, \beta_{1,m}\right) = \sum_{\mu,\nu=1}^L C_{\mu\nu} \xi_m^{*\mu} \zeta_{m-1}^{\nu} (\beta_{2,m}^* + \beta_{1,m}) \end{cases}$$
(4.1.7)

Before focusing our attention on bosons, we compute the integrals each of the Grassmann generators $\xi_m^{*\mu}$, ξ_m^{μ} . We have

$$\begin{split} I &= \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu} \xi_{m}^{\mu}} \right] \left\langle \zeta_{m} \mid \xi_{m} \right\rangle \left\langle \xi_{m} \mid \zeta_{m-1} \right\rangle \exp\left(-\frac{i}{\hbar} \delta t \, H_{F}\left(\zeta_{m}^{*}, \xi_{m}\right)\right) \exp\left(-\frac{i}{\hbar} \delta t \, H_{int}\left(\xi_{m}^{*}, \beta_{2,m}^{*}, \zeta_{m-1}, \beta_{1,m}\right)\right) \right) \\ &= \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu} \xi_{m}^{\mu}} \right] \exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu} \xi_{m}^{\mu}\right) \exp\left(\sum_{\mu=1}^{L} \xi_{m}^{*\mu} \zeta_{m-1}^{\mu}\right) \exp\left(-\frac{i}{\hbar} \delta t \, \sum_{\mu=1}^{L} E_{F,\mu} \zeta_{m}^{*\mu} \xi_{m}^{\mu}\right) \right) \\ &\times \exp\left(-\frac{i}{\hbar} \delta t \, \sum_{\mu,\nu=1}^{L} C_{\mu\nu} \xi_{m}^{*\mu} \zeta_{m-1}^{\nu} (\beta_{2,m}^{*} + \beta_{1,m})\right) \right) \\ &= \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu} \xi_{m}^{\mu}} \right] \exp\left(\sum_{\mu=1}^{L} \left(1 - \frac{i}{\hbar} \delta t \, E_{F,\mu}\right) \zeta_{m}^{*\mu} \xi_{m}^{\mu}\right) \exp\left(\sum_{\mu,\nu=1}^{L} \left(\delta_{\mu\nu} - (\beta_{2,m}^{*} + \beta_{1,m}) \frac{i}{\hbar} \delta t \, C_{\mu\nu}\right) \xi_{m}^{*\mu} \zeta_{m-1}^{\nu}\right) \right)$$

$$(4.1.8)$$

with $\delta_{\mu\nu}$ the Kronecker delta. The application of formula (3.2.46) yields

$$I = \exp\left(\sum_{\mu,\nu=1}^{L} \left[\left(\mathbb{1} - \frac{i}{\hbar} \delta t \, \mathbf{E} \right) \left(\mathbb{1} - (\beta_{2,m}^* + \beta_{1,m}) \frac{i}{\hbar} \delta t \, \mathbf{C} \right) \right]_{\mu\nu} \zeta_m^{*\mu} \zeta_{m-1}^{\nu} \right)$$
(4.1.9)

with **E** the matrix diag $(E_{F,1}, \ldots, E_{F,L})$ and **C** the matrix containing the coefficients $C_{\mu\nu}$. Since the limit for $M \to \infty$ has been taken, δt is infinitesimal and we can further develop the matrix product, yielding

$$1 - \frac{i}{\hbar} \delta t \mathbf{E} - (\beta_{2,m}^* + \beta_{1,m}) \frac{i}{\hbar} \delta t \mathbf{C} + \mathcal{O}(\delta t^2)$$
(4.1.10)

where the terms of order δt^2 and higher can be neglected. In the limit where M goes to infinity, we can thus write

$$I = \exp\left(\sum_{\mu,\nu=1}^{L} \left[\mathbb{1} - \frac{i}{\hbar} \delta t \,\mathbf{E} - (\beta_{2,m}^* + \beta_{1,m}) \frac{i}{\hbar} \delta t \,\mathbf{C}\right]_{\mu\nu} \zeta_m^{*\mu} \zeta_{m-1}^{\nu}\right)$$
(4.1.11)

which can be split into a purely fermionic part and a part containing bosonic variables using the BCH formula (3.3.4):

$$I = \exp\left(\sum_{\mu=1}^{L} \left(1 - \frac{i}{\hbar} \delta t \, E_{F,\mu}\right) \zeta_m^{*\mu} \zeta_{m-1}^{\mu}\right) \exp\left(-\frac{i}{\hbar} \delta t \, \sum_{\mu,\nu=1}^{L} (\beta_{2,m}^* + \beta_{1,m}) C_{\mu\nu} \zeta_m^{*\mu} \zeta_{m-1}^{\nu}\right)$$
(4.1.12)

4.2 Elimination of the bosonic degrees of freedom

We now turn to the bosonic degrees of freedom. The three bosonic variables β_3 , β_2 and β_1 and their complex conjugates need to be integrated over in every elementary propagators. The integration over β_2 and β_2^* can be performed in each elementary propagator separately and will thus come first. Then, β_1 and β_3 will both be treated simultaneously for the whole propagator using a recurrence approach. We first re-write the elementary propagator by using the formula for the scalar product between two coherent states and by replacing the Hamiltonians involving bosonic variables by their expression:

$$\left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1} \right\rangle = \exp\left(\sum_{\mu=1}^{L} \left(1 - \frac{i}{\hbar}\delta t\,E_{F,\mu}\right)\zeta_{m}^{*\mu}\zeta_{m-1}^{\mu}\right) \int d\left[\beta_{3,m},\beta_{2,m},\beta_{1,m}\right] e^{-\left(|\beta_{3,m}|^{2} + |\beta_{2,m}|^{2} + |\beta_{1,m}|^{2}\right)} \times \exp\left(\beta_{3,m}^{*}\beta_{2,m}\right) \exp\left(-\frac{i}{\hbar}\delta t\,E_{B}\beta_{3,m}^{*}\beta_{2,m}\right) \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu,\nu=1}^{L}(\beta_{2,m}^{*} + \beta_{1,m})C_{\mu\nu}\zeta_{m}^{*\mu}\zeta_{m-1}^{\nu}\right) \left|\beta_{3,m}\rangle\langle\beta_{1,m}\right|$$

$$(4.2.1)$$

To simplify the expression above along with the upcoming calculations, we introduce some notations for factors that are constants with respect to the bosonic variables:

$$\begin{cases}
-\frac{i}{\hbar}\delta t \sum_{\mu,\nu=1}^{L} C_{\mu\nu}\zeta_{m+1}^{*\mu}\zeta_{m}^{\nu} \to F_{m} \\
\frac{i}{\hbar}\delta tE_{B} \to B \\
1-B \to D
\end{cases}$$
(4.2.2)

The elementary propagator now reads

$$\left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}\right) \right| \zeta_{m-1} \right\rangle = \exp\left(\sum_{\mu=1}^{L} \left(1 - \frac{i}{\hbar} \delta t \, E_{F,\mu}\right) \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu}\right) \int d\left[\beta_{3,m}, \beta_{2,m}, \beta_{1,m}\right] e^{-(|\beta_{3,m}|^{2} + |\beta_{2,m}|^{2} + |\beta_{1,m}|^{2})} \times \exp\left(\beta_{2,m}^{*} \beta_{1,m} + D\beta_{3,m}^{*} \beta_{2,m} + F_{m-1}(\beta_{2,m}^{*} + \beta_{1,m})\right) |\beta_{3,m}\rangle \langle\beta_{1,m}|$$
(4.2.3)

In order to lighten the equations, the purely fermionic exponential in front of the bosonic integrals will be ignored until the bosonic degrees of freedom have been integrated over.

Integration over $\beta_{2,m}$

Now that the elementary propagator is written in a simplified form, we apply the formula (3.1.21) in the case of only one bosonic mode and an independent term:

$$\int \frac{d\alpha^* d\alpha}{2i\pi} e^{-a|\alpha|^2} \exp\left(b\alpha^* + c\alpha + d\right) = \frac{1}{a} \exp\left(\frac{bc}{a} + d\right),\tag{4.2.4}$$

where α is a complex variable, $a \in \mathbb{R}$, a > 0, and b, c, d are constants. We identify the coefficients in front of $|\beta_{2,m}|^2$, $\beta_{2,m}^*$, $\beta_{2,m}$, $\beta_{2,m}$ and the independent term in (4.2.3):

$$\begin{cases} a = 1 \\ b = (F_{m-1} + \beta_{1,m}) \\ c = D\beta_{3,m}^* \\ d = -|\beta_{3,m}|^2 - |\beta_{1,m}|^2 + F_{m-1}\beta_{1,m} \end{cases}$$
(4.2.5)

We thus have

$$\int d\left[\beta_{2,m}\right] e^{-\left(|\beta_{3,m}|^2 + |\beta_{2,m}|^2 + |\beta_{1,m}|^2\right)} \exp\left(\beta_{2,m}^* \beta_{1,m} + D\beta_{3,m}^* \beta_{2,m} + F_{m-1}(\beta_{2,m}^* + \beta_{1,m})\right)$$

= $e^{-\left(|\beta_{3,m}|^2 + |\beta_{1,m}|^2\right)} \exp\left(DF_{m-1}\beta_{3,m}^* + F_{m-1}\beta_{1,m} + D\beta_{3,m}^* \beta_{1,m}\right)$ (4.2.6)

Integration over $\beta_{3,m}, \beta_{1,m}$

We are now left with the integrals over $\beta_{3,m}$ and $\beta_{1,m}$ for all m. This calculation however is a bit more involved, since the mth elementary propagator contains the operator $|\beta_{3,m}\rangle \langle \beta_{1,m}|$. Thus, we see the appearance of terms containing one variable from the mth elementary propagator and one from the m - 1th, coming from the scalar products between $\langle \beta_{1,m} |$ and $|\beta_{3,m-1}\rangle$. To handle this case, we will consider the whole propagator at once. It currently reads

$$K(\zeta_{M}\alpha_{M}, t_{M}; \zeta_{0}\alpha_{0}, t_{0}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \int \left[\prod_{\mu=1}^{L} d\zeta_{m}^{*\mu} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu}\zeta_{m}^{\mu}} \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{\mu=1}^{L} \left(1 - \frac{i}{\hbar} \delta t \, E_{F,\mu} \right) \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu} \right) \right] \\ \times \langle \alpha_{M} | \prod_{m=1}^{M} \left[\int d[\beta_{3,m}, \beta_{1,m}] e^{-\left(|\beta_{3,m}|^{2} + |\beta_{1,m}|^{2}\right)} \exp\left(DF_{m-1}\beta_{3,m}^{*} + F_{m-1}\beta_{1,m} + D\beta_{3,m}^{*}\beta_{1,m} \right) |\beta_{3,m}\rangle \langle \beta_{1,m} | \right] |\alpha_{0}\rangle$$

$$(4.2.7)$$

with again the notation $|\zeta_f \alpha_f \rangle \rightarrow |\zeta_M \alpha_M \rangle$ and $|\zeta_i \alpha_i \rangle \rightarrow |\zeta_0 \alpha_0 \rangle$. Omitting the fermionic closure relations and the purely fermionic exponentials, the quantity we need to compute is

$$I_{M}(\alpha_{M}^{*},\alpha_{0}) \equiv \langle \alpha_{M} | \prod_{m=1}^{M} \left[\int d\left[\beta_{3,m},\beta_{1,m}\right] e^{-\left(|\beta_{3,m}|^{2} + |\beta_{1,m}|^{2}\right)} \exp\left(DF_{m-1}\beta_{3,m}^{*} + F_{m-1}\beta_{1,m} + D\beta_{3,m}^{*}\beta_{1,m}\right) |\beta_{3,m}\rangle \langle \beta_{1,m}| \right] |\alpha_{0}\rangle$$

$$(4.2.8)$$

The result of the M integrals will be obtained by recurrence. To understand how exactly we can construct a recurrence, we need to take a closer look at the above expression. Consider first the case M = 1. We have

$$I_{1}(\alpha_{M}^{*},\alpha_{0}) \equiv \langle \alpha_{M} | \int d\left[\beta_{3,1},\beta_{1,1}\right] e^{-\left(|\beta_{3,1}|^{2}+|\beta_{1,1}|^{2}\right)} \exp\left(DF_{0}\beta_{3,1}^{*}+F_{0}\beta_{1,1}+D\beta_{3,1}^{*}\beta_{1,1}\right) |\beta_{3,1}\rangle \langle \beta_{1,1} | \alpha_{0}\rangle$$

$$= \int d\left[\beta_{3,1},\beta_{1,1}\right] e^{-\left(|\beta_{3,1}|^{2}+|\beta_{1,1}|^{2}\right)} \exp\left(DF_{0}\beta_{3,1}^{*}+F_{0}\beta_{1,1}+D\beta_{3,1}^{*}\beta_{1,1}+\alpha_{M}^{*}\beta_{3,1}+\beta_{1,1}^{*}\alpha_{i}\right)$$
(4.2.9)

If we now compute $I_2(\alpha_M^*, \alpha_0)$, we see that the expression for $I_1(\alpha_M^*, \alpha_0)$ occurs in it but with the variable $\beta_{1,2}^*$ taking the role of α_M^* :

$$\begin{split} I_{2}(\alpha_{M}^{*},\alpha_{0}) \\ &= \langle \alpha_{M} | \int d\left[\beta_{3,2},\beta_{1,2}\right] e^{-\left(|\beta_{3,2}|^{2}+|\beta_{1,2}|^{2}\right)} \exp\left(DF_{1}\beta_{3,2}^{*}+F_{1}\beta_{1,2}+D\beta_{3,2}^{*}\beta_{1,2}\right) |\beta_{3,2}\rangle \langle \beta_{1,2}| \\ &\times \int d\left[\beta_{3,1},\beta_{1,1}\right] e^{-\left(|\beta_{3,1}|^{2}+|\beta_{1,1}|^{2}\right)} \exp\left(DF_{0}\beta_{3,1}^{*}+F_{0}\beta_{1,1}+D\beta_{3,1}^{*}\beta_{1,1}\right) |\beta_{3,1}\rangle \langle \beta_{1,1} | \alpha_{0}\rangle \\ &= \int d\left[\beta_{3,2},\beta_{1,2}\right] e^{-\left(|\beta_{3,2}|^{2}+|\beta_{1,2}|^{2}\right)} \exp\left(DF_{1}\beta_{3,2}^{*}+F_{1}\beta_{1,2}+D\beta_{3,2}^{*}\beta_{1,2}+\alpha_{f}^{*}\beta_{3,2}\right) \\ &\times \langle \beta_{1,2} | \int d\left[\beta_{3,1},\beta_{1,1}\right] e^{-\left(|\beta_{3,1}|^{2}+|\beta_{1,1}|^{2}\right)} \exp\left(DF_{0}\beta_{3,1}^{*}+F_{0}\beta_{1,1}+D\beta_{3,1}^{*}\beta_{1,1}\right) |\beta_{3,1}\rangle \langle \beta_{1,1} | \alpha_{0}\rangle \\ &= \int d\left[\beta_{3,2},\beta_{1,2}\right] e^{-\left(|\beta_{3,2}|^{2}+|\beta_{1,2}|^{2}\right)} \exp\left(DF_{1}\beta_{3,2}^{*}+F_{1}\beta_{1,2}+D\beta_{3,2}^{*}\beta_{1,2}+\alpha_{f}^{*}\beta_{3,2}\right) I_{1}(\beta_{1,2}^{*},\alpha_{0}) \tag{4.2.10}$$

Applying the same reasoning to I_3 , I_4 etc up to I_M would show that $I_M(\alpha_M^*, \alpha_0)$ is in fact given by

$$I_{M}(\alpha_{M}^{*},\alpha_{0}) = \int d\left[\beta_{3,M},\beta_{1,M}\right] e^{-\left(|\beta_{3,M}|^{2}+|\beta_{1,M}|^{2}\right)} \exp\left(DF_{M-1}\beta_{3,M}^{*}+F_{M-1}\beta_{1,M}+D\beta_{3,M}^{*}\beta_{1,M}+\alpha_{f}^{*}\beta_{3,M}\right) I_{M-1}(\beta_{1,M}^{*},\alpha_{M})$$

$$(4.2.11)$$

It is using this recursive formula that we will obtain the expression for $I_M(\alpha_M^*, \alpha_0)$. The main ingredient we need for this calculation is the following formula¹ obtained by applying (4.2.4) twice to an exponential function of the bosonic variables α and β :

$$\int \frac{d\alpha^* d\alpha}{2i\pi} \int \frac{d\beta^* d\beta}{2i\pi} e^{-(|\alpha|^2 + |\beta|^2)} \exp\left(b_\alpha \alpha^* + b_\beta \beta^* + c_\alpha \alpha + c_\beta \beta + c_{\alpha^*\beta} \alpha^* \beta + d\right)$$

= exp ($b_\alpha c_\alpha + b_\beta c_\beta + c_{\alpha^*\beta} b_\beta c_\alpha + d$) (4.2.12)

The details for obtaining this formula are worked out in appendix B. We now put it to work. Starting from the expression for $I_M(\alpha_M^*, \alpha_0)$, equation (4.2.11), and putting $\alpha \to \beta_{3,1}$, $\beta \to \beta_{1,1}$, we can identify every coefficient except for b_β and d. Before computing them, we summarize the coefficients we already know:

$$\begin{cases} b_{\alpha} = DF_{M-1}, \quad b_{\beta} = ?\\ c_{\alpha} = \alpha_{f}^{*}, \quad c_{\beta} = F_{M-1}\\ c_{\alpha^{*}\beta} = D\\ d = ? \end{cases}$$

$$(4.2.13)$$

Once we know every coefficient, we can straightforwardly compute $I_M(\alpha_M^*, \alpha_0)$ using (4.2.12). The coefficients b_β and d require the knowledge of $I_{M-1}(\beta_{1,M}^*, \alpha_0)$, since I_{M-1} contains $\beta_{1,M}^*$ and might contain an independent term. The expression for I_{M-1} is given by the recursive formula (4.2.11):

$$I_{M-1}(\beta_{1,M}^*,\alpha_0) = \int d\left[\beta_{3,M-1},\beta_{1,M-1}\right] e^{-\left(|\beta_{3,M-1}|^2 + |\beta_{1,M-1}|^2\right)} \times \exp\left(DF_{M-2}\beta_{3,M-1}^* + F_{M-2}\beta_{1,M-1} + D\beta_{3,M-1}^*\beta_{1,M-1} + \beta_{1,M}^*\beta_{3,M-1}\right) I_{M-2}(\beta_{1,M-1}^*,\alpha_0)$$
(4.2.14)

Since it is an integral of the form (4.2.12), we can again search for the set of coefficients that intervene in the formula (4.2.12). Denoting them by primed constants, we find

$$\begin{cases}
b'_{\alpha} = DF_{M-2}, & b'_{\beta} = ? \\
c'_{\alpha} = \beta^{*}_{1,M}, & c'_{\beta} = F_{M-2} \\
c'_{\alpha^{*}\beta} = D \\
D' = ?
\end{cases}$$
(4.2.15)

where again, the coefficients b'_{β} and d' are unknown. We can however plug them in the right hand side of (4.2.12) without replacing b'_{β} and d', yielding

$$I_{M-1}(\beta_{1,M}^*,\alpha_0) = \exp\left(DF_{M-2}\beta_{1,M}^* + b'_{\beta}F_{M-2} + Db'_{\beta}\beta_{1,M}^* + d'\right)$$
(4.2.16)

The coefficients we are searching for to compute I_M are the coefficient in front of $\beta_{1,M}^*$ and the independent term. We thus find

$$\begin{cases} b_{\beta} = Db'_{\beta} + DF_{M-2} \\ d = d' + b'_{\beta}F_{M-2} \end{cases}$$
(4.2.17)

With these recursive formulae, we shall prove that the general form of the coefficients b_{β} and d for all M is in fact

$$\begin{cases} b_{\beta} = \sum_{k=0}^{M-2} D^{M-k-1} F_k + D^{M-1} \alpha_0 \\ d = \sum_{k=0}^{M-2} D^k F_k \alpha_0 + \sum_{k=0}^{M-3} \sum_{l=k+1}^{M-2} D^{l-k} F_k F_l \end{cases}$$
(4.2.18)

¹This formula is a particular case of a more general formula shown in appendix B. This simplified version is obtained by recognizing that in our context, some coefficients will always have trivial values. This discussion is presented in more details in the appendix.

The base case is given by $I_1(\alpha_M^*, \alpha_0)$. Identifying the coefficient in front of $\beta_{1,1}^*$ and the independent term in (4.2.9), we find

$$M = 1: \begin{cases} b_{\beta} = \alpha_0 \\ d = 0 \end{cases}$$
(4.2.19)

which is consistent with the postulated formulae. Let's now assume that these formulae are correct for M-1 and prove that they hold for M. Starting with b_{β} , we have, using the recurrence hypothesis:

$$b'_{\beta} = \sum_{k=0}^{M-3} D^{M-k-2} F_k + D^{M-2} \alpha_0$$
(4.2.20)

Using equation (4.2.17), we compute

$$b_{\beta} = Db'_{\beta} + DF_{M-2}$$

$$= D\left(\sum_{k=0}^{M-3} D^{M-k-2}F_{k} + D^{M-2}\alpha_{0}\right) + DF_{M-2}$$

$$= \sum_{k=0}^{M-3} D^{M-k-1}F_{k} + D^{M-1}\alpha_{0} + DF_{M-2}$$

$$= \sum_{k=0}^{M-2} D^{M-k-1}F_{k} + D^{M-1}\alpha_{0},$$
(4.2.22)

which is indeed what is given by (4.2.18). For d, we have:

$$d' = \sum_{k=0}^{M-3} D^k F_k \alpha_0 + \sum_{k=0}^{M-4} \sum_{l=k+1}^{M-3} D^{l-k} F_k F_l$$
(4.2.23)

Using again equation (4.2.17), we find

$$d = d' + F_{M-2}b'_{\beta}$$

$$= \sum_{k=0}^{M-3} D^{k}F_{k}\alpha_{0} + \sum_{k=0}^{M-4} \sum_{l=k+1}^{M-3} D^{l-k}F_{k}F_{l} + F_{M-2} \left(\sum_{k=0}^{M-3} D^{M-k-2}F_{k} + D^{M-2}\alpha_{0}\right)$$

$$= \sum_{k=0}^{M-2} D^{k}F_{k}\alpha_{0} + \sum_{k=0}^{M-4} \sum_{l=k+1}^{M-3} D^{l-k}F_{k}F_{l} + \sum_{k=0}^{M-3} D^{M-k-2}F_{k}F_{M-2}$$

$$= \sum_{k=0}^{M-2} D^{k}F_{k}\alpha_{0} + \sum_{k=0}^{M-3} \sum_{l=k+1}^{M-2} D^{l-k}F_{k}F_{l}$$

$$(4.2.24)$$

To obtain the last equality, we realize that the sum containing F_{M-2} corresponds to the M-2 terms with l = M-2. D^{M-k-2} thus becomes D^{l-k} , and the second and third sums can be merged, extending both ranges by 1. This is illustrated in figure 4.2. Equation (4.2.18) is proven.

We have thus obtained the explicit expression for all coefficient required to compute $I_M(\alpha_M^*, \alpha_0)$, summarized below

$$\begin{cases} b_{\alpha} = DF_{M-1}, \quad b_{\beta} = \sum_{k=0}^{M-2} D^{M-k-1} + F_k D^{M-1} \alpha_0 \\ c_{\alpha} = \alpha_f^*, \quad c_{\beta} = F_{M-1} \\ c_{\alpha^*\beta} = D \\ d = \sum_{k=0}^{M-2} D^k F_k \alpha_0 + \sum_{k=0}^{M-3} \sum_{l=k+1}^{M-2} D^{l-k} F_k F_l \end{cases}$$
(4.2.25)

$\downarrow l,k ightarrow$	0	1	2	3	4
0					
1	X				
2	X	X			
3	X	X	X		
4	X	X	X	X	

Figure 4.2: Pair of values k, l covered by the simple sum (in green) and the double sum (in red) in the third line of equation (4.2.24), illustrating that the single sum extends the double sum and that the two can be merged.

These expressions can be plugged back into the right hand side of formula (4.2.12) to obtain:

$$I_{M}(\alpha_{M}^{*},\alpha_{0}) = \exp\left(F_{M-1}\left(\sum_{k=0}^{M-2} D^{M-k-1}F_{k} + D^{M-1}\alpha_{0}\right) + DF_{M-1}\alpha_{M}^{*} + D\left(\sum_{k=0}^{M-2} D^{M-k-1}F_{k} + D^{M-1}\alpha_{0}\right)\alpha_{M}^{*}\right)$$

$$\times \exp\left(\sum_{k=0}^{M-2} D^{k}F_{k}\alpha_{0} + \sum_{k=0}^{M-3} \sum_{l=k+1}^{M-2} D^{l-k}F_{k}F_{l}\right)$$

$$= \exp\left(\left(D^{M-1}F_{M-1} + \sum_{k=0}^{M-2} D^{k}F_{k}\right)\alpha_{0} + \left(DF_{M-1} + D\sum_{k=0}^{M-2} D^{M-k-1}F_{k}\right)\alpha_{M}^{*}\right)$$

$$\times \exp\left(D^{M}\alpha_{0}\alpha_{M}^{*} + \sum_{k=0}^{M-2} D^{M-k-1}F_{k}F_{M-1} + \sum_{k=0}^{M-3} \sum_{l=k+1}^{M-3} D^{l-k}F_{k}F_{l}\right)$$

$$(4.2.26)$$

Using the same argument as we used for merging the single sum and the double sum in the expression of d, we obtain the expression for the bosonic part of the mixed propagator containing M elementary propagators, between the initial bosonic coherent state $|\alpha_0\rangle$ and the final bosonic coherent state $|\alpha_M\rangle$, after integration on the bosonic degrees of freedom:

$$I_M(\alpha_M^*, \alpha_0) = \exp\left(\sum_{m=1}^M D^{m-1} F_{m-1}\alpha_0 + \sum_{m=1}^M D^{M-m-1} F_{m-1}\alpha_M^* + D^M \alpha_0 \alpha_M^* + \sum_{m=1}^{M-1} \sum_{m'=m+1}^M D^{m-m'} F_{m-1} F_{m'-1}\right)$$
(4.2.27)

where we have made the change $k \to m-1$ and $l \to m'-1$, applying an offset of -1 for them to match with the product $\prod_{m=1}^{M}$ in the propagator. Inserting back the values for D and F_i , we finally obtain

$$I_{M}(\alpha_{M}^{*},\alpha_{0}) = \exp\left[-\frac{i}{\hbar}\delta t\sum_{m=1}^{M}\left(1-\frac{i}{\hbar}\delta tE_{B}\right)^{m-1}\sum_{\mu,\nu=1}^{L}C_{\mu\nu}\zeta_{m}^{*\mu}\zeta_{m-1}^{\nu}\alpha_{0} + \left(1-\frac{i}{\hbar}\delta tE_{B}\right)^{M}\alpha_{0}\alpha_{M}^{*}\right) - \frac{i}{\hbar}\delta t\sum_{m=1}^{M}\left(1-\frac{i}{\hbar}\delta tE_{B}\right)^{M-m-1}\sum_{\mu,\nu=1}^{L}C_{\mu\nu}\zeta_{m}^{*\mu}\zeta_{m-1}^{\nu}\alpha_{M}^{*} - \frac{1}{\hbar^{2}}\delta t^{2}\sum_{m=1}^{M-1}\sum_{m'=m+1}^{M}\left(1-\frac{i}{\hbar}\delta tE_{B}\right)^{m'-m}\left(\sum_{\mu,\nu=1}^{L}C_{\mu\nu}\zeta_{m}^{*\mu}\zeta_{m-1}^{\nu}\right)\left(\sum_{\mu,\nu=1}^{L}C_{\mu\nu}\zeta_{m'}^{*\mu}\zeta_{m'-1}^{\nu}\right)\right]$$
(4.2.29)

We can now write the propagator (4.1.4) by bringing back the fermionic closure relations and the purely fermionic exponentials:

$$K(\zeta_{M}\alpha_{M}, t_{M}; \zeta_{0}\alpha_{0}, t_{0}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} d\zeta_{m}^{*\mu} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu}\zeta_{m}^{\mu}} \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{\mu=1}^{L} \left(1 - \frac{i}{\hbar} \delta t \, E_{F,\mu}\right) \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu} \right) \right] I_{M}(\alpha_{f}^{*}, \alpha_{i})$$

$$(4.2.30)$$

In order to better compare this expression to a purely fermionic system, we also replace $I_M(\alpha_f^*, \alpha_i)$ by its expression, yielding

$$K(\zeta_{f}\alpha_{f}, t_{f}; \zeta_{i}\alpha_{i}, t_{i}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \int \prod_{\mu=1}^{L} \left[d\zeta_{m}^{*\mu} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu}\zeta_{m}^{\mu}} \right]$$

$$\times \exp\left(\left(1 - \frac{i}{\hbar} \delta t E_{B} \right)^{M} \alpha_{f}^{*} \alpha_{i} \right) \prod_{m=1}^{M} \left[\exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu} \right) \exp\left(-\frac{i}{\hbar} \delta t \sum_{\mu=1}^{L} E_{F,\mu} \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu} \right) \right]$$

$$\times \exp\left(-\frac{i}{\hbar} \delta t \left(\left(1 - \frac{i}{\hbar} \delta t E_{B} \right)^{m-1} \alpha_{i} + \left(1 - \frac{i}{\hbar} \delta t E_{B} \right)^{M-m-1} \alpha_{f}^{*} \right) \sum_{\mu,\nu=1}^{L} C_{\mu\nu} \zeta_{m}^{*\mu} \zeta_{m-1}^{\nu} \right) \right]$$

$$\times \exp\left(-\frac{1}{\hbar^{2}} \delta t^{2} \sum_{m=1}^{M-1} \sum_{m'=m+1}^{M} \left(1 - \frac{i}{\hbar} \delta t E_{B} \right)^{m'-m} \left(\sum_{\mu,\nu=1}^{L} C_{\mu\nu} \zeta_{m}^{*\mu} \zeta_{m-1}^{\nu} \right) \left(\sum_{\mu,\nu=1}^{L} C_{\mu\nu} \zeta_{m'}^{*\mu} \zeta_{m'-1}^{\nu} \right) \right)$$

$$(4.2.31)$$

We verify that setting the coupling $C_{\mu\nu}$ between the fermions and the bosonic field to 0 and performing the integrals on the fermionic degrees of freedom (which are exactly the same as in section 3.3) yields the propagator (3.3.25) obtained in the case of non-interacting bosonic and fermionic fields in section 3.3. When the coupling is non-zero, we can compare this propagator to the propagator obtained in the case of a purely fermionic system with two-body interactions. This allows us to verify that the above propagator contains a two-body interaction between fermions as we would expect. If the two propagators can be related in terms of their dynamics, we hope that eliminating the fermions from the propagator as was done for the bosons in the above calculations could give sensible results as well.

4.3 Comparison with a purely fermionic interacting system

The obtained result is to be compared with the result obtained for a strictly fermionic interacting system. A standard Hamiltonian for describing such systems is given by the sum of a one body component for the interaction with the potential wells, and a two-body component responsible for interactions between particles:

$$\hat{H} = \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu} + \sum_{\mu,\nu,\rho,\sigma=1}^{L} D_{\mu\nu\rho\sigma} \hat{c}_{\mu}^{\dagger} \hat{c}_{\nu}^{\dagger} \hat{c}_{\rho} \hat{c}_{\sigma}$$
(4.3.1)

The two body part is the effective equivalent of the term $\sum_{\mu,\nu=1}^{L} C_{\mu\nu} \hat{c}^{\dagger}_{\mu} \hat{c}_{\nu} (\hat{b}^{\dagger} + \hat{b})$ in (4.1.1). It is responsible for two fermions in state $|\phi_{\rho}\rangle$ and $|\phi_{\sigma}\rangle$ to interact and transition to states $|\phi_{\mu}\rangle$ and $|\phi_{\nu}\rangle$, whereas the equivalent term in (4.1.1) allows two fermions to interact via a boson. The path integral expression for the propagator between coherent states $|\zeta_i\rangle \equiv |\zeta_0\rangle$ and $|\zeta_f\rangle \equiv |\zeta_M\rangle$ reads

$$K(\zeta_f, t_f; \zeta_i, t_i) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} d\zeta_m^{*\mu} d\zeta_m^{\mu} e^{-\zeta_m^{*\mu} \zeta_m^{\mu}} \right] \prod_{m=1}^{M} \left[\left\langle \zeta_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}\right) \left| \zeta_{m-1} \right\rangle \right] \right]$$
(4.3.2)

We first compute the elementary propagator in the same way as was done before, by splitting the exponential into a one body and a two-body part and inserting a fermionic closure relationship between the two:

$$\left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1} \right\rangle = \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \left\langle \zeta_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu=1}^{L} E_{F,\mu}\hat{c}_{\mu}^{\dagger}\hat{c}_{\mu}\right) \right| \xi_{m} \right\rangle \\ \times \left\langle \xi_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu,\nu,\rho,\sigma=1}^{L} D_{\mu\nu\rho\sigma}\hat{c}_{\mu}^{\dagger}\hat{c}_{\nu}^{\dagger}\hat{c}_{\rho}\hat{c}_{\sigma}\right) \right| \zeta_{m-1} \right\rangle \\ = \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu} d\xi_{m}^{\mu} e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu=1}^{L} E_{F,\mu}\zeta_{m}^{*\mu}\xi_{m}^{\mu}\right) \exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu}\xi_{m}^{\mu}\right) \\ \times \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu,\nu,\rho,\sigma=1}^{L} D_{\mu\nu\rho\sigma}\xi_{m}^{*\mu}\xi^{*\nu_{m}}\zeta_{m-1}^{\sigma}\zeta_{m-1}^{\sigma}\right) \exp\left(\sum_{\mu=1}^{L} \xi_{m}^{*\mu}\zeta_{m-1}^{\mu}\right)$$
(4.3.3)

where a property similar to the action of exponentials of one-body Hamiltonians (3.3.14) was used for the two-body fermionic Hamiltonian. A reader who would not be convinced should consult appendix D where a proof for this

property is presented. Let **A** and **B** twos square matrices of order *L* such that $\mathbf{A}_{\mu\nu}\mathbf{B}_{\rho\sigma} = -\frac{i}{\hbar}\delta t \mathbf{D}_{\mu\nu\rho\sigma}$ and **E** be the diagonal matrix diag $(E_{F,1}, \ldots, E_{F,L})$. We have to compute the quantity

$$\int \prod_{\mu=1}^{L} \left[d\xi_m^{*\mu} d\xi_m^{\mu} e^{-\xi_m^{*\mu} \xi_m^{\mu}} \right] \exp\left(\sum_{\mu=1}^{L} \left(\mathbb{1} - \frac{i}{\hbar} \delta t \, \mathbf{E} \right)_{\mu} \zeta_m^{*\mu} \xi_m^{\mu} \right)$$

$$\times \exp\left(\sum_{\mu,\nu,\rho,\sigma=1}^{L} \mathbf{A}_{\mu\nu} \mathbf{B}_{\rho\sigma} \xi_m^{*\mu} \xi^{*\nu_m} \zeta_{m-1}^{\rho} \zeta_{m-1}^{\sigma} \right) \exp\left(\sum_{\mu=1}^{L} \xi_m^{*\mu} \zeta_{m-1}^{\mu} \right)$$
(4.3.4)

The integral is computed using (3.2.48), yielding

$$\left\langle \zeta_m \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1} \right\rangle = \exp\left(\sum_{\mu=1}^L \left(\mathbbm{1} - \frac{i}{\hbar}\delta t\,\mathbf{E}\right)_\mu \zeta_m^{*\mu} \zeta_{m-1}^\mu\right) \\ \times \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu,\nu,\rho,\sigma=1}^L \left(\left(\mathbbm{1} - \frac{i}{\hbar}\delta t\,\mathbf{E}\right)\mathbf{A}\left(\mathbbm{1} - \frac{i}{\hbar}\delta t\,\mathbf{E}\right)\right)_{\mu\nu} \mathbf{B}_{\rho\sigma} \zeta_m^{*\mu} \zeta_m^{*\nu} \zeta_{m-1}^\rho \zeta_m^\sigma\right)$$
(4.3.5)

Inserting the expression for the elementary propagator back into the total propagator (4.3.2), we finally find

$$K(\zeta_{f}, t_{f}; \zeta_{i}, t_{i}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} d\zeta_{m}^{*\mu} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu} \zeta_{m}^{\mu}} \right] \prod_{m=1}^{M} \left[\exp\left(-\frac{i}{\hbar} \delta t \sum_{\mu=1}^{L} E_{F,\mu} \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu}\right) \\ \times \exp\left(\sum_{\mu=1}^{L} \zeta_{m}^{*\mu} \zeta_{m-1}^{\mu}\right) \exp\left(-\frac{i}{\hbar} \delta t \sum_{\mu,\nu,\rho,\sigma=1}^{L} \left(\left(\mathbbm{1} - \frac{i}{\hbar} \delta t \mathbf{E}\right) \mathbf{A} \left(\mathbbm{1} - \frac{i}{\hbar} \delta t \mathbf{E}\right) \right)_{\mu\nu} \mathbf{B}_{\rho\sigma} \zeta_{m}^{*\mu} \zeta_{m}^{*\nu} \zeta_{m-1}^{\rho} \zeta_{m-1}^{\sigma} \right) \right]$$
(4.3.6)

Expressions (4.2.31) and (4.3.6) will now be compared. We first notice that the two expressions have the same fermionic one-body part with the exception of a cross-site term in the propagator (4.2.31). This term comes from the interaction between the fermions and the bosonic field. We also notice the appearance of the purely bosonic term $\exp\left(\left(1-\frac{i}{\hbar}\delta t E_B\right)^M \alpha_f^* \alpha_i\right)$, which corresponds to what was obtained in section 3.3 for the bosonic part of the mixed path-integral in the case of non-interacting bosonic and fermionic fields. In a more physical sense, this bosonic term is interpreted as the probability of transition from state $|\alpha_i\rangle$ to $|\alpha_f\rangle$ in the case where the fields do not interact. Both propagators also contain two-body terms. However, the two-body term obtained from the elimination of the bosons is recognized as being non-local in time, in the sense that it couples fermionic variables from different time indices m and m'. The appearance of a non-local two-body interaction is an expected effect of the elimination of a field, in the same manner as the elimination of the electromagnetic field gives rise to a retarded potential expressed from the charged particles that generate the field [47]. In this case, the difference between the purely fermionic propagator and the mixed propagator can be understood in the following way: in the purely fermionic case, the interaction is assumed to be instantaneous since the two pairs of creation and annihilation operators responsible for the transitions are packed together at the same time index m. In the mixed case however, the bosons mediating the interaction need to be created at one time step in order to affect a fermion at another time step, which gives rise to an effect that is not local in time.

Further analysis would require a strategy to correctly handle the initial and final state of the bosonic field. One could think of taking both states to be the vacuum of the bosonic field, meaning that the eigenvalues α_i and α_f^* are very close² to 0. In that case, the additional purely bosonic term as well as the cross-site one body terms vanish, leaving an expression that has the same form as the purely fermionic propagator (4.3.6) in the case of the one-body part. The two-body part in (4.2.31) is however still non-local in time and the two-body terms of each propagator cannot be related by a mere choice of coefficient

One could argue that taking the initial and final bosonic states to be vacuum states is arbitrary, and has very little generality since such case would not appear in practice. And one would be right. A better strategy would be to integrate over the initial and final bosonic states with a weight corresponding to the probability of finding the bosonic field in each state, *i.e.* to perform a statistical mean. One could also re-express the result in terms of bosonic Fock states by inserting a closure relation on bosonic Fock states at the beginning and end of the propagator if such states are more suitable for a given problem. Neither of these discussion are presented here, but they could perhaps be treated in a future work. We will for now content ourselves with a fermionic propagator that contains both a one body interaction and a two-body interaction as one would expect from a system of fermions interacting via bosons.

 $^{^{2}}$ In practical cases, the quantum fluctuations make it impossible to reach exactly 0 particles. Such fluctuations are however often negligible in many-body systems.

Chapter 5

From a Mixed to a Bosonic Propagator

Now that the elimination of the bosons in the mixed system has been shown to yield an interacting fermionic system as expected, the same calculations will now be carried out for removing the fermionic degrees of freedom from the system. The remaining degrees of freedom being purely bosonic and thus complex, one could apply, for instance, a stationary-phase approximation without further complications. We mention that stationary-phase approximations can be more directly applied to fermionic systems using a different kind of fermionic coherent states [18], namely Klauder coherent states. Introduced by J.R. Klauder in [48], those coherent states have complex eigenvalues rather than Grassmannian and they therefore have a more direct physical interpretation, at the cost of them not being eigenvectors of the annihilation operator anymore. Those will not be discussed here but present a promising way to semiclassical approximation for the considered Hamiltonian is written out. The fermionic degrees of freedom are then eliminated by computing every fermionic (Grassmannian) integral. The resulting object is a bosonic path integral containing reminiscences of the fermionic system such as the energy of the fermionic site $E_{F,\mu}$. The application of semi-classical methods to the resulting path integral are then discussed.

5.1 Path integral formulation

Again, the Hamiltonian considered is the mixed Hamiltonian containing both fermionic particles and bosons carrying interactions between them, as discussed in section 1.2. We now consider N bosonic modes instead of just one. As a reminder, the Hamiltonian reads:

$$\hat{H} = \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu} + \sum_{n=1}^{N} E_{B,n} \hat{b}_{n}^{\dagger} \hat{b}_{n} + \sum_{n=1}^{N} \sum_{\mu,\nu=1}^{L} C_{\mu\nu n} \hat{c}_{\mu}^{\dagger} \hat{c}_{\nu} (\hat{b}_{n}^{\dagger} + \hat{b}_{n})$$
(5.1.1)

Let $|\zeta_i \alpha_i\rangle$ and $|\zeta_f \alpha_f\rangle$ be the initial and final states of the mixed system. The first step we need to perform, namely dividing the time range into smaller time steps, is exactly the same as in the previous chapter, so we start directly from (4.1.3) and insert both a fermionic and bosonic closure relation between each exponential:

$$K(\zeta_{f}\alpha_{f}, t_{f}; \zeta_{i}\alpha_{i}, t_{i}) = \lim_{M \to \infty} \left\langle \zeta_{f}\alpha_{f} \left| \prod_{m=1}^{M} \exp\left(-\frac{i}{\hbar}\Delta t \,\hat{H}\right) \right| \zeta_{i}\alpha_{i} \right\rangle$$
$$= \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} \left[d\zeta_{m}^{*\mu} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu}\zeta_{m}^{\mu}} \right] \int \prod_{n=1}^{N} \left[\frac{d\alpha_{m}^{n*} d\alpha_{m}^{n}}{2i\pi} e^{-|\alpha_{m}^{n}|^{2}} \right] \right] \prod_{m=1}^{M} \left[\left\langle \alpha_{m}\zeta_{m} \right| \exp\left(-\frac{i}{\hbar}\Delta t \,\hat{H}\right) \right| \alpha_{m-1}\zeta_{m-1} \right\rangle \right]$$
(5.1.2)

Since the limit for M goes to infinity has already been taken, the exponential of \hat{H} can be split into three exponentials. We are first interested in computing the elementary propagator. We again do so by inserting the appropriate closure relations between the three exponentials:

$$\left\langle \zeta_m \alpha_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}\right) \right| \zeta_{m-1} \alpha_{m-1} \right\rangle = \left\langle \zeta_m \alpha_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}_F\right) \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}_B\right) \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}_{int}\right) \right| \zeta_{m-1} \alpha_{m-1} \right\rangle$$

$$= \int \prod_{\mu=1}^L \left[d\xi_m^{*\mu} d\xi_m^\mu e^{-\xi_m^{*\mu} \xi_m^\mu} \right] \int \prod_{n=1}^N \left[\frac{d\beta_m^{n*} d\beta_m^n}{2i\pi} e^{-|\beta_m^n|^2} \right] \left\langle \zeta_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}_F\right) \right| \xi_m \right\rangle$$

$$\times \left\langle \alpha_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}_B\right) \right| \beta_m \right\rangle \left\langle \xi_m \beta_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}_{int}\right) \right| \zeta_{m-1} \alpha_{m-1} \right\rangle$$

$$(5.1.3)$$

We draw the reader's attention to the fact that the bosonic and fermionic states and operators belong to distinct spaces. If the freedom taken in the notation of state vectors brings confusion, we hope that the summary of notations presented in appendix A can clear it up. The action of exponentials of one-body Hamiltonians on coherent states has already been exposed in section

By virtue of (3.3.9) and (3.3.14), we let each exponential act on the vectors, yielding

$$\left\langle \zeta_{m}\alpha_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t \,\hat{H}\right) \right| \zeta_{m-1}\alpha_{m-1} \right\rangle = \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu}d\xi_{m}^{\mu}e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*}d\beta_{m}^{n}}{2i\pi}e^{-|\beta_{m}^{n}|^{2}} \right] \exp\left(-\frac{i}{\hbar}\delta t \,H_{F}(\zeta_{m}^{*},\xi_{m})\right) \\ \times \left\langle \zeta_{m} \left| \xi_{m} \right\rangle \exp\left(-\frac{i}{\hbar}\delta t \,H_{B}(\alpha_{m}^{*},\beta_{m})\right) \left\langle \alpha_{m} \left| \beta_{m} \right\rangle \exp\left(-\frac{i}{\hbar}\delta t \,H_{int}(\xi_{m}^{*},\beta_{m}^{*},\zeta_{m-1},\alpha_{m-1})\right) \left\langle \xi_{m}\beta_{m} \left| \zeta_{m-1}\alpha_{m-1} \right\rangle \right. \right.$$

$$(5.1.4)$$

with

$$\begin{cases}
H_F(\zeta_m^*, \xi_m) = \sum_{\mu=1}^{L} E_{F,\mu} \zeta_m^{*\mu} \xi_m^{\mu} \\
H_B(\alpha_m^*, \beta_m) = \sum_{n=1}^{N} E_{B,n} \alpha_m^{*n} \beta_m^n \\
H_{int}(\xi_m^*, \beta_m^*, \zeta_{m-1}, \alpha_{m-1}) = \sum_{n=1}^{N} \sum_{\mu,\nu=1}^{L} C_{\mu\nu n} \xi_m^{*\mu} \zeta_{m-1}^{\nu} (\beta_m^{*n} + \alpha_{m-1}^n)
\end{cases}$$
(5.1.5)

To perform the integration over each β_m^n and β_m^{*n} , we use formula (3.1.21). If we omit terms that do not contain β_m^n or β_m^{*n} , what is left to compute is the quantity

$$I_{B} \equiv \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*} d\beta_{m}^{n}}{2i\pi} \right] \exp\left(-\frac{i}{\hbar} \delta t \, H_{B}(\alpha_{m}^{*}, \beta_{m})\right) \langle \alpha_{m} | \beta_{m} \rangle \exp\left(-\frac{i}{\hbar} \delta t \, H_{int}(\xi_{m}^{*}, \beta_{m}^{*}, \zeta_{m-1}, \alpha_{m-1})\right) \langle \beta_{m} | \alpha_{m-1} \rangle$$

$$= \int \prod_{n=1}^{N} \left[\frac{d\beta_{m}^{n*} d\beta_{m}^{n}}{2i\pi} \right] \exp\left(-\frac{i}{\hbar} \delta t \, H_{B}(\alpha_{m}^{*}, \beta_{m})\right) \exp\left(\sum_{n=1}^{N} \alpha_{m}^{*n} \beta_{m}^{n}\right)$$

$$\times \exp\left(-\frac{i}{\hbar} \delta t \, H_{int}(\xi_{m}^{*}, \beta_{m}^{*}, \zeta_{m-1}, \alpha_{m-1})\right) \exp\left(\sum_{n=1}^{N} \beta_{m}^{*n} \alpha_{m-1}^{n}\right)$$
(5.1.6)

The coefficients in front of each term in $|\beta_m^n|^2$, β_m^{*n} and β_m^n are identified:

$$\begin{cases}
 a_n = 1 \\
 b_n = -\frac{i}{\hbar} \delta t \sum_{\mu,\nu=1}^{L} C_{\mu\nu n} \xi_m^{*\mu} \zeta_{m-1}^{\nu} + \alpha_{m-1}^n \\
 c_n = \left(1 - \frac{i}{\hbar} \delta t E_{B,n}\right) \alpha_m^{*n}
\end{cases}$$
(5.1.7)

The application of formula (3.1.21) yields

$$I_{B} = \exp\left(\sum_{n=1}^{N} \left(-\frac{i}{\hbar} \delta t \sum_{\mu,\nu=1}^{L} C_{\mu\nu n} \xi_{m}^{*\mu} \zeta_{m-1}^{\nu} + \alpha_{m-1}^{n}\right) \left(1 - \frac{i}{\hbar} \delta t E_{B,n}\right) \alpha_{m}^{*n}\right)$$
$$= \exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t E_{B,n}\right) \left[\left(-\frac{i}{\hbar} \delta t \sum_{\mu,\nu=1}^{L} C_{\mu\nu n} \xi_{m}^{*\mu} \zeta_{m-1}^{\nu} \alpha_{m}^{*n}\right) + \alpha_{m}^{*n} \alpha_{m-1}^{n}\right]\right)$$
(5.1.8)

The elementary propagator now reads

$$\left\langle \zeta_{m}\alpha_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1}\alpha_{m-1} \right\rangle = \int \prod_{\mu=1}^{L} \left[d\xi_{m}^{*\mu}d\xi_{m}^{\mu}e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}} \right] \exp\left(-\frac{i}{\hbar}\delta t\,H_{F}(\zeta_{m}^{*},\xi_{m})\right) \\ \times \left\langle \zeta_{m} \left| \xi_{m} \right\rangle \left\langle \xi_{m} \left| \zeta_{m-1} \right\rangle \exp\left(\sum_{n=1}^{N} \left(1-\frac{i}{\hbar}\delta t\,E_{B,n}\right) \left[\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu,\nu=1}^{L} C_{\mu\nu n}\xi_{m}^{*\mu}\zeta_{m-1}^{\nu}\alpha_{m}^{*n}\right) + \alpha_{m}^{*n}\alpha_{m-1}^{n} \right] \right)$$
(5.1.9)

5.2 Elimination of the fermionic degrees of freedom

What remains to be computed in this elementary propagator is the integral over the Grassmannian variables $\xi_m^{*\mu}$ and ξ_m^{μ} for all μ 's. Those integrals are performed using formula (3.2.46). In order to better identify the matrices for the application of this formula, we develop the scalar products and replace $H_F(\zeta_m^*, \xi_m)$ by its expression. We also isolate the purely bosonic part of this expression and put it at the beginning:

$$\left\langle \zeta_{m}\alpha_{m} \left| \exp\left(-\frac{i}{\hbar}\delta t\,\hat{H}\right) \right| \zeta_{m-1}\alpha_{m-1} \right\rangle = \exp\left(\sum_{n=1}^{N}\left(1-\frac{i}{\hbar}\delta t\,E_{B,n}\right)\alpha_{m}^{*n}\alpha_{m-1}^{n}\right) \\ \times \int\prod_{\mu=1}^{L}\left[d\xi_{m}^{*\mu}d\xi_{m}^{\mu}e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}}\right] \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{\mu=1}^{L}E_{F,\mu}\zeta_{m}^{*\mu}\xi_{m}^{\mu}\right) \exp\left(\sum_{\mu=1}^{L}\zeta_{m}^{*\mu}\xi_{m}^{\mu}\right) \\ \times \exp\left(\sum_{\mu=1}^{L}\xi_{m}^{*\mu}\zeta_{m-1}^{\mu}\right) \exp\left(-\frac{i}{\hbar}\delta t\,\sum_{n=1}^{N}\left(1-\frac{i}{\hbar}\delta t\,E_{B,n}\right)\sum_{\mu,\nu=1}^{L}C_{\mu\nu n}\xi_{m}^{*\mu}\zeta_{m-1}^{\nu}\alpha_{m}^{*n}\right) \\ = \exp\left(\sum_{n=1}^{N}\left(1-\frac{i}{\hbar}\delta t\,E_{B,n}\right)\alpha_{m}^{*n}\alpha_{m-1}^{n}\right)\int\prod_{\mu=1}^{L}\left[d\xi_{m}^{*\mu}d\xi_{m}^{\mu}e^{-\xi_{m}^{*\mu}\xi_{m}^{\mu}}\right] \\ \times \exp\left(\sum_{\mu,\nu=1}^{L}\Phi_{\mu\nu}\zeta_{m}^{*\mu}\xi_{m}^{\mu}\right)\exp\left(\sum_{\mu\nu}^{L}\Theta(\alpha_{m}^{*})_{\mu\nu}\xi_{m}^{*\mu}\zeta_{m-1}^{\nu}\right)$$
(5.2.1)

with the matrices

$$\begin{cases} \Phi = \left(\mathbb{1} - \frac{i}{\hbar} \delta t \, \mathbf{E}\right) \\ \Theta(\alpha_m^*) = \left(\mathbb{1} - \frac{i}{\hbar} \delta t \, \sum_{n=1}^N \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_m^{*n} \mathbf{C}_n \right) \end{cases}$$
(5.2.2)

where \mathbf{C}_n is the set of $L \times L$ matrices obtained by considering $(C_{\mu\nu n})_{\mu\nu}$ for a given n and \mathbf{E} is again the diagonal matrix diag $(E_{F,1}, \ldots, E_{F,L})$. Applying formula (3.2.46), the final result for the elementary propagator is

$$\left\langle \zeta_m \alpha_m \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}\right) \right| \zeta_{m-1} \alpha_{m-1} \right\rangle = \exp\left(\sum_{n=1}^N \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_m^{*n} \alpha_{m-1}^n\right) \exp\left(\sum_{\mu,\nu=1}^L (\Phi \Theta(\alpha_m^*))_{\mu\nu} \zeta_m^{*\mu} \zeta_{m-1}^\nu\right)$$
(5.2.3)

We can now compute the total propagator of the system. As a reminder, it is given by

$$K(\zeta_{f}\alpha_{f}, t_{f}; \zeta_{i}\alpha_{i}, t_{i})$$

$$= \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} \left[d\zeta_{m}^{*\mu} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu} \zeta_{m}^{\mu}} \right] \int \prod_{n=1}^{N} \left[\frac{d\alpha_{m}^{n*} d\alpha_{m}^{n}}{2i\pi} e^{-|\alpha_{m}^{n}|^{2}} \right] \right] \prod_{m=1}^{M} \left[\left\langle \alpha_{m} \zeta_{m} \left| \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H}\right) \right| \alpha_{m-1} \zeta_{m-1} \right\rangle \right]$$

$$= \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{\mu=1}^{L} \left[d\zeta_{m}^{*\mu} d\zeta_{m}^{\mu} e^{-\zeta_{m}^{*\mu} \zeta_{m}^{\mu}} \right] \int \prod_{n=1}^{N} \left[\frac{d\alpha_{m}^{n*} d\alpha_{m}^{n}}{2i\pi} e^{-|\alpha_{m}^{n}|^{2}} \right] \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \right]$$

$$\times \prod_{m=1}^{M} \left[\exp\left(\sum_{\mu,\nu=1}^{L} \left(\Phi\Theta(\alpha_{m}^{*})\right)_{\mu\nu} \zeta_{m}^{*\mu} \zeta_{m-1}^{\nu}\right) \right]$$
(5.2.4)

We wish to eliminate the fermionic degrees of freedom, and therefore we compute each integral over the variables $\zeta_m^{*\mu}$ and ζ_m^{μ} . If we first take a look at the case for M = 2, we find

$$K_{2}(\zeta_{2}\alpha_{2}, t_{2}; \zeta_{0}\alpha_{0}, t_{0}) = \int \prod_{\mu=1}^{L} d\zeta_{1}^{*\mu} d\zeta_{1}^{\mu} e^{-\zeta_{1}^{*\mu}\zeta_{1}^{\mu}} \int \prod_{n=1}^{N} \frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \\ \times \prod_{m=1}^{2} \left[\exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \right] \exp\left(\sum_{\mu,\nu=1}^{L} (\Phi\Theta(\alpha_{2}^{*}))_{\mu\nu} \zeta_{2}^{*\mu} \zeta_{1}^{\nu}\right) \exp\left(\sum_{\mu,\nu=1}^{L} (\Phi\Theta(\alpha_{1}^{*}))_{\mu\nu} \zeta_{1}^{*\mu} \zeta_{0}^{\nu}\right)$$
(5.2.5)

Applying formula (3.2.46) yet again yields

$$K_{2}(\zeta_{2}\alpha_{2}, t_{2}; \zeta_{0}\alpha_{0}, t_{0}) = \int \prod_{n=1}^{N} \left[\frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \right] \prod_{m=1}^{2} \left[\exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \right] \\ \times \exp\left(\sum_{\mu,\nu=1}^{L} (\Phi\Theta(\alpha_{2}^{*}) \Phi\Theta(\alpha_{1}^{*}))_{\mu\nu} \zeta_{2}^{*\mu} \zeta_{0}^{\nu}\right)$$
(5.2.6)

In the same way as we computed the propagator in the example of section 3.3, we notice that the $m + 1^{th}$ approximation to the propagator can be obtained from the m^{th} with the formula

$$K_{m}(\zeta_{m}\alpha_{m}, t_{m}; \zeta_{0}\alpha_{0}, t_{0}) = \int \prod_{\mu=1}^{L} \left[d\zeta_{m-1}^{*\mu} d\zeta_{m-1}^{\mu} e^{-\zeta_{m-1}^{*\mu}\zeta_{m-1}^{\mu}} \right] \int \prod_{n=1}^{N} \left[\frac{d\alpha_{m-1}^{n*} d\alpha_{m-1}^{n}}{2i\pi} e^{-|\alpha_{m-1}^{n}|^{2}} \right]$$
$$\times \exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \exp\left(\sum_{\mu,\nu=1}^{L} (\Phi\Theta(\alpha_{m}^{*}))_{\mu\nu} \zeta_{m}^{*\mu} \zeta_{m-1}^{\nu}\right)$$
$$\times K_{m-1}(\zeta_{m-1}\alpha_{m-1}, t_{m-1}; \zeta_{0}\alpha_{0}, t_{0}) \tag{5.2.7}$$

Using this recursive formula and the case for M = 2, we are easily convinced that the M^{th} approximation to the propagator is given by

$$K_{M}(\zeta_{M}\alpha_{M}, t_{M}; \zeta_{0}\alpha_{0}, t_{0}) = \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^{N} \frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \right] \\ \times \exp\left(\sum_{\mu,\nu=1}^{L} \left(\prod_{m=1}^{M} \Phi \Theta(\alpha_{M-m+1}^{*})\right)_{\mu\nu} \zeta_{M}^{*\mu} \zeta_{0}^{\nu}\right)$$
(5.2.8)

Note that the matrix product is defined in a time-ordered way. The limit for M goes to infinity of the above quantity yields the exact propagator for the mixed system where all the fermionic degrees of freedom except for the initial and final state have been eliminated

$$K(\zeta_f \alpha_f, t_f; \zeta_i \alpha_i, t_i) = \lim_{M \to \infty} K_M(\zeta_M \alpha_M, t_M; \zeta_0 \alpha_0, t_0)$$
(5.2.9)

with the usual conventions $|\zeta_f \alpha_f \rangle \equiv |\zeta_M \alpha_M \rangle$, $|\zeta_i \alpha_i \rangle \equiv |\zeta_0 \alpha_0 \rangle$ and the corresponding notation for t_f , t_i .

5.3 The limit of infinitesimal time steps

Let us now discuss this expression. We first notice that the one-body term of this bosonic propagator is the same as in the purely bosonic propagator computed in section 3.3, which is a good sign since we do not expect the fermionic field to influence the single-body dynamics of the bosonic field. However, a property of this propagator is that the matrix product in the second line contains *n*-body bosonic terms for all *n* between 1 and *M*. Indeed, since each Θ can be decomposed into the sum of an identity matrix and a matrix containing a bosonic degree of freedom, we have for instance, for M = 2:

$$\Phi\Theta(\alpha_2)\Phi\Theta(\alpha_1) = \Phi\left(\mathbb{1} + \sum_{n=1}^N e_n \alpha_2^{*n} \mathbf{C}_n\right) \Phi\left(\mathbb{1} + \sum_{n=1}^N e_n \alpha_1^{*n} \mathbf{C}_n\right)$$
(5.3.1)

with $e_n = -\frac{i}{\hbar}\delta t \left(-\frac{i}{\hbar}\delta t E_{B,n} + 1\right)$. As a reminder, Φ is a purely fermionic term. This expression thus features terms in order 0, 1 and 2 in bosonic variables. It is straightforward to extend this reasoning to any M, yielding terms in order M in bosonic variables. This seems like a major setback for the application of existing semiclassical results, since to our knowledge none appear to be appropriate to handle *n*-body terms with *n* getting arbitrarily big as Mgoes to infinity. A way out of this problem is to recall that as M goes to infinity, δt also becomes infinitesimal, allowing for neglecting terms of order δt^2 and higher. Formally, we can write

$$\lim_{M \to \infty} \prod_{m=1}^{M} \left[\Phi \Theta(\alpha_{M-m+1}^*) \right] = \lim_{M \to \infty} \exp\left(\ln \left(\prod_{m=1}^{M} \Phi \Theta(\alpha_{M-m+1}^*) \right) \right) = \exp\left(\sum_{m=1}^{\infty} \ln \left(\Phi \Theta(\alpha_m^*) \right) \right)$$
(5.3.2)

Note that because the matrices Φ and $\Theta(\alpha_m^*)$ do not commute in general, the third equality is only possible in the limit where δt is infinitesimal. Outside of this limit, the passage from the logarithm of a product to a sum of logarithm would involve commutators that could not be neglected. In our case however, we safely neglect them and proceed. Recalling the expressions for Φ and $\Theta(\alpha_m^*)$ given in (5.2.2), we have

$$\ln\left(\Phi\Theta(\alpha_m^*)\right) = \ln\left[\left(\mathbb{1} - \frac{i}{\hbar}\delta t\,\mathbf{E}\right)\left(\mathbb{1} - \frac{i}{\hbar}\delta t\,\sum_{n=1}^N\left(1 - \frac{i}{\hbar}\delta t\,E_{B,n}\right)\alpha_m^{*n}\mathbf{C}_n\right)\right]$$
$$= \ln\left[\mathbb{1} - \frac{i}{\hbar}\delta t\,\mathbf{E} - \frac{i}{\hbar}\delta t\,\sum_{n=1}^N\alpha_m^{*n}\mathbf{C}_n + \mathcal{O}(\delta t^2)\right]$$
(5.3.3)

Since in the limit where M goes to infinity δt is infinitesimal, we can expand the logarithm to first order in δt , yielding

$$\ln\left(\Phi\Theta(\alpha_m^*)\right) \approx -\frac{i}{\hbar} \delta t \,\mathbf{E} - \frac{i}{\hbar} \delta t \sum_{n=1}^N \alpha_m^{*n} \mathbf{C}_n \tag{5.3.4}$$

and we have

$$\lim_{M \to \infty} \prod_{m=1}^{M} \left[\Phi \Theta(\alpha_m^*) \right] = \lim_{M \to \infty} \exp\left(-\frac{i}{\hbar} \delta t \sum_{m=1}^{M} \left(\mathbf{E} + \sum_{n=1}^{N} \alpha_m^{*n} \mathbf{C}_n \right) \right)$$
(5.3.5)

Since $\delta t = \frac{t_f - t_i}{M}$ and because **E** doesn't depend on the time index *m*, the fermionic term can be re-written as

$$-\frac{i}{\hbar}\frac{(t_f - t_i)}{M}\sum_{m=1}^{M} \mathbf{E} = -\frac{i}{\hbar}\frac{(t_f - t_i)}{M}\mathbf{E}\sum_{m=1}^{M} 1 = -\frac{i}{\hbar}(t_f - t_i)\mathbf{E}$$
(5.3.6)

Let's now go back to our mixed propagator (5.2.8). In the limit where M goes to infinity, we are allowed to insert the above results, yielding

$$K(\zeta_{f}\alpha_{f}, t_{f}; \zeta_{i}\alpha_{i}, t_{i}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^{N} \frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \right] \\ \times \exp\left(\sum_{\mu,\nu=1}^{L} \left[\exp\left(-\frac{i}{\hbar} (t_{f} - t_{i}) \mathbf{E} - \frac{i}{\hbar} \delta t \, \sum_{m=1}^{M} \sum_{n=1}^{N} \alpha_{m}^{*n} \mathbf{C}_{n}\right) \right]_{\mu\nu} \zeta_{f}^{*\mu} \zeta_{i}^{\nu} \right)$$
(5.3.7)

We verify that in the case where there is no interaction between the bosonic and fermionic field, *i.e.* C_n is a null matrix for all n, we recover the propagators (3.3.35) and (3.3.36) which represented a mixed system with no interactions. The fermionic part of this affirmation is immediate since $\mathbf{E}_{\mu\nu} = E_{F,\mu}\delta_{\mu\nu}$. The bosonic part requires to compute the same integrals as was done in the development for the bosonic part of the mixed system with no interaction in chapter 3.

We conclude this section with a discussion on the practical use of this propagator and prospects for application of semiclassical approximations. The first challenge to overcome in order to relate this propagator to the propagator of the interacting fermionic system is the handling of the Grassmannian generators ζ_f^* and ζ_i . A solution is to use the fact that fermionic coherent states form an (over)complete base of the fermionic Fock state. Unlike fermionic coherent states, fermionic Fock states represent physical states of the fermionic part of the system. One could then, for instance, project this propagator on two Fock states and integrate over the two remaining Grassmann generators ζ_f^* and ζ_i as if they formed a closure relation. In the case where the initial and final state of the fermions is not known, an alternative solution could be to perform the previous step followed with a statistical mean over the fermionic Fock states. Although the semiclassical theory of this propagator will not be developed here, we can already discuss prospects on its application. Once the initial and final fermionic states have been eliminated, the first step is to define an effective Hamiltonian for the bosonic field. Using this Hamiltonian, a Lagrangian could be defined using the transformation (3.3.37) as was done for the mixed system without interaction in chapter 3. In order to define the said Hamiltonian, one has to treat the sum over m in the matrix product. In an ideal case, the terms relative to different time indices could be separated as was the case in the example at the end of chapter 3. However, like the final result of chapter 4, this sum is non-local in time, as can be seen by developing the exponential containing the sum into its power series. Note that this sum is guaranteed to converge in the limit where M goes to infinity thanks to the prefactor δt . The treatment of this term is the next challenge in order to successfully apply a stationary phase approximation to this propagator.

To end this chapter, we propose a brief discussion on the limit of small interactions between the fermions and the bosonic field. Although this case is not general, some interesting physical intuitions can be recovered and it could represent a more accessible first target for future applications of semiclassical approximations.

5.4 The limit of small interactions

In the limit where the interaction between the bosonic field and the fermions is weak, i.e the coefficients of \mathbf{C}_n are small as compared to the fermionic and bosonic energies $E_{F,\mu}$ and $E_{B,n}$, we have

$$\exp\left(-\frac{i}{\hbar}\delta t\sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_{m}^{*n}\mathbf{C}_{n}\right)\approx\mathbf{1}-\frac{i}{\hbar}\delta t\sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_{m}^{*n}\mathbf{C}_{n}$$
(5.4.1)

In that case, we can express the total propagator of the mixed system using the propagator of the fermionic system without interaction. First, notice that since δt is infinitesimal, we can use the BCH formula (3.3.4) to split the exponential, yielding

$$\exp\left(\sum_{\mu,\nu=1}^{L}\left[\exp\left(-\frac{i}{\hbar}(t_{f}-t_{i})\mathbf{E}\right)\left(1-\frac{i}{\hbar}\delta t\sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_{m}^{*n}\mathbf{C}_{n}\right)\right]_{\mu\nu}\zeta_{f}^{*\mu}\zeta_{i}^{\nu}\right)$$

$$=\exp\left(\sum_{\mu,\nu=1}^{L}\left[\exp\left(-\frac{i}{\hbar}(t_{f}-t_{i})\mathbf{E}\right)-\exp\left(-\frac{i}{\hbar}(t_{f}-t_{i})\mathbf{E}\right)\frac{i}{\hbar}\delta t\sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_{m}^{*n}\mathbf{C}_{n}\right]_{\mu\nu}\zeta_{f}^{*\mu}\zeta_{i}^{\nu}\right)$$

$$=\exp\left(\sum_{\mu=1}^{L}\exp\left(-\frac{i}{\hbar}(t_{f}-t_{i})E_{F,\mu}\right)\zeta_{M}^{*\mu}\zeta_{i}^{\mu}\right)\exp\left(\sum_{\mu,\nu=1}^{L}\left[-\exp\left(-\frac{i}{\hbar}(t_{f}-t_{i})\mathbf{E}\right)\frac{i}{\hbar}\delta t\sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_{m}^{*n}\mathbf{C}_{n}\right]_{\mu\nu}\zeta_{f}^{*\mu}\zeta_{i}^{\nu}\right)$$

$$=K^{F}(\zeta_{f},t_{f};\zeta_{i},t_{i})\exp\left(\sum_{\mu,\nu=1}^{L}\left[-\exp\left(-\frac{i}{\hbar}(t_{f}-t_{i})\mathbf{E}\right)\frac{i}{\hbar}\delta t\sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_{m}^{*n}\mathbf{C}_{n}\right]_{\mu\nu}\zeta_{f}^{*\mu}\zeta_{i}^{\nu}\right)$$
(5.4.2)

where the exponential acts as a perturbation since C_n is small for all n. The total propagator in the limit of small interactions can thus approximately be written as

$$K(\zeta_f \alpha_f, t_f; \zeta_i \alpha_i, t_i) \approx K^F(\zeta_f, t_f; \zeta_i, t_i) K^P(\zeta_f \alpha_f, t_f; \zeta_i \alpha_i, t_i)$$
(5.4.3)

with K^F the propagator of the fermionic field with no interactions between fermions, and K^P the term containing the bosonic part of the propagator and the perturbation

$$K^{P}(\zeta_{f}\alpha_{f}, t_{f}; \zeta_{i}\alpha_{i}, t_{i}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^{N} \frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \right] \prod_{m=1}^{M} \left[\exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n}\right) \right] \\ \times \exp\left(\sum_{\mu,\nu=1}^{L} \left[-\exp\left(-\frac{i}{\hbar} (t_{f} - t_{i}) \mathbf{E}\right) \frac{i}{\hbar} \delta t \, \sum_{m=1}^{M} \sum_{n=1}^{N} \alpha_{m}^{*n} \mathbf{C}_{n} \right]_{\mu\nu} \zeta_{f}^{*\mu} \zeta_{i}^{\nu} \right)$$
(5.4.4)

We can develop the mixed part of the perturbation as

$$\left[-\exp\left(-\frac{i}{\hbar}(t_f - t_i)\mathbf{E}\right)\frac{i}{\hbar}\delta t \sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_m^{*n}\mathbf{C}_n\right]_{\mu\nu}$$
$$=\sum_{m=1}^{M}\sum_{n=1}^{N}\left[-\exp\left(-\frac{i}{\hbar}(t_f - t_i)\mathbf{E}\right)\frac{i}{\hbar}\delta t \,\alpha_m^{*n}\mathbf{C}_n\right]_{\mu\nu}$$
(5.4.5)

In that case, in the limit where M goes to infinity, we can separate the exponential

$$\exp\left(\sum_{m=1}^{M}\sum_{n=1}^{N}\sum_{\mu,\nu=1}^{L}\left[-\exp\left(-\frac{i}{\hbar}(t_{f}-t_{i})\mathbf{E}\right)\frac{i}{\hbar}\delta t\,\alpha_{m}^{*n}\mathbf{C}_{n}\right]_{\mu\nu}\zeta_{f}^{*\mu}\zeta_{i}^{\nu}\right)$$
(5.4.6)

into m exponentials using the BCH formula (3.3.4) and the fact that Grassmann pairs commute with each other. The exponential relative to each time index m can then be merged with the exponentials of the first line, yielding

$$K^{P}(\zeta_{f}\alpha_{f}, t_{f}; \zeta_{i}\alpha_{i}, t_{i}) = \lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{n=1}^{N} \frac{d\alpha_{1}^{n*} d\alpha_{1}^{n}}{2i\pi} e^{-|\alpha_{1}^{n}|^{2}} \right] \times \prod_{m=1}^{M} \left[\exp\left(\sum_{n=1}^{N} \left(1 - \frac{i}{\hbar} \delta t \, E_{B,n}\right) \alpha_{m}^{*n} \alpha_{m-1}^{n} + \sum_{n=1}^{N} \sum_{\mu,\nu=1}^{L} \left[-\exp\left(-\frac{i}{\hbar} (t_{f} - t_{i}) \mathbf{E}\right) \frac{i}{\hbar} \delta t \, \alpha_{m}^{*n} \mathbf{C}_{n} \right]_{\mu\nu} \zeta_{f}^{*\mu} \zeta_{i}^{\nu} \right) \right]$$

$$(5.4.7)$$

This propagator is now local in time, and so is the total propagator (5.4.3). Now that there is no coupling between terms from different time indices, one could define an effective Hamiltonian as was done in section 3.3 and from it, a Lagrangian. We mention however that the Grassmannian variables ζ_f^* and ζ_i still need to be eliminated, for instance by projecting the propagator on fermionic Fock states as described in the end of the previous section.

Chapter 6

Summary and outlook

Our goal was to re-express the dynamics of an interacting fermionic system using bosonic degrees of freedom. Starting from a mixed system on a lattice containing fermions interacting via bosons, we first obtained a propagator in coherent state representation that contains only fermionic degrees of freedom and the initial and final bosonic states. This propagator was shown to correspond to a system of interacting fermions with a two-body interaction which is non-local in time. Then, starting from the same mixed system, we obtained a propagator expressed with only bosonic degrees of freedom except for the initial and final state of the fermionic field. No approximations were made yet except in the last section of chapter 5 where a discussion for small couplings between the bosonic field and the fermions was made. Furthermore, very few assumptions were made in the choice of the Hamiltonian. All the results except for those of section 5.4 are therefore both exact and quite general. A promising prospect of application of a semiclassical approach was also presented in the context of small coupling between the bosonic field and the fermions.

In the context of this work, a symbolic manipulation tool in the form of a Python library was also developed in order to treat expressions of Grassmann generators which are anti-commuting numbers. This tool allows to compute the power series of functions such as exponentials of Grassmann generators, the integral over Grassmann variables and the product of terms containing Grassmann generators. It also allows for the comparison of such terms. These features allowed to numerically show some formulae used in this work in an automated way in cases where exhaustive algebraic derivations were out of reach. An algebraic proof for these formulae would however be welcome.

In order to apply semiclassical approximations on this propagator, work still has to be done. First, the integration of bosonic degrees of freedom must be extended to more than one bosonic mode. This is necessary in order to find the proper correspondence between the mixed propagator where bosons have been eliminated and the mixed propagator where fermions have been eliminated. Second, general ways of handling the initial and final states of the bosonic and fermionic field have to be developed. Since the system we considered was very generic, there also remains a lot of freedom in the choice of the coupling constants of the Hamiltonian. In future works, this freedom has to be used to relate the purely fermionic propagator to the purely bosonic one. This freedom could also be exploited to investigate if the appropriate choice of constants for the bosonic propagator obtained from the mixed system would allow to match predictions from other models such as the Fermi-Hubbard model for the dynamics of the fermions. Another challenge to be tackled in a future work is the treatment of the non-locality in time of the bosonic propagator obtained, since semiclassical methods do not to our knowledge cover such case. Outside of the limit of small interactions, this could be tackled for instance by searching for a way to transform the non-local interaction into an effective local interaction that would likely be time-dependent.

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Appendix A

Summary of shorthands and notations

Coherent states are used extensively in this work. The closure relations in coherent state representation can already appear lengthy. In addition, they are used in the context of path integrals, which requires to use a large amount of indices and closure relations. This has lead to the simplification of some cumbersome notations and the introduction of shorthands. Although most of them are natural, they are all presented in this appendix.

A.1 Eigenvalue notations

Working with path integrals implies that several indices have to be used. In particular, state vectors are often labeled with a "time slice" index. Since each vector is also associated with several eigenvalues, a choice had to be made. The notation that was finally is the following:

$$\hat{a}_k \left| \eta_m \right\rangle = \eta_m^k \left| \eta_m \right\rangle \tag{A.1.1}$$

with $|\eta\rangle$ a generic coherent state and \hat{a}_k a generic annihilation operator. In order to avoid any confusion, powers of the eigenvalues will always be denoted using parenthesis, such as in

$$\hat{a}_k \hat{a}_k \left| \eta_m \right\rangle = \left(\eta_m^k \right)^2 \left| \eta_m \right\rangle \tag{A.1.2}$$

A.2 Notations of operators and coherent states in the mixed space

Since this work mixes bosonic and fermionic coherent states, it appears necessary to be able to quickly distinguish between the two. For this purpose, the Greek letters α , β and γ are exclusively used for bosonic coherent states, and the letters ζ , ξ and χ for fermionic coherent states.

Working in a mixed space also implies that each vector and operator has to be considered as a tensor product of a quantity from both spaces. For instance, in the total space, a bosonic coherent state $|\alpha\rangle$ is written as $\hat{\mathbb{1}}_F \otimes |\alpha\rangle$, and the one-body fermionic Hamiltonian \hat{H}_F is written as $\hat{H}_F \otimes \hat{\mathbb{1}}_B$. The operators $\hat{\mathbb{1}}_B$ and $\hat{\mathbb{1}}_F$ are the identity operator in the bosonic and fermionic space respectively. However, writing out all tensor products for operators and vectors that are mainly restricted to one space or the other would lead to an enormous amount of identity operators and tensor products.

A more economical approach is to use notations that make clear which quantity belongs to which space, allowing to omit the tensor products in most cases. The first ingredient towards this approach is the introduction of notations distinguishing between fermionic and bosonic vectors. The other ingredient is the use of distinct notations for bosonic and fermionic creation and annihilation operators, the former being denoted \hat{b}_k^{\dagger} , \hat{b}_k and the latter \hat{c}_{μ}^{\dagger} , \hat{c}_{μ} . Since each operator in this work is written in second quantization form as detailed in section 1.1, they can all be written unambiguously without the use of tensor products. Some illustrative examples are presented below.

The first example is the sum of a purely fermionic Hamiltonian and a purely bosonic Hamiltonian, such as the one-body Hamiltonians \hat{H}_F and \hat{H}_B presented in section 1.2. In the mixed space, it reads

$$\hat{H}_F \otimes \hat{\mathbb{1}}_B + \hat{\mathbb{1}}_F \otimes \hat{H}_B = \left(\sum_{\mu=1}^L E_{F,\mu} \hat{c}_{\mu}^{\dagger} \hat{c}_{\mu}\right) \otimes \hat{\mathbb{1}}_B + \hat{\mathbb{1}}_F \otimes \left(\sum_{n=1}^N E_{B,n} \hat{b}_n^{\dagger} \hat{b}_n\right)$$
(A.2.1)

	Creation and annihilation operators	Coherent states	
Bosons:	$\hat{b}_k^\dagger { m and} \hat{b}_k$	$ lpha angle, eta angle, \gamma angle$	
Fermions:	$\hat{c}^{\dagger}_{\mu} { m and} \hat{c}_{\mu}$	$ \zeta angle, \xi angle, \chi angle$	

Table A.1: Summary of the notations of vectors and operators for bosons and fermions.

Remembering the convention for creation and annihilation operators in table A.1, the tensor products can be omitted since the information about the space to which each Hamiltonian belongs is contained in the use of \hat{b} or \hat{c} . Thus, this sum is simply written as

$$\hat{H}_F + \hat{H}_B = \sum_{\mu=1}^{L} E_{F,\mu} \hat{c}^{\dagger}_{\mu} \hat{c}_{\mu} + \sum_{n=1}^{N} E_{B,n} \hat{b}^{\dagger}_n \hat{b}_n$$
(A.2.2)

Another interesting example is the way the Hamiltonian responsible for the interaction between the fermions and the bosonic field is written. It is given in the mixed space by

$$\hat{H}_{int} = \sum_{n=1}^{N} \sum_{\mu,\nu=1}^{L} C_{\mu\nu n} \hat{c}^{\dagger}_{\mu} \hat{c}_{\nu} \otimes \left(\hat{b}^{\dagger}_{n} + \hat{b}_{n} \right)$$
(A.2.3)

The tensor product is again unnecessary and will be denoted by the usual product, giving

$$\hat{H}_{int} = \sum_{n=1}^{N} \sum_{\mu,\nu=1}^{L} C_{\mu\nu n} \hat{c}^{\dagger}_{\mu} \hat{c}_{\nu} \left(\hat{b}^{\dagger}_{n} + \hat{b}_{n} \right)$$
(A.2.4)

Turning our attention to vectors, we consider the quantity

$$(\langle \zeta | \otimes \langle \alpha |)(|\xi \rangle \otimes \hat{1}_B) \equiv \langle \zeta | \otimes \langle \alpha | |\xi \rangle \otimes \hat{1}_B$$
(A.2.5)

We would first like to draw the attention of the reader to the fact that the bra $\langle \alpha |$ and the ket $|\xi\rangle$ do not form a scalar as they are from different space. In order to avoid confusion, a space is inserted between the two. This lead to a rather inelegant expression. Omitting the tensor products will allow for avoiding it in most cases. In this specific situation, this inner product would be written as

$$\langle \zeta \alpha \,|\, \xi \rangle = \langle \zeta \,|\, \xi \rangle \,\langle \alpha | \tag{A.2.6}$$

It might still happen that a bra from one space faces a ket from the other space. In that case, the notation $\langle \zeta | \alpha \rangle$ will still be used, and will be understood as a shorthand for $\langle \zeta | \otimes | \alpha \rangle$. We end these examples with a more intricate case, mixing operators and vectors. Suppose that we want to simplify the notation of the quantity

$$\langle \zeta | \otimes \hat{\mathbb{1}}_B \ \hat{H}_F \otimes \hat{H}_B \ | \xi \rangle \otimes \hat{\mathbb{1}}_B \tag{A.2.7}$$

The fermionic part yields a scalar and the quantity will be written as

$$\left\langle \zeta \left| \hat{H}_F \left| \xi \right\rangle \hat{H}_B \right.$$
 (A.2.8)

A.3 Shorthands and notations for integrals

This section introduces, we hope, all of the notations for integrals that could cause confusion and disturb the reader's peaceful reading. We begin by mentioning that exponentials coming from closure relations will always be written in the e^{\cdots} form in order to distinguish them from other exponentials:

Closure exponential: $e^{\alpha^* \alpha}$ Other exponential: $\exp(\alpha_m^* \alpha_{m-1})$

In the context of coherent states, and especially used along with path integrals, integrals very often appear as pairs. An example is given by the coherent state closure relations (3.1.19) and (3.2.45). We will present the shorthands in the context of bosonic closure relations, but they all naturally extend to fermionic closure relations. The rigorous definition of the bosonic closure relation over bosonic modes denoted by an index k is

$$\prod_{k} \left[\int_{-\infty}^{+\infty} \int_{-\infty}^{\infty} \frac{d\Re(\alpha_k) d\Im(\alpha_k)}{\pi} e^{-|\alpha_k|^2} \right] |\alpha\rangle \langle \alpha| = \hat{\mathbb{1}}$$
(A.3.1)

We will instead use the notation

$$\prod_{k} \left[\int \frac{d\alpha_{k}^{*} d\alpha_{k}}{2i\pi} e^{-|\alpha_{k}|^{2}} \right] |\alpha\rangle \langle \alpha| = \hat{\mathbb{1}},$$
(A.3.2)

keeping in mind that the rigorous definition for measure and limits of the integration is given in A.3.1. In this work, we always write the product inside of the integral:

$$\prod_{k} \left[\int \frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] \to \int \prod_{k} \left[\frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right]$$
(A.3.3)

When some simplification is welcome and it is obvious that an integral corresponds to a closure relation, the notation

$$\int \prod_{k} \left[\frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] \to \int \prod_{k} \left[d[\alpha^{k}] e^{-|\alpha^{k}|^{2}} \right]$$
(A.3.4)

is adopted. When several closure relations are inserted at once, we merely combine them in one notation:

$$\int \prod_{k} \left[\frac{d\alpha^{*k} d\alpha^{k}}{2i\pi} e^{-|\alpha^{k}|^{2}} \right] \int \prod_{k'} \left[\frac{d\beta^{*k'} d\beta^{k'}}{2i\pi} e^{-|\beta^{k'}|^{2}} \right] \to \int \prod_{k} \left[d[\alpha^{k}, \beta^{k}] e^{-\left(|\alpha^{k}|^{2} + |\beta^{k}|^{2}\right)} \right]$$
(A.3.5)

A common expression in the context of path integrals and occurring in this work is the integral over all paths relating states $|\alpha_i\rangle$ and $|\alpha_f\rangle$. When a little simplification is welcome, these integrals will often be written as:

$$\lim_{M \to \infty} \prod_{m=1}^{M-1} \left[\int \prod_{k} \frac{d\alpha_m^{*k} d\alpha_m^k}{2i\pi} \right] \to \int_{\alpha_i}^{\alpha_f} D[\alpha(t)]$$
(A.3.6)

The same notation is used for fermions by replacing the integrals over the complex variables α^k by Grassmannian integrals as those shown in section 3.2. The denominator is also removed as it is not part of the fermionic closure relation (3.2.45).

Appendix B

Gaussian integral and related formulae

The Gaussian integral is a well-known result. Let $a \in \mathbb{R}$, a > 0 and $b, d \in \mathbb{C}$ three constants, and x a real parameter. We have :

$$\int_{-\infty}^{+\infty} e^{-(ax^2 + bx + d)} dx = e^{b^2/4a} \sqrt{\frac{\pi}{a}}$$
(B.0.1)

Starting from this formula, we derive three results that were frequently used in dealing with the integration over bosonic (complex) variables.

B.1 Integrating over one complex variable and its conjugate

Let $a \in \mathbb{R}$, a > 0, and $b, c, d \in \mathbb{C}$ four constants. Let α be a complex variable (often being the eigenvalue associated to a coherent state). We then have :

$$\int \frac{d\alpha^* d\alpha}{2i\pi} e^{-a|\alpha|^2} \exp\left(b\alpha^* + c\alpha + d\right) = \frac{1}{a} \exp\left(\frac{bc}{a} + d\right)$$
(B.1.1)

Proof. First, we use the rigorous definition of the integration measure and limits to write the integral over α^* and α as integrals over the real parameters $\Re(\alpha)$ and $\Im(\alpha)$:

$$\int \frac{d\alpha^* d\alpha}{2i\pi} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{d\Re(\alpha)d\Im(\alpha)}{\pi}$$
(B.1.2)

Let $x \equiv \Re(\alpha), y \equiv \Im(\alpha)$. The integral can be re-written as

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{dx \, dy}{\pi} \exp\left(-a(x+iy)(x-iy) + b(x-iy) + c(x+iy) + d\right)$$

$$= \frac{e^d}{\pi} \int_{-\infty}^{+\infty} \exp\left(-\left(ax^2 - (b+c)x\right)\right) dx \int_{-\infty}^{+\infty} \exp\left(-\left(ay^2 - (ic-ib)y\right)\right) dy$$

$$= \frac{e^d}{\pi} \sqrt{\frac{\pi}{a}} \exp\left(\frac{(b+c)^2}{4a}\right) \sqrt{\frac{\pi}{a}} \exp\left(\frac{i^2(c-b)^2}{4a}\right)$$

$$= \frac{e^d}{a} \exp\left(\frac{1}{4a}(b^2 + 2bc + c^2 - c^2 + 2bc - b^2)\right)$$
(B.1.3)

$$=\frac{1}{a}\exp\left(\frac{bc}{a}+d\right) \tag{B.1.4}$$

B.2 Integrating over N complex variables and their conjugates

Formula (B.1.1) can be easily generalized for N integrals in cases where there is no coupling between variables. In particular, this case appear when considering closure relations with more than one bosonic mode in the context of the evaluation of the propagator. Suppose that we have to compute an integral of the form

$$\int \prod_{n=1}^{N} \left[\frac{d\alpha^{*n} d\alpha^{n}}{2i\pi} e^{-a_{n}|\alpha^{n}|^{2}} \right] \exp\left(\sum_{n=1}^{N} \left[b_{n} \alpha^{*n} + c_{n} \alpha^{n} \right] \right)$$
(B.2.1)

The result is easily computed by splitting the exponentials. We have

$$\int \prod_{n=1}^{N} \left[\frac{d\alpha^{*n} d\alpha^{n}}{2i\pi} e^{-a_{n}|\alpha^{n}|^{2}} \right] \prod_{n=1}^{N} \exp\left(b_{n} \alpha^{*n} + c_{n} \alpha^{n}\right)$$
$$= \prod_{n=1}^{N} \left[\int \frac{d\alpha^{*n} d\alpha^{n}}{2i\pi} e^{-a_{n}|\alpha^{n}|^{2}} \exp\left(b_{n} \alpha^{*n} + c_{n} \alpha^{n}\right) \right]$$

Applying N times formula (B.1.1) yields

$$\int \prod_{n=1}^{N} \left[\frac{d\alpha^{*n} d\alpha^n}{2i\pi} e^{-a_n |\alpha^n|} \right] \exp\left(\sum_{n=1}^{N} b_n \alpha^{*n} + c_n \alpha^n\right) = \frac{1}{\prod_{n=1}^{N} a_n} \exp\left(\sum_{n=1}^{N} \frac{b_n c_n}{a_n}\right)$$
(B.2.2)

B.3 Integrating over two complex variables and their conjugate

By using equation (B.1.1), one can obtain a formula for a general integral form that occurs in propagator computations. Even though the proof is a bit involved, this result proves itself very useful for the computation of the mixed path integral where bosonic variables are integrated over.

Let $a_{\alpha}, a_{\beta} \in \mathbb{R}, a_{\alpha}, a_{\beta} > 0$ two constants. Let α, β two complex variables. Every other symbol in the equation is a complex constant. We have :

$$\int \frac{d\alpha^* d\alpha}{2i\pi} \int \frac{d\beta^* d\beta}{2i\pi} e^{-\left(a_{\alpha}|\alpha|^2 + a_{\beta}|\beta|^2\right)} \exp\left(b_{\alpha}\alpha^* + b_{\beta}\beta^* + c_{\alpha}\alpha + c_{\beta}\beta + c_{\alpha^*\beta}\alpha^*\beta + c_{\alpha\beta^*}\alpha\beta^* + d\right)$$
$$= \frac{1}{a_{\alpha}a_{\beta} - c_{\alpha^*\beta}c_{\alpha\beta^*}} \exp\left(\frac{1}{a_{\alpha}a_{\beta} - c_{\alpha^*\beta}c_{\alpha\beta^*}} \left(a_{\alpha}b_{\beta}c_{\beta} + a_{\beta}b_{\alpha}c_{\alpha} + c_{\alpha^*\beta}b_{\beta}c_{\alpha} + c_{\alpha\beta^*}b_{\alpha}c_{\beta}\right) + d\right)$$
(B.3.1)

Proof. We first use equation (B.1.1) on one of the complex variables, for instance β . We identify the coefficients in front of the β 's in (B.3.1):

$$\begin{cases} a_1 = a_\beta \\ b_1 = b_\beta + c_{\alpha\beta^*}\alpha \\ c_1 = c_\beta + c_{\alpha^*\beta}\alpha^* \\ d_1 = -a_\alpha |\alpha|^2 + b_\alpha \alpha^* + c_\alpha \alpha + d \end{cases}$$
(B.3.2)

Applying (B.1.1), we obtain

$$\int \frac{d\alpha^* d\alpha}{2i\pi} \int \frac{d\beta^* d\beta}{2i\pi} e^{-(a_\alpha |\alpha|^2 + a_\beta |\beta|^2)} \exp\left(b_\alpha \alpha^* + b_\beta \beta^* + c_\alpha \alpha + c_\beta \beta + c_{\alpha^*\beta} \alpha^* \beta + c_{\alpha\beta^*} \alpha \beta^* + d\right)$$

$$= \int \frac{d\alpha^* d\alpha}{2i\pi} e^{-a_\alpha |\alpha|^2} \frac{1}{a_\beta} \exp\left(\frac{1}{a_\beta} \left(b_\beta + c_{\alpha\beta^*} \alpha\right) \left(c_\beta + c_{\alpha^*\beta} \alpha^*\right) + \left(b_\alpha \alpha^* + c_\alpha \alpha + d\right)\right)$$

$$= \int \frac{d\alpha^* d\alpha}{2i\pi} \frac{1}{a_\beta} \exp\left(-(a_\alpha - \frac{1}{a_\beta} c_{\alpha^*\beta} c_{\alpha\beta^*})|\alpha|^2 + (b_\alpha + \frac{1}{a_\beta} b_\beta c_{\alpha^*\beta})\alpha^* + (c_\alpha - \frac{1}{a_\beta} c_\beta c_{\alpha\beta^*})\alpha + d + \frac{1}{a_\beta} b_\beta c_\beta\right)$$

We can again identify the coefficients in front of the integrated variable :

$$\begin{cases} a_2 = a_{\alpha} - \frac{1}{a_{\beta}} c_{\alpha^* \beta} c_{\alpha \beta^*} \\ b_2 = b_{\alpha} + \frac{1}{a_{\beta}} b_{\beta} c_{\alpha^* \beta} \\ c_2 = c_{\alpha} + \frac{1}{a_{\beta}} c_{\beta} c_{\alpha \beta^*} \\ d_2 = d + \frac{1}{a_{\beta}} b_{\beta} c_{\beta} \end{cases}$$
(B.3.3)

Applying (B.1.1) a second time, we find

$$\int \frac{d\alpha^* d\alpha}{2i\pi} \frac{1}{a_\beta} \exp\left(\left(a_\alpha - \frac{1}{a_\beta} c_{\alpha^*\beta} c_{\alpha\beta^*}\right)|\alpha|^2 + \left(b_\alpha + \frac{1}{a_\beta} b_\beta c_{\alpha^*\beta}\right)\alpha^* + \left(c_\alpha + \frac{1}{a_\beta} c_\beta c_{\alpha\beta^*}\right)\alpha + d + \frac{1}{a_\beta} b_\beta c_\beta\right)$$
$$= \frac{1}{a_\beta} \frac{1}{a_\alpha - \frac{1}{a_\beta} c_{\alpha^*\beta} c_{\alpha\beta^*}} \exp\left(\frac{1}{a_\alpha - \frac{1}{a_\beta} c_{\alpha^*\beta} c_{\alpha\beta^*}}\left(b_\alpha + \frac{1}{a_\beta} b_\beta c_{\alpha^*\beta}\right)\left(c_\alpha + \frac{1}{a_\beta} c_\beta c_{\alpha\beta^*}\right) + d + \frac{1}{a_\beta} b_\beta c_\beta\right)$$

The prefactor can in fact be re-written as $\frac{1}{a_{\alpha}a_{\beta}-c_{\alpha^{*}\beta}c_{\alpha\beta^{*}}}$. Let's now take interest in the exponent. We have :

$$\begin{aligned} &\frac{a_{\beta}}{a_{\beta}} \frac{1}{a_{\alpha} - \frac{1}{a_{\beta}} c_{\alpha^{*}\beta} c_{\alpha\beta^{*}}} \left(b_{\alpha} + \frac{1}{a_{\beta}} b_{\beta} c_{\alpha^{*}\beta} \right) \left(c_{\alpha} + \frac{1}{a_{\beta}} c_{\beta} c_{\alpha\beta^{*}} \right) + d + \frac{1}{a_{\beta}} b_{\beta} c_{\beta} \\ &= \frac{1}{a_{\alpha} a_{\beta} - c_{\alpha^{*}\beta} c_{\alpha\beta^{*}}} a_{\beta} \left(b_{\alpha} c_{\alpha} + \frac{1}{a_{\beta}} b_{\alpha} c_{\beta} c_{\alpha\beta^{*}} + \frac{1}{a_{\beta}} b_{\beta} c_{\alpha} c_{\alpha^{*}\beta} + \frac{1}{a_{\beta}^{2}} b_{\beta} c_{\beta} c_{\alpha^{*}\beta} c_{\alpha\beta^{*}} \right) + d + \frac{1}{a_{\beta}} b_{\beta} c_{\beta} \\ &= \frac{1}{a_{\alpha} a_{\beta} - c_{\alpha^{*}\beta} c_{\alpha\beta^{*}}} \left(a_{\beta} b_{\alpha} c_{\alpha} + b_{\alpha} c_{\beta} c_{\alpha\beta^{*}} + b_{\beta} c_{\alpha} c_{\alpha^{*}\beta} + \frac{1}{a_{\beta}} b_{\beta} c_{\beta} c_{\alpha^{*}\beta} c_{\alpha\beta^{*}} + \frac{1}{a_{\beta}} b_{\beta} c_{\beta} (a_{\alpha} a_{\beta} + c_{\alpha^{*}\beta} c_{\alpha\beta^{*}}) \right) + d \\ &= \frac{1}{a_{\alpha} a_{\beta} - c_{\alpha^{*}\beta} c_{\alpha\beta^{*}}} \left(a_{\alpha} b_{\beta} c_{\beta} + a_{\beta} b_{\alpha} c_{\alpha} + c_{\alpha^{*}\beta} b_{\beta} c_{\alpha} + c_{\alpha\beta^{*}} b_{\alpha} c_{\beta} \right) + d \end{aligned}$$

Putting together the two results, we have :

$$\int \frac{d\alpha^* d\alpha}{2i\pi} \int \frac{d\beta^* d\beta}{2i\pi} e^{-(a_{\alpha}|\alpha|^2 + a_{\beta}|\beta|^2)} \exp\left(b_{\alpha}\alpha^* + b_{\beta}\beta^* + c_{\alpha}\alpha + c_{\beta}\beta + c_{\alpha^*\beta}\alpha^*\beta + c_{\alpha\beta^*}\alpha\beta^* + d\right)$$

$$= \frac{1}{a_{\alpha}a_{\beta} - c_{\alpha^*\beta}c_{\alpha\beta^*}} \exp\left(\frac{1}{a_{\alpha}a_{\beta} - c_{\alpha^*\beta}c_{\alpha\beta^*}} \left(a_{\alpha}b_{\beta}c_{\beta} + a_{\beta}b_{\alpha}c_{\alpha} + c_{\alpha^*\beta}b_{\beta}c_{\alpha} + c_{\alpha\beta^*}b_{\alpha}c_{\beta}\right) + d\right)$$

Note that in most use cases, this result can be greatly simplified. Indeed, since in our use case the variables come from closure relations, the situation where both $\alpha^*\beta$ and $\alpha\beta^*$ appear in a term never occurs, since it would require an expression of the form $|\alpha\rangle \langle \alpha | e^{\hat{O}} | \beta \rangle \langle \beta | e^{\hat{O}'} | \alpha \rangle \langle \alpha |$. Thus, there is at least one null coefficient between $c_{\alpha^*\beta}$ and $c_{\alpha\beta^*}$. In this work, the closure relation on what we call α is always inserted to the left of the one on β , and thus $c_{\alpha\beta^*} = 0$. The prefactors then reduces to $1/a_{\alpha}a_{\beta}$. Furthermore, a_{α} and a_{β} both come from and only from the normalisation of the closure relation. Thus, they are both equal to one in all cases and can be omitted. We finally arrive to a more practical formula :

$$\int \frac{d\alpha^* d\alpha}{2i\pi} \int \frac{d\beta^* d\beta}{2i\pi} e^{-\left(|\alpha|^2 + |\beta|^2\right)} \exp\left(b_\alpha \alpha^* + b_\beta \beta^* + c_\alpha \alpha + c_\beta \beta + c_{\alpha^*\beta} \alpha^* \beta + d\right)$$

= exp ($b_\alpha c_\alpha + b_\beta c_\beta + c_{\alpha^*\beta} b_\beta c_\alpha + d$) (B.3.4)

Appendix C

Numeric tools developed in the context of this work

Working with Grassmann numbers requires the development of new formulae, since they differ from complex numbers in several ways, such as their anti-commutation or the definition of the Grassmannian integral. This appendix will not recall or summarize basic properties of Grassmann numbers, since this is done in detail in the first part of section 3.2. Instead, we will focus here on the original tool that allowed us to numerically check some formulae for which algebraic proofs could not be obtained. This tool is a small Python¹ library as of yet unnamed, and a non-exhaustive list of its characteristics and possibilities will be exposed in this appendix. The library can be found in the following GitHub repository: https://github.com/Anatel-Phys/GrassmannLibrary.

C.1 The code's core

The concept of the library is to allow symbolic manipulation of expressions containing ordinary numbers and Grassmann numbers. The user starts by writing a string representing the expression they want to compute or simplify. A function is provided to convert them into a form that can be used by the library, which is a list of terms. The user can then manipulate those expressions, multiply them, apply Grassmann integration on them, eliminate the terms with Grassmann duplicates (*i.e.* null terms) etc. Other tools are available such as tools to help the user generate strings for specific Grassmann functions, tools to generate exponentials of any expression of Grassmann generators etc. A few example of use of the code will now be presented. Note that the actual name of the library's functions will not be used, since it might change in the future. In the same spirit, the outputs of the various functions presented might not be exactly the same as that of the actual function from the library, although it will likely be equivalent. This chapter thus cannot be used as a tutorial for the library. For this purpose, a tutorial file is included in the library.

Here is a simple example of a correctly formatted string and how the code converts it. It contains the expression $1 + A\xi$ with A a complex number and ξ a Grassmann generator, and is represented in the following way for the library:

convert("(+1 +A.g_xi)") \rightarrow [['+', '1'], ['+', 'A', 'g_xi']]

The prefix g indicates that the variable ξ is a Grassmann generator. This form can now be manipulated using various functions from the library. The function multiply allows for multiplying two expressions stored in such form. Suppose that we want to compute the square of the above expression. We have

e = [['+', '1'], ['+', 'A', 'g_xi']] e_sq = multiply(e, e) e_sq → [['+', '1'], ['+', '2', 'A', 'g_xi'], ['+', 'A', 'A', 'g_xi', 'g_xi']]

This function however does not take into account the properties of Grassmann generators. This is the role of the function remove_dupe, which works exactly as one would expect:

correct_e_sq = remove_dupe(sq_e, sq_e)
corect_e_sq → [['+', '1'], ['+', '2', 'A', 'g_xi']]

 $^{^{1}}$ When the scale of use of the library grew, it became evident that a more efficient programming language would have been appropriate. This might be a work for the future.
The last important feature of the library is the ability to integrate over Grassmann generatorss. This is done quite straightforwardly with a single function that applies the integration rules (3.2.23):

```
e = [['+', '1'], ['+', 'A', 'g_xi']]
int_e = integrate(e, xi)
int_e → [['+', 'A']]
```

The integrate function can integrate over several generators at once and takes care of the anti-commutation of Grassmann generators. Recall that the Grassmann integration properties (3.2.23) require the integrated generator to be exactly to the right of the symbolic integral. Computing the integral $\int d\xi \int d\zeta \xi\zeta$ then yields

```
e = [['+', 'g_xi', 'g_zeta']]
int_e = integrate(e, [xi, zeta])
int_e → [['-', '1']]
```

as expected. The functionalities as presented above do not yet seem to allow for more than what could be done by hand. However, as the set of Grassmann generators considered grows, exhaustive calculations rapidly become beyond the reach of someone doing the calculations by hand, even if they are very brave. This will be discussed in section C.3. But first, let us take a look at the original algorithm used to compute integrals over several Grassmann generators.

C.2 Algorithm for multiple Grassmann integrals

From a computational point of view, the main difficulty in computing multiple Grassmannian in an effective way is to keep track of the minus signs brought by the permutations required to bring each Grassmannian generator in front of the expression in the order implied by the integrals (see section 3.2 for a reminder on Grassmannian integration). For instance, say we have to compute

$$\int d\xi_1 \int d\xi_2 \,\xi_3 \xi_2 \xi_1 \tag{C.2.1}$$

It is done by bringing ξ_2 in front of the product, computing the corresponding integral, and then doing the same for ξ_1 . Extensively, the computation goes as follow:

$$\int d\xi_1 \int d\xi_2 \,\xi_3 \xi_2 \xi_1 = -\int d\xi_1 \int d\xi_2 \,\xi_2 \xi_3 \xi_1 = -\int d\xi_1 \,\xi_3 \xi_1 = \int d\xi_1 \xi_1 \xi_3 = \xi_3 \tag{C.2.2}$$

The algorithm chosen to compute integrals over Grassmann generators takes a list of Grassmann generators and a term of the form $C\xi_1 \cdots \xi_N$ with C any ordinary (complex or real) number. Each generator we integrate over can occur either 0 or 1 time in the integrated term, since the square of a Grassmann generators is 0. We also do not need to deal with functions of Grassmann generators in the integration function since every function of Grassmann generators can be expanded into a finite power series.

The algorithm first checks if each Grassmann generator we integrate over is present in the integrated term. If not, the result of the integral is 0. If they are all present, then looking at (C.2.2) can easily convince us that the result will be the initial integrated term where the Grassmann generators we integrate over have been removed, up to a sign. This sign is what is computed next by the algorithm. It first computes the position of each generator we integrate over in the integrated term in order of integration and adds this position minus 1 to a list. Applied to the above example, we would have:

$$\int d\xi_1 \int d\xi_2 \,\xi_3 \xi_2 \xi_1 \longrightarrow (1,2) \tag{C.2.3}$$

because ξ_2 is in second position and ξ_1 in third. Note that the resulting list corresponds to the number of permutation required to bring each generators in front of the product, which justifies the decrement by 1. The next step is to iterate over the indices in the list and decrement them by 1 for each smaller index that comes before it in the list. This step corresponds to removing from the permutation count the cases where a generators would be permuted with a generators that has already been integrated over. In our example, the index 3 is greater than 2 and is thus decreased by 1, yielding

$$(1,2) \longrightarrow (1,1) \tag{C.2.4}$$

The final result is obtained by summing every indices and computing the parity of the sum. Here the sum is an even number, meaning that the sign of the integral is '+'. This is indeed what was obtained by hand in (C.2.2). A more involved example is presented below consider the integral

$$\int d\xi_1 \int d\xi_5 \int d\xi_3 \,\xi_1 \xi_2 \xi_3 \xi_4 \xi_5 \xi_6 \tag{C.2.5}$$

The position of each generator we integrate over is computed in order of integration and decreased by 1, yielding

$$\int d\xi_1 \int d\xi_5 \int d\xi_3 \,\xi_1 \xi_2 \xi_3 \xi_4 \xi_5 \xi_6 \longrightarrow (2,4,0) \tag{C.2.6}$$

Since 2 is smaller than 4 and comes before it in the list, we decrease the index 4 by one, giving the final list (2,3,0). The sum of each element of this list gives 5 which is odd, and the final result of this integration is thus

$$\int d\xi_1 \int d\xi_5 \int d\xi_3 \,\xi_1 \xi_2 \xi_3 \xi_4 \xi_5 \xi_6 = -\xi_2 \xi_4 \xi_6 \tag{C.2.7}$$

One advantage of this algorithm is that it does not require to compute any actual swap between generatorss, thus being more efficient in term of space than a sorting algorithm.

C.3 Perspectives on large scale applications

What makes the treatment of Grassmann generators different from that of ordinary number is the fact that they are symbolic quantities. A term is not a number but a list of symbols. Furthermore, the order of these symbols matter since we are dealing with anti-commuting numbers. Simplifying functions of Grassmann generators amounts to computing the non-zero terms of their power series, and there is no notion of convergence. One then has to deal with an amount of symbols that can be quite large. For instance, the treatment of a fermionic system with L sites requires at least L Grassmann generators. The computation of, for instance, power series with an increasing L rapidly gets out of hand as will be seen.

Over the course of this work, the use of this library shifted from a quick verification of elementary calculations to large-scale computation of elementary propagators. This was principally allowed by the creation of functions that compute the power series development of exponentials of arbitrarily large expressions, and the use of recursion. For instance, suppose you have to compute the power series development of the exponential

$$\exp\left(\sum_{\mu=1}^{L}\xi_{\mu}\right) \tag{C.3.1}$$

It is given by

$$\exp\left(\sum_{\mu=1}^{L}\xi_{\mu}\right) = \sum_{p=1}^{\infty}\frac{1}{p!}\left(\sum_{\mu=1}^{L}\xi_{\mu}\right)^{p}$$
(C.3.2)

Because there is L different Grassmannian generator in this exponential, the power series expansion of the exponential will stop at the term of order L. Indeed, a term of order L + 1 would contain a duplicate of at least one of the Grassmann generators. But one still has to compute each term up to order L, giving a computational complexity of $\mathcal{O}(L^L)$ for obtaining the power series. What is important to realize in order to reduce the complexity of this operation is that most of the terms in the power series contain duplicates of Grassmann generators and are actually null. Starting from there, computing the terms of the power series in a recursive way appear to reduce the computational complexity of several orders of magnitude. An efficient algorithm can then be described by the following pseudo-code:

```
function EXPONENTIALPOWERSERIES(term)

PowerSeries = new List

PowerSeries.append(1)

p = 1

while termP != Null do

termP = termP * term / p

RemoveDuplicates(termP)

PowerSeries.append(termP)

p = p + 1

end while

return PowerSeries

end function
```

This algorithm removes the Grassmann duplicates as they occur in the term of order p. The term of order p + 1 is then computed using the term of order p which has been cleansed of its duplicates, meaning that no

useless product is computed. This approach can be generalized to any product of quantities containing Grassmann generators. The idea is to always remove the duplicates in one product before multiplying it with another term in order to avoid any useless computations. This approach represents a major improvement in performance. For example, the expression

$$\left(\sum_{\mu=1}^{L}\xi_{\mu}\right)^{p} \tag{C.3.3}$$

contains L^p possible terms but only $\frac{L!}{(L-p)!}$ non-zero terms. Plugging in values to give an idea, we find that for L = 10 and p = 6, there is 1.000.000 possible terms but "only" 151.200 non-zero terms. The next step is to reassemble terms that are similar up to a permutation. This would further decrease the quickly increasing number of possible terms since there is only $\frac{L!}{p!(L-p)!}$ different terms possible up to a permutation. In the given examples, it reduces the number of non-zero terms to only 210. This could make up for a huge difference in, for instance, the RAM required to perform computation of power series, which occur a lot in the treatment of functions of Grassmann generators. This is still a work in progress at the time of writing.

Using this technique for computing the power series of exponentials, one essentially has the tools to compute the quantities occurring in the path integral formulation to the quantum propagator. It was using this technique that the formulae (3.2.46) and (3.2.48) were verified numerically for several values of L. Those verification were made by using comparison tools between the exhaustive development using Grassmann rules, and the postulated formula. We conclude this section by mentioning that this tool does not replace algebraic tools and rigorous proofs for results involving Grassmann generators. Obtaining such proofs for the formulae that were only numerically tested would of course be an improvement.

Appendix D

Miscellaneous proofs

D.1 Exponential of a sum of commuting quantities

In this work, expression containing sums of Grassmannian pairs occur very frequently. In order to prove some properties of exponentials of Grassmann pairs, it is sometimes required to split the exponential of a sum into a product of exponentials. We here show that this operation is indeed correct. Because Grassmann pairs commute, it suffice to show that in general, the exponential of a sum of commuting objects can be split into a product of exponentials. In other words, that we have

$$\exp\left(\mathbf{A} + \mathbf{B}\right) = \exp\left(\mathbf{A}\right)\exp\left(\mathbf{B}\right) \tag{D.1.1}$$

with A, B two generic quantities that commute.

Proof. We begin by expanding the exponential into its power series:

$$\exp\left(\mathbf{A} + \mathbf{B}\right) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\mathbf{A} + \mathbf{B}\right)^n \tag{D.1.2}$$

Since A and B commute, we can use the binomial theorem to write

$$\left(\mathbf{A} + \mathbf{B}\right)^{n} = \sum_{k=0}^{n} \binom{n}{k} \mathbf{A}^{k} \mathbf{B}^{n-k} = \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} \mathbf{A}^{k} \mathbf{B}^{n-k}$$
(D.1.3)

Plugging this result back into the power series (D.1.2) yields

$$\exp\left(\mathbf{A} + \mathbf{B}\right) = \sum_{n=0}^{\infty} \sum_{k=0}^{n} \frac{\mathbf{A}^{k}}{k!} \frac{\mathbf{B}^{n-k}}{(n-k)!}$$
(D.1.4)

We can permute the order of summation:

$$\sum_{n=0}^{\infty} \sum_{k=0}^{n} \frac{\mathbf{A}^{k}}{k!} \frac{\mathbf{B}^{n-k}}{(n-k)!} = \sum_{k=0}^{\infty} \sum_{n=k}^{\infty} \frac{\mathbf{A}^{k}}{k!} \frac{\mathbf{B}^{n-k}}{(n-k)!}$$
(D.1.5)

Letting m = n - k, we finally have

$$\sum_{k=0}^{\infty} \sum_{n=k}^{\infty} \frac{\mathbf{A}^k}{k!} \frac{\mathbf{B}^{n-k}}{(n-k)!} = \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \frac{\mathbf{A}^k}{k!} \frac{\mathbf{B}^m}{(m)!} = \left(\sum_{k=0}^{\infty} \frac{\mathbf{A}}{k!}\right) \left(\sum_{m=0}^{\infty} \frac{\mathbf{B}}{m!}\right)$$
(D.1.6)

Recognizing the power series, we thus have proven that for two commuting objects \mathbf{A} and \mathbf{B} ,

$$\exp\left(\mathbf{A} + \mathbf{B}\right) = \exp\left(\mathbf{A}\right)\exp\left(\mathbf{B}\right) \tag{D.1.7}$$

D.2 Position-conjugate momentum relation for coherent eigenvalues

We want to prove that the eigenvalues associated to coherent states and their complex conjugate are equivalent to a position and momentum if both multiplied by a factor $\sqrt{i\hbar}$. Here, we will only prove the bosonic case. As a reminder, coherent states are defined as right eigenvalues of the annihilation operator:

$$\hat{b} \left| \alpha \right\rangle = \alpha \left| \alpha \right\rangle \tag{D.2.1}$$

We first write the definition of the creation and annihilation operators in terms of the position and momentum operators coming from the correspondence between bosonic particles and harmonic oscillators:

$$\hat{b} = \frac{1}{\sqrt{2m\hbar\omega}} (\hat{q} + i\hat{p}) \tag{D.2.2}$$

$$\hat{b}^{\dagger} = \frac{1}{\sqrt{2m\hbar\omega}} (\hat{q} - i\hat{p}) \tag{D.2.3}$$

with ω the angular frequency of the bosonic mode considered. Inverting these relations, we find that

$$\hat{q} = \sqrt{\frac{m\hbar\omega}{2}}(\hat{b} + \hat{b}^{\dagger}) \tag{D.2.4}$$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{b} - \hat{b}^{\dagger}), \qquad (D.2.5)$$

We can compute the expectation values of these operators in the coherent state representation:

$$q_{\alpha} = \langle \alpha \,|\, \hat{q} \,|\, \alpha \rangle = \sqrt{\frac{m\hbar\omega}{2}} (\alpha + \alpha^*) \tag{D.2.6}$$

$$p_{\alpha} = \langle \alpha \,|\, \hat{p} \,|\, \alpha \rangle = i \sqrt{\frac{m\hbar\omega}{2}} (\alpha - \alpha^*) \tag{D.2.7}$$

Writing the complex number α as its real and imaginary part, we find

$$q_{\alpha} = \sqrt{2m\hbar\omega}\Re(\alpha) \tag{D.2.8}$$

$$p_{\alpha} = i\sqrt{2m\hbar\omega}\Im(\alpha) \tag{D.2.9}$$

We thus see that the value of the position and momentum in coherent state representation relates to the real and imaginary part of the coherent eigenvalue respectively. By considering α and α^* as distinct generators, we can associate the information on the position to α and the information on the momentum to α^* . The origin of the factor $\sqrt{i\hbar}$ lies in the fact that a position-momentum couple of operators in quantum mechanics satisfies to the commutation relation

$$\hat{q}, \hat{p}] = i\hbar \tag{D.2.10}$$

In the case of the creation and annihilation operator, we have

$$[\hat{b}, \hat{b}^{\dagger}] = 1$$
 (D.2.11)

We thus need to somehow multiply them in order to make the right hand side be equal to $i\hbar$. We do so by arbitrarily multiplying both of them by $\sqrt{i\hbar}$, which is applied to the eigenvalues as well.

D.3 Exponential of two pairs of fermionic creation/annihilation operators

In chapter 3, the action of the exponential of a pair of creation and annihilation operators was derived. A very similar result can be obtained for two pairs of such operators. We expose here this result in the case of fermions since the bosonic case do not occur in this work. Suppose that we have a generic two-body Hamiltonian expressed in second quantization in the generic form

$$\hat{H}_{TB} = \sum_{\mu,\nu,\rho,\sigma=1}^{L} D_{\mu\nu\rho\sigma} \hat{c}^{\dagger}_{\mu} \hat{c}^{\dagger}_{\nu} \hat{c}_{\rho} \hat{c}_{\sigma}$$
(D.3.1)

In the path integral theory of such Hamiltonian, we would encounter quantities such as

$$\left\langle \xi \left| \exp\left(-\frac{i}{\hbar}\delta t \, \hat{H}_{TB}\right) \right| \chi \right\rangle$$
 (D.3.2)

with δt an infinitesimal time step and $|\xi\rangle$, $|\chi\rangle$ two fermionic coherent states. We can expand the exponential to first order in δt , yielding

$$\left\langle \xi \left| \exp\left(-\frac{i}{\hbar}\delta t \, \hat{H}_{TB}\right) \right| \chi \right\rangle = \left\langle \xi \left| \left(\hat{\mathbb{1}} - \frac{i}{\hbar}\delta t \, \hat{H}_{TB}\right) \right| \chi \right\rangle = \left\langle \xi \left| \left(\hat{\mathbb{1}} - \frac{i}{\hbar}\delta t \, \sum_{\mu,\nu,\rho,\sigma=1}^{L} D_{\mu\nu\rho\sigma} \hat{c}^{\dagger}_{\mu} \hat{c}^{\dagger}_{\nu} \hat{c}_{\rho} \hat{c}_{\sigma}\right) \right| \chi \right\rangle$$
(D.3.3)

Recall the eigenvalue notations introduced in chapter 3, which are summarized in appendix A. Using the fact that fermionic coherent states are right eigenstates of annihilation operators and left eigenstates of creation operators, along with the anti-commutation rules (3.2.30), we have

$$\left\langle \xi \left| \hat{c}_{\mu}^{\dagger} \hat{c}_{\nu}^{\dagger} \hat{c}_{\rho} \hat{c}_{\sigma} \right| \chi \right\rangle = \left\langle \xi \left| \xi^{*\mu} \hat{c}_{\nu}^{\dagger} \hat{c}_{\rho} \chi^{\sigma} \right| \chi \right\rangle = \left\langle \xi \left| (-1)^{2} \hat{c}_{\nu}^{\dagger} \xi^{*\mu} \chi^{\sigma} \hat{c}_{\rho} \right| \chi \right\rangle = \left\langle \xi \left| (-1)^{4} \xi^{*\mu} \xi^{*\nu} \chi^{\rho} \chi^{\sigma} \right| \chi \right\rangle$$
(D.3.4)

Inserting this result back in (D.3.3) yields

$$\left\langle \xi \left| \left(1 - \frac{i}{\hbar} \delta t \sum_{\mu,\nu,\rho,\sigma=1}^{L} D_{\mu\nu\rho\sigma} \hat{c}^{\dagger}_{\mu} \hat{c}^{\dagger}_{\nu} \hat{c}_{\rho} \hat{c}_{\sigma} \right) \right| \chi \right\rangle = \left\langle \xi \left| \left(1 - \frac{i}{\hbar} \delta t \sum_{\mu,\nu,\rho,\sigma=1}^{L} D_{\mu\nu\rho\sigma} \xi^{*\mu} \xi^{*\nu} \chi^{\rho} \chi^{\sigma} \right) \right| \chi \right\rangle$$
(D.3.5)

We recognize the term with the sum as being the Hamiltonian (D.3.1) where the creation and annihilation operators have been replaced by the corresponding left and right eigenvalues respectively. We naturally denote it with $H_{TB}(\xi^*, \zeta)$. Since δt is infinitesimal, we can write the expression in parenthesis back in exponential form:

$$\left\langle \xi \left| \left(1 - \frac{i}{\hbar} \delta t \, H_{TB}(\xi^*, \zeta) \right) \right| \chi \right\rangle = \left\langle \xi \left| \exp\left(-\frac{i}{\hbar} \delta t \, H_{TB}(\xi^*, \zeta) \right) \right| \chi \right\rangle \tag{D.3.6}$$

We thus finally have

$$\left\langle \xi \left| \exp\left(-\frac{i}{\hbar}\delta t \, \hat{H}_{TB}\right) \right| \chi \right\rangle = \left\langle \xi \left| \exp\left(-\frac{i}{\hbar}\delta t \, H_{TB}(\xi^*,\zeta)\right) \right| \chi \right\rangle \tag{D.3.7}$$

with

$$H_{TB}(\xi^*, \zeta) = \sum_{\mu, \nu, \rho, \sigma = 1}^{L} D_{\mu\nu\rho\sigma} \xi^{*\mu} \xi^{*\nu} \chi^{\rho} \chi^{\sigma}$$
(D.3.8)