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Open Quantum Systems and Ultracold Atoms

Matteo Sighinolfi

Under the supervision of:
Dr. Alessio Recati
and
Dr. Pietro Faccioli

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A chiunque mi abbia sostenuto ed aiutato,
senza di voi questo non sarebbe stato possibile.

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Introduction

The main topic of this thesis is the development of theoretical techniques for the description of the dynamics of impurities in a larger system, in the sense of number of degrees of freedom. This is the well known impurity problem, paradigmatic to different fields of physics from solid state to neutron stars and standard model. A very interesting analogy is possible between the impurity problem and Open Quantum Systems: indeed, the latter are large systems composed of a large environment and a small subsystem of interest, i.e. the typical situation for the impurity problem. The development of this analogy will be discussed throughout the thesis, that is organized in three main Chapters.

In Chapter 1 the theoretical foundations necessary for a complete understanding of all the presented results is given. The definition of Open Quantum System (OQS) and the properties of it are discussed in Section 1.1. A first possible strategy to solve the desired dynamics using master equations, such as the so-called Lindblad equation, is presented in Section 1.2 with the main details and a possible application to Quantum Brownian motion.

OQS can be studied also with the path integral technique, that turns out being extremely useful to focus on the desired dynamics of the subsystem/impurity. The characteristic dynamics of an OQS can also involve out of equilibrium processes, therefore a more suitable formalism than the standard quantum field theory should be employed. A particular formalism well suited for the systems discussed here is the so-called Keldysh formalism for quantum field theory. Section 1.3 is devoted to the introduction to Keldysh formalism for non-interacting systems of bosons and fermions. All the main properties and differences with equilibrium field theory are discussed, while details on interactions are discussed in the next Chapters.

To conclude, it should be kept in mind that this theoretical introduction has not the goal of be extensive. The goal is to be consistent and give the reader all the necessary tools to understand the remaining Chapters of this work and the results presented within them. The reader interested in a more deep discussion can find additional material in Ref. [1] for the discussion on OQS and master equations and in Ref. [2] for the Keldysh formalism.

In Chapter 2 the Keldysh formalism introduced in the previous chapter is used to study the first system of interest. This system is composed of heavy impurities interacting with a bath of light fermions. This system is a typical OQS, indeed the dynamics of the impurities is the one of greater interest and the degrees of freedom of the bath are much more than the ones of the impurities. Due to the extremely large number of degrees of freedom of the bath, an approach involving master equations is not the best possible way to describe the system and Keldysh formalism has to be used to obtain an effective equation of motion for the impurities. The derivation of this equation of motion is the subject of the first part of the Chapter, in which all the relevant details of the procedure are discussed and only a small part of it can be found in Appendix A. The final equation of motion will be stochastic and semiclassical: stochastic because a consequence of tracing out the bath degrees of freedom is that some information on the whole system are lost and semiclassical because the equation of motion will be classical but with coefficients that reflect the underlying quantum nature of the bath. This equation is the

so-called generalized Langevin equation.

The analysis on the effective stochastic semiclassical equation of motion is then carried out and interesting results are found: the bath induces on the impurities an attractive interaction and during their motion impurities experience a viscosity of the medium that depends on the relative distance between impurities. While this fact is general and independent of the interaction considered, the focus in this Chapter is on the case where the interaction between impurities and bath is contact-like. Another interesting point is that the equation of motion is quite general in form, while some approximations made are directly impacting on the quantum coefficients: therefore, when a refined approximation is made, only the quantum coefficients have to be updated without modifying the form of the equation itself. Moreover, when the interplay between the strength of the impurity-bath coupling and the temperature is favorable, a bound state of impurities is admissible. The study of the main properties of the bound state, i.e. radius and lifetime, is possible thanks to the numerical implementation of the equation of motion with a stochastic version of the Verlet algorithm, discussed in this Chapter.

Finally, some possible further developments and extension, like inclusion of the effective mass of impurities in our model, are discussed. The whole chapter is an extended discussion on the results and on the method presented in Ref. [3].

In Chapter 3, a system where polarons are coherently coupled to a non-interacting impurity level via a Rabi coupling is studied, in order to find a theoretical description for the experiment presented in Ref. [4]. As in the previous Chapter, the Keldysh formalism is employed to describe the dynamics of the system, but instead of generalized Langevin equation a set of kinetic equations for the populations in the different levels is obtained. While some parts of the theory are tailored for the particular system described in the experiment, the approach is general and can be extended to different systems where a quasiparticle and a coherent drive are present at the same time.

The larger part of the Chapter is devoted to the description of the microscopical Hamiltonian and of the various approximations needed and assumptions made in the path to the desired kinetic equations. Some smaller and more technical part are moved to Appendix B to facilitate the reading, without affecting the understanding of the final equations. In the next part of the chapter, numerical results for the static polaron properties and for the dynamics are discussed. It is important to remember that the final kinetic equations are a model for the system that does not need any external fitting parameters and are therefore a good candidate for the description of the dynamics. Finally, some future perspectives are reported.

The work presented in detail in this Chapter will be illustrated in a future work [5] mainly focused on the final kinetic equations.

The very last part of this thesis is used to draw some conclusions on the methodology employed and on future perspectives.

Chapter 1

Theoretical introduction

1.1 Open Quantum Systems

1.1.1 Isolated and closed systems

Quantum mechanics describes the evolution in time of a closed system with the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle , \tag{1.1}$$

where $|\Psi(t)\rangle$ is the state vector of Hilbert space $\mathcal{H}$ that describes the system and $H(t)$ is the Hamiltonian (generally time-dependent) of the system. The solution of the Schrödinger equation can be represented with a unitary time evolution operator $U(t, t_0)$ which action is

$$|\Psi(t)\rangle = U(t, t_0) |\Psi(t_0)\rangle , \tag{1.2}$$

i.e. $U(t, t_0)$ transforms the state at some initial time t_0 $|\Psi(t_0)\rangle$ into the state $|\Psi(t)\rangle$ at time t. If Eq. (1.2) is inserted into Schrödinger equation, an equation for the time evolution operator is obtained

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t) U(t, t_0), \tag{1.3}$$

with the initial condition[1] $U(t_0, t_0) = I$. The operator $U(t, t_0)$ is unitary, i.e. $U(t, t_0) U^\dagger(t, t_0) = U^\dagger(t, t_0) U(t, t_0) = I$.

If the Hamiltonian H of the system is time-independent, then Eq. (1.3) can be easily solve and the well known expression

$$U(t, t_0) = \exp\left(-\frac{i}{\hbar} H(t - t_0) \right) , \tag{1.4}$$

is obtained. When the Hamiltonian of the system is time-independent and Eq. (1.4) holds the system is defined as *isolated*. When the dynamics of the system can be formulated in terms of a time-dependent generator $H(t)$ the system is defined as *closed* and the time evolution operator of the system can be represented as

$$U(t, t_0) = T_\leftarrow \exp\left(-\frac{i}{\hbar} \int_{t_0}^{t} ds\, H(s) \right) , \tag{1.5}$$

where $T_\leftarrow$ is the time-ordering operator that orders time-dependent operators in such a way that time arguments increase form right to left (as indicated by the direction of the arrow).

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[1] In this Chapter the identity matrix of arbitrary dimension is labelled as I. Dimensions will be specified only when they are relevant for the understanding of the equations.

The state vector $|\Psi(t)\rangle$ (or the corresponding wave function Ψ) is not the only way to describe a system. Indeed, the density matrix ρ can be used

$$\rho = \sum_i w_i |\Psi_i\rangle \langle \Psi_i|, \tag{1.6}$$

where Ψ_i are the elements of an arbitrary basis of the Hilbert space $\mathcal{H}$, w_i are coefficients of the decomposition such that $w_i \geq 0$ and $\sum_i w_i = 1$ and the sum spans over $\mathcal{H}$.

The density matrix ρ is a positive definite operator and when diagonalized its eigenvalues p_i are equal to or greater than zero. Density matrix has only a countable number of eigenvalues $p_i > 0$ and the only possible accumulation point is 0. After the diagonalization ρ is written as

$$\rho = \sum_i p_i |\phi_i\rangle \langle \phi_i|. \tag{1.7}$$

It is straightforward to include time dependence in the density matrix, assuming that at initial time t_0 the state of the system described by $H(t)$ is characterized via the density matrix

$$\rho(t_0) = \sum_i w_i |\Psi_i(t_0)\rangle \langle \Psi_i(t_0)|. \tag{1.8}$$

After the evolution from t_0 to t, the state of the system is given by

$$\rho(t) = \sum_i w_i U(t, t_0) |\Psi_i(t_0)\rangle \langle \Psi_i(t_0)| U^\dagger(t, t_0), \tag{1.9}$$

or in a more concise way

$$\rho(t) = U(t, t_0)\rho(t_0)U^\dagger(t, t_0). \tag{1.10}$$

The equation of motion of the density matrix, known as the von Neumann equation, is then obtained through a differentiation with respect to time

$$\frac{\partial}{\partial t}\rho(t) = -\frac{i}{\hbar}[H(t), \rho(t)], \tag{1.11}$$

Up to now only closed and isolated system have been discussed. The time evolution of both is described by a unitary operator $U(t, t_0)$ and the main difference is that the Hamiltonian of an isolated system is time-independent, conversely to the time-dependent Hamiltonian of closed system.

1.1.2   Open systems

In quantum mechanics a system S with Hilbert space $\mathcal{H}_S$ is said to be open if it is coupled to another quantum system B, called the *environment*, with Hilbert space $\mathcal{H}_B$. The total system $S + B$ is assumed to be closed, so its dynamics is described by a unitary operator. Usually, S is labelled as the *subsystem* (or reduced system).

In most cases, studying the dynamics of whole system $S + B$ is extremely complicated (or practically impossible). Indeed, the environment B can have infinite degrees of freedom so an exact treatment requires the solution of an infinite hierarchy of coupled equation of motion. A strategy different from solving the Schrödinger equation for $S + B$ is necessary, and an efficient one is to focus only on the dynamics of the subsystem S that usually is the most relevant one from a physical point of view. However, the dynamics of S is in general not described by a unitary operator, as it is determined by its own internal dynamics and interaction with B.

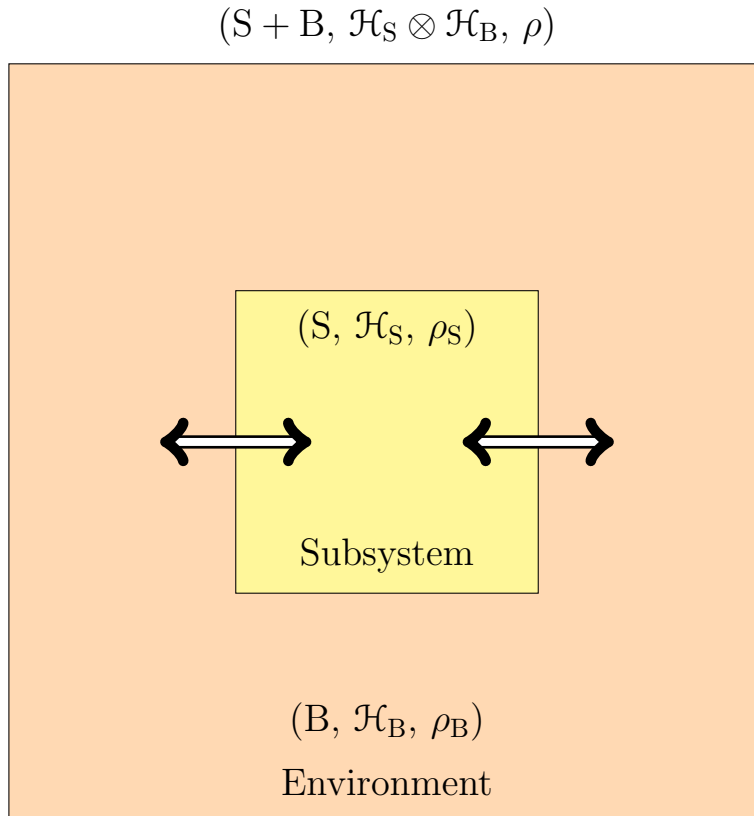$$(S + B, \; \mathcal{H}_S \otimes \mathcal{H}_B, \; \rho)$$

Figure 1.1. Schematic representation of open quantum system, with a subsystem (yellow) and an environment (orange) interacting.

To describe the dynamics of the subsystem, the first step is writing the Hilbert space of the total system $S + B$ as the tensor product space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$. The total time-dependent Hamiltonian is of the form

$$H(t) = H_S \otimes I_B + I_S \otimes H_B + \hat{H}_I(t), \tag{1.12}$$

where H_S is the self (or free) Hamiltonian of S, H_B is the self Hamiltonian of B and $\hat{H}_I(t)$ is the Hamiltonian that describes the interaction between S and B and I_S and I_B are the identity operator of respectively $\mathcal{H}_S$ and $\mathcal{H}_B$. A pictorial representation of this type of system is shown in Fig. 1.1 where the interaction is depicted by arrows. By construction, all the observable of physical interest are encoded in the subsystem, therefore all of them are of the form

$$A = O \otimes I_B, \tag{1.13}$$

where O acts on the Hilbert space $\mathcal{H}_S$.

The subsystem can be singled out with a partial trace operation. This operation allows to write the subsystem density matrix ρ_S as

$$\rho_S = \mathrm{tr}_B \rho, \tag{1.14}$$

where tr_B labels a trace over the Hilbert space $\mathcal{H}_B$. The importance of defining S such that all the physical quantities are described by operators of the form Eq. (1.13) is clear: indeed, for a generic observable C defined on $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ the expectation value is

$$\langle C \rangle = \mathrm{tr}\{C\rho\}, \tag{1.15}$$

while for an observable of the form Eq. (1.13) the expectation value is

$$\langle A \rangle = \mathrm{tr}_S\{A\rho_S\}. \tag{1.16}$$

The reduced density matrix is therefore the key quantity to determine the expectation value of quantities of physical interest. This matrix can be written exploiting Eq. (1.10) as

$$\rho_{\text{S}}(t) = \text{tr}_{\text{B}}\{U(t, t_0)\rho(t_0)U^\dagger(t, t_0)\}, \tag{1.17}$$

since the total density matrix ρ evolves unitarily and with $U(t, t_0)$ time evolution operator of the whole system $S + B$. From the Von Neumann equation for ρ the equation of motion for ρ_{S} is obtained

$$\frac{d}{dt}\rho_{\text{S}}(t) = -\frac{i}{\hbar}\text{tr}_{\text{B}}[H(t), \rho(t)]. \tag{1.18}$$

As said before, Eq. (1.18) is complicated due to the large number of degrees of freedom and approximations are therefore needed to solve it. One of the most prominent difficulties in all the approximation schemes is the description of the so-called *memory effects* that are due to the interaction. Intuitively, they can be seen as a measure of how long correlations due to interaction last.

To conclude this section, a comment on terminology is necessary. With *environment* is labelled any system in contact with a subsystem of interest, while the term *reservoir* is used when the environment has infinite degrees of freedom. Finally, a *bath* is defined as a reservoir at thermal equilibrium.

In the rest of this work open quantum systems will be denoted with OQS, and they will always be of a type like the one depicted in Fig 1.1.

1.2   Quantum master equations

As discussed before, the dynamics of all relevant physical quantities of an OQS can be reconstructed with the time-evolved subsystem density matrix $\rho_{\text{S}}(t)$. The equation whose solution is $\rho_{\text{S}}(t)$ is usually referred as a Quantum Master Equation (QME). In this section two particular QMEs are presented, the Lindblad equation and the master equation for the quantum Brownian motion. For both of them the approximation schemes are presented and a microscopical derivation is sketched in its relevant details.

1.2.1   Lindblad equation

The principal example of QME is obtained in the frame of Quantum Markov process. A stochastic process (classical or quantum) is defined Markovian if memory effects are negligible in the description of the dynamics of the quantity under examination, e.g. ρ_{S} in an OQS. A memory effect is the necessity to describe how the dynamics of the subsystem modify the environment.

Consider Eq. (1.18): to describe the time evolution of the reduced density matrix the knowledge of the total density matrix $\rho(t)$ is in principle required. This is complicated because it is necessary to address memory effect, or at least approximate them reasonably. However, if correlation times of the environment are small it is possible to introduce dynamical maps to describe $\rho_{\text{S}}(t)$. Small environment correlation times means that memory effects in the environment disappear on a timescale faster than the typical time for the evolution of the subsystem.

Suppose that the system is in an uncorrelated initial state at $t = 0$, $\rho(0) = \rho_{\text{S}}(0) \otimes \rho_{\text{B}}$ and ρ_{B} is a generic reference state of the environment. The transformation of the subsystem from $\rho_{\text{S}}(0)$ to $\rho_{\text{S}}(t)$ can be described as

$$\rho_{\text{S}}(0) \mapsto \rho_{\text{S}}(t) = V(t)\rho_{\text{S}}(0) \equiv \text{tr}_{\text{B}}\{U(t, 0)[\rho_{\text{S}}(0) \otimes \rho_{\text{B}}]U^\dagger(t, 0)\}. \tag{1.19}$$

In the approximation of neglecting memory effects, the reference state can be regarded as fixed at time t. Therefore, Eq. (1.19) describes a map, called *dynamical map*

$$V(t) : \mathcal{S}(\mathcal{H}_{\text{S}}) \to \mathcal{S}(\mathcal{H}_{\text{S}}), \tag{1.20}$$

where $\mathcal{S}(\mathcal{H}_S)$ is the space of reduced density matrices. The dynamical map can be completely characterized in terms of operators related to $\mathcal{H}_S$. Environment density matrix ρ_B can be decomposed as

$$\rho_B = \sum_i \eta_i |\phi_i\rangle \langle \phi_i|, \tag{1.21}$$

where the sum runs over $\mathcal{H}_B$, $|\phi_i\rangle$ are elements of an orthonormal bases and η_i such that $\eta_i \geq 0$ $\forall i$ and $\sum_i \eta_i = 1$. It is therefore possible to write

$$V(t)\rho_S = \sum_{i,j} W_{ij}(t)\rho_S W_{ij}^\dagger(t), \tag{1.22}$$

where

$$W_{ij}(t) = \sqrt{\eta_j} \langle \phi_i| U(t,0) |\phi_j\rangle \in \mathcal{H}_S. \tag{1.23}$$

Operators W_{ij} satisfy the condition

$$\sum_{ij} W_{ij}^\dagger(t)W_{ij}(t) = I_S, \tag{1.24}$$

from which is possible to conclude that

$$\text{tr}_S\{V(t)\rho_S\} = 1. \tag{1.25}$$

Therefore, a dynamical map is a trace preserving, completely positive and convex-linear operation.

The Markovian hypothesis of neglecting memory effects has consequences on the properties of the dynamical map $V(t)$. Indeed, if the parameter family of dynamical maps $\{V(t)|t \geq 0\}$ is considered, where $V(0)$ has the role of identity, for a Markovian it holds that

$$V(t_1)V(t_2) = V(t_1 + t_2) \quad t_1, t_2 \geq 0. \tag{1.26}$$

The one-parameter family of dynamical maps forms a semigroup, i.e. a group without inverse transformation, for which a generator $\mathcal{L}$ exists. The generator allows to represent the semigroup in exponential form

$$V(t) = e^{\mathcal{L}t}. \tag{1.27}$$

Inserting Eq. (1.27) inside Eq. (1.19) after a derivation the following equation for the dynamics of the reduced density matrix is obtained

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t), \tag{1.28}$$

that is called the *Markovian master equation*. For a dynamical semigroup that describes a Markovian master equation the most general form for the generator $\mathcal{L}$ can be determined to be [1]

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S = -i[H, \rho_S] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right), \tag{1.29}$$

where $N = \dim \mathcal{H}_S$, H is the total Hamiltonian, operators A_k are called Lindblad operators and γ_k are called relaxation rates, because their dimension is of an inverse time and they are related to decay modes of the open system. Eq. (1.29) is known as the *Gorini–Kossakowski—Sudarshan-–Lindblad equation*, or simply Lindblad equation.

In literature an alternative form of the Lindblad equation is also present. It is obtained through the definition of the dissipator $\mathcal{D}(\rho_S)$ as

$$\mathcal{D}(\rho_S) \equiv \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right), \tag{1.30}$$

and so the Lindblad equation now takes the form

$$\frac{d}{dt}\rho_S(t) = -i[H, \rho_S(t)] + \mathcal{D}(\rho_S(t)). \tag{1.31}$$

Now, a microscopic derivation with instructive intent of Eq. (1.29) is presented. This is useful because all the necessary approximations to obtain it are discussed. The total Hamiltonian of the OQS under examination is

$$H = H_S + H_B + H_I, \tag{1.32}$$

where H_B and H_S are the free Hamiltonians of environment and subsystem respectively. It is more convenient to work in the interaction picture where the Von Neumann equation for the total density matrix holds

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H_I(t), \rho(t)], \tag{1.33}$$

and from now on in this derivation $\hbar = 1$ for convenience. The integral form of the von Neumann equation is

$$\rho(t) = \rho(0) - i \int_0^t ds \ [H_I(t), \rho(t)], \tag{1.34}$$

and combining Eq. (1.33) and Eq. (1.34) after a partial trace over the environment one has

$$\frac{d}{dt}\rho_S(t) = -i\mathrm{tr}_B[H_I(t), \rho(0)] - \int_0^t ds \ \mathrm{tr}_B[H_I(t), [H_I(s), \rho(s)]]. \tag{1.35}$$

Up to now the equation is exact, indeed on the right-hand side of the last equation $\rho(t)$ is still present. The first approximation is now introduced: consider a situation of weak coupling between environment and subsystem. It is therefore possible to consider the environment as weakly affected by the interaction and write the total density matrix at any instant t as

$$\rho(t) \approx \rho_S(t) \otimes \rho_B. \tag{1.36}$$

Eq (1.36) is usually referred as the *Born approximation* and once inserted in Eq. (1.34) gives the equation

$$\frac{d}{dt}\rho_S(t) = - \int_0^t ds \ \mathrm{tr}_B[H_I(t), [H_I(s), \rho_S(s) \otimes \rho_B]], \tag{1.37}$$

under the simplifying and not restrictive assumption $\mathrm{tr}_B[H_I(t), \rho(0)] = 0$. The equation for $\rho_S(t)$ is now closed. It is possible to further simplify this integro-differential equation in the *Markov approximation*, i.e. performing the substitution $\rho_S(s) \to \rho_S(t)$. This means that at any instant the time evolution of the subsystem is only determined by the state of the subsystem at the present time. In this way memory effects, that are considered when inside the integral on the right-hand side $\rho_S(s)$ is present, are neglected. In this way the Redfield equation is obtained

$$\frac{d}{dt}\rho_S(t) = - \int_0^t ds \ \mathrm{tr}_B[H_I(t), [H_I(s), \rho_S(t) \otimes \rho_B]]. \tag{1.38}$$

Redfield equation is local in time, but the dynamics of the reduced system is not yet described by a dynamical semigroup, because $\rho_S(t)$ depends on the choice of the initial state. This problem

can be tackled with the change of variable $s \to t - s$ and setting the upper integration limit to infinity. This is the second part of the Markov approximation and gives a Markovian QME

$$\frac{d}{dt}\rho_{\mathrm{S}}(t) = \int_0^\infty ds \ \mathrm{tr}_{\mathrm{B}}[H_{\mathrm{I}}(t), [H_{\mathrm{I}}(t-s), \rho_{\mathrm{S}}(t) \otimes \rho_{\mathrm{B}}]]. \tag{1.39}$$

The change of variable that leads to Eq. (1.39) is justified as long as the integrand vanishes fast enough for $s \gg \tau_{\mathrm{B}}$, where τ_{B} is the typical environment correlation time. Therefore, Markov approximation is valid if the timescale τ_{R} for the change of ρ_{S} is large when compared to τ_{B}. The Markovian approximation therefore implies that the equation for $\rho_{\mathrm{S}}(t)$ describes a dynamics coarse-grained in time, where environmental correlation of timescale τ_{B} are not resolved.

Up to now, the overall performed approximation is known as *Born- Markov approximation.* Even if Eq. (1.39) describes Markovian master equation it is not guaranteed that it also describes a generator of a dynamical semigroup, i.e. it is not possible to state that $d\rho_{\mathrm{S}}(t)/dt = \mathcal{L}\rho_{\mathrm{S}}(t)$. A further approximation is indeed necessary, known as the *secular*, or rotating wave, approximation. To describe the secular approximation is useful to write H_{I} in the Schrödinger picture in the most general form

$$H_{\mathrm{I}} = \sum_\alpha A_\alpha \otimes B_\alpha, \tag{1.40}$$

with A_α and B_α Hermitian operators. Now suppose that H_{S} has a discrete spectrum of eigenvalues ε, associated to projectors $\Pi(\varepsilon)$. It is therefore possible to define the operators

$$A_\alpha(\omega) = \sum_{\varepsilon' - \varepsilon = \omega} \Pi(\varepsilon) A_\alpha \Pi(\varepsilon'), \tag{1.41}$$

where the sum runs over all ε, ε' that satisfy the condition $\varepsilon' - \varepsilon = \omega$. Operators $A_\alpha(\omega)$ have the following properties

$$\sum_\omega A_\alpha(\omega) = \sum_\omega A_\alpha^\dagger(\omega) = A_\alpha \tag{1.42}$$

$$[H_{\mathrm{S}}, A_\alpha^\dagger(\omega)] = +\omega A_\alpha^\dagger(\omega) \tag{1.43}$$

$$[H_{\mathrm{S}}, A_\alpha(\omega)] = -\omega A_\alpha(\omega) \tag{1.44}$$

$$[H_{\mathrm{S}}, A_\alpha^\dagger(\omega)A_\beta(\omega)] = 0 \tag{1.45}$$

$$A_\alpha^\dagger(\omega) = A_\alpha(-\omega). \tag{1.46}$$

By definition, $A_\alpha(\omega)$ and $A_\alpha^\dagger(\omega)$ are eigenoperators of H_{S} belonging to frequencies $\pm\omega$. The interaction picture representation of them is

$$e^{iH_{\mathrm{S}}t} A_\alpha(\omega) e^{-iH_{\mathrm{S}}t} = e^{-i\omega t} A_\alpha(\omega) \tag{1.47}$$

$$e^{iH_{\mathrm{S}}t} A_\alpha^\dagger(\omega) e^{-iH_{\mathrm{S}}t} = e^{+i\omega t} A_\alpha^\dagger(\omega). \tag{1.48}$$

Now turn back to Eq. (1.39), that is in interaction picture. The projection defined above leads to the following form of $H_{\mathrm{I}}(t)$ in interaction picture

$$H_{\mathrm{I}}(t) = \sum_{\alpha,\omega} e^{-i\omega t} A_\alpha(\omega) \otimes B_\alpha(t), \tag{1.49}$$

with

$$B_\alpha(t) = e^{iH_{\mathrm{B}}t} B_\alpha e^{-iH_{\mathrm{B}}t}. \tag{1.50}$$

Now the condition $\mathrm{tr}_{\mathrm{B}}[H_{\mathrm{I}}(t), \rho(0)] = 0$ is equivalent to assume that the environment average of $B_\alpha(t)$ vanish, i.e.

$$\langle B_\alpha(t) \rangle \equiv \mathrm{tr}_{\mathrm{B}}\{B_\alpha(t)\rho_{\mathrm{B}}\} = 0. \tag{1.51}$$

It is now possible to rewrite, after a bit of algebra, the Markovian QME Eq. (1.39) as

$$\frac{d}{dt}\rho_{\rm S}(t) = \sum_{\omega,\omega'}\sum_{\alpha,\beta} e^{i(\omega'-\omega)t}\Gamma_{\alpha\beta}(\omega)(A_\beta(\omega)\rho_{\rm S}(t)A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega')A_\beta(\omega)\rho_{\rm S}(t)) + {\rm h.c.},\qquad(1.52)$$

where h.c. is the Hermitian conjugate. The quantity $\Gamma_{\alpha\beta}(\omega)$ is defined as

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds\; e^{i\omega s}{\rm tr_B}\{B_\alpha^\dagger(t)B_\beta(t-s)\}.\qquad(1.53)$$

It is possible to define the environment correlation function

$$\langle B_\alpha^\dagger(t)B_\beta(t-s)\rangle = {\rm tr_B}\{B_\alpha^\dagger(t)B_\beta(t-s)\},\qquad(1.54)$$

from which is evident the $\Gamma_{\alpha\beta}$ is the one-sided Fourier transform of this correlation function, i.e. the transformation with only positive ω components. In principle $\Gamma_{\alpha\beta}$ should also depend on time t, but this dependence can be neglected if $\rho_{\rm B}$ is a stationary state of the environment, i.e. $[H_{\rm B}, \rho_{\rm B}] = 0$.

Eq. (1.52) is close to the Lindblad equation, Eq. (1.29). To reach this form it is first necessary to perform another approximation. The subsystem has an intrinsic evolution on a timescale of order $\tau_{\rm S}$. This timescale is defined by $|\omega - \omega'|^{-1}$ for $\omega \neq \omega'$. If $\tau_{\rm S}$ is small compared to $\tau_{\rm R}$, the typical evolution time described by the Markovian QME, all the terms with $\omega \neq \omega'$ in the sum inside Eq. (1.52) oscillate rapidly due to the presence of $\exp(i(\omega'-\omega)t)$. Neglecting these oscillating terms is the core of the secular approximation. Note that here the relevant scale to define the rapidity of the oscillations is $\tau_{\rm R}$.

After the secular approximation the QME has the form

$$\frac{d}{dt}\rho_{\rm S}(t) = \sum_\omega\sum_{\alpha,\beta}\Gamma_{\alpha\beta}(\omega)(A_\beta(\omega)\rho_{\rm S}(t)A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega')A_\beta(\omega)\rho_{\rm S}(t)) + {\rm h.c.}.\qquad(1.55)$$

It is now useful to decompose $\Gamma_{\alpha\beta}$ as

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + iS_{\alpha\beta}(\omega).\qquad(1.56)$$

The imaginary part of Γ is a Hermitian matrix by definition and the real part is

$$\gamma_{\alpha\beta}(\omega) = \int_{-\infty}^\infty ds\; e^{i\omega s}\langle B_\alpha(s)B_\beta^\dagger(0)\rangle.\qquad(1.57)$$

It is possible to demonstrate that the matrix $\gamma_{\alpha\beta}(\omega)$ is positive. This can be proved using Bochner's theorem, which states that the Fourier transform of a function $g(s)$ is positive if $g(s)$ is of positive type, that here is valid because all the correlation functions $\langle B_\alpha(s)B_\beta^\dagger(0)\rangle$ are positive [6]. This fact will have importance in the last steps of the derivation of the Lindblad equation.

The above definitions of $S_{\alpha\beta}$ and $\gamma_{\alpha\beta}$ lead to

$$\frac{d}{dt}\rho_{\rm S}(t) = -i\left[\sum_\omega\sum_{\alpha,\beta}S_{\alpha\beta}(\omega)A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_{\rm S}(t)\right] +$$

$$+\sum_\omega\sum_{\alpha,\beta}\gamma_{\alpha\beta}(\omega)\left(A_\beta(\omega)\rho_{\rm S}(t)A_\alpha^\dagger(\omega) - \frac{1}{2}\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_{\rm S}(t)\}\right).\qquad(1.58)$$

In this equation, the first term on the right-hand side is known as the Lamb shift Hamiltonian H_{LS}

$$H_{\text{LS}} = \sum_\omega \sum_{\alpha,\beta} S_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega), \tag{1.59}$$

that commutes with the self-Hamiltonian of the subsystem, i.e. $[H_{\text{LS}}, H_{\text{S}}] = 0$. The second term of Eq. (1.58) has the form of a dissipator

$$\mathcal{D}(\rho_{\text{S}}(t)) = \sum_\omega \sum_{\alpha,\beta} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega)\rho_{\text{S}}(t)A_\alpha^\dagger(\omega) - \frac{1}{2}\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_{\text{S}}(t)\} \right), \tag{1.60}$$

therefore the QME can be written in the form

$$\frac{d}{dt}\rho_{\text{S}}(t) = -i[H_{\text{LS}}, \rho_{\text{S}}(t)] + \mathcal{D}(\rho_{\text{S}}(t)). \tag{1.61}$$

This form is extremely close to Eq. (1.31), although there are some differences in the dissipator. Moreover, this last equation is in interaction picture while the Lindblad equation is in Schrödinger picture.

The two generators become the same if one diagonalizes the matrices $\gamma_{\alpha\beta}(\omega)$. This diagonalization is possible because these matrices are positive. The Schrödinger picture is obtained adding H_{S} to H_{LS} thanks to eigenoperators properties. With these two operations the standard form of a Lindblad equation Eq. (1.29) is restored.

To conclude, some comments on the approximation scheme are appropriate. The adopted scheme is composed as follows:

1. Weak coupling expansion to second order in interaction of the total Hamiltonian,

2. Born approximation that assumes $\rho(t) = \rho_{\text{S}}(t) \otimes \rho_{\text{B}}$,

3. Markov approximation (locality in time and time integration to infinity), valid if $\tau_{\text{R}} \gg \tau_{\text{B}}$. The last two points combined are the Born-Markov approximation.

4. Secular approximation (neglect rapidly oscillating modes), valid if $\tau_{\text{R}} \gg \tau_{\text{S}}$.

Up to now, only Markovian situation were discussed. Non Markovian situations, where memory effects are important, are more involved and deriving a master equation is not trivial. It was however demonstrated by Hall *et al.* [7] that also for non Markovian systems under fairly general conditions a master equation of a form close to the Lindblad one can be found and used for the characterization of non Markovianity.

The Lindblad equation that was derived using Born-Markov and secular approximation is

$$\frac{d}{dt}\rho_{\text{S}}(t) = -\frac{i}{\hbar}[H, \rho_{\text{S}}(t)] + \sum_k \gamma_k \left(A_k\rho_{\text{S}}(t)A_k^\dagger - \frac{1}{2}\{A_k^\dagger A_k, \rho_{\text{S}}(t)\} \right), \tag{1.62}$$

where γ_k are positive constant relaxation rates. The form of Eq. (1.62) is non-unique because γ_k and A_k can be chosen in infinitely different ways due to different Kraus decomposition of completely positive maps that forms the dynamical semigroup used to derive the Lindblad equation.

Note that because of Born-Markov approximation the Lindblad equation is local in time. This locality defines a Markovian process, that has no memory effects. An alternative form for a master equation is [8, 9]

$$\frac{d}{dt}\rho_{\text{S}}(t) = -\frac{i}{\hbar}[H_{\text{S}}, \rho_{\text{S}}(t)] + \int_0^t ds \mathcal{K}_{s,t}\rho_{\text{S}}(t), \tag{1.63}$$

where $\mathcal{K}_{s,t}$ is a linear map where the effect of the environment on the system are encoded and that is known as memory kernel. The Born-Markov approximation is equivalent to $\mathcal{K}_{s,t} \approx \mathcal{K}_t \delta(s-t)$. It has been demonstrated [10, 11] that even when memory effects are present it is possible to describe the time evolution of ρ_S via a linear map

$$\frac{d}{dt}\rho_S(t) = \Lambda_t \rho_S(t), \tag{1.64}$$

and Λ_t is a linear map such that $\Lambda_t \rho$ is Hermitian and traceless for any ρ. An important condition to derive Eq. (1.64) is that the evolution of ρ_S is invertible, i.e. an equilibrium state is reached in a finite time. In the work of Hall *et al.* [7] discussed here it is demonstrated that any Master equation of the form given by Eq. (1.64) can be cast in a Lindblad-like form that is similar to Eq. (1.62)

$$\frac{d}{dt}\rho_S(t) = -\frac{i}{\hbar}[H(t), \rho_S(t)] + \sum_k \gamma_k(t)\left(A_k(t)\rho_S(t)A_k^\dagger(t) - \frac{1}{2}\{A_k^\dagger(t)A_k(t), \rho_S(t)\}\right), \tag{1.65}$$

where $H(t)$ is Hermitian and the operators $A_k(t)$ form an orthonormal basis of traceless operators,

$$\mathrm{tr}[A_j^\dagger(t)A_k(t)] = \delta_{jk} \quad \mathrm{tr}A_k(t) = 0. \tag{1.66}$$

Some points of Eq. (1.65) are relevant and must be pointed out:

1. Relaxation rates $\gamma_k(t)$ and operators $A_k(t)$ are now time-dependent,

2. Relaxation rates are uniquely determined,

3. Relaxation rates can be negative.

So it is possible to write, under some fairly general conditions, a Lindblad-like equation also for non Markovian systems.

1.2.2 Quantum Brownian motion

In this section Quantum Brownian motion (QBM) and the corresponding quantum master equation are treated. The main difference with the Markovian process that was governed by the Lindblad equation is that the approximation scheme involved in the derivation of the QME is different. The differences and their consequences will be discussed in this section.

Consider the Caldeira-Leggett model [12], that describes a particle of mass m with coordinate x and momentum p inside a potential $V(x)$. The free particle Hamiltonian is

$$H_S = \frac{p^2}{2m} + V(x). \tag{1.67}$$

In this model, the environment is a bath modeled as a large number of harmonic oscillators of frequencies ω_n and masses m_n

$$H_B = \sum_n \left(\frac{1}{2m_n}p_n^2 + \frac{1}{2}m_n\omega_n^2 x_n^2\right), \tag{1.68}$$

and the sum runs over the number of oscillators and x_n and p_n are the corresponding conjugate coordinates of the oscillators.

The coupling between bath and particle in the Caldeira-Leggett model is assumed to be linear between the coordinates of particle and oscillators. The corresponding interaction Hamiltonian is

$$H_I = -x\sum_n \kappa_n x_n \equiv -xB, \tag{1.69}$$

where κ_n are coupling constants. It is useful to introduce a counter term Hamiltonian H_C

$$H_C = x^2 \sum_n \frac{\kappa_n^2}{2m_n\omega_n^2}. \tag{1.70}$$

The introduction of the counter term is not mandatory but is convenient because the interaction term Eq. (1.69) leads to a renormalization of $V(x)$. Through the insertion of H_C this renormalization is compensated and therefore $V(x)$ will involve physical frequencies of the motion of the particle.

The total Hamiltonian with the counter term is

$$H = H_S + H_B + H_I + H_C, \tag{1.71}$$

and it is important to remember that H_C is of quadratic order in coupling constant κ_n. This fact has relevant consequences in the adopted approximation scheme.

Now, suppose that the coupling is weak, so that the Born-Markov approximation is feasible. In this situation and in the Schrödinger picture the equation for ρ_S is

$$\frac{d}{dt}\rho_S(t) = \frac{i}{\hbar}[H_S + H_C, \rho_S(t)] + \mathcal{K}\rho_S(t), \tag{1.72}$$

where

$$\mathcal{K}\rho_S(t) = -\frac{1}{\hbar^2}\int_0^\infty ds\, \mathrm{tr_B}[H_I, [H_I(-s), \rho_S(t) \otimes \rho_B]]. \tag{1.73}$$

Note that this expression can be derived from Eq. (1.39) after a transformation from interaction to Schrödinger picture. It is also important to notice that in the weak coupling limit the counter term is not involved in $\mathcal{K}\rho_S(t)$, otherwise the expansion in orders of κ_n would not be consistent. The time dependence in the operator $H_I(-s)$ denotes an interaction picture operator with respect to the Hamiltonian $H_0 = H_S + H_B$. The reference state is considered to be a thermal state at inverse temperature $\beta = 1/k_B T$, i.e.

$$\rho_B = \frac{e^{-\beta H_B}}{\mathrm{tr_B} e^{-\beta H_B}}. \tag{1.74}$$

Note that Eq. (1.73) can be rewritten as

$$\mathcal{K}\rho_S(t) = \frac{1}{\hbar^2}\int_0^\infty ds\, \left(\frac{i}{2}D(s)[x, \{x(-s), \rho_S(t)\}] - \frac{1}{2}D_1(s)[x, [x(-s), \rho_S(t)]]\right), \tag{1.75}$$

where the dissipation $D(s)$ and noise kernel $D_1(s)$ have been inserted. These to functions are defined as

$$D(s) \equiv i\mathrm{tr_B}[B, B(-s)], \tag{1.76}$$
$$D_1(s) \equiv \mathrm{tr_B}\{B, B(-s)\}. \tag{1.77}$$

Dissipation and noise kernel are therefore bath correlation functions. They can be expressed in terms of the bath spectral density $J(\omega)$ as

$$D(s) = 2\hbar \int_0^\infty d\omega\, J(\omega)\sin(\omega s), \tag{1.78}$$

$$D_1(s) = 2\hbar \int_0^\infty d\omega\, J(\omega)\coth\left(\frac{\beta\hbar\omega}{2}\right)\cos(\omega s). \tag{1.79}$$

The properties of $\mathcal{K}$ as written in Eq. (1.75) strongly depend on $J(\omega)$ that determines D and D_1. The spectral function is clearly model dependent and should be carefully defined in order to

obtain reasonable physics. In the Caldeira-Leggett model [12] one wants to obtain an irreversible dynamics, therefore $J(\omega)$ is phenomenologically modelled as a smooth function of ω

$$J(\omega) = \frac{2m\gamma}{\pi}\omega\frac{\Omega^2}{\Omega^2 + \omega^2}, \tag{1.80}$$

where the high frequency cutoff Ω accounts for the renormalization of physical parameters at high frequencies. A spectral density linear for small ω like the one defined in Eq. (1.80) is said to be *Ohmic*. The parameter γ labels a frequency independent damping.

With the last expression of $J(\omega)$ it is possible to derive explicit expression for D and $D1$. These expressions are

$$D(s) = 2m\gamma\hbar\Omega^2 e^{-\Gamma|s|}\mathrm{sign}s, \tag{1.81}$$

$$D_1(s) = \frac{4m\gamma}{\beta}\Omega^2 \sum_{n=-\infty}^{\infty} \frac{\Omega e^{-\Omega|s|} - |\nu_n|e^{-|\nu_n||s|}}{\Omega^2 - \nu_n^2}, \tag{1.82}$$

where the Matsubara frequencies $\nu_n = 2\pi n/\beta\hbar$ are used. It is now possible to discuss correlation times τ_B of the bath: from correlation functions

$$\tau_\mathrm{B} = \max\left\{\frac{1}{\Omega}, \frac{\beta\hbar}{2\pi}\right\}, \tag{1.83}$$

and the condition for the applicability of the Born-Markov approximation $\tau_\mathrm{B} \ll \tau_\mathrm{R}$ is equivalent to

$$\frac{\hbar}{\tau_\mathrm{R}} = \hbar\gamma \ll \frac{\hbar}{\tau_\mathrm{B}} = \min\left\{\hbar\Omega, \frac{2\pi}{\beta}\right\}. \tag{1.84}$$

The approximation scheme is now different from the one used to derive the Lindblad equation: indeed in the Lindblad case the condition for the secular approximation is that $\tau_\mathrm{S} \ll \tau_\mathrm{R}$, while now the evolution of the subsystem with timescale τ_S is slow compared to the bath correlation time τ_B. Therefore, the condition is $\tau_\mathrm{B} \ll \tau_\mathrm{S}$ and it is equivalent to

$$\frac{\hbar}{\tau_\mathrm{S}} = \hbar\omega_0 \ll \min\left\{\hbar\Omega, \frac{2\pi}{\beta}\right\}. \tag{1.85}$$

This last condition denies the possibility of performing a secular approximation, but on the other hand it is possible to approximate $x(-s)$ inside Eq. (1.75) in the following way

$$x(-s) = e^{-iH_\mathrm{S}s/\hbar}xe^{iH_\mathrm{S}s/\hbar} \approx x - \frac{p}{m}s \tag{1.86}$$

With these approximations all the commutators and anticommutators inside $\mathcal{K}\rho_\mathrm{S}(t)$ are not dependent on time s and can be factorized out of the integral. Moreover, all the remaining four integrals that involve $D(s)$, $D_1(s)$ and their product with s can be carried out analytically[2]. One of these integrals will exactly cancel the counter term Hamiltonian H_C, another one can be neglected because it involves a term ω_0/Ω that is small in the limits considered here. This leads to the *Caldeira-Leggett master equation*

$$\frac{d}{dt}\rho_\mathrm{S}(t) = -\frac{i}{\hbar}[H_\mathrm{S}(t), \rho_\mathrm{S}(t)] - \frac{i\gamma}{\hbar}[x, \{p, \rho_\mathrm{S}(t)\}] - \frac{2m\gamma}{\beta\hbar^2}[x, [x, \rho_\mathrm{S}(t)]]. \tag{1.87}$$

In this equation, the first term describes the free evolution of the particle. The second term is a dissipative term that comes from the dissipation kernel $D(s)$. Finally, the third term is responsible for thermal fluctuations, and is indeed proportional to the temperature, and it is

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[2]The full calculation is not particularly instructive and therefore is not reported here, but it can be found in Sec. 3.6.2 of Ref. [1].

related to the noise kernel $D_1(s)$. It is important to remember that Caldeira-Leggett master equation can be derived in the weak coupling (second order expansion in the coupling constant) and high temperature limit (small β). Eq. (1.87) can also be cast into Lindblad form with the addition of a term that is small in the high temperature limit.

With Caldeira-Leggett master equation it is possible to derive Ehrenfest equations for the first and second moments of coordinate and momentum of the Brownian particle. These equations are

$$\frac{d}{dt}\langle x \rangle = \frac{1}{m}\langle p \rangle, \tag{1.88}$$

$$\frac{d}{dt}\langle p \rangle = -\langle V'(x) \rangle - 2\gamma\langle p \rangle, \tag{1.89}$$

$$\frac{d}{dt}\langle x^2 \rangle = \frac{1}{m}\langle px + xp \rangle, \tag{1.90}$$

$$\frac{d}{dt}\langle px + xp \rangle = \frac{2}{m}\langle p^2 \rangle - 2\langle xV'(x) \rangle - 2\gamma\langle px + xp \rangle, \tag{1.91}$$

$$\frac{d}{dt}\langle p^2 \rangle = -\langle pV'(x) + V'(x)p \rangle - 4\gamma\langle p^2 \rangle + \frac{4m\gamma}{\beta}. \tag{1.92}$$

For a free Brownian particle, $V = 0$, the solutions for the first moments are

$$\langle x(t) \rangle = \langle x(0) \rangle + \frac{1}{2m\gamma}(1 - e^{-2\gamma t})\langle p(0) \rangle, \tag{1.93}$$

$$\langle p(t) \rangle = e^{-2\gamma t}\langle p(0) \rangle, \tag{1.94}$$

which means that the initial position is asymptotically displaced by the value $\langle \dot{x}(0) \rangle/2\gamma$ while initial momentum decays over a timescale $1/2\gamma$. The second momenta are defined as

$$\sigma_x^2(t) = \langle x^2(t) \rangle - \langle x(t) \rangle^2, \tag{1.95}$$

$$\sigma_p^2(t) = \langle p^2(t) \rangle - \langle p(t) \rangle^2, \tag{1.96}$$

$$\sigma_{px}^2(t) = \langle \{p(t), x(t)\} \rangle - 2\langle x(t) \rangle\langle p(t) \rangle, \tag{1.97}$$

and can be determined analytically. In the long time limit $\gamma t \gg 1$ where initial conditions are no longer relevant one has the asymptotic results

$$\sigma_x^2 \to \frac{1}{m\gamma\beta}t, \tag{1.98}$$

$$\sigma_p^2 \to \frac{m}{\beta}, \tag{1.99}$$

$$\sigma_{px}^2 \to \frac{1}{\gamma\beta}. \tag{1.100}$$

Note that the position uncertainty increases with square root of time as in classical Brownian motion and momentum uncertainty approaches a value close to the one given by the thermal equilibrium.

Caldeira-Leggett master equation is not the only possible way to describe quantum Brownian motion: indeed thanks to the linear coupling between the bath and the particle is possible to derive the exact Heisenberg equations of motion for the bath and the particle and solve. Considering the complete model with also the counter term Hamiltonian, the exact Heisenberg

equations of motion are

$$\dot{x}(t) = \frac{1}{m}p(t), \tag{1.101}$$

$$\dot{p}(t) = -V_C'(x(t)) + \sum_n \kappa_n x_n(t), \tag{1.102}$$

$$\dot{x}_n(t) = \frac{1}{m}p_n(t), \tag{1.103}$$

$$\dot{p}_n(t) = -m_n\omega_n^2 x_n(t) + \kappa_n x(t), \tag{1.104}$$

where $V_C = V + H_C$. To better understand the process involved it is useful to write the equations for the coordinate of the Brownian particle x and of the bath oscillator $x_n(t)$

$$m\ddot{x}(t) + V_C'(x(t)) - \sum_n \kappa_n x_n(t) = 0, \tag{1.105}$$

$$m\ddot{x}_n(t) + m_n\omega_n^2 x_n(t) - \kappa_n x(t) = 0, \tag{1.106}$$

from which it is clear that the bath oscillators are driven by a force that depends linearly on the position of the particle $x(t)$. Up to now the equation are coupled, but it is possible to close the equation for $x(t)$ solving the equation for $x_n(t)$ in terms of $x(t)$ itself and substituting the result inside Eq. (1.105). The best way to do this is to write the initial coordinate of the bath oscillators using the creation and annihilation operators of the bath b_n and $b_n^\dagger$

$$x_n(0) = \sqrt{\frac{\hbar}{2m_n\omega_n}}(b_n + b_n^\dagger), \tag{1.107}$$

with a representation for $p_n(0)$ that comes from canonical commutation relations. The solution of Eq. (1.106) can be written employing the interaction picture representation of b_n and $b_n^\dagger$ as

$$x_n(t) = \sqrt{\frac{\hbar}{2m_n\omega_n}}(e^{-i\omega_n t}b_n + e^{i\omega_n t}b_n^\dagger) + \frac{\kappa_n}{m_n\omega_n}\int_0^t ds \ \sin(\omega_n(t-s))x(s), \tag{1.108}$$

that gives for Eq. (1.105) the form

$$\ddot{x}(t) + \frac{1}{m}V_C'(x(t)) - \frac{1}{m}\sum_n \frac{\kappa_n^2}{m_n\omega_n}\int_0^t ds \ \sin(\omega_n(t-s))x(s) = \frac{1}{m}\sum_n \kappa_n\sqrt{\frac{\hbar}{2m_n\omega_n}}(e^{-i\omega_n t}b_n + e^{i\omega_n t}b_n^\dagger) \tag{1.109}$$

On the right-hand side of Eq. (1.109) it is possible to recognize the bath operator B in interaction picture, i.e.

$$B(t) = \sum_n \kappa_n\sqrt{\frac{\hbar}{2m_n\omega_n}}(e^{-i\omega_n t}b_n + e^{i\omega_n t}b_n^\dagger). \tag{1.110}$$

From definition of the dissipation kernel given in Eq. (1.78) it is possible to write Eq. (1.109) as

$$\ddot{x}(t) + \frac{1}{m}V_C'(x(t)) - \frac{1}{\hbar m}\int_0^t ds \ D(t-s)x(s) = \frac{1}{m}B(t). \tag{1.111}$$

Now it is possible to define the damping kernel $\gamma(t-s)$ in relation to the spectral density $J(\omega)$ as

$$\gamma(t-s) = \frac{2}{m}\int_0^\infty d\omega \ \frac{J(w)}{\omega}\cos(\omega(t-s)), \tag{1.112}$$

and this definition leads to the following relations

$$\frac{d}{dt}\gamma(t-s) = -\frac{1}{\hbar m}D(t-s), \tag{1.113}$$

$$\gamma(0) = \frac{1}{m}\sum_n \frac{\kappa_n^2}{m_n\omega_n^2}. \tag{1.114}$$

The equation of motion for $x(t)$ in terms of the damping kernel can be written as

$$\ddot{x}(t) + \frac{1}{m}V'(x(t)) + \frac{d}{dt}\int_0^t ds\ \gamma(t-s)x(s) = \frac{1}{m}B(t), \tag{1.115}$$

where taking the time derivative outside the integral on the left-hand side results in the cancellation of the counter term thanks to $\gamma(0)$. Eq. (1.115) is a quantum analogue of a classical stochastic equation of motion with damping kernel $\gamma(t-s)$ and stochastic force $B(t)$. Memory effects are encoded in the kernel, as can be understood from its time dependence, while the statistical properties of the stochastic force $B(t)$ depend on the initial total distribution.

To better understand the connection with the classical Brownian motion, consider for example an Ohmic spectral density of the form Eq. (1.80) with infinite cutoff, i.e. $\Omega \to \infty$. It is straightforward to derive that

$$\gamma(t) = 4\gamma\delta(t), \tag{1.116}$$

and from this expression of the dissipation kernel derive then the Heisenberg equations for $x(t)$ and $p(t)$

$$\dot{x}(t) = \frac{1}{m}p(t), \tag{1.117}$$

$$\dot{p}(t) = -V'(x(t)) - 2m\gamma\dot{x}(t) + B(t). \tag{1.118}$$

These equations are identical to the classical equations for the Brownian motion with the presence of the usual friction term $-2m\gamma\dot{x}$.

The stochastic force $B(t)$ is still undefined. For consistency, consider a factorized initial state as done in the derivation of the Caldeira-Leggett master equation. In this scenario it was already shown that the correlation function of the bath operator is equal to the noise kernel, i.e. $D_1(t-t) = \langle\{B(t), B(t')\}\rangle$ which for an Ohmic spectral density is given by

$$D_1(t-t') = \frac{4m\gamma\hbar}{\pi}\int_0^\Omega d\omega\ \omega\coth\left(\frac{\beta\hbar\omega}{2}\right)\cos(\omega(t-t')), \tag{1.119}$$

that in the high temperature limit where for all relevant frequencies $2/\beta \gg \hbar\omega$ can be approximated as

$$D_1(t-t') \approx \frac{4m\gamma\hbar}{\pi}\frac{2}{\beta\hbar}\int_0^\infty d\omega\ \cos(\omega(t-t')) = 8\frac{m\gamma}{\beta}\delta(t-t'), \tag{1.120}$$

and the $\hbar$ terms is no longer present. Therefore, the noise present in the high temperature regime is the same of the classical scenario.

Interestingly, similar Heisenberg equations can be used to describe the dynamics of a single Bose polaron [13] using the Frölich Hamiltonian [14]. In this case, the bath is a Bose-Einstein condensate and the weak coupling regime is considered, so that the coupling between the particle and the bath is still linear in position. However, it is difficult to extend this approach to systems with bath dimensionality greater than one for numerical reasons, or to strongly interacting systems with non-linear coupling for theoretical reasons.

1.3 Introduction to out of equilibrium quantum field theory

The master equation approach previously described is not the only possible way to study open quantum systems. Indeed, a different approach based on quantum field theory (QFT) [15, 16, 17] techniques is possible starting from the formalism of out of equilibrium QFT, derived by Keldysh and others. In this thesis this out of equilibrium formalism is referred as *Keldysh formalism* for sake of brevity and for consistency with the literature. Other authors, such as

Schwinger, Kadanoff, Baym, Larkin and Ovchinnikov developed important contributions too, see e.g. Refs. [18, 19, 20, 21, 22].

The importance of a method based on QFT is huge when in the typical systems under examination many body physics is present and the number of degrees of freedom starts to grow. Indeed, in these situations a master equation approach is extremely complicated, regardless of the approximations adopted. Finally, the Keldysh formalism is general enough to be adapted to the study of open quantum systems (for example, the usual partial trace over the degrees of freedom of the environment can be treated with the typical QFT machinery).

1.3.1   Closed time contour

Consider a quantum many body system with a time-dependent Hamiltonian $H(t)$. Suppose that in a distant past, labelled as $t = -\infty$, the state of the system was the one described by the density matrix $\rho(-\infty)$. Assume also that the time dependence of the Hamiltonian is such that in this distant past no interactions were present. Interactions are then switched on adiabatically before observation and in general ρ is driven out of equilibrium (for example, this can happen if time-dependent external fields are present in the Hamiltonian).

The evolution of the total density matrix is described by the Von Neumann equation Eq. (1.11) (with $\hbar = 1$)

$$\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)]. \tag{1.121}$$

The time evolution of the total density matrix can be described with the help of the unitary operators defined in Section 1.1.1 with now $t_0 = -\infty$

$$\rho(t) = U(t, -\infty)\rho(-\infty)U(-\infty, t). \tag{1.122}$$

In Schrödinger picture the expectation value for an arbitrary observable A at time t is

$$\langle A\rangle(t) = \frac{1}{\text{tr}\rho(t)}\text{tr}\{U(-\infty, t)AU(t, -\infty)\rho(-\infty)\}, \tag{1.123}$$

where the evolution of the initial state is both forward and backward. Indeed, reading the trace at the numerator from right to left, the initial state is $\rho(-\infty)$, a time evolution toward time t is applied, the observable A is evaluated, then another evolution back to $-\infty$ is applied. The denominator is necessary for normalization.

Usually in equilibrium QFT forward-backward evolution is not needed because some mathematical tricks, together with some physical assumptions on the adiabatic switching of interactions, are applicable both at zero and finite temperature formalism [23] and only the forward evolution is considered. These tricks can not be applied to the non-equilibrium scenario and therefore also the backward evolution (and not only the forward) is necessary. Anyway, there is a better way to write Eq. (1.123) extending the evolution to $+\infty$ thanks to the trivial identities $U(t, +\infty)U(+\infty, t) = I$ and $U(-\infty, t)U(t, +\infty) = U(-\infty, +\infty)$. Putting them into Eq. (1.123) and exploiting the cyclic property of the trace

$$\langle A\rangle(t) = \frac{1}{\rho(-\infty)}\text{tr}\{U(-\infty, +\infty)U(+\infty, t)AU(t, -\infty)\rho(-\infty)\}, \tag{1.124}$$

where in the denominator there is $\rho(-\infty)$ because von Neumann equation does not change the trace of ρ. Now the forward-backward evolution goes from $-\infty$ to $+\infty$ and back and this particular time contour, depicted in Fig. (1.2), is labelled as $\mathcal{C}$. In this contour the observable is inserted in the forward evolution process, but this choice is arbitrary.
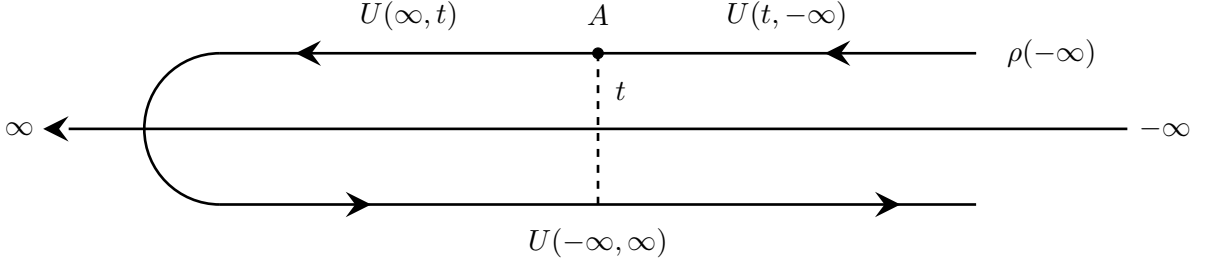
Figure 1.2. Representation of the closed time contour used for the evaluation of $\langle A \rangle(t)$.

The Keldysh formalism for QFT is formulated over the contour $\mathcal{C}$, in order to deal with non-equilibrium processes where the backward evolution can not be reabsorbed thanks to mathematical tricks.

It is useful to define the quantity

$$U_{\mathcal{C}} = U(-\infty, \infty)U(\infty, -\infty), \tag{1.125}$$

such that the partition function Z can be defined as

$$Z \equiv \frac{\mathrm{tr}\{U_{\mathcal{C}}\rho(-\infty)\}}{\mathrm{tr}\rho(-\infty)}, \tag{1.126}$$

and if the total Hamiltonian $H(t)$ is the same on the forward and backward branches of the contour then $U_{\mathcal{C}} = I$ and $Z = 1$. Observables have to be inserted in some point of $\mathcal{C}$ to be evaluated and this can be done modifying $H(t)$ with the help of an external source $V(t)$ as

$$H_V^{\pm}(t) = H(t) \pm AV(t), \tag{1.127}$$

where $\pm$ is referred to the forward (backward) branch. Now that the total Hamiltonian is different on the branches the closed-contour evolution operator $U_{\mathcal{C}}$ is no longer equal to the identity and the partition function becomes non trivial and dependent on V

$$Z[V] = \frac{1}{\mathrm{tr}\rho(-\infty)}\mathrm{tr}\{U_{\mathcal{C}}[V]\rho(-\infty)\}, \tag{1.128}$$

where now $U_{\mathcal{C}}$ clearly depends on the external source. With the help of Eq. (1.124) it is possible to demonstrate that Z plays the role of generating function for the observables, i.e.

$$\langle A \rangle(t) = \frac{i}{2}\left.\frac{\delta Z[V]}{\delta V(t)}\right|_{V=0}, \tag{1.129}$$

where δ denotes the functional derivative. The situation is different from the expression from the equilibrium scenario where the functional derivative involves the logarithm of the partition function: the absence of the logarithm is also due to the fact that $Z[V = 0] = 1$.

1.3.2 Bosonic scenario

After the introduction of the closed time contour, the next step is the derivation of the evolution operator $U_{\mathcal{C}}$ in path integral formalism, starting from systems where bosons are considered. In this way, the representation of the generating function Z is also obtained, from which it is possible to obtain all the desired observables through the proper functional derivative. This path integral derivation on the closed time contour is the core of the Keldysh formalism and it is discussed in detail to highlight the differences with the equilibrium QFT. A key concept in this derivation is the one of coherent states, i.e. eigenstates of the bosonic annihilation operator.

Since coherent states are largely discussed in QFT, they are not introduced in detail here, but further information on coherent states and many body systems can be found in any standard textbook, see e.g. Ref. [24, 25].

The first thing to do is to describe with path integral formalism the partition function Z defined in Eq. (1.126). One defines $2N$ point on $\mathcal{C}$ such that $t_1 = t_{2N} = -\infty$ and $t_N = t_{N+1} = +\infty$. Because of this choice, $2N - 2$ intervals have been defined. At each point j it is possible to insert an identity exploiting the coherent state basis

$$I = \int d[\bar{\phi}_j, \phi_j] \; e^{-|\phi_j|^2} \left| \phi_j \right\rangle \left\langle \phi_j \right|, \tag{1.130}$$

where $\left| \phi_j \right\rangle$ is the coherent state and $d[\bar{\phi}_j, \phi_j] = d(\mathrm{Re}\phi_j) d(\mathrm{Im}\phi_j)/\pi$. The numerator of Eq. (1.126) becomes

$$\mathrm{tr}(U_\mathcal{C}\rho(-\infty)) = \left\langle \phi_{2N} \right| U_{-\delta t} \left| \phi_{2N-1} \right\rangle \cdots \left\langle \phi_{N+2} \right| U_{-\delta t} \left| \phi_{N+1} \right\rangle \left\langle \phi_{N+1} \right| I \left| \phi_N \right\rangle \left\langle \phi_N \right| U_{\delta t} \left| \phi_{N-1} \right\rangle \cdots$$
$$\cdots \left\langle \phi_2 \right| U_{\delta t} \left| \phi_1 \right\rangle \left\langle \phi_1 \right| \rho(-\infty) \left| \phi_{2N} \right\rangle, \tag{1.131}$$

where $U_{\pm \delta t} \equiv U(t \pm \delta t, t)$ Note that no time evolution is present between t_N and t_{N+1} because the points are indistinguishable by definition, $\rho(-\infty)$ is evaluated on ϕ_1 and ϕ_{2N} and the use of $U_{+\delta t}$ or $U_{-\delta t}$ depends on the branch considered ($+$ for the forward and $-$ for the backward evolution). The matrix elements defined in Eq. (1.131) can be approximated to linear order in δt for any normal ordered[3] Hamiltonian as

$$\left\langle \phi_j \right| U_{\pm \delta t} \left| \phi_{j-1} \right\rangle \approx \left\langle \phi_j \right| (1 \mp iH(b^\dagger, b))\delta t \left| \phi_{j-1} \right\rangle \approx e^{\bar{\phi}_j \phi_{j-1}} e^{\mp iH(\bar{\phi}_j, \phi_{j-1})\delta t}, \tag{1.132}$$

where $b^\dagger (b)$ is the bosonic creation (annihilation) operator. Now all the exponential factors can be collected together and the partition function can be written as

$$Z = \frac{1}{\mathrm{tr}\rho(-\infty)} \int \prod_{j=1}^{2N} d[\bar{\phi}_j, \phi_j] \; \exp \left(i \sum_{i,j=1}^{2N} \bar{\phi}_i G_{ij}^{-1} \phi_j \right). \tag{1.133}$$

The matrix iG_{ij}^{-1} has a particular form: it possesses non-null elements on the diagonal and lower sub-diagonal, but also the element $(1, 2N)$, i.e. the upper right corner, is different from 0. This particular form can be written as

$$iG_{ij}^{-1} \equiv \begin{pmatrix} -1 & & \cdots & & & & \chi \\ h_- & -1 & \cdots & & & & \\ & & \cdots & & & & \\ \hline & & & 1 & -1 & \cdots & \\ & & & & h_+ & -1 & \cdots \\ & & & & & & h_+ & -1 \end{pmatrix}, \tag{1.134}$$

where the lines divide the matrix in blocks of $N \times N$ elements, $h_\pm = 1 \pm \left\langle \phi_j \right| H(\bar{\phi}_j, \phi_{j-1}) \left| \phi_{j-1} \right\rangle \delta t$ and $\chi = \left\langle \phi_1 \right| \rho(-\infty) \left| \phi_{2N} \right\rangle$. If the system is considered to be at equilibrium at initial time (choice that is not restrictive on the possibility of treating non-equilibrium dynamics) the denominator of Z can be computed. This term is therefore a constant and can be omitted without any confusion or ambiguity. In this case, also χ can be determined analytically.

While the derivation started before can be carried out with a generic Hamiltonian, everything is clearer if a toy model Hamiltonian that has a single quantum state with energy ε_0 is considered

$$H(b^\dagger, b) = \varepsilon_0 b^\dagger b, \tag{1.135}$$

---

[3]A Hamiltonian is defined as normally ordered if all the annihilation operators are on the right of all the creation operators

and the initial equilibrium density matrix can be proven to be

$$\rho(-\infty) = \exp[-\beta(\varepsilon_0 - \mu)b^\dagger b], \tag{1.136}$$

where μ is the chemical potential and $\beta = 1/T$ is the inverse temperature ($k_B = 1$ in this Chapter). The denominator of Z is

$$\mathrm{tr}\rho(-\infty) = \frac{1}{1 - \rho(\varepsilon_0)}, \tag{1.137}$$

with $\rho(\varepsilon_0) = e^{-\beta(\varepsilon_0 - \mu)}$. With this toy model it is also possible to prove that $\chi = \rho(\varepsilon_0)$.

Now, note that the integral present in Eq. (1.133) is a generalization of a Gaussian integral of type

$$\int \prod_{j=1}^N d[\bar{z}_j, z_j]\, e^{-\sum_{ij}^N \bar{z}_i A_{ij} z_j + \sum_j^N \bar{z}_j J_j + \bar{J}_j z_j} = \frac{e^{\sum_{ij}^N \bar{J}_i (A^{-1})_{ij} J_j}}{\det A}, \tag{1.138}$$

where J_j is a complex vector and $d[\bar{z}_j, z_j] = d(\mathrm{Re}z_j)d(\mathrm{Im}z_j)/\pi$. With this identity Eq. (1.133) is given by

$$Z = \frac{1}{\rho(-\infty)} \frac{1}{\det\left[iG^{-1}\right]}. \tag{1.139}$$

In the toy model of Eq. (1.135) the determinant can be easily computed, exploiting that now $h_\pm = 1 \pm i\varepsilon_0 \delta t$ and in the continuum limit $N \to \infty$

$$\begin{aligned}
\det\left[iG^{-1}\right] &= 1 - \rho(\varepsilon_0)(h_- h_+)^{N-1} = 1 - \rho(\varepsilon_0)(1 + \varepsilon_0^2(\delta t)^2)^{N-1} \\
&\approx 1 - \rho(\varepsilon_0)e^{\varepsilon_0^2(\delta t)^2(N-1)} \xrightarrow{N\to\infty} 1 - \rho(\varepsilon_0),
\end{aligned} \tag{1.140}$$

where $(\delta t)^2 N \to 0$ if $N \to \infty$ because $\delta t N$ is kept constant and therefore $\delta t^2 \sim N^{-2}$ as standard procedure in constructing the path integral formalism. With the last result it immediately follows that $Z = 1$ as it should be for Hamiltonians that are equals on the forward and backward branch and therefore the path integral construction is consistent.

The $N \to \infty$ limit allows writing formally Z in continuum notation

$$Z = \int \mathbf{D}[\bar{\phi}(t), \phi(t)]\, e^{iS[\bar{\phi}, \phi]}, \tag{1.141}$$

where the integration measure is defined as

$$\mathbf{D}[\bar{\phi}(t), \phi(t)] = \frac{1}{\mathrm{tr}\rho(-\infty)} \prod_{j=1}^{2N} d[\bar{\phi}_j, \phi_j], \tag{1.142}$$

and note that the trace over the initial density matrix can be absorbed without ambiguity in the integration measure. The continuum expression of the action $S[\bar{\phi}, \phi]$ is derived starting from the discrete version

$$S[\bar{\phi}, \phi] = \sum_{j=2}^{2N} \left[i\bar{\phi}_j \frac{\phi_j - \phi_{j-1}}{\delta t_j} - \varepsilon_0 \bar{\phi}_j \phi_{j-1}\right] \delta t_j + i\bar{\phi}_1 \left[\phi_1 - i\rho(\varepsilon_0)\phi_{2N}\right], \tag{1.143}$$

where $\delta t_j \equiv t_j - t_{j-1} = \pm\delta t$ on the forward or backward branches. In continuum notation the substitution $\phi_j \to \phi(t)$ is made and in the first square bracket it is possible to recognize the discrete expression of a derivative. Therefore, the action can be formally written as

$$S[\bar{\phi}, \phi] = \int_{\mathfrak{C}} dt\, \bar{\phi}(t)G^{-1}\phi(t), \tag{1.144}$$

where the continuum version of the discrete operator G^{-1} is

$$G^{-1} = i\partial_t - \varepsilon_0, \tag{1.145}$$

and $\int_{\mathfrak{C}} dt$ means that the integration is considered over the whole time contour.

Apparently, the boundary element in the upper-right corner of G^{-1} is not included in the continuum notation. However, this element has to be considered when the inverse operator G is determined to define it uniquely.

Going back to the continuum version of the action, the integration over the whole contour $\mathfrak{C}$ can be conveniently substituted with a different notation where the fields are split in two components living on the different branches. The forward component is then labelled with $\phi^+(t)$ and the backward with $\phi^-(t)$ and the action becomes

$$S[\bar{\phi}, \phi] = \int_{-\infty}^{\infty} dt \ \left[\bar{\phi}^+(t)(i\partial_t - \varepsilon_0)\phi^+(t) - \bar{\phi}^-(t)(i\partial_t - \varepsilon_0)\phi^-(t)\right], \tag{1.146}$$

and the relative minus sign is a consequence of the reverse integration direction in the backward branch. It has to be noticed that the forward and backward components of the field are not unrelated: indeed the off-diagonal elements of the discretized matrix version of G^{-1} in Eq. (1.134) establish a relation between components that live on different branch. This fact is somehow hidden by the continuum notation, but this inconvenience will disappear after the formal introduction of the Green functions and of their Keldysh-rotated version.

Now, a deeper look into G^{-1} and its inverse is necessary. The starting point are correlators, i.e. quantities like $\langle \phi\bar{\phi} \rangle$. Correlators can be computed using properties of Gaussian integrals [25] in discrete notation as

$$\langle \phi_i \bar{\phi}_j \rangle \equiv \int \mathbf{D}[\bar{\phi}, \phi] \ \phi_i \bar{\phi}_j \exp\left(i \sum_{k,l=1}^{2N} \bar{\phi}_k G_{kl}^{-1} \phi_l\right) = iG_{ij}. \tag{1.147}$$

After an explicit inversion of G^{-1} given in Eq (1.134) and the splitting on the time branches, 4 different correlators are defined: two of them involve fields on the same branch and the other involve fields on different branches. After the continuum limit, these 4 correlators for the considered toy model can be calculated

$$\langle \phi^+(t)\bar{\phi}^-(t') \rangle = iG^<(t,t') = n_{\mathrm{B}}(\varepsilon_0)e^{i\varepsilon_0(t-t')}, \tag{1.148a}$$

$$\langle \phi^-(t)\bar{\phi}^+(t') \rangle = iG^>(t,t') = (1 + n_{\mathrm{B}}(\varepsilon_0))e^{i\varepsilon_0(t-t')}, \tag{1.148b}$$

$$\langle \phi^+(t)\bar{\phi}^+(t') \rangle = iG^{\mathrm{T}}(t,t') = \theta(t - t')iG^>(t,t') + \theta(t' - t)iG^<(t,t'), \tag{1.148c}$$

$$\langle \phi^-(t)\bar{\phi}^-(t') \rangle = iG^{\tilde{\mathrm{T}}}(t,t') = \theta(t - t')iG^<(t,t') + \theta(t' - t)iG^>(t,t'), \tag{1.148d}$$

where $n_{\mathrm{B}}(\varepsilon_0)$ is the boson occupation number defined as

$$n_{\mathrm{B}}(\varepsilon_0) = \frac{\rho(\varepsilon_0)}{1 - \rho(\varepsilon_0)}. \tag{1.149}$$

In Eqs. (1.148a)-(1.148d) the symbols $<$ ($>$) are used for a correlator where the first time argument is taken before (after) the second, while T and $\tilde{T}$ labels the time ordering and anti-time ordering operation. The following properties hold

$$[G^{<(>)}]^\dagger = -G^{<(>)} \quad [G^{\mathrm{T}}]^\dagger = -G^{\tilde{\mathrm{T}}}, \tag{1.150}$$

where in the Hermitian conjugation also the change of time arguments is involved. The above correlators are the well known Green's functions (GFs) and can be defined in the continuum notation consistently as

$$\langle \phi^{\pm}(t)\bar{\phi}^{\pm}(t')\rangle = \int \mathbf{D}[\bar{\phi}, \phi]\; \phi^{\pm}(t)\bar{\phi}^{\pm}(t')e^{iS[\bar{\phi}, \phi]}. \tag{1.151}$$

The 4 GFs defined in Eqs. (1.148a)-(1.148d) are not independent: indeed for any $t \neq t'$ the relation

$$G^{<}(t, t') + G^{>}(t, t') - G^{\mathrm{T}}(t, t') - G^{\tilde{\mathrm{T}}}(t, t') = 0, \tag{1.152}$$

holds. The above relation is not valid for $t = t'$, but this pathological point has no consequences on the rest of the formalism and can be safely ignored. Note that, even if Eq. (1.152) was derived for a toy model, it is completely general. Using the above equality, it is possible to perform a rotation of the fields, known as *Keldysh rotation*, that gives only 3 GFs different from zero and automatically account for the correlations between fields living on different branches. This rotation is performed defining the fields

$$\phi^{\mathrm{cl}}(t) = \frac{1}{\sqrt{2}}(\phi^{+}(t) + \phi^{-}(t)), \tag{1.153a}$$

$$\phi^{\mathrm{q}}(t) = \frac{1}{\sqrt{2}}(\phi^{+}(t) - \phi^{-}(t)), \tag{1.153b}$$

and the same for conjugated fields. The superscripts cl and q that stand for classical and quantum components are commonly used in literature and the same is done here. The reason behind this labelling is that it can be shown that for any field with $\phi^{\mathrm{q}} = 0$ the total action will be null, i.e. $S[\phi^{\mathrm{cl}}, 0] = 0$, meaning that the evolution on the forward branch is exactly canceled by the evolution on the backward branch. This reflects the fact that the fields on the two branches are the same and it is not a specificity of the toy model but it is valid for any bosonic action.

After the rotation, the new Keldysh-rotated GFs can be described in a matrix structure, with $\alpha, \beta = (cl, q)$

$$\langle \phi^{\alpha}(t)\bar{\phi}^{\beta}(t')\rangle \equiv iG^{\alpha\beta}(t, t') = \begin{pmatrix} iG^{\mathrm{K}}(t, t') & iG^{\mathrm{R}}(t, t') \\ iG^{\mathrm{A}}(t, t') & 0 \end{pmatrix}, \tag{1.154}$$

where the superscripts R, A and K label the retarded, advanced and Keldysh component of the GF. Their definition is

$$G^{\mathrm{R}}(t, t') = \theta(t - t')(G^{>}(t, t') - G^{<}(t, t')), \tag{1.155a}$$

$$G^{\mathrm{A}}(t, t') = \theta(t' - t)(G^{<}(t, t') - G^{>}(t, t')), \tag{1.155b}$$

$$G^{\mathrm{K}}(t, t') = G^{<}(t, t') + G^{>}(t, t'), \tag{1.155c}$$

for $t \neq t'$. It also follows from the definition of $G^{<}$, $G^{>}$, G^{T} and $G^{\tilde{\mathrm{T}}}$ that

$$G^{\mathrm{A}} = (G^{\mathrm{R}})^{\dagger} \quad G^{\mathrm{K}} = -(G^{\mathrm{K}})^{\dagger}, \tag{1.156}$$

where the Hermitian conjugation involves as before complex conjugation and exchange of time arguments.

The structure of the matrix G in Eq. (1.154) is a consequence of the Keldysh rotation procedure, but it is also directly related to the presence of the closed time contour. Indeed, the price to pay for working on the closed time contour is a sort of proliferation of Green functions with respect to the equilibrium case. As a trade-off, this allows to treat with less ambiguity non-equilibrium situations.
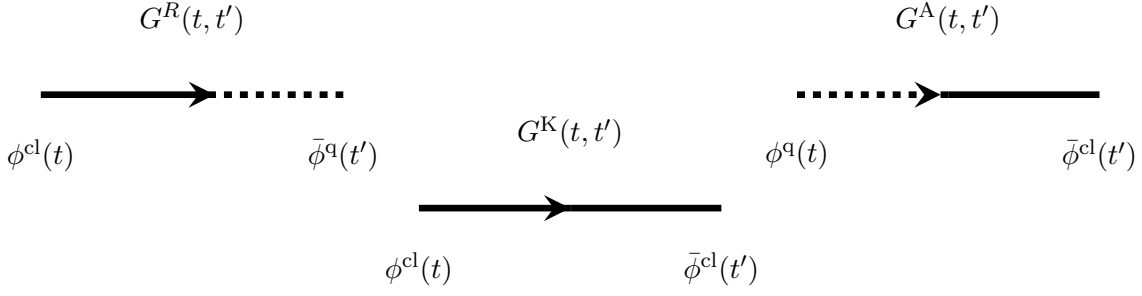
$$G^R(t,t')$$

$$G^A(t,t')$$

$$\phi^{\mathrm{cl}}(t) \qquad\qquad \bar{\phi}^{\mathrm{q}}(t')$$

$$G^{\mathrm{K}}(t,t')$$

$$\phi^{\mathrm{q}}(t) \qquad\qquad \bar{\phi}^{\mathrm{cl}}(t')$$

$$\phi^{\mathrm{cl}}(t) \qquad\qquad \bar{\phi}^{\mathrm{cl}}(t')$$

Figure 1.3. Graphical representation of the 3 different GFs. The solid line denotes a classical component ϕ^{cl} while the dashed line denotes the quantum component ϕ^{q}.

A small discussion for the equal time case $t = t'$ is now necessary. It can be shown that

$$G^{\mathrm{R}}(t,t') + G^{\mathrm{A}}(t,t') = G^{\mathrm{T}}(t,t') - G^{\tilde{\mathrm{T}}}(t,t'), \tag{1.157}$$

and because at $t = t'$ time ordering and anti-time ordering are equivalent one has

$$G^{\mathrm{R}}(t,t) + G^{\mathrm{A}}(t,t) = 0. \tag{1.158}$$

In energy representation after a Fourier transform

$$\int \frac{d\omega}{2\pi} \left[G^{\mathrm{R}}(\omega) + G^{\mathrm{A}}(\omega) \right] = 0. \tag{1.159}$$

Note however that from Eqs. (1.155a-1.155b)

$$G^{\mathrm{R}}(t,t) - G^{\mathrm{A}}(t,t) = -i, \tag{1.160}$$

and this is not a specific property of the toy model but a general one being related to commutation relation of bosonic annihilation and creation operators, indeed it is due to the fact that $G^{\mathrm{R}} - G^{\mathrm{A}} = -i\langle bb^\dagger - b^\dagger b \rangle = -i$ at equal times. One also obtains that in energy representation

$$\int d\omega \left[G^{\mathrm{R}}(\omega) - G^{\mathrm{A}}(\omega) \right] = -2\pi i. \tag{1.161}$$

It should be noticed that in practical calculations G^{R} and G^{A} at equal times never appear alone, but always as a sum or as a difference in the different scenarios investigated in this thesis. Therefore, the general properties described by Eq. (1.159) and Eq. (1.161) are enough to treat the equal time situation without ambiguities and the continuum notation can be safely extended to the equal time case. A graphical representation for the retarded, advanced and Keldysh components of the bosonic GFs is given in Fig 1.3, where the classical component of the bosonic field is denoted with a full line and the quantum component with a dashed line. The arrows are pointing from the annihilation to the creation operator.

In the simple toy model currently under consideration, the GFs can be computed analytically in position and momentum space. Their expressions are

$$G^{\mathrm{R}}(t-t') = -i\theta(t-t')e^{-i\varepsilon_0(t-t')} \xrightarrow{\mathrm{FT}} G^{\mathrm{R}}(\omega) = (\omega - \varepsilon_0 + i0)^{-1}, \tag{1.162}$$

$$G^{\mathrm{A}}(t-t') = i\theta(t'-t)e^{-i\varepsilon_0(t-t')} \xrightarrow{\mathrm{FT}} G^{\mathrm{A}}(\omega) = (\omega - \varepsilon_0 - i0)^{-1}, \tag{1.163}$$

$$G^{\mathrm{K}}(t-t') = -i[2n_{\mathrm{B}}(\varepsilon_0)+1]e^{-i\varepsilon_0(t-t')} \xrightarrow{\mathrm{FT}} G^{\mathrm{K}}(\omega) = -2\pi i[2n_{\mathrm{B}}(\omega)+1]\delta(\omega - \varepsilon_0), \tag{1.164}$$

where the arrows label a Fourier transform. The dependence on the time difference $t - t'$ in position space (and the corresponding frequency ω dependence in momentum space) is a consequence of the toy model, that is invariant under time translations. The occupation number is present only in the Keldysh component, while the retarded and advanced GFs give information on the spectrum of the system. In thermal equilibrium, where the occupation number is given by Eq. (1.149) the Keldysh component in momentum space has the form

$$G^{\mathrm{K}}(\omega) = \coth\left(\frac{\beta(\omega - \mu)}{2}\right)[G^{\mathrm{R}}(\omega) - G^{\mathrm{A}}(\omega)]. \tag{1.165}$$

This last equation is the well known fluctuation-dissipation relation. This relation is not characteristic of the toy model, but is a general property of systems in thermal equilibrium where correlation functions and response functions are directly related.

In continuum notation and after the Keldysh rotation, the action $S[\bar{\phi}, \phi]$ is written in terms of the retarded, advanced and Keldysh inverse GFs as

$$S[\phi^{\mathrm{cl}}, \phi^{\mathrm{q}}] = \iint dt dt' \; (\bar{\phi}^{\mathrm{cl}}(t'), \bar{\phi}^{\mathrm{q}}(t')) \begin{pmatrix} 0 & [G^{-1}]^{\mathrm{A}}(t,t') \\ [G^{-1}]^{\mathrm{R}}(t,t') & [G^{-1}]^{\mathrm{K}}(t,t') \end{pmatrix} \begin{pmatrix} \phi^{\mathrm{cl}}(t') \\ \phi^{\mathrm{q}}(t') \end{pmatrix}. \tag{1.166}$$

Off-diagonal elements of the G^{-1} matrix can be obtained from the condition $[G^{-1}]^{\mathrm{R/A}} \circ G^{\mathrm{R/A}} = I$, where $\circ$ labels convolution operation. It follows that these off- diagonal components can be derived directly from matrix inversion, i.e. $[G^{-1}]^{\mathrm{R/A}} = [G^{\mathrm{R/A}}]^{-1}$. In momentum space the inversion is trivial and one has

$$[G^{-1}]^{\mathrm{R/A}}(\omega) = \omega - \varepsilon_0 \pm i0 \xrightarrow{\text{FT}} [G^{-1}]^{\mathrm{R/A}}(t - t') = \delta(t - t')(i\partial_{t'} - \varepsilon_0 \pm i0). \tag{1.167}$$

For the non-interacting toy model under consideration the Keldysh component of the inverse matrix G^{-1} is infinitesimally small and it is just a regularization element responsible for the convergence of the integral. In interacting models this element is on the contrary different from zero, in the sense that it is no longer a regularization term.

The form of the action given by Eq. (1.166), i.e. the causality structure reflected in the position of the elements of the matrix G^{-1}, is general for every bosonic action, regardless of the model under consideration. Of course the bosonic fields and the Green functions are model dependent, but causality structure is not. This causality structure is written here for convenience

$$G^{-1} = \begin{pmatrix} 0 & [G^{\mathrm{A}}]^{-1} \\ [G^{\mathrm{R}}]^{-1} & [G^{\mathrm{K}}]^{-1} \end{pmatrix}, \tag{1.168}$$

where the two off-diagonal elements are mutually Hermitian conjugated and the only non-zero diagonal element is anti-Hermitian. Note also that the causality structure of Eq. (1.168) is determined by the Keldysh rotation that gives Eq. (1.154).

Before proceeding, an additional discussion on the Keldysh component of the GF is needed. As stated before, the anti-Hermitian Green function G^{K} is related to occupation number at equilibrium. For this reason it is useful to parametrize it with the help of the Hermitian matrix F through the relation

$$G^{\mathrm{K}} = G^{\mathrm{R}} \circ F - F \circ G^{\mathrm{A}}, \tag{1.169}$$

where in the toy model[4] $F = F(t, t')$. The Wigner transformation, see Appendix B, of the function F is called the distribution function. At equilibrium in the bosonic scenario it is possible to show that

$$F(\omega) = 1 + 2n_{\mathrm{B}}(\omega). \tag{1.170}$$

---

[4] In general F depend also on the spatial coordinates, i.e. $F = F(\mathbf{r}, t, \mathbf{r}', t')$.

Therefore this distribution function, together with the retarded and advanced GFs, can be used to study the dynamics of a system since the first one gives information on the populations (both in equilibrium or out of it) while the second ones on the spectrum.

As a conclusion to this introductory part for bosonic fields, consider the slightly more complicated system made of bosons of mass m inside a box. Single particle states are labelled by vector $\mathbf{k}$ and the energies are given by $\varepsilon(\mathbf{k}) = \mathbf{k}^2/2m$. In absence of an external potential the Hamiltonian is

$$H = \sum_{\mathbf{k}} \omega(\mathbf{k}) b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}, \tag{1.171}$$

where $b_{\mathbf{k}}$ ($b_{\mathbf{k}}^{\dagger}$) are annihilation (creation) operators of particles with wavenumbers $\mathbf{k}$. The initial density matrix is supposed to be the equilibrium one, i.e. $\rho_0 = \exp[-\beta(H - \mu N)]$ where N is the particle number operator defined as $N = \sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$. The coherent states needed for the construction of the path integral are now also labelled by the wavenumber, so in the discrete notation one has $\phi_j(\mathbf{k}, t)$. After the passage to continuum notation and the Keldysh rotation one obtains the fields $\phi^{\mathrm{cl}}(\mathbf{k}, t)$ and $\phi^{\mathrm{q}}(\mathbf{k}, t)$. The action is

$$S[\phi^{\mathrm{cl}}, \phi^{\mathrm{q}}] = \sum_{\mathbf{k}} \int dt \, (\bar{\phi}^{\mathrm{cl}}(\mathbf{k}, t), \bar{\phi}^{\mathrm{q}}(\mathbf{k}, t)) \begin{pmatrix} 0 & i\partial_t - \omega(\mathbf{k}) - i0 \\ i\partial_t - \omega(\mathbf{k}) + i0 & 2i0F(\omega(\mathbf{k})) \end{pmatrix} \begin{pmatrix} \phi^{\mathrm{cl}}(\mathbf{k}, t) \\ \phi^{\mathrm{q}}(\mathbf{k}, t) \end{pmatrix}. \tag{1.172}$$

Also for this system, the Keldysh component is pure regularization because no interactions are present.

The corresponding GFs in momentum space are

$$G^{\mathrm{R}}(\omega, \mathbf{k}) = (\omega - \omega(\mathbf{k}) + i0)^{-1}, \tag{1.173}$$
$$G^{\mathrm{A}}(\omega, \mathbf{k}) = (\omega - \omega(\mathbf{k}) - i0)^{-1}, \tag{1.174}$$
$$G^{\mathrm{K}}(\omega, \mathbf{k}) = -2\pi i F(\omega)\delta(\omega - \omega(\mathbf{k})). \tag{1.175}$$

In position space the action S is

$$S[\phi^{\mathrm{cl}}, \phi^{\mathrm{q}}] = \int dt \int d\mathbf{r} \, (\bar{\phi}^{\mathrm{cl}}(\mathbf{r}, t), \bar{\phi}^{\mathrm{q}}(\mathbf{r}, t)) \begin{pmatrix} 0 & i\partial_t + \nabla_{\mathbf{r}}^2/2m - i0 \\ i\partial_t + \nabla_{\mathbf{r}}^2/2m + i0 & 2i0F \end{pmatrix} \begin{pmatrix} \phi^{\mathrm{cl}}(\mathbf{r}, t) \\ \phi^{\mathrm{q}}(\mathbf{r}, t) \end{pmatrix}. \tag{1.176}$$

Up to now, only non-interacting toy models have been discussed. Interactions are treated directly in Chapter 2 and 3 where other important concepts such as self-energies are introduced.

1.3.3   Fermionic scenario

The same construction for the path integral representation of Z of the bosonic scenario can be carried out when the particles involved in the system are fermions. What happens is that due to the different statics involved some details are different, e.g. the causality structure of the matrix of Green functions. Also for fermions the theory used to introduce the formalism is a free one and interactions will be treated in detail in Chapter 3.

The main difference between bosons and fermions is in the different statistics each type of particle obeys. This is encoded in the fact that while bosonic creation and annihilation operators follow the so-called canonical commutation relations (CCR) [26], the fermionic ones obey canonical anticommutation relations (CAR). CAR are defined with the help of fermionic creation and annihilation operators $f^{\dagger}$ and f as

$$\{f^{\dagger}, f\} = \{f, f^{\dagger}\} = I, \tag{1.177}$$

where the hat accent for operators is understood. Before the introduction of the path integral formalism, a small recap on properties of f and $f^\dagger$ could be helpful. Consider a single quantum level: due to Pauli exclusion principle, this level can contain zero or one fermion, i.e. is described by states $|0\rangle$ and $|1\rangle$. This consideration is valid for any state, therefore the many body state is spanned by the orthonormal basis $\{|0\rangle, |1\rangle\}$. Creation and annihilation operators therefore act on the element of the basis in the following way

$$f|0\rangle = 0 \ f^\dagger|0\rangle = |1\rangle \ f|1\rangle = |0\rangle \ f^\dagger|1\rangle = 0 \tag{1.178}$$

Notice also that the operators have the properties that $(f)^2 = (f^\dagger)^2 = 0$ and $f^\dagger f|n\rangle = |n\rangle$ with $n = 0, 1$.

The construction of the coherent states needed for the formulation of the path integral formalism is different because of Eq. (1.177). Indeed, an *anticommuting algebra* is now needed to find an eigenstate of f. This can be done introducing Grassmann numbers denoted as ψ, ψ' that follow the multiplication rules

$$\psi\psi' = -\psi'\psi \quad (\psi)^2 = 0. \tag{1.179}$$

An extremely important property holds for the Taylor expansion of functions of one or more variables, e.g. $f(\psi)$ and $f(\psi_1, \psi_2)$, that becomes exact with a finite number of terms

$$f(\psi) = f_0 + f_1\psi \quad f(\psi_1, \psi_2) = f_{00} + f_{10}\psi_1 + f_{01}\psi_2 + f_{11}\psi_1\psi_2, \tag{1.180}$$

where f_i and f_{ij} are real or complex coefficients and the generalization to more variables is straightforward. The definition of the derivative on the Grassmann algebra is now natural

$$\frac{\partial\psi}{\partial\psi} = 1 \quad \frac{\partial f(\psi)}{\partial\psi} = f_1. \tag{1.181}$$

Also the derivative is anticommuting as can be seen directly from

$$\frac{\partial}{\partial\psi_1}\frac{\partial}{\partial\psi_2}f(\psi_1, \psi_2) = -f_{11} = -\frac{\partial}{\partial\psi_2}\frac{\partial}{\partial\psi_1}f(\psi_1, \psi_2), \tag{1.182}$$

integration on Grassmann variables is *defined* as

$$\int d\psi \ 1 = 0 \quad \int d\psi \ \psi = 1, \tag{1.183}$$

and this definition can not be derived from first principles.

Now it is possible to define fermionic coherent states in analogy with the bosonic ones, i.e. as eigenstates of the annihilation operator. These eigenstates must be a linear combination of $|0\rangle$ and $|1\rangle$ but no linear combination with real or complex numbers is possible. This combination is on the other hand possible if Grassmann numbers are involved. Indeed, thanks to Taylor expansion property the state $|\psi\rangle$ that parametrizes the Grassmann number ψ can be immediately written as

$$|\psi\rangle = |0\rangle - \psi|1\rangle = (1 - \psi f^\dagger)|0\rangle = e^{-\psi f^\dagger}|0\rangle, \tag{1.184}$$

and it is immediate to show that $f|\psi\rangle = \psi|\psi\rangle$ because for convention Grassmann numbers and $f, f^\dagger$ anticommute

$$\{\psi, f\} = \{\psi, f^\dagger\} = 0. \tag{1.185}$$

Thus the right eigenstate $|\psi\rangle$ defined in Eq. (1.184) is the desired fermionic coherent state, obtained with the help of Grassmann algebra. The left eigenstate $\langle\psi|$ is

$$\langle\psi| = \langle 0|e^{-f\bar{\psi}}, \tag{1.186}$$

and $\bar{\psi}$ is a Grassmann number completely unrelated to ψ. Therefore, the superposition of two fermionic coherent states is

$$\langle\psi|\psi'\rangle = e^{\bar{\psi}\psi'}, \tag{1.187}$$

and the following equality in the coherent state representation, analogue to Eq. (1.130), holds

$$I = \iint d\bar{\psi}d\psi \; e^{-\bar{\psi}\psi} \langle\psi|\psi\rangle, \tag{1.188}$$

where the integration order has a role due to the anticommuting multiplication rules. For any normal ordered operator the matrix elements on the coherent state basis are given by

$$\langle\psi| H(f^\dagger, f) |\psi'\rangle = H(\bar{\psi}, \psi')e^{\bar{\psi}\psi'}, \tag{1.189}$$

and the Gaussian integration over sets of independent Grassmann variables is

$$Z[\bar{\chi}, \chi] = \int \prod_{j=1}^{N}[d\bar{\psi}_j d\psi_j] \; e^{-\sum_{i,j=1}^{N}\bar{\psi}_i A_{ij}\psi_j + \sum_{j=1}^{N}(\bar{\psi}_j\chi_j + \bar{\chi}_j\psi_j)} = \det A \; e^{\sum_{i,j=1}^{N}\bar{\chi}_i(A^{-1})_{ij}\chi_j}, \tag{1.190}$$

where A_{ij} is a complex invertible matrix and $\bar{\chi}_j$ and χ_j are two sets of independent Grassmann variables also independent on $\bar{\psi}_i$ and ψ_i. Note that, in contrast with Eq. (1.138) the determinant of the invertible matrix is now at the numerator (and not at the denominator) of the right-hand side of the equation. This is due to the specific properties of multiplication and integration for the Grassmann numbers.

Now all the ingredients for the construction of the path integral are present. Also for the fermionic scenario it is useful to consider a toy model with

$$H = \varepsilon_0 f^\dagger f, \tag{1.191}$$

with ε_0 the characteristic energy of the model. If the system is in thermal equilibrium at initial time, the equilibrium density matrix has a trace

$$\mathrm{tr}\rho(-\infty) = \mathrm{tr}\rho_0 = 1 + \rho(\varepsilon_0) \tag{1.192}$$

The algebra behind the construction of the path integral is now the same used in Chapter 1.3.2 with the only difference lying in the presence of Grassmann variables. After the continuum limit the partition function is now written as

$$Z = \int \mathbf{D}[\bar{\psi}, \psi] \; e^{iS[\bar{\psi},\psi]} = \int \mathbf{D}[\bar{\psi}, \psi] \; \exp\left(i \int_{\mathbb{C}} dt \; \bar{\psi}(t)G^{-1}\psi(t)\right). \tag{1.193}$$

The fields ψ and $\bar{\psi}$ are again split between the two branches and the action for the toy model Eq. 1.191 acquires the form

$$S[\bar{\psi}, \psi] = \int_{-\infty}^{\infty} dt \; \left[\bar{\psi}^+(t)(i\partial_t - \varepsilon_0)\psi^+(t) - \bar{\psi}^-(t)(i\partial_t - \varepsilon_0)\psi^-(t)\right], \tag{1.194}$$

where the meaning of ψ^+ and ψ^- is the same used before. A difference between the fermionic and bosonic scenario is encoded in the Green functions. Indeed, their definition is the same given in Eqs. (1.148a)-(1.148d) applied to the ψ fields, but their expressions are different. For the present toy model,

$$\langle\psi^+(t)\bar{\psi}^-(t')\rangle = iG^<(t, t') = -n_{\mathrm{F}}(\varepsilon_0)e^{-i\varepsilon_0(t-t')}, \tag{1.195a}$$

$$\langle\psi^-(t)\bar{\psi}^+(t')\rangle = iG^>(t, t') = (1 - n_{\mathrm{F}}(\varepsilon_0))e^{-i\varepsilon_0(t-t')}, \tag{1.195b}$$

$$\langle\psi^+(t)\bar{\psi}^+(t')\rangle = iG^{\mathrm{T}}(t, t') = \theta(t - t')iG^>(t, t') + \theta(t' - t)iG^<(t, t'), \tag{1.195c}$$

$$\langle\psi^-(t)\bar{\psi}^-(t')\rangle = iG^{\tilde{\mathrm{T}}}(t, t') = \theta(t - t')iG^<(t, t') + \theta(t' - t)iG^>(t, t'). \tag{1.195d}$$

These functions are different from their bosonic counterparts in the presence of the fermionic occupation number $n_F = \rho(\varepsilon_0)/1 + \rho(\varepsilon_0)$ and in the minus sign in front of this occupation number in the expressions for $G^{<(>)}$. Fermionic Green functions are not independent too, therefore a Keldysh rotation can be performed in order to eliminate one of them and restore the correlation between fields living on different branches as done for the bosons.

A key difference in the Keldysh rotation procedure is that, contrary to what happens to bosons, ψ and $\bar{\psi}$ are defined in two independent ways and not as complex conjugated. This is done because ψ and $\bar{\psi}$ used in the construction of the path integral are two independent Grassmann fields and have to be treated consequently. Keldysh rotation for fermions is defined as [22]

$$\psi_1(t) = \frac{1}{\sqrt{2}}(\psi^+(t) + \psi^-(t)) \quad \psi_2(t) = \frac{1}{\sqrt{2}}(\psi^+(t) - \psi^-(t)), \tag{1.196}$$

$$\bar{\psi}_1(t) = \frac{1}{\sqrt{2}}(\bar{\psi}^+(t) - \bar{\psi}^-(t)) \quad \bar{\psi}_2(t) = \frac{1}{\sqrt{2}}(\bar{\psi}^+(t) + \bar{\psi}^-(t)). \tag{1.197}$$

The components of the Keldysh rotated fields are no longer defined as classical or quantum, because Grassmann field can not have a classical meaning because of their anticommutative nature under multiplication. The rotated matrix of Green functions is given by

$$- i\langle \psi_a(t)\bar{\psi}_b(t)\rangle = G_{ab}(t, t') = \begin{pmatrix} G^R(t, t') & G^K(t, t') \\ 0 & G^A(t, t') \end{pmatrix}, \tag{1.198}$$

where $a, b = 1, 2$. The retarded, advanced and Keldysh components are defined in the same way of the bosonic ones. The different causality structure is a consequence of the different rotation, and it is also possible to prove that the same causality structure hold for the matrix of inverse GFs

$$G^{-1}(t, t') = \begin{pmatrix} [G^R]^{-1}(t, t') & [G^K]^{-1}(t, t') \\ 0 & [G^A]^{-1}(t, t') \end{pmatrix}. \tag{1.199}$$

Finally, the analytical GFs for the toy model in time and frequency space are

$$G^R(t - t') = -i\theta(t - t')e^{-i\varepsilon_0(t-t')} \xrightarrow{\text{FT}} G^R(\omega) = (\omega - \varepsilon_0 + i0)^{-1}, \tag{1.200}$$

$$G^A(t - t') = i\theta(t' - t)e^{-i\varepsilon_0(t-t')} \xrightarrow{\text{FT}} G^A(\omega) = (\omega - \varepsilon_0 - i0)^{-1}, \tag{1.201}$$

$$G^K(t - t') = -i[1 - 2n_F(\varepsilon_0)]e^{-i\varepsilon_0(t-t')} \xrightarrow{\text{FT}} G^K(\omega) = -2\pi i[1 - 2n_F(\omega)]\delta(\omega - \varepsilon_0). \tag{1.202}$$

In thermal equilibrium, fermionic occupation number is given by the Fermi-Dirac distribution

$$n_F(\omega) = \left(1 + e^{\beta(\omega - \mu)}\right)^{-1}, \tag{1.203}$$

the expressions of $G^K(\omega)$ contains the fluctuation-dissipation relation for fermions

$$G^K(\omega) = \tanh\left(\frac{\beta(\omega - \mu)}{2}\right)[G^R(\omega) - G^A(\omega)]. \tag{1.204}$$

A parametrization of G^K with the introduction of a Hermitian matrix F like in Eq. (1.169) is possible also for fermions in the same manner. The difference is that in equilibrium the distribution function F has the value

$$F(\omega) = 1 - 2n_F(\omega). \tag{1.205}$$

Also for fermions is possible to define a general structure for the action as done for bosons: the differences are the presence of the fields $(1, 2)$ instead of (cl, q) and the different causality structure of the inverse GFs matrix.

Another important difference has to be considered: indeed fermions always have a spin index and this has to be considered in the construction of the general form of the action. However, spin index can be included directly without changing the structure of the path integral construction because spin behaves in the same manner on the two branches and does not need a Keldysh rotation. Therefore, a Grassmann field with a spin index can be split and decomposed in the same manner described in Eqs. (1.196)-(1.197) simply adding the spin index itself. In conclusion, the general form for a system of fermions with spin index σ is (sum over repeated indices understood)

$$S[\bar{\psi}, \psi] = \iint dx\, dx'\; \bar{\psi}_{a,\sigma}(x)[G^{-1}_{\sigma,\sigma'}(x, x')]^{ab}\psi_{b,\sigma'}(x'). \tag{1.206}$$

Now it can be helpful to introduce a new toy model with an energy that is dependent on momentum and spin. The Hamiltonian of this new toy model is

$$H = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\sigma}(\mathbf{k}) f_{\sigma}^{\dagger}(\mathbf{k}) f_{\sigma}(\mathbf{k}), \tag{1.207}$$

where for example $\sigma = \uparrow, \downarrow$ and the energy is

$$\varepsilon_{\sigma}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} + H_{\mathrm{Z}}\sigma, \tag{1.208}$$

and H_{Z} is a Zeeman magnetic field. The action has the form Eq. (1.206) and the retarded, advanced and Keldysh components in momentum space are

$$G^{\mathrm{R(A)}}_{\sigma,\sigma'}(\omega, \mathbf{k}) = \delta_{\sigma,\sigma'}(\omega - \varepsilon_{\sigma}(\mathbf{k}) + \pm i0)^{-1} \tag{1.209}$$

$$G^{\mathrm{K}}_{\sigma,\sigma'}(\omega, \mathbf{k}) = -2\pi i \delta_{\sigma,\sigma'} F(\omega)\delta(\omega - \varepsilon_{\sigma}(\mathbf{k})). \tag{1.210}$$

A more detailed discussion on GFs when spin and Zeeman fields are present in the system will be given in Chapter 3. Now it is only relevant to see that spin index does not play a fundamental role in the form of the action (only an additional sum over spin index is needed) while it affect in a more deep way the GFs.

A small comment now on the GFs discussed and calculated in the bosonic and fermionic scenarios. All the GFs have been derived for systems with no interaction: while in these non-interacting systems the actions are called *free*, the GFs are conventionally called *bare*. The reason behind the name "bare" is that usually interaction are said to be responsible for a "dressing" of the GFs, so the name bare is justified in this sense. Another convention that will be adopted from now on throughout this work is the use of the subscript "0" to label free actions and bare Green functions. Therefore, an action like the one in Eq. (1.206) will be called $S_0[\bar{\psi}, \psi]$ in the remaining part of this thesis.

Chapter 2

Impurities in a quantum bath and bound states

2.1 Theoretical setup

The system under examination is composed by a bath of degenerate Fermi atoms and a small number N of impurities. The fermions of the bath are characterized by their chemical potential μ and mass m, while the mass m_I of the impurities is much larger, so that $m_\text{I}/m \gg 1$. Moreover, the bath is at low but finite temperature T. At the energy scales considered, particles interact only via s-wave scattering and therefore the interaction between the atoms of the bath can be neglected. It is also assumed that there is no direct interaction between the impurities. In the language of open quantum systems, the impurities plays the role of the subsystem: indeed, they have much fewer degrees of freedom than the bath and their dynamics is the main point of interest in the theoretical description and numerical implementation.

The interaction between the bath and the impurities is modeled as a contact potential of strength g. Contact potentials have to be treated properly to avoid divergences, but they also make the theoretical derivation easier and are therefore a suitable choice for describing this type of systems. Another important assumption is that the de Broglie wavelength of the impurities at the considered temperature, $\lambda = \hbar\sqrt{2\pi/m_\text{I}k_\text{B}T}$, is small compared to the typical inter-particle distance and therefore impurities can be treated as classical objects. This assumption will be justified in Sec 2.4 when all the numerical parameters will be introduced.

Impurities are described in first quantization and coordinate representation, while the bath of degenerate fermions is treated using quantum field theory. The Hamiltonian that models the system is

$$\hat{H} = \hat{H}_\text{F} + \hat{H}_\text{I} + \hat{V}, \tag{2.1}$$

where $\hat{H}_\text{F}$ and $\hat{H}_\text{I}$ are respectively the Hamiltonians of the bath and of the impurities and $\hat{V}$ is the interaction potential given by

$$\hat{H}_\text{I} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m_\text{I}} \tag{2.2}$$

$$\hat{H}_\text{F} = \int d\mathbf{x}\, \hat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\hat{\nabla}^2 - \mu \right) \hat{\Psi}(\mathbf{x}) \tag{2.3}$$

$$\hat{V} = g \sum_{i=1}^{N} \int d\mathbf{x}\, \hat{\Psi}^\dagger(\mathbf{x})\, \delta(\hat{\mathbf{q}}_i - \mathbf{x})\, \hat{\Psi}(\mathbf{x}). \tag{2.4}$$
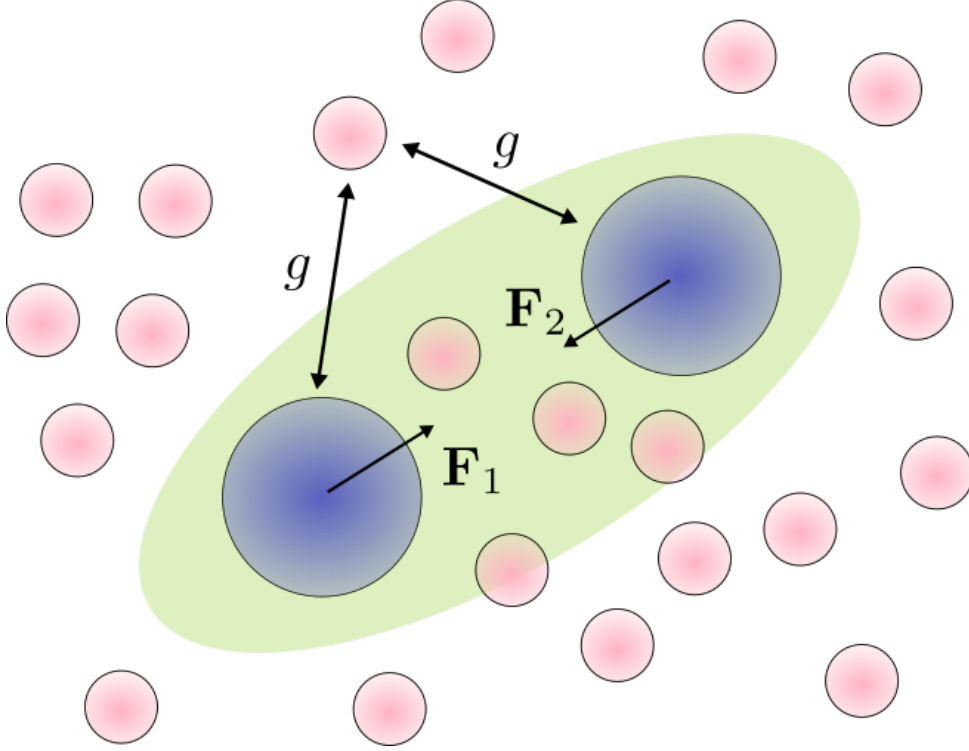
Figure 2.1. Two heavy impurities (violet) in a bath of fermions (pink): the bare impurity-bath interaction g is responsible for the induced forces between impurities $\mathbf{F}_{1;2}$ and for the low friction region (green).

Here, $\hat{\mathbf{q}}_i$ and $\hat{\mathbf{p}}_i$ are the position and momentum operators of the i-th impurity, while $\hat{\Psi}(\mathbf{x})$ and $\hat{\Psi}^\dagger(\mathbf{x})$ are the annihilation and creation operators associated with the fermions of the bath. The dimensionality of the Hamiltonians is not specified yet and it will be set later.

In the situation considered, the impurities are initially decoupled from the bath, i.e. $\hat{V}$ is not present. Impurities are initially at positions $\mathbf{Q}_i = (\mathbf{q}_1(t_i), \ldots, \mathbf{q}_N(t_i))$ then at $t = t_i$ the interaction is turned on and the total density matrix of the system $\rho(t)$ starts evolving under the action of the complete Hamiltonian $\hat{H}$, Eq. (2.1). The initial density matrix can be factorized as $\rho(t_i) = \rho_\mathrm{I}(t_i) \otimes \rho_F(t_i)$, where $\rho_\mathrm{I}(t_i) = |\mathbf{Q}_i\rangle \langle \mathbf{Q}_f|$ and ρ_F is the density matrix of the fermions of the bath. The most important quantity to determine is the probability to have a configuration $\mathbf{Q}_f = (\mathbf{q}_1(t_f), \ldots, \mathbf{q}_N(t_f))$ at time $t = t_f$, denoted as $P(\mathbf{Q}_f, t_f | \mathbf{Q}_i, t_i)$. This transition probability is given by

$$P(\mathbf{Q}_f, t_f | \mathbf{Q}_i, t_i) = \mathrm{Tr}\left\{ (|\mathbf{Q}_f\rangle \langle \mathbf{Q}_f| \otimes I_\mathrm{F}) \rho(t) \right\}, \tag{2.5}$$

where $t \equiv t_f - t_i$ and I_F is the identity matrix defined on the fermionic degrees of freedom. In Eq. (2.5) it is evident that tracing out the bath degrees of freedom is necessary to obtain the desired probability, and this operation is done using path integral representation. Indeed, the transition probability can be written as

$$P(\mathbf{Q}_f, t_f | \mathbf{Q}_i, t_i) = \int_{\mathbf{Q}_i}^{\mathbf{Q}_f} \mathcal{D}\mathbf{Q} \int \mathcal{D}\xi \int \mathcal{D}\xi^* \, e^{\frac{i}{\hbar} S[\mathbf{Q}, \xi, \xi^*]}. \tag{2.6}$$

where $\xi(t, \mathbf{x})$ and $\xi^*(t, \mathbf{x})$ are Grassmann coherent field variables. The functional at the exponent

is obtained directly from the total Hamiltonian $\hat{H}$ and it is given by

$$S[\mathbf{Q}, \xi, \xi^*] = \int_{\mathbb{C}} dt' \left\{ \frac{m_\mathrm{I}}{2} \sum_{j=1}^{N} \dot{\mathbf{q}}_j^2(t') + \right.$$
$$\left. \int d\mathbf{x}\, \xi^*(t', \mathbf{x}) \left(i\hbar \partial_{t'} - \frac{\hbar^2 \nabla^2}{2m} - \mu(T) + \rho_\mathrm{I}(t', \mathbf{x}) \right) \xi(t', \mathbf{x}) \right\}, \quad (2.7)$$

where $\mathbb{C}$ labels an integral on the Keldysh contour and $\rho_\mathrm{I}(t, \mathbf{x}) = g \sum_{i=1}^{N} \delta(\mathbf{q}_i(t) - \mathbf{x})$ is the instantaneous impurity density.

After an integration over the Grassmann fields in Eq. (2.6), the formal result obtained is

$$P(\mathbf{Q}_f, t_f | \mathbf{Q}_i, t_i) = \int_{\mathbf{Q_i}}^{\mathbf{Q_F}} D\mathbf{Q}\ e^{\frac{i}{\hbar} \Phi_{\mathbb{C}}[\mathbf{Q}]} e^{i \frac{m_\mathrm{I}}{2\hbar} \sum_{j=1}^{N} \int_{\mathbb{C}} dt'\, \dot{\mathbf{q}}_j^2}, \quad (2.8)$$

where $\Phi_{\mathbb{C}}[\mathbf{Q}]$ is the so-called Feynman-Vernon influence functional [27]. The meaning of $\Phi_{\mathbb{C}}[\mathbf{Q}]$ can be understood directly from the last equation for $P(\mathbf{Q}_f, t_f | \mathbf{Q}_i, t_i)$: indeed, in the exponent of the path integral the last term describe the free dynamics of the impurities related to $\hat{H}_\mathrm{I}$, while all the contributions from $\hat{H}_\mathrm{F}$ and $\hat{V}$ are encoded in $\Phi_{\mathbb{C}}[\mathbf{Q}]$. This description is general and no approximations have been done so far, but computing and using the exact expression of the influence functional is generally extremely complicated. Also in this system, with non-interacting bath and contact interaction, some approximations are desirable.

Integral over Grassmann fields can be carried out analytically with standard techniques for Grassmann fields, see e.g. Sec. 1.5 of Ref. [25], and therefore the influence functional in Eq. (2.8) is formally given by

$$i\Phi_{\mathbb{C}}[\mathbf{Q}] = \mathrm{Tr} \left[\log \left(i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu(T) + \rho_\mathrm{I}(t, \mathbf{x}) \right) \right]. \quad (2.9)$$

Before starting the chain of approximations that is fundamental in the calculations of this chapter, a small clarifying comment is useful. The goal of the manipulations is to obtain a simpler form of the exponent in the path integral for the transition probability: in this way it will be possible to build an analogy between this system and a classical one and derive the semiclassical equations of motion for the impurities.

The first step is to expand the logarithm in the expression of $\Phi_{\mathbb{C}}[\mathbf{Q}]$ in Taylor series to obtain terms of order zeroth, first etc. in powers of the impurity density ρ_I. The first three terms of the expansion are

$$\log \left(i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu(T) + \rho_\mathrm{I}(t, \mathbf{x}) \right) = \log \left(i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu(T) \right) + \log \left(1 + \frac{\rho_\mathrm{I}(t, \mathbf{x})}{i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu(T)} \right) =$$
$$= \log \left(i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu(T) \right) + \frac{\rho_\mathrm{I}(t, \mathbf{x})}{i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu(T)} + \frac{1}{2} \left(\frac{\rho_\mathrm{I}(t, \mathbf{x})}{i\hbar \partial_t - \frac{\hbar^2 \nabla^2}{2m} - \mu(T)} \right)^2 + \ldots \quad (2.10)$$

Truncating the expansion at second order is justified when the density of impurities is small. Note that, since the expansion in Eq. (2.10) only consider ρ_I, also strongly interacting impurities in some limits can be described within this approximation.

Inserting Eq. (2.10) in Eq. (2.9) three terms are obtained: the first term is of order 0 in ρ_I, does not depend on the configuration of impurities $\mathbf{Q}$ and therefore can be reabsorbed in the integration measure. The second term is of first order in ρ_I and gives this contribution to the

influence functional

$$\text{Tr}\left(\frac{\rho_{\text{I}}(t,\mathbf{x})}{i\hbar\partial_t - \frac{\hbar^2\nabla^2}{2m} - \mu(T)}\right) = \iint_{\mathcal{C}} dxdy \ \langle y| \frac{1}{i\hbar\partial_t - \frac{\hbar^2\nabla^2}{2m} - \mu(T)} |y\rangle \langle y| \rho_{\text{I}} |x\rangle =$$
$$= \iint_{\mathcal{C}} dxdy \ \delta(x-y)\rho_{\text{I}}(x)G_{\mathcal{C}}(x-y), \tag{2.11}$$

where $G_{\mathcal{C}}$ is the fermionic propagator on the Keldysh contour. Using the explicit form of ρ_{I}, a constant energy shift that does not affect the dynamics of the system is obtained. Finally, the last term, of second order is ρ_{I}, is

$$\text{Tr}\left(\frac{\rho_{\text{I}}(t,\mathbf{x})}{i\hbar\partial_t - \frac{\hbar^2\nabla^2}{2m} - \mu(T)}\right)^2 = \iiiint_{\mathcal{C}} dxdydy'dy'' \ \langle x| \frac{1}{i\hbar\partial_t - \frac{\hbar^2\nabla^2}{2m} - \mu(T)} |y'\rangle \langle y'| \rho_{\text{I}} |y\rangle \times$$
$$\times \langle y| \frac{1}{i\hbar\partial_t - \frac{\hbar^2\nabla^2}{2m} - \mu(T)} |y''\rangle \langle y''| \rho_{\text{I}} |x\rangle =$$
$$= \iiiint_{\mathcal{C}} dxdydy'dy'' \ G_{\mathcal{C}}(x-y')\rho_{\text{I}}(y)\delta(y'-y)G_{\mathcal{C}}(y-y'')\delta(x-y'')\rho_{\text{I}}(x) =$$
$$= \iint_{\mathcal{C}} dxdy \ \rho_{\text{I}}(x)G_{\mathcal{C}}(x-y)G_{\mathcal{C}}(y-x)\rho_{\text{I}}(y). \tag{2.12}$$

The resulting expression for the transition probability with the zeroth order contribution reabsorbed in the integration measure and the constant energy shift neglected is, with all variables split on the branches of the contour,

$$P(\mathbf{Q}_f,t|\mathbf{Q}_i,0) = \int_{\mathbf{Q}_i}^{\mathbf{Q_f}} \mathcal{D}\mathbf{Q}' \int_{\mathbf{Q}_i}^{\mathbf{Q_f}} \mathcal{D}\mathbf{Q}'' \ e^{i\Phi(\mathbf{Q}',\mathbf{Q}'')} \ e^{i\frac{m_{\text{I}}}{2\hbar}\sum_{j=1}^{N}\int_0^t dt'\left(\dot{\mathbf{q}}_j'^2 - \dot{\mathbf{q}}_j''^2\right)}, \tag{2.13}$$

with

$$\Phi(\mathbf{Q}',\mathbf{Q}'') = \frac{i}{2}\sum_{a,b=\pm} \iint_0^t dt'dt'' \iint dxdy \ \rho_a(t',\mathbf{x})\Delta_{ab}(t'-t'',\mathbf{x}-\mathbf{y}) \ \rho_b(t'',\mathbf{y}). \tag{2.14}$$

In the last expression, a and b are the branches of the Keldysh contour $\mathcal{C}$, primed variables are referred to the forward branch, double primed branch to the backward. Moreover, from now on the impurity density is labelled as ρ instead of ρ_{I} for sake of brevity without any ambiguity. In the free term of the action $\dot{\mathbf{q}}_j'^2 - \dot{\mathbf{q}}_j''^2$ the relative minus sign is a direct consequence of the splitting onto the two branches as explained in Chapter 1. The key term in Eq. (2.14) is Δ_{ab}, i.e. the entries of the 2×2 matrix $\Delta_{\mathcal{C}}$, defined as

$$\Delta_{\mathcal{C}}(x-y) = G_{\mathcal{C}}(x-y)G_{\mathcal{C}}(y-x). \tag{2.15}$$

The four entries are defined through the time ordering operation on the Keldysh contour and are given by, in analogy with the Green function defined in the previous Chapter

$$\Delta_{++}(t,\mathbf{x}) = \Delta_{\text{T}}(t,\mathbf{x}) = iD^{\text{T}}(t,\mathbf{x}) \tag{2.16}$$
$$\Delta_{+-}(t,\mathbf{x}) = -\Delta_{<}(t,\mathbf{x}) = -iD^{<}(t,\mathbf{x}) \tag{2.17}$$
$$\Delta_{-+}(t,\mathbf{x}) = -\Delta_{>}(t,\mathbf{x}) = -iD^{>}(t,\mathbf{x}) \tag{2.18}$$
$$\Delta_{--}(t,\mathbf{x}) = \Delta_{\tilde{\text{T}}}(t,\mathbf{x}) = iD^{\tilde{\text{T}}}(t,\mathbf{x}). \tag{2.19}$$

In these expressions, $D^{>}(t,\mathbf{x}), D^{<}(t,\mathbf{x})$ and $D^{\text{T}}(t,\mathbf{x})$ are the standard fermionic polarization propagators of many-body theory [24, 28], i.e. bubble-like diagrams. However, the explicit form of Δ is not strictly necessary to derive the equation of motion for the impurities. Therefore, the derivation of the above equations will be carried out using only general properties of the propagators, the explicit form of which will be used only when strictly necessary.
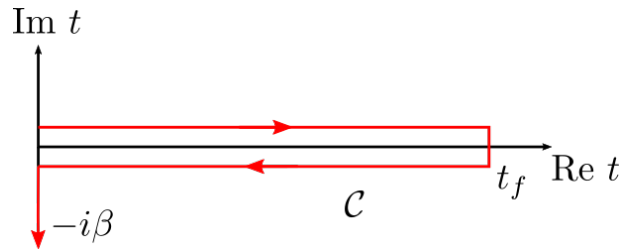
Figure 2.2. Keldysh contour with the vertical piece for the initial average over degrees of freedom of the bath.

2.2 Effective stochastic dynamics of heavy impurities

Starting from Eq (2.14) it is now possible to derive the desired stochastic equation of motion for the impurities. This is done using different approximations justified by physical properties.

2.2.1 Small frequency expansion

Impurities considered in this system are heavy, therefore their dynamics is expected to be slow compared with the typical timescales of the bath. Then, it is possible to expand Δ_{ab} in frequency around $\omega = 0$

$$\Delta_{ab}(t, \mathbf{x}) = \int \frac{d\omega}{2\pi} \, e^{-i\omega t} \left(\sum_{n=0}^{\infty} \frac{\omega^n}{n!} \, F_{ab}^{(n)}(x) \right) = F_{ab}^{(0)}(\mathbf{x}) + i\frac{d}{dt}\delta(t)F_{ab}^{(1)}(\mathbf{x}) + \dots, \qquad (2.20)$$

where

$$F_{ab}^{(0)}(\mathbf{x} - \mathbf{y}) \;\equiv\; \Delta_{ab}(\omega = 0, \mathbf{x} - \mathbf{y}) \qquad (2.21)$$

$$F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \;\equiv\; \lim_{\omega \to 0} \frac{d}{d\omega} \Delta_{ab}(\omega, \mathbf{x} - \mathbf{y}), \qquad (2.22)$$

and the dots denote higher order terms in the Taylor expansion that are not considered. Note that the first term of the expansion corresponds to the infinite mass limit of the impurities when they are frozen in their position.

It is useful to recall some properties of propagators Δ_{ab} and introduce the retarded propagator Δ_{R} to better work with Eq. (2.20). The retarded propagator is defined as

$$\Delta_{\mathrm{R}}(x - y) = \Delta_{\mathrm{T}}(x - y) - \theta(t_x - t_y)\Delta_{<}(x - y), \qquad (2.23)$$

and by definition

$$\Delta_{\mathrm{T}}(x - y) = (\Delta_{\tilde{\mathrm{T}}}(x - y))^* \qquad (2.24)$$

$$\Delta_{\mathrm{T}}(x - y) = \Delta_{\mathrm{T}}(y - x) \qquad (2.25)$$

$$\Delta_{>}(x - y) = \Delta_{<}(y - x). \qquad (2.26)$$

Now, a slightly different version of the closed-time contour is used here. In this version, also a vertical piece [29], that represents the initial average over the degrees of freedom of the bath, is included, Fig 2.2. Thanks to the presence of the vertical piece, on which the impurities are not propagating on by construction, the Kubo-Martin-Schwinger (KMS) relation is satisfied, implying that

$$\Delta_{<}(t, \mathbf{x}) = \Delta_{>}(t - i\beta, \mathbf{x}) \quad \text{if} \quad 0 \le \mathrm{Im}\, t \le \beta. \qquad (2.27)$$

KMS relation is extremely important because in it are encoded information on the thermodynamic properties of our system, like the equilibrium of the bath. In momentum space it has the form

$$\widetilde{\Delta}_<(\omega, \mathbf{x}) = e^{-\beta\omega}\widetilde{\Delta}_>(\omega, \mathbf{x}), \tag{2.28}$$

where $\widetilde{\Delta}$ is the Fourier transform in frequency space of Δ. Indeed,

$$\widetilde{\Delta}_<(\omega, \mathbf{x}) = \int_\infty^\infty dt\ e^{-i\omega t}\Delta_<(t, \mathbf{x}) = \int_{-\infty+i\beta}^{\infty+i\beta} dt\ e^{i\omega t}\Delta_<(t, \mathbf{x}) =$$

$$= e^{-\beta\omega}\int_{-\infty}^\infty du\ e^{i\omega u}\Delta_>(u, \mathbf{x}) = e^{-\beta\omega}\widetilde{\Delta}_>(\omega, \mathbf{x}). \tag{2.29}$$

Moreover, the spectral density σ can be written as $\sigma(\omega, \mathbf{k}) = \widetilde{\Delta}_>(\omega, \mathbf{k}) - \widetilde{\Delta}_<(\omega, \mathbf{k})$ and therefore from Eq. (2.28)

$$\widetilde{\Delta}_<(\omega, \mathbf{k}) = \frac{\sigma(\omega, \mathbf{k})}{e^{\beta\omega} - 1}. \tag{2.30}$$

Another useful formulation is

$$\sigma(\omega, \mathbf{k}) = (1 - e^{-\beta\omega})\Delta_>(\omega, \mathbf{k}) = (e^{\beta\omega} - 1)\Delta_<(\omega, \mathbf{k}), \tag{2.31}$$

and it is also useful to remember that σ is odd in ω, i.e. $\sigma(-\omega, \mathbf{k}) = -\sigma(\omega, \mathbf{k})$.

Finally, from Eq. (2.23) in momentum space it follows that $\sigma(\omega, \mathbf{k}) = 2\mathrm{Re}\widetilde{\Delta}_\mathrm{R}(\omega, \mathbf{k})$. It is now evident that only Δ_R is needed to compute the influence functional: this is possible because the bath considered is at equilibrium, i.e. on the timescales relevant for the dynamics of heavy impurities particles of the bath thermalize back to equilibrium state. Note that this is also in agreement with the Keldysh-rotated GFs introduced in Chapter 1, where at equilibrium the Keldysh component can be expressed only in terms of the imaginary part of the retarded component.

With the previously described properties of Δ_{ab} it can be proved that $F_{ab}^{(1)}$ is odd in position space, indeed

$$F_{ab}^{(1)}(\mathbf{x}-\mathbf{y}) = \lim_{\omega\to 0}\frac{d}{d\omega}\widetilde{\Delta}_{ab}(\omega, \mathbf{x}-\mathbf{y}) = \lim_{\omega\to 0}\frac{d}{d\omega}\int_{-\infty}^\infty dt\ e^{i\omega t}\Delta_{ab}(t, \mathbf{x}-\mathbf{y}) = i\int_{-\infty}^\infty dt\ t\Delta_{ab}(t, \mathbf{x}-\mathbf{y}) =$$

$$\overset{u=-t}{=} -i\int_{-\infty}^\infty du\ u\Delta_{ab}(-u, \mathbf{x}-\mathbf{y}) = -i\int_{-\infty}^\infty dt\ t\Delta_{ba}(-t, \mathbf{y}-\mathbf{x}) = -F_{ba}^{(1)}(\mathbf{y}-\mathbf{x}), \tag{2.32}$$

where the fact that $\Delta_{ab}(x-y) = \Delta_{ba}(y-x)$ has been used. Thanks to convolution theorem, the Fourier transform in frequency of Δ_T can be written as

$$\widetilde{\Delta}_\mathrm{T}(\omega, \mathbf{x}) = \int_{-\infty}^\infty d\eta\ \left\{\left[\pi\delta(\eta-\omega) + \frac{i}{\eta-\omega}\right]\widetilde{\Delta}_>(\eta, \mathbf{x}) + \left[\pi\delta(\eta-\omega) - \frac{i}{\eta-\omega}\right]\widetilde{\Delta}_<(\eta, \mathbf{x})\right\} =$$

$$= \pi(\widetilde{\Delta}_>(\omega, \mathbf{x}) + \widetilde{\Delta}_<(\omega, \mathbf{x})) + i\int_{-\infty}^\infty d\eta\ \frac{\sigma(\eta, \mathbf{x})}{\eta-\omega}, \tag{2.33}$$

and after a differentiation with respect to ω of Eq. (2.33) it follows that

$$F_{11}^{(1)}(\mathbf{x}-\mathbf{y}) = F_{22}^{(1)}(\mathbf{x}-\mathbf{y}) = 0 \tag{2.34}$$

The properties of $F_{ab}^{(1)}$ will be used to deal with the form of the influence functional. The first

step is inserting the expansions of Eq. (2.21,2.22) inside Eq. (2.14)

$$\Phi(\mathbf{Q}', \mathbf{Q}'') = \frac{i}{2} \sum_{a,b=\pm} I(\mathbf{Q}', \mathbf{Q}'') \tag{2.35}$$

$$I(\mathbf{Q}', \mathbf{Q}'') = \iint_0^t dt' dt'' \iint d\mathbf{x} d\mathbf{y} \; \rho_a(t', \mathbf{x}) \Delta_{ab}(t' - t'', \mathbf{x} - \mathbf{y}) \; \rho_b(t'', \mathbf{y}) =$$

$$= \iint_0^t dt' dt'' \iint d\mathbf{x} d\mathbf{y} \; \rho_a(t', \mathbf{x}) \left(F_{ab}^{(0)}(\mathbf{x} - \mathbf{y}) \delta(t' - t'') + i F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \frac{d}{d(t' - t'')} \delta(t' - t'') \right) \rho_b(t'', \mathbf{y}) =$$

$$= \int_0^t du \iint d\mathbf{x} d\mathbf{y} \; \rho_a(u, \mathbf{x}) \left[F_{ab}^{(0)}(\mathbf{x} - \mathbf{y}) \rho_b(u, \mathbf{y}) + i \int_{u-t}^u ds \; \left(\frac{d}{ds} \delta(s) \right) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \rho_b(u - s, \mathbf{y}) \right] =$$

$$= \alpha + \alpha'. \tag{2.36}$$

The term α' can be calculated via an integration by parts

$$\alpha' = i \int_0^t du \iint d\mathbf{x} d\mathbf{y} \left\{ \left[\rho_a(u, \mathbf{x}) \delta(s) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \rho_b(u - s, \mathbf{y}) \right]_{s=u-t}^{s=u} + \right.$$

$$\left. -i \int_{u-t}^u ds \; \rho_a(u, \mathbf{x}) \delta(s) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \frac{d}{ds} \rho_b(u - s, \mathbf{y}) \right\} = \alpha_0' + \alpha_1'$$

$$\alpha_1' = i \int_0^t du \int_{u-t}^u ds \iint d\mathbf{x} d\mathbf{y} \; \rho_a(u, \mathbf{x}) \delta(s) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \frac{d}{du} \rho_b(u - s, \mathbf{y}) =$$

$$= i \int_0^t du \iint d\mathbf{x} d\mathbf{y} \rho_a(u, \mathbf{x}) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \frac{d}{du} \rho_b(u, \mathbf{y})$$

$$\alpha_0' = i \int_0^t du \iint d\mathbf{x} d\mathbf{y} \; \rho_a(u, \mathbf{x}) \delta(u) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \rho_b(0, \mathbf{y}) - \rho_a(u, \mathbf{x}) \delta(u - t) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \rho_b(t, \mathbf{y}) =$$

$$= i \iint d\mathbf{x} d\mathbf{y} \; \rho_a(0, \mathbf{x}) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \rho_B(0, \mathbf{y}) - \rho_a(t, \mathbf{x}) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \rho_B(t, \mathbf{y}) = 0, \tag{2.37}$$

where the last equality is a consequence of Eq. (2.32,2.34). The influence functional therefore has the form

$$\Phi(\mathbf{Q}', \mathbf{Q}'') = \frac{i}{2} \sum_{a,b=\pm} \int_0^t du \iint d\mathbf{x} d\mathbf{y} \; \left[\rho_a(u, \mathbf{x}) F_{ab}^{(0)}(\mathbf{x} - \mathbf{y}) \rho_b(u, \mathbf{y}) + \right.$$

$$\left. i \rho_a(u, \mathbf{x}) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \frac{d}{du} \rho_b(u, \mathbf{y}) \right]. \tag{2.38}$$

The next step is using the explicit expression of ρ inside the above expression for the influence functional. It is convenient to separate $\Phi(\mathbf{Q}', \mathbf{Q}'')$ in two different terms, one without and one with the total time derivative of ρ. The first term, the one without the time derivative, is

$$\iint d\mathbf{x} d\mathbf{y} \; \rho_a(u, \mathbf{x}) F_{ab}^{(0)}(\mathbf{x} - \mathbf{y}) \rho_b(u, \mathbf{y}) =$$

$$= g^2 \sum_{i,j=1}^N \iint d\mathbf{x} d\mathbf{y} \; \delta(\mathbf{x} - \mathbf{q}_{i,a}(u)) F_{ab}^{(0)}(\mathbf{x} - \mathbf{y}) \delta(\mathbf{y} - \mathbf{q}_{j,b}(u)) =$$

$$= \sum_{i,j=1}^N F_{ab}^{(0)}(\mathbf{q}_{i,a}(u) - \mathbf{q}_{j,b}(u)). \tag{2.39}$$

In the second term, the explicit expression for the time derivative is

$$\frac{d}{du} \rho_b(u, \mathbf{y}) = g \sum_{j=1}^N \dot{\mathbf{q}}_{j,b} \frac{\partial}{\partial q_{j,b}} \delta(\mathbf{q}_{j,b} - \mathbf{y}), \tag{2.40}$$

so the term inside the influence functional is

$$i \iint d\mathbf{x} d\mathbf{y} \; \rho_a(u, \mathbf{x}) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \frac{d}{du} \rho_b(u, \mathbf{y}) =$$

$$= ig^2 \sum_{i,j=1}^{N} \iint d\mathbf{x} d\mathbf{y} \; \delta(\mathbf{x} - \mathbf{q}_{i,a}(u)) F_{ab}^{(1)}(\mathbf{x} - \mathbf{y}) \dot{\mathbf{q}}_{j,b} \frac{\partial}{\partial q_{j,b}} \delta(\mathbf{q}_{j,b} - \mathbf{y}) =$$

$$= -ig^2 \sum_{i,j=1}^{N} \int d\mathbf{y} \; F_{ab}^{(1)}(\mathbf{q}_{i,a}(u) - \mathbf{y}) \frac{\partial}{\partial y} \delta(\mathbf{q}_{j,b} - \mathbf{y}) \dot{\mathbf{q}}_{j,b}(u) =$$

$$= ig^2 \sum_{i,j=1}^{N} \frac{\partial}{\partial q_{j,b}} F_{ab}^{(1)}(\mathbf{q}_{i,a} - \mathbf{q}_{j,b}) \dot{\mathbf{q}}_{j,b}(u) \tag{2.41}$$

Finally, thanks to Eq. (2.32,2.34), the influence functional becomes

$$\Phi(\mathbf{Q}', \mathbf{Q}'') = \frac{ig^2}{2} \sum_{i,j=1}^{N} \int_0^t du \left\{ F_{\mathrm{T}}^{(0)}(\mathbf{q}_{i,1} - \mathbf{q}_{j,1}) + F_{\tilde{T}}^{(0)}(\mathbf{q}_{i,2} - \mathbf{q}_{j,2}) - F_{<}^{(0)}(\mathbf{q}_{i,1} - \mathbf{q}_{j,2}) + \right.$$
$$\left. - F_{>}^{(0)}(\mathbf{q}_{i,2} - \mathbf{q}_{j,1}) - i\dot{\mathbf{q}}_{j1} \frac{\partial}{\partial \mathbf{q}_{j,1}} F_{>}^{(1)}(\mathbf{q}_{i,2} - \mathbf{q}_{j,1}) - i\dot{\mathbf{q}}_{j2} \frac{\partial}{\partial \mathbf{q}_{j,2}} F_{<}^{(1)}(\mathbf{q}_{i,1} - \mathbf{q}_{j,2}) \right\}. \tag{2.42}$$

At this point, it is convenient to introduce the so-called complex potential $\mathcal{V}(\mathbf{x} - \mathbf{y})$:

$$i\mathcal{V}(\mathbf{x} - \mathbf{y}) \equiv F_{\mathrm{T}}^{(0)}(\mathbf{x} - \mathbf{y}) = V(\mathbf{x} - \mathbf{y}) + iW(\mathbf{x} - \mathbf{y}), \tag{2.43}$$

A direct relation between $\mathcal{V}$ and the retarded polarization propagator can be derived for this system. Thanks to Eq. (2.28,2.32) it is proved that

$$F_{<}^{(0)}(\mathbf{k}) = F_{>}^{(0)}(\mathbf{k}) \tag{2.44}$$

$$F_{<}^{(1)}(\mathbf{k}) = -F_{>}^{(1)}(\mathbf{k}). \tag{2.45}$$

From this directly follows that

$$\partial_\omega \Delta_<(\omega, \mathbf{k}) = \partial_\omega (e^{-\beta\omega} \Delta_>(\omega, \mathbf{k})) = e^{-\beta\omega}(-\beta \Delta_>(\omega, \mathbf{k}) + \partial_\omega \Delta_>(\omega, \mathbf{k})) \xrightarrow{\omega \to 0}$$

$$\xrightarrow{\omega \to 0} \quad F_{<}^{(1)}(\mathbf{k}) = -\beta F_{>}^{(0)}(\mathbf{k}) + F_{>}^{(1)}(\mathbf{k}) = -\beta F_{>}^{(0)}(\mathbf{k}) - F_{<}^{(1)}(\mathbf{k}), \tag{2.46}$$

and the useful relation

$$F_{<}^{(1)}(\mathbf{k}) = -\frac{\beta}{2} F_{<}^{(0)}(\mathbf{k}) = -\frac{\beta}{2} F_{>}^{(0)}(\mathbf{k}) = -F_{>}^{(1)}(\mathbf{k}), \tag{2.47}$$

is derived. Remembering that $\sigma(\omega, \mathbf{k}) = 2\mathrm{Re}\widetilde{\Delta}_\mathrm{R}(\omega, \mathbf{k})$ the small frequency expansion of $\mathrm{Re}\widetilde{\Delta}_R$ is

$$\mathrm{Re}\widetilde{\Delta}_R(\omega, \mathbf{k}) = A^\mathrm{R}(\mathbf{k}) + \omega B^\mathrm{R}(\mathbf{k}) = \omega B^\mathrm{R}(\mathbf{k}), \tag{2.48}$$

where $A^\mathrm{R}(\mathbf{k}) = 0$ because $\sigma(\omega, \mathbf{k})$ is odd in ω. It immediately follows that

$$\widetilde{\Delta}_<(\omega, \mathbf{k}) = \frac{2}{e^{\beta\omega} - 1} \mathrm{Re}\widetilde{\Delta}_\mathrm{R}(\omega, \mathbf{k}), \tag{2.49}$$

and thus

$$F_{<}^{(0)}(\mathbf{k}) = \lim_{\omega \to 0} \frac{2}{e^{\beta\omega} - 1} \mathrm{Re}\widetilde{\Delta}_R(\omega, \mathbf{k}) = \frac{2}{\beta} B^\mathrm{R}(\mathbf{k}) \tag{2.50}$$

$$F_{<}^{(1)}(\mathbf{k}) = -B^\mathrm{R}(\mathbf{k}). \tag{2.51}$$

It is now possible to conclude that

$$F_{\mathrm{T}}^{(0)}(\mathbf{k}) = \lim_{\omega \to 0}(\mathrm{Re}\widetilde{\Delta}_{\mathrm{R}}(\omega, \mathbf{k}) + i\mathrm{Im}\widetilde{\Delta}_{\mathrm{R}}(\omega, \mathbf{k}) + \widetilde{\Delta}_<(\omega, \mathbf{k})) = i\mathrm{Im}\widetilde{\Delta}_{\mathrm{R}}(\omega = 0, \mathbf{k}) + F_<^{(0)}(\mathbf{k}) =$$

$$= i\mathrm{Im}\widetilde{\Delta}_{\mathrm{R}}(\omega = 0, \mathbf{k}) + \frac{2}{\beta}B^{\mathrm{R}}(\mathbf{k}) = i\mathcal{V}(\mathbf{k}). \tag{2.52}$$

So, the complex potential $\mathcal{V}$ is written in terms of the retarded propagator Δ_{R} as a consequence of bath properties. The complex potential itself is divided in a real and an imaginary part

$$\mathcal{V}(\mathbf{x} - \mathbf{y}) = V(\mathbf{x} - \mathbf{y}) + iW(\mathbf{x} - \mathbf{y}), \tag{2.53}$$

and the real and imaginary potentials V and W can be written in terms of the retarded polarization propagator D^{R} as

$$V(\mathbf{x} - \mathbf{y}) = \mathrm{Im}\Delta_{\mathrm{R}}(\omega = 0, \mathbf{x} - \mathbf{y}) = \mathrm{Re}D^{\mathrm{R}}(\omega = 0, \mathbf{x} - \mathbf{y}) \tag{2.54}$$

$$W(\mathbf{x} - \mathbf{y}) = -\frac{2}{\beta}\lim_{\omega \to 0}\frac{1}{\omega}\mathrm{Re}\Delta_{\mathrm{R}}(\omega, \mathbf{x} - \mathbf{y}) = \frac{2}{\beta}\lim_{\omega \to 0}\frac{1}{\omega}\mathrm{Im}D^{\mathrm{R}}(\omega, \mathbf{x} - \mathbf{y}). \tag{2.55}$$

The purpose of having introduced the complex potential is to write $\Phi(\mathbf{Q}', \mathbf{Q}'')$ in terms of V and W, because later it will become clear how real and imaginary potentials affect the dynamics. Inserting the equalities $F_F^{(0)} = i\mathcal{V}$, $F_{\tilde{F}}^{(0)} = -i\mathcal{V}^*$ and $F_<^{(0)} = -W$ in Eq. (2.42) the influence functional becomes

$$\Phi(\mathbf{Q}', \mathbf{Q}'') = \frac{ig^2}{2}\sum_{i,j=1}^{N}\int_0^t du\,\{i\mathcal{V}(\mathbf{q}_{i,1} - \mathbf{q}_{j,1}) - i\mathcal{V}^*(\mathbf{q}_{i,2} - \mathbf{q}_{j,2}) + W(\mathbf{q}_{i,1} - \mathbf{q}_{j,2}) +$$

$$+W(\mathbf{q}_{i,2} - \mathbf{q}_{j,1}) + i\frac{\beta}{2}\dot{\mathbf{q}}_{j,1}\frac{\partial}{\partial\mathbf{q}_{j,1}}W(\mathbf{q}_{i,2} - \mathbf{q}_{j,1}) - i\frac{\beta}{2}\dot{\mathbf{q}}_{j,2}\frac{\partial}{\partial\mathbf{q}_{j,2}}W(\mathbf{q}_{i,1} - \mathbf{q}_{j,2})\}, \tag{2.56}$$

since $W(\mathbf{q}_{i,1} - \mathbf{q}_{j,2}) = W(\mathbf{q}_{i,2} - \mathbf{q}_{j,1})$ and $W(\mathbf{x}) = W(-\mathbf{x})$ for symmetry reasons and

$$\dot{\mathbf{q}}_{j,1}\frac{\partial}{\partial\mathbf{q}_{j,1}}W(\mathbf{q}_{i,2} - \mathbf{q}_{j,1}) = -\dot{\mathbf{q}}_{j,1}\frac{\partial}{\partial\mathbf{q}_{i,2}}W(\mathbf{q}_{i,2} - \mathbf{q}_{j,1}) = -\dot{\mathbf{q}}_{i,1}\frac{\partial}{\partial\mathbf{q}_{j,2}}W(\mathbf{q}_{j,2} - \mathbf{q}_{1,1}). \tag{2.57}$$

After a permutation of indices i and j the final form of $\Phi(\mathbf{Q}', \mathbf{Q}'')$ is obtained

$$\Phi(\mathbf{Q}', \mathbf{Q}'') = \frac{g^2}{2}\sum_{i,j=1}^{N}\int_0^t du\,\{\mathcal{V}^*(\mathbf{q}_{i,2} - \mathbf{q}_{j,2}) - \mathcal{V}(\mathbf{q}_{i,1} - \mathbf{q}_{j,1}) + 2iW(\mathbf{q}_{i,1} - \mathbf{q}_{j,2}) +$$

$$+\frac{\beta}{2}(\dot{\mathbf{q}}_{i,1} + \dot{\mathbf{q}}_{j,2})\frac{\partial}{\partial\mathbf{q}_{j,2}}W(\mathbf{q}_{i,1} - \mathbf{q}_{j,2})\}. \tag{2.58}$$

2.2.2   Classical limit

The next approximation made is to consider the classical limit for the dynamics of the impurities. In order to implement this approximation, in Eq. (2.42) the change of variables

$$\mathbf{r}_i = \frac{1}{2}(\mathbf{q}_{i,1} + \mathbf{q}_{i,2}) \qquad \mathbf{y}_i = \mathbf{q}_{i,1} - \mathbf{q}_{i,2}, \tag{2.59}$$

is performed. With this change of variables the free part of the action takes the form, see Eq. (2.13),

$$S_0[\mathbf{r}, \mathbf{y}] = \frac{m_{\mathrm{I}}}{\hbar}\sum_{i=1}^{N}\int_0^t du\,\dot{\mathbf{r}}_i \cdot \dot{\mathbf{y}}_i = \frac{m_{\mathrm{I}}}{\hbar}\sum_{i=1}^{N}\int_0^t du\,\ddot{\mathbf{r}}_i \cdot \mathbf{y}_i, \tag{2.60}$$

after an integration by parts. Therefore inside the transition probability there is the term

$$\exp\left(\frac{im_{\mathrm{I}}}{\hbar}\sum_{i=1}^{N}\int_0^t du\,\ddot{\mathbf{r}}_i\cdot\mathbf{y}_i\right),\tag{2.61}$$

and the dominant contribution to the path integral is expected to come from the functional region where the time integral in the exponent is small (or at most order unity). To estimate this region, please note that $\int_0^t du\,\ddot{\mathbf{r}}_i\cdot\mathbf{y}_i\sim\sqrt{k_{\mathrm{B}}T/m_{\mathrm{I}}}|\mathbf{y}_i|$, where $\sqrt{k_{\mathrm{B}}T/m_{\mathrm{I}}}$ is the average thermal velocity of the impurities. Then, the stationary phase condition implies $|\mathbf{y}_i|\lesssim\sqrt{1/m_{\mathrm{I}}k_{\mathrm{B}}T}$. In the limit of heavy impurities considered here, fluctuations of $|\mathbf{y}_i|$ become small compared to all relevant length scales and thus the influence functional can be expanded to second order in $\mathbf{y}_i$. The new variables $\mathbf{r}_i$ and $\mathbf{y}_i$ are inserted in Eq. (2.58) and the influence functional is expanded, but this procedure is too long to be reported here and therefore it is discussed in Appendix A. It is also better to define the rescaled imaginary potential W_{R} as

$$W_{\mathrm{R}}(\mathbf{x}-\mathbf{y})=\frac{\beta}{2}W(\mathbf{x}-\mathbf{y}),\tag{2.62}$$

for an easier understanding. The resulting transition probability is

$$P(\mathbf{R}_f,t|\mathbf{R}_i,0)=\int_{\mathbf{R}_i}^{\mathbf{R}_f}\mathcal{D}\mathbf{R}\int_0^0\mathcal{D}\mathbf{Y}\exp\left\{-\frac{i}{\hbar}\int_0^t dt'\,[\mathbf{y}_i\,(m_{\mathrm{I}}\ddot{\mathbf{r}}_i+\Gamma_{ij}(\mathbf{R})\dot{\mathbf{r}}_j-\mathbf{F}_i(\mathbf{R}))+\right.$$
$$\left.-\frac{1}{2}\mathbf{y}_i\frac{2}{\beta}\Gamma_{ij}(\mathbf{R})\mathbf{y}_j\right]\right\},\tag{2.63}$$

where $\mathbf{R}=(\mathbf{r}_1,\ldots,\mathbf{r}_N)^T$, $\mathbf{Y}=(\mathbf{y}_1,\ldots,\mathbf{y}_N)^T$, the sum over repeated indices $i,j=1,\ldots,N$ is understood and $\mathbf{F}_i(\mathbf{R})$ and $\Gamma_{ij}(\mathbf{R})$ respectively are

$$\mathbf{F}_i(\mathbf{R})=-g^2\sum_{j=i}^{N}\nabla V(\mathbf{r}_i-\mathbf{r}_j)\tag{2.64}$$

$$\Gamma_{ij}(\mathbf{R})=g^2\mathcal{H}_{W_{\mathrm{R}}}(\mathbf{r}_i-\mathbf{r}_j),\tag{2.65}$$

where $\mathcal{H}_{W_{\mathrm{R}}}$ is the Hessian of W_{R} defined in Eq. (2.62). Gaussian integral in Eq. (2.63) can be carried out analytically leading to

$$P(\mathbf{R}_f,t|\mathbf{R}_i,0)=\int_{\mathbf{R}_i}^{\mathbf{R}_f}\mathcal{D}\mathbf{R}\,e^{-\int_0^t d\tau\left(m_{\mathrm{I}}\ddot{\mathbf{R}}-m_{\mathrm{I}}\Gamma(\mathbf{R})\dot{\mathbf{R}}-\mathbf{F}(\mathbf{R})\right)^2},\tag{2.66}$$

that is the desired path integral over all possible trajectories for the transition probability between two configuration of impurities. The relative statistical weight of $\mathbf{R}(t)$ trajectories is determined by the functional at the exponent, which does not explicitly depend on $\hbar$. Indeed, this exponent corresponds to an action of Onsager-Machlup type [30], which characterizes path integral representation of propagators in classical Fokker-Planck dynamics.

A consequence of this conclusion is that the dynamics of the impurities can be described with a Langevin equation: indeed it is possible to prove that a Langevin dynamics generates a path integral expression for the transition probability $P(\mathbf{R}_f,t|\mathbf{R}_i,0)$ like the one in Eq. (2.66), see e.g. Ref [2, 31, 32]. Therefore, in the classical limit the dynamics of the impurities is described by the following equation:

$$m_{\mathrm{I}}\ddot{\mathbf{r}}_i=-\Gamma_{ij}(\mathbf{R})\dot{\mathbf{r}}_j+\mathbf{F}_i(\mathbf{R})+\boldsymbol{\Psi}_i(\mathbf{R},t),\tag{2.67}$$

that is called the generalized Langevin equation (GLE). On the left-hand side there is the resulting force on the i-th impurity, on the right-hand side there are three different terms:

viscosity, force and noise. The force term $\mathbf{F}_i(\mathbf{R})$ is defined in Eq. (2.64) and describe the force between impurities generated by the real potential V. The viscosity $\Gamma_{ij}(\mathbf{R})$ is given in Eq. (2.65) and describe the deterministic viscous effect of the medium on the impurities. Finally, the noise term $\boldsymbol{\Psi}_i(\mathbf{R}, t)$ is responsible for the stochastic part of the dynamics, being related to random thermal fluctuations. Viscosity and noise term also satisfy fluctuation-dissipation relation (FDR)

$$\langle \boldsymbol{\Psi}_i(\mathbf{R}, t) \rangle = 0 \tag{2.68}$$

$$\langle \boldsymbol{\Psi}_i(\mathbf{R}, t) \otimes \boldsymbol{\Psi}_j(\mathbf{R}, t') \rangle = \frac{2}{\beta} \Gamma_{ij}(\mathbf{R}) \delta(t - t'). \tag{2.69}$$

The definition of "generalized" for this Langevin equation is used because both viscosity and noise depend on the configuration of the impurities, contrary to the standard Langevin dynamics. Note also that in the FDR the noise is Markovian, as a consequence of the approximations made so far.

The GLE for this system is a semiclassical equation. Indeed, the description of the dynamics is based on a purely classical equation typical of a diffusion process but the quantum properties of the system are now encoded in the three terms on the right-hand side. It is also interesting to note that in the whole derivation made so far the specific form of $\mathcal{V}$ was not specified because it is not necessary. This point is of key importance, because it makes explicit that a derivation of $\mathcal{V}$ within a better approximation can be inserted directly into the GLE without any additional manipulation.

Generalized Langevin equation is derived for a generic case with N impurities, but now the focus is moved to two specific situations, the one impurity and the two impurity scenario. The first one is an instructive case also used to better understand the formalism, while the second contains the main numerical results of this treatment.

2.2.3 One impurity scenario

The first situation considered is the one impurity case, because it is the simplest one described by the model. Because $N = 1$, the notation is simplified as $\mathbf{R} = \mathbf{r}_1 \equiv \mathbf{r}$. The force term disappears, indeed $\nabla V(0) = 0$ because of symmetry properties and Newton third law. On the other hand, the viscosity now only has a constant contribution given by $\Gamma_{11}(0) \equiv \gamma$, so the GLE is

$$m_{\mathrm{I}} \ddot{\mathbf{r}} = -\gamma \dot{\mathbf{r}} + \boldsymbol{\Psi}(t), \tag{2.70}$$

that corresponds to the equation of Brownian motion with white noise that is no longer dependent on the configuration. Therefore, in the long time limit the squared displacement grows linearly and the kinetic energy thermalizes with the bath as for standard Brownian motion [33].

What is described here is useful also in the generic multi-impurities scenario: indeed, now it is even clearer that all the force terms are only present when other impurities are considered. Moreover, each impurity feels a constant friction term γ and a configuration-dependent friction term that is present only in the multi-impurities scenario because sensitive to the modification of the bath due to the presence of the other impurities. Also in the $N > 1$ scenario it is possible to engineer a situation with N independent Brownian motions are present: if the impurities are distant enough force and configuration-dependent viscosity terms are both expected to become negligible in absence of long-range interactions.

2.2.4 Two impurities scenario

When two impurities are present in the system, interesting effects appear. The two GLEs of the impurities are

$$m_I \ddot{\mathbf{r}}_1 = -(\gamma \dot{\mathbf{r}}_1 + \Gamma_{12}(\mathbf{r}_1 - \mathbf{r}_2)\dot{\mathbf{r}}_2) + \mathbf{F}_1(\mathbf{r}_1 - \mathbf{r}_2) + \mathbf{\Psi}_1(\mathbf{r}_1 - \mathbf{r}_2, t) \tag{2.71}$$

$$m_I \ddot{\mathbf{r}}_2 = -(\Gamma_{21}(\mathbf{r}_1 - \mathbf{r}_2)\dot{\mathbf{r}}_1 + \gamma \dot{\mathbf{r}}_2) - \mathbf{F}_1(\mathbf{r}_1 - \mathbf{r}_2) + \mathbf{\Psi}_2(\mathbf{r}_1 - \mathbf{r}_2, t), \tag{2.72}$$

and $\Gamma_{11}(0) = \Gamma_{22}(0) = \gamma$ as before. Indeed, all the $\Gamma_{ii}(0)$ terms have to be equal because they represent the constant viscosity of the bath. It is however convenient to combine the above equations to obtain equations for the center of mass, $\mathbf{r}_{CM} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, and for the relative distance between the impurities, $\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2$

$$m_I \ddot{\mathbf{r}}_{CM} = -(\gamma + \Gamma_{12}(\mathbf{s}))\dot{\mathbf{r}}_{CM} + \frac{1}{2}\eta_+(\mathbf{s}, t) \tag{2.73}$$

$$m_I \ddot{\mathbf{s}} = -(\gamma - \Gamma_{12}(\mathbf{s}))\dot{\mathbf{s}} + 2\mathbf{F}_1(\mathbf{s}) + \eta_-(\mathbf{s}, t), \tag{2.74}$$

where the Gaussian noises are defined as

$$\eta_\pm(\mathbf{s}, t) = \mathbf{\Psi}_1(\mathbf{s}, t) \pm \mathbf{\Psi}_2(\mathbf{s}, t). \tag{2.75}$$

It is useful to analyze how Eq. (2.73,2.74) behave for different values of the relative distance $\mathbf{s}$. When the relative distance is small, the effective friction $(\gamma - \Gamma_{12}(\mathbf{s}))$ in Eq. (2.74) diminishes and the motion of $\mathbf{s}$ becomes underdamped. On the other hand, in the same regime the motion of the center of mass experiences an increase in the effective friction and become overdamped. Finally, when $\mathbf{s}$ is large both $\mathbf{F}_1$ and Γ_{12} vanish and the motions of the two impurities become independent, each one described by a single particle equation like Eq. (2.70).

Interestingly, while this result is in strong analogy with the literature about heavy particles in incompressible fluids [34, 35, 36], when the same approach is adopted for the dynamics of heavy quarks diffusing in an ultra-relativistic quark-gluon plasma [32], Γ_{12} has opposite sign. This sign difference is due to the presence of heavy quarks and anti-quarks -that play the role of different impurities- that couple differently with the bath through a Debye-screened Coulomb interaction.

2.3 Complex potential

In the previous discussion, no details of the complex potential $\mathcal{V}$ have been discussed: indeed, only general symmetry properties have been used in the derivation of the complete GLE, Eq. (2.67). It is now time to discuss the details of $\mathcal{V}$, that depend on the nature of the bath (bosonic or fermionic) and on the interactions between impurities and the bath and between particles of the bath themselves. Also, the fact that the quantum nature of the system is encoded in $\mathcal{V}$ will become evident as it will be shown how considering a bath made of fermions or bosons change can drastically change the final GLE.

In the system under examination a bath of free fermions at finite temperature T in 3 dimensions is considered. From the definition of $\Delta_{\mathcal{C}}$ in Eq. (2.15) it is clear that to compute D^R are necessary two Green functions of the bath, i.e. G^R, that form a bubble diagram. When the bath is made of free fermions and it is spherically symmetric, $D^R(\omega, \mathbf{k})$ is known analytically even at finite temperature [28]. Therefore, $V(\mathbf{k})$ and $W(\mathbf{k})$ only depend on the modulus of the momentum, $k = |\mathbf{k}|$ and are given by

$$\frac{\mathrm{Re}D^{\mathrm{R}}(\omega,k)}{N} = -k_{\mathrm{F}} \int_0^\infty dq \, \frac{q}{k} f_{\mathrm{FD}}(q,T) \frac{1}{2} \left(\log\left|\frac{q/k_{\mathrm{F}} - \nu_-}{q/k_{\mathrm{F}} + \nu_-}\right| - \log\left|\frac{q/k_{\mathrm{F}} - \nu_+}{q/k_{\mathrm{F}} + \nu_+}\right| \right), \tag{2.76}$$

$$\frac{\mathrm{Im}D^{\mathrm{R}}(\omega,k)}{N} = -\frac{\pi}{v_{\mathrm{F}}k} \left(\omega + \frac{k_{\mathrm{B}}T}{\hbar} \log\frac{1 + e^{\beta(\nu_-^2 \varepsilon_{\mathrm{F}} - \mu)}}{1 + e^{\beta(\nu_+^2 \varepsilon_{\mathrm{F}} - \mu)}} \right), \tag{2.77}$$

where k_{F} is the Fermi momentum, μ the chemical potential of the bath (with dependence on temperature T not specified for sake of brevity) and

$$\nu_\pm = \frac{\omega}{kv_{\mathrm{F}}} \pm \frac{k}{2k_{\mathrm{F}}} \tag{2.78}$$

$$v_{\mathrm{F}} = \frac{k_{\mathrm{F}}}{m} \tag{2.79}$$

$$N = \frac{mk_{\mathrm{F}}}{2\pi^2\hbar^2}. \tag{2.80}$$

Now, the derivation of $V(k)$ and $W(k)$ can be made according to their definitions, Eq. (2.54,2.55). The real potential $V(k)$ is

$$
\begin{aligned}
V(k) &= -Nk_{\mathrm{F}} \int_0^\infty dq \, \frac{q}{k} f_{\mathrm{FD}}(q,T) \frac{1}{2} \lim_{\omega \to 0} \left(\log\left|\frac{q/k_{\mathrm{F}} - \nu_-}{q/k_{\mathrm{F}} + \nu_-}\right| - \log\left|\frac{q/k_{\mathrm{F}} - \nu_+}{q/k_{\mathrm{F}} + \nu_+}\right| \right) = \\
&= -\frac{mk_{\mathrm{F}}^2}{2\pi^2\hbar^2} \int_0^\infty dq \, \frac{q}{k} f_{\mathrm{FD}}(q,T) \frac{1}{2} \left(\log\left|\frac{q/k_{\mathrm{F}} + k/2k_{\mathrm{F}}}{q/k_{\mathrm{F}} - k/2k_{\mathrm{F}}}\right| - \log\left|\frac{q/k_{\mathrm{F}} - k/2k_{\mathrm{F}}}{q/k_{\mathrm{F}} + k/2k_{\mathrm{F}}}\right| \right) = \\
&= -\frac{mk_{\mathrm{F}}^2}{2\pi^2\hbar^2} \int_0^\infty dq \, \frac{q}{k} f_{\mathrm{FD}}(q,T) \log\left|\frac{q + k/2}{q - k/2}\right|,
\end{aligned}
\tag{2.81}
$$

while the rescaled imaginary potential $W_{\mathrm{R}}(k)$ is

$$
\begin{aligned}
W_{\mathrm{R}}(k) &= -\frac{N\pi}{v_{\mathrm{F}}k} \left(1 + \frac{k_{\mathrm{B}}T}{\hbar} \lim_{\omega \to 0} \frac{1}{\omega} \log\frac{1 + e^{\beta(\nu_-^2 \varepsilon_{\mathrm{F}} - \mu)}}{1 + e^{\beta(\nu_+^2 \varepsilon_{\mathrm{F}} - \mu)}} \right) = \\
&= -\frac{mk_{\mathrm{F}}}{2\pi v_{\mathrm{F}}\hbar^2 k} \left(1 - \frac{e^{\beta\varepsilon_{\mathrm{F}}(k^2/4k_{\mathrm{F}}^2 - \mu/\varepsilon_{\mathrm{F}})}}{1 + e^{\beta\varepsilon_{\mathrm{F}}(k^2/4k_{\mathrm{F}}^2 - \mu/\varepsilon_{\mathrm{F}})}} \right) = \\
&= -\frac{m^2}{2\pi\hbar^2 k} \frac{e^{\beta\varepsilon_{\mathrm{F}}(\mu/\varepsilon_{\mathrm{F}} - k^2/4k_{\mathrm{F}}^2)}}{1 + e^{\beta\varepsilon_{\mathrm{F}}(\mu/\varepsilon_{\mathrm{F}} - k^2/4k_{\mathrm{F}}^2)}}.
\end{aligned}
\tag{2.82}
$$

After a Fourier transformation, the expressions of real and imaginary potential in position space are obtained: they are already written depending on the distance $\mathbf{s}$ between two particles as in Eq. (2.67). Spherical symmetry also implies that also position space the dependence is only on the modulus of the distance, $s = |\mathbf{s}|$

$$V(s) = -\frac{mk_{\mathrm{F}}}{4\pi^4\hbar^2} \int dk \, \frac{\sin(ks)}{s} \int dq \, f_{\mathrm{FD}}(q,T) q \times \log\left|\frac{q + k/2}{q - k/2}\right| \tag{2.83}$$

$$W_{\mathrm{R}}(s) = -\frac{m^2}{4\pi^3\hbar^3} \int dk \, f_{\mathrm{FD}}(k/2,T) k \frac{\sin(ks)}{ks}. \tag{2.84}$$

Note that both real and imaginary potential are even in s and they vanish in the limit 0 for $s \to \infty$, as it is expected, while their limit is non-vanishing for $s \to 0$. For finite values of s, they both exhibit an oscillatory behavior and the dependence on temperature is encoded only in

the Fermi-Dirac distribution function f_{FD}. The spatial dependence of V and of $\mathcal{H}_{W_{\text{R}}}$ is shown in Fig. 2.3, while the spatial dependence of W_{R} is not shown because it does not affect the equations of motion or any relevant parameter of the dynamics. In the remaining part of this section, the different force and viscosity terms entering the equation of motion for the single and double impurity scenario will be analyzed.

2.3.1   One impurity

The single impurity equation of motion, Eq. (2.70), is

$$m_{\text{I}}\ddot{\mathbf{r}} = -\gamma\dot{\mathbf{r}} + \boldsymbol{\Psi}(t), \tag{2.85}$$

and the most interesting quantity here is the symmetric 3×3 matrix γ, that is defined as

$$\gamma = \Gamma_{11}(\mathbf{s})|_{s=0}, \tag{2.86}$$

as it follows from the definition Eq. (2.65). The starting point in the derivation of the explicit form of γ is the explicit form of $\Gamma_{11}(\mathbf{s})$, given by

$$\Gamma_{11}^{ij}(\mathbf{s}) = -\frac{m^2 g^2}{4\pi^3 \hbar^3 s^2} \int_0^\infty dq\, q \left\{ h(q,s)\left(\delta_{ij} - \frac{3s_i s_j}{s^2}\right) - \frac{s_i s_j}{s} q \sin(qs) \right\} f_{\text{FD}}(q/2), \tag{2.87}$$

where s_i and s_j are components of $\mathbf{s}$ and

$$h(q,s) = \cos(qs) - \sin(qs)/(qs) \tag{2.88}$$

The notation in Eq. (2.87) is a bit sloppy, because Γ_{11} is evaluated at zero distance by definition. However, it is more convenient to momentarily maintain this notation to compute the $\mathbf{s} \to 0$ limit analytically. This limit is calculated separately for $i = j$ and $i \neq j$: for the latter the relevant terms inside Eq. (2.87) are

$$\frac{1}{s^2}h(q,s)\left(-3\frac{s_i s_j}{s^2}\right) - \frac{s_i s_j}{s^3}q\sin(qs) = -\frac{3s_i s_j}{s^4}\left(\cos(qs) - \frac{\sin(qs)}{qs}\right) - \frac{s_i s_j}{s^3}q\sin(qs) =$$

$$= -3\frac{s_i s_j}{s^4}\left(1 - \frac{(qs)^2}{2} - 1 + \frac{(qs)^2}{6}\right) - \frac{s_i s_j}{s^3}q\left(qs - \frac{(qs)^3}{6}\right) =$$

$$= s_i s_j \frac{q^2}{s^2} - s_i s_j \frac{q^2}{s^2} + s_i s_j \frac{q^4}{6} \xrightarrow{s\to 0} \quad 0, \tag{2.89}$$

while for $i = j$

$$\frac{1}{s^2}h(q,s)\left(1 - 3\frac{s_i^2}{s^2}\right) - \frac{s_i^2}{s^3}q\sin(qs) = \frac{s^2 - 3s_i^2}{s^4}\left(\cos(qs) - \frac{\sin(qs)}{qs}\right) - \frac{s_i^2}{s^3}q\sin(qs) =$$

$$= \frac{s^2 - 3s_i^2}{s^4}\left(1 - \frac{(qs)^2}{2} - 1 + \frac{(qs)^2}{6}\right) - \frac{s_i^2}{s^3}q\left(qs - \frac{(qs)^3}{6}\right) =$$

$$= -\frac{1}{3}q^2 + s_i^2\frac{q^2}{s^2} - s_i^2\frac{q^2}{s^2} + s_i^2\frac{q^4}{6} \xrightarrow{s\to 0} \quad -\frac{1}{3}q^2. \tag{2.90}$$

Therefore, it is proved that γ is a diagonal matrix, because only $i = j$ terms are different from 0 and equal, since the final result does not depend on i. This means that, considering a system of reference with origin on the impurity, the medium is equally viscous in all possible directions and a spherical symmetry is present. Now it is possible to move on with the calculations

$$\lim_{s\to 0}\Gamma_{11}^{ii}(\mathbf{s}) = -\frac{mg^2}{4\pi^3\hbar^3}\int_0^\infty dq\, q\left(-\frac{1}{3}q^3\right)f_{\text{FD}}(q/2) = \frac{mg^2}{12\pi^3\hbar^3}\int_0^\infty dq\, q^3 f_{\text{FD}}(q/2) = \frac{mg^2}{12\pi^3\hbar^3}I_q$$

$$I_q = \int_0^\infty dq\, q^3\left(1 + e^{\beta(\hbar^2 q^2/8m - \mu)}\right)^{-1} = \int_0^\infty dq\, q^3\frac{e^{\beta\mu}}{e^{\beta\mu} + e^{\beta\hbar^2 q^2/8m}} = z\int_0^\infty dq\, \frac{q^3}{z + e^{\beta\hbar^2 q^2/8m}},$$

where $z = e^{\beta\mu}$. Making the change of variable $k = \hbar q\sqrt{\beta/8m}$ a new form for I_q is obtained

$$I_q = \left(\frac{8m}{\beta}\right)^2 \frac{1}{\hbar^4} z \int_0^\infty dk \, \frac{k^3}{z + e^{k^2}} = -\frac{32m^2}{\beta^2} \frac{1}{\hbar^4} \text{Li}_2(-z), \tag{2.91}$$

where the definition of Fermi-Dirac integrals has been used and Li_2 is the dilogarithm [37]. Finally, the expression for the desired constant single impurity friction at finite temperature γ is

$$\gamma = -\frac{8m^4 g^2}{3\hbar^7 \pi^3} (k_B T)^2 \text{Li}_2(-e^{\beta\mu(T)}). \tag{2.92}$$

The zero temperature limit for γ can be derived analytically, considering also the first finite temperature contribution

$$\lim_{T \to 0} \gamma = \lim_{T \to 0} -\frac{8m^4}{3\hbar^7 \pi^3} \left(\frac{2\pi\hbar^2}{m_r} a\right)^2 \varepsilon_F^2 \left(\frac{T}{T_F}\right)^2 \text{Li}_2(e^{\beta\mu(T)})$$

$$= -\frac{8\hbar k_F^2}{3\pi} \left(\frac{m}{m_r} k_F a\right)^2 \lim_{T \to 0} \left(\frac{T}{T_F}\right)^2 \text{Li}_2(e^{\beta\mu(T)}) =$$

$$= \frac{4\hbar k_F^2}{3\pi} \left(\frac{m}{m_r} k_F a\right)^2 \left(\frac{T}{T_F}\right)^2 \left(\frac{\pi^2}{3} + \frac{T_F^2}{T^2}\right) = \frac{4\hbar k_F^2}{3\pi} \left(\frac{m}{m_r} k_F a\right)^2 \left(1 + \frac{T^2}{T_F^2} \frac{\pi^2}{3}\right), \tag{2.93}$$

where g is expressed in terms of the more physical s-wave scattering length $g = 2\pi\hbar^2 a/m_r$, $m_r = m_I m/(m_I + m)$ is the reduced mass, ε_F is the Fermi energy and $T_F = \varepsilon_F/k_B$ is the Fermi temperature. The most compact form of the zero temperature limit is

$$\gamma_{T \to 0} = \frac{4\hbar k_F^2}{3\pi} \left(\frac{m}{m_r} k_F a\right)^2 \left(1 + \frac{T^2}{T_F^2} \frac{\pi^2}{3}\right). \tag{2.94}$$

The $T \to 0$ limit of the constant friction coefficient γ is the most interesting quantity to discuss: in Eq. (2.94) it is clear that this limit is finite, a non-trivial result. The physical meaning is that a slowly moving impurity in a bath of fermions dissipates energy, a result that is the opposite of the one obtained in an interacting bosonic bath, where in 3 dimension $\gamma \propto T^7$ [38] and therefore a moving impurity can not dissipate energy at $T = 0$. This is because for Landau criterion [39] a particle moving in a superfluid can not dissipate energy if it is slower than the critical velocity c, corresponding to the speed of sound. For fermions there is no such thing as the critical velocity of superfluid, so even a slow impurity dissipates energy. The reason behind the absence of a critical velocity is that fermions in 3 dimensions have particle-hole excitation with broad energy spectrum, so at any velocity the bath is excited.

Interestingly, the same result of Eq. (2.94) can be obtained considering that the energy dissipated per unit time by a particle moving at velocity V is $\dot{E} = -F_V V$ [39, 40].

$$\dot{E} = -\int_{-\infty}^\infty \frac{d\mathbf{k}}{(2\pi)^3} \int_{-\infty}^\infty \frac{d\omega}{2\pi} \, 2\pi S(\omega, \mathbf{k}) \frac{n}{2N} \omega 2\pi g^2 \delta(\omega - k_z V) =$$

$$= -\frac{ng^2}{2N} \frac{1}{(2\pi)^2} \int_{-\infty}^\infty d\mathbf{k} \, S(k_z V, k) k_z V = -F_V V. \tag{2.95}$$

The drag force F_V can be written as

$$F_V = \frac{ng^2}{8N\pi^2} \int_{-\infty}^\infty d\mathbf{k} \, S(k_z V, \mathbf{k}) k_z = \frac{ng^2}{4N\pi} \iint_{-\infty}^\infty dk_\perp dk_z k_\perp k_z \, S(k_z V, \sqrt{k_z^2 + k_\perp^2}), \tag{2.96}$$

and Eq. (2.96) can be integrated by parts using the explicit expression of the dynamical structure factor $S(k_z V, \sqrt{k_z^2 + k_\perp^2})$. For fermions this expression is given in Ref. [41], Sec. 2.

$$S(\omega, \mathbf{k}) = \frac{\nu(0)}{2} \frac{\omega}{k v_F} \quad \text{if} \quad 0 \leq \omega \leq k v_F - \frac{k^2}{2m}, \tag{2.97}$$

that gives the conditions $0 \leq k_z \leq 2m v_F$ and $0 \leq k_\perp \leq \sqrt{(2m v_F)^2 - k_z^2}$ in the small velocity limit. Integral is the calculated as

$$\frac{\nu(0)V}{2v_F} \int_0^{2m v_F} dk_z \ k_z^2 \int_0^{\sqrt{(2m v_F)^2 - k_z^2}} dk_\perp \frac{k_\perp}{\sqrt{k_z^2 + k_\perp^2}} = \frac{8}{3} \nu(0) m V k_F^3. \tag{2.98}$$

Finally, using $\nu(0) = 3mN/k_F^2$ (see [41]) and $n = k_F^3/6\pi^2$ the expression of F_V is obtained

$$F_V = \frac{ng^2}{4N\pi} \frac{8}{3} \nu(0) m V k_F^3 = \frac{3mN}{k_F^2} \frac{k_F^3}{6\pi^2} \frac{g^2}{N\pi} \frac{2}{3} m k_F^3 V =$$

$$= \frac{m^2 k_F^4}{3\pi^3} g^2 V = \frac{4k_F^2}{3\pi} \left(k_F a \frac{m}{m_r} \right)^2 V = \gamma_{T=0} V. \tag{2.99}$$

Now, comparing Eq. (2.99) with Eq. (2.94) we see that the same result for the friction coefficient at $T = 0$ is obtained (the missing $\hbar$ term is due to the fact that in the last derivation $\hbar = 1$). This connection between the statistical structure factor $S(\omega, \mathbf{k})$ gives also a useful insight on why γ vanishes for phonons at $T = 0$ as pointed out before: indeed the dynamical structure factor in presence of single low energy phonon mode is [39]

$$S(\omega, \mathbf{q}) = S_\mathbf{k} \delta(\omega - c|\mathbf{k}|), \tag{2.100}$$

where c is the speed of sound. Therefore, in agreement with the Landau criterion, the drag force vanishes for any impurity with speed $V < c$.

2.3.2   Two impurities

In the previous section the single particle friction coefficient γ has been discussed. On the other hand, when two impurities are present in the system, the equation of motion for the distance $\mathbf{s}$ and for the center of mass $\mathbf{r}_{CM}$, Eq. (2.73,2.74) also contain other terms different from γ. As before, these equations are written again here

$$m_I \ddot{\mathbf{r}}_{CM} = -(\gamma + \Gamma_{12}(\mathbf{s})) \dot{\mathbf{r}}_{CM} + \frac{1}{2} \eta_+(\mathbf{s}, t) \tag{2.101}$$

$$m_I \ddot{\mathbf{s}} = -(\gamma - \Gamma_{12}(\mathbf{s})) \dot{\mathbf{s}} + 2\mathbf{F}_1(\mathbf{s}) + \eta_-(\mathbf{s}, t), \tag{2.102}$$

The main ingredients of the above equations are $\mathbf{F}_i(\mathbf{R})$ and $\Gamma_{ij}(\mathbf{R})$. After all the proper differentiations their expressions are

$$\mathbf{F}_1^i(\mathbf{s}) = \frac{mg^2}{16\pi^4 \hbar^2} \frac{s_i}{s^2} \int_0^\infty dq \ qh(q, s) \int_0^\infty dk k f_{FD}(k/2) \log \left| \frac{k+q}{k-q} \right|, \tag{2.103}$$

$$\Gamma_{12}^{ij}(\mathbf{s}) = \alpha(s)\delta_{ij} + \beta(s) \frac{s_i s_j}{s^2} \tag{2.104}$$

$$\alpha(s) = -\frac{m^2 g^2}{4\pi^3 \hbar^3 s^2} \int_0^\infty dq \ qh(q, s) f_{FD}(q/2)$$

$$\beta(s) = \frac{m^2 g^2}{4\pi^3 \hbar^3 s^2} \int_0^\infty dq \ q(3h(q, s) + qs \sin(qs)) f_{FD}(q/2)$$
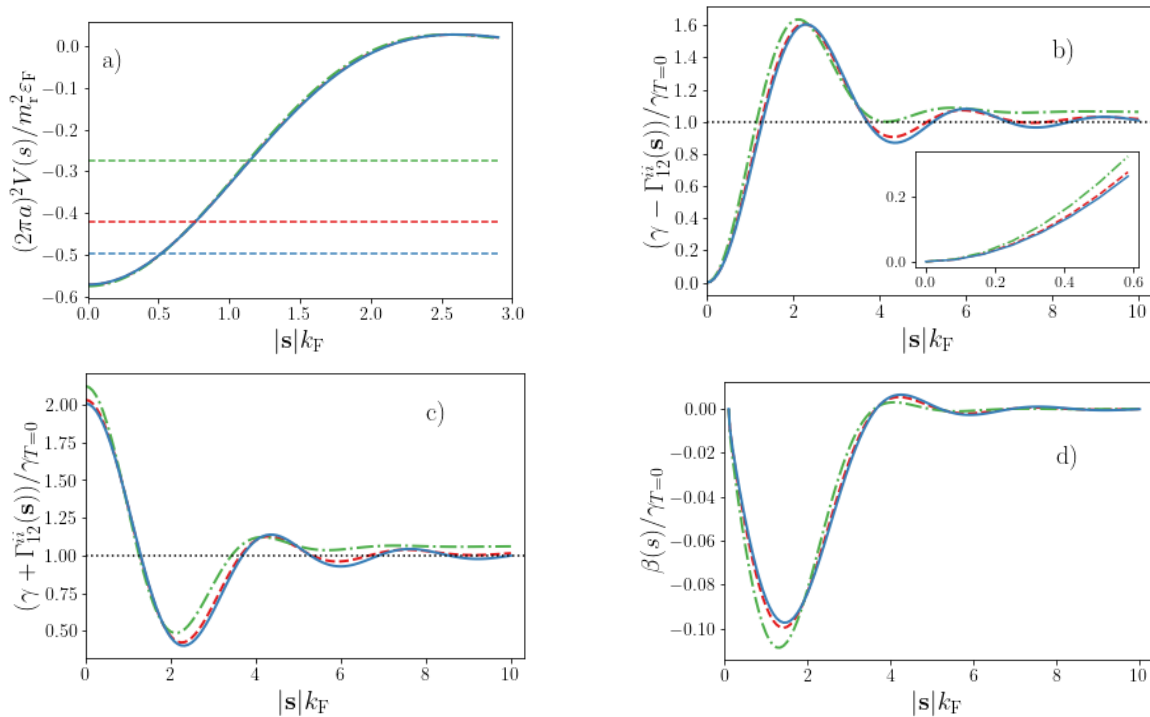
$$\tag{2.105}$$

Figure 2.3. Spatial dependencies for $k_\mathrm{F}a = 0.19$ and $T/T_\mathrm{F} = 0.2, 0.1, 0.05$ (dotted-dashed green, dashed red, solid blue lines). Panel a): real potential $V(\mathbf{s})$, the horizontal dashed lines are $V(s=0) + 3k_\mathrm{B}T/2$ and their intersection with potential lines gives the typical size of the bound state radius r_b, further details in Sec 2.4. $V(s)$ is not visible for $T/T_\mathrm{F} = 0.1$ because hidden by the other lines. Panel b): Difference between γ of Eq. (2.92) and the diagonal component of the viscosity matrix $\gamma - \Gamma_{12}^{ii}$ in units of $\gamma_{T=0}$, Eq. (2.94), i.e. Eq. (2.94) for $T = 0$. When $|\mathbf{s}|k_\mathrm{F} \gtrsim 6$ the oscillations decay because the contribution of Γ_{12}^{ii} vanishes. Inset: small s behavior. Panel c): Sum between γ and the diagonal component of the viscosity matrix $\gamma + \Gamma_{12}^{ii}$ in units of $\gamma_{T=0}$. The behavior of the oscillations is the same of the previous panel. The horizontal dotted lines in panels c) and d) reiterate that at large distance mutual friction Γ_{12} is irrelevant and only the single-impurity friction γ is present. The deviation at large distance is captured by Eq. (2.94) Panel d): Off-diagonal component $\beta(\mathbf{s})$ of the friction coefficient matrix Γ_{12}^{ij} in units of $\gamma_{T=0}$. Also here the oscillatory behavior vanishes for $|\mathbf{s}|k_\mathrm{F} \gtrsim 6$.

where $h(q,s)$ is defined in Eq. (2.88) and Γ_{12}^{ij} has been written in order to encode the off-diagonal component in $\beta(\mathbf{s})$.

The presence of the second impurity in the system strongly modifies the equations of motion: both the relative and the center of mass motions are Brownian-like with distance-dependent friction and not decoupled from each other. Notice that for both the center of mass and relative motion the friction matrix is in general non-diagonal and that while in the diagonal component are present both the single-impurity friction γ and the multi-impurity friction Γ_{ij}, in the off-diagonal component only the latter is present. As discussed above, both $\nabla V(\mathbf{s})$ and $\Gamma_{12}^{ij}(\mathbf{s})$ vanish in the limit for $s \to \infty$ and when this happens each impurity follows an independent Brownian motion like the one described in Eq. (2.70).

The presence of distance-dependent friction is due to the breaking of spherical symmetry of the one impurity scenario that happens when the second impurity is added: indeed, now there is a preferred direction along the relative distance vector $\mathbf{s}$ and the system has cylindrical symmetry. This symmetry argument has physical grounds based on polarization effects: indeed, each impurity modifies the bath in its proximity affecting the possible collisions between other

impurities and bath fermions. Since friction is related to the imaginary part of $\mathcal{V}$ that accounts for collisions, when more than one impurity is present in the system friction has to depend on the configuration of impurities as observed here.

Until this moment, only the limits for $s \to 0$ and $s \to \infty$ at finite T for both $\mathbf{F}(\mathbf{s})$ and $\Gamma_{12}(\mathbf{s})$ have been discussed. When an arbitrary distance $\mathbf{s}$ is considered, the integral over momentum q in Eq. (2.83), and so in Eq. (2.103), leads to a divergence. This divergence arises from the fact that a simple bubble diagram, without any renormalization process, is considered. A complete renormalization procedure for V is not the scope of this treatment, therefore a physical cutoff Λ for the integral over q and a renormalization of the s-wave scattering length a [42, 43] are instead used

$$ 4k_{\mathrm{F}}a = \left(\frac{\hbar^2}{2m_{\mathrm{r}}} \frac{\pi}{gk_{\mathrm{F}}} + \frac{\Lambda}{\pi k_{\mathrm{F}}} \right)^{-1} . \tag{2.106} $$

From now on, the interaction will be therefore no longer characterized by the bare coupling constant g but by the renormalized scattering length $k_{\mathrm{F}}a$ of the above equation. In Fig. 2.3 a) the induced real potential, which clearly has a weak temperature dependence, is shown. The weak dependence is compatible with the fact that temperatures mainly affects collision, that are however characterized by the imaginary potential W and not by V. In Fig. 2.3 also Γ_{12} is shown: in panels b) and c) the underdamped (overdamped) character of the motion for small relative distance (center of mass coordinates) of Eqs. (2.73,2.74) is visible, while the off-diagonal component $\beta(\mathbf{s})$ is on the other hand shown in Fig. 2.3 d)

Interestingly, if g is not renormalized as prescribed by Eq. (2.106) and the upper integration bound Λ of the momentum integral is modified, $V(s)$ shows a much stronger dependence on Λ than $W(s)$: in particular, $V(0)$ depends linearly on Λ, while for small values of s the dependence is more complicated but still strong[1]. A different possible strategy to deal with divergences is to use some resummation schemes, like the ladder one [24] or others, to go beyond the 1 particle-hole approximation adopted here.

Finally, note that in the $T = 0$ limit for V the RKKY interaction [44, 45, 46] is recovered because $V(s)$ is by construction a finite temperature version of it. Finding a RKKY-like induced interaction is not particularly surprising for this system since the impurity-bath interaction is of density-density type.

2.4   Numerical implementation and results

The equation of motion for an arbitrary number of impurities, Eq. (2.67), is a stochastic equation. When more than one impurity is present in the system, the equation has to be solved numerically. As usual in stochastic dynamics, more than one trajectory has to be simulated, in order to obtain average quantities. In this Section the focus is on the results obtained simulating 1000 trajectories for the dynamics of two impurities at different scattering length and temperature.

2.4.1   Stochastic-Verlet algorithm

The numerical solution of a stochastic equation is obtained through proper algorithms: in this work the so-called stochastic-Verlet algorithm [47], modeled on the standard Verlet algorithm [48], is used. The standard Verlet algorithm was derived for non-stochastic systems

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[1]Empirically, it can be verified that this dependence is proportional to $\mathrm{Si}(\Lambda s)$, with Si the sine-integral function.

that satisfy Hamilton equations for coordinate $\mathbf{q}$ and momentum $\mathbf{p}$

$$\dot{\mathbf{q}} = \frac{\mathbf{p}}{m} \tag{2.107}$$

$$\dot{\mathbf{p}} = \mathbf{F}(\mathbf{q}), \tag{2.108}$$

and for any dynamical variable $A(\mathbf{q}, \mathbf{p})$ the equation of motion can be written

$$\dot{A} = \mathcal{L}A, \tag{2.109}$$

with formal solution

$$A(\mathbf{q}_t, \mathbf{p}_t) = e^{\mathcal{L}t}A(\mathbf{q}, \mathbf{p}), \tag{2.110}$$

where $\mathcal{L}$ is the general deterministic propagator

$$\mathcal{L} = \dot{\mathbf{q}}\frac{\partial}{\partial\mathbf{q}} + \dot{\mathbf{p}}\frac{\partial}{\partial\mathbf{p}}. \tag{2.111}$$

This propagator can be written as the sum of propagators for the coordinate and the momentum update, respectively $\mathcal{L} = \mathcal{L}^{(q)} + \mathcal{L}^{(p)}$, with $\mathcal{L}^{(q)} = \dot{\mathbf{q}}\partial_{\mathbf{q}}$ and $\mathcal{L}^{(p)} = \dot{\mathbf{p}}\partial_{\mathbf{p}}$. These new propagators act as

$$e^{\mathcal{L}^{(q)}t}\mathbf{q} = \mathbf{q}_t^{(q)} = \mathbf{q} + \frac{\mathbf{p}}{m}t \tag{2.112}$$

$$e^{\mathcal{L}^{(q)}t}\mathbf{p} = \mathbf{p}_t^{(q)} = \mathbf{p} \tag{2.113}$$

$$e^{\mathcal{L}^{(p)}t}\mathbf{q} = \mathbf{q}_t^{(p)} = \mathbf{q} \tag{2.114}$$

$$e^{\mathcal{L}^{(p)}t}\mathbf{p} = \mathbf{p}_t^{(p)} = \mathbf{p} + \mathbf{F}(\mathbf{q})t, \tag{2.115}$$

and it is possible to decompose the action of the general propagator in an approximated form that involves only the direct action of coordinate and momentum update, like

$$e^{\mathcal{L}t} = e^{\mathcal{L}^{(q)}t/2}e^{\mathcal{L}^{(p)}t}e^{\mathcal{L}^{(q)}t/2} + o(t^3). \tag{2.116}$$

This particular decomposition is the cornerstone of the Verlet algorithm: indeed, the time evolution from t_0, where $(\mathbf{q}_0, \mathbf{p}_0)$ is known, to $t_0 + \Delta t$ is obtained in three steps:

1. Update the coordinate $\mathbf{q}_0$ to half of the desired timestep $\Delta t/2$: the intermediate coordinate $\mathbf{q}_+$ is obtained

2. Update the momentum $\mathbf{p}_0$ to $\mathbf{p}_{\Delta t}$ using $\mathbf{q}_+$

3. Update intermediate coordinate $\mathbf{q}_+$ to the finale coordinate $\mathbf{q}_{\Delta t}$ using $\mathbf{p}_{\Delta t}$.

This procedure can be applied to both deterministic and stochastic dynamics. In the stochastic case this algorithm works well for the Ornstein-Uhlenbeck (OU) process [33] that in one dimension is described by the equation

$$\dot{p} = -\gamma\frac{p}{m} + F + \sqrt{2k_\mathrm{B}T\gamma}\phi(t), \tag{2.117}$$

where γ is the friction coefficient, F is the force term and the noise $\phi(t)$ is a Gaussian white noise with

$$\langle\phi(t)\rangle = 0 \qquad \langle\phi(t)\phi(t')\rangle = \delta(t - t'). \tag{2.118}$$

The OU process can also be written in the form

$$dp = -\gamma\frac{p}{m}dt + Fdt + \sqrt{2k_\mathrm{B}T\gamma}d\phi(t) \tag{2.119}$$

which has an exact solution given by [33]

$$p_{t+\Delta t} = p_t e^{-\alpha} + \frac{m}{\gamma} F(1 - e^{-\alpha}) + \sqrt{mk_BT(1 - e^{-2\alpha})}\phi_t, \tag{2.120}$$

with $\alpha = \gamma\Delta t/m$.

It is now possible to write the explicit procedure of the stochastic-Verlet algorithm with F and α that depend on the coordinate q. Following the steps defined above the discrete time evolution from t to $t + \Delta t$ for an OU process at second order in Δt is given by

$$q_{t_+} = q_t + \frac{1}{2m}p_t\Delta t \tag{2.121}$$

$$p_{t+\Delta t} = p_t(1 - \alpha(q_{t_+})) + F(q_{t_+})\Delta t + \sqrt{2mk_BT\alpha(q_{t_+})}\phi_t \tag{2.122}$$

$$q_{t+\Delta t} = q_{t_+} + \frac{1}{2m}p_{t+\Delta t}\Delta t. \tag{2.123}$$

Note that the updates described by Eq. (2.121-2.123) come from a decomposition of $\mathcal{L}$ like the one of Eq. (2.116), the only difference being a proper momentum update for the OU process. Also, all the exponential function are substituted with their expansion at first order in Δt, because they are computationally expansive when α shows a dependence on the coordinate as in this case. Another advantage of this algorithm is that friction and force evaluation, that are the most computationally expansive processes in the algorithm, are required only once per timestep.

Now the algorithm of Eq. (2.121-2.123) has to be applied to the system with two impurities. The problem is that the algorithm described above is valid for 1-dimensional process, while the system of equations that has to be solved is made of two coupled 3-dimensional equations, Eq. (2.71, 2.72). It is indeed more convenient to work with the form of the GLE where each impurity position is explicitly described than the one with relative distance and center of mass in the numerical implementation.

Anyway, it is still possible to use the one-dimensional algorithm after some manipulations. The first step is finding the matrix M for the change of coordinates that makes the matrix Γ_{12} diagonal: in this way 6 equations like Eq. (2.117) are obtained. As second step, the previously found change of coordinates is applied and the forward time evolution procedure of Eq. (2.121-2.123) is computed, obtaining the coordinates and the momenta at $t + \Delta t$ in the new basis. Finally, the inverse transformation $M^T = M^{-1}$ is applied to return to the original Cartesian coordinates. The procedure is analogous at the next time step, with a new matrix M that has to be found.

2.4.2   Results of the numerical simulations

Now that the algorithm is defined, the results of numerical simulation are discussed. A mass ratio m_I/m consistent with the hypothesis of heavy impurities and the condition on the ratio between the de Broglie thermal wavelength and the inter-particle spacing $2\pi/k_F$ has to be chosen. The value considered for the mass ratio is $m_I/m = 30$, close to mixtures realized experimentally, like the ^{133}Cs-^{6}Li one where the mass ratio is 22.17 [49]. Moreover, with this value also the condition $\lambda k_F/2\pi < 1$ is satisfied for $T/T_F = 0.05, 0.1, 0.2$. In the system with two impurities, a bound state of typical size r_b is possible [32], where r_b is estimated matching the average kinetic energy provided by the coupling with the bath and the mediated interaction, $(k_Fa)^2V(r_b) \propto 3k_BT/2$. This condition means that the impurity pair is in thermal equilibrium with the bath and their average distance is therefore fixed by temperature and scattering length, providing a classical analogue to the notion of bound state. As expected, an increase in temperature (scattering length) leads to a larger (smaller) r_b, see Fig 2.3 a). The process of bound state formation, i.e.
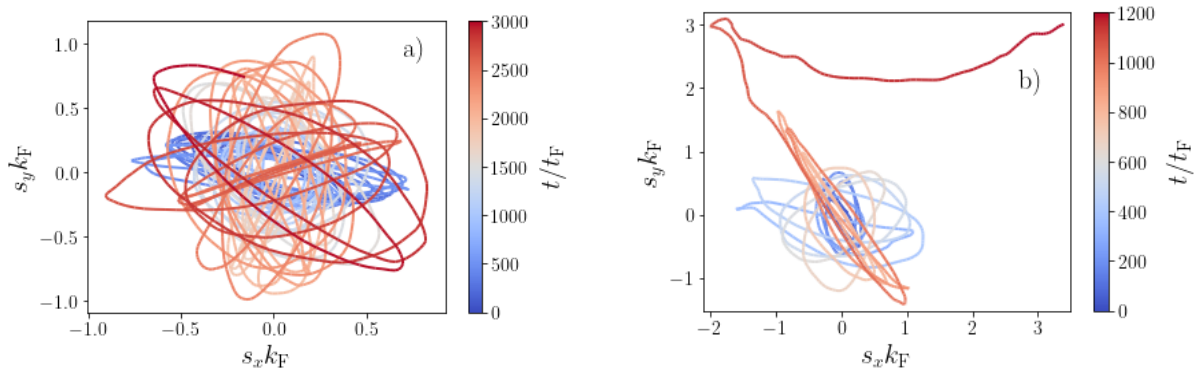
Figure 2.4.   Two representative trajectories generated by the GLE from a configuration with relative distance r_b, $k_F a = 0.19$ and $T/T_F = 0.05$. Color map labels the time and components s_x and s_y are shown. Note that the motion of the impurities is also not confined on a plane due to noise. In the trajectory reported in panel a), the impurities remain in the bound state up to $t = 3000\, t_F$. In panel b): the dissociation of bound state starts at $t \simeq 1000\, t_F$. The motion of the bound state becomes quasi one-dimensional in this case, as a consequence of angular momentum dissipation.

impurities that are initially far apart and come eventually closer up to r_b, is not the case study of these simulations: on the contrary, the focus is on the dissociation process.

With the stochastic Verlet algorithm previously explained, 1000 independent simulations for the time evolutions of the impurities are performed. Initially, impurities are at rest with an initial random position $\mathbf{r}_1$, $\mathbf{r}_2$ with the constraint $|\mathbf{r}_1 - \mathbf{r}_2| = r_b$. Time is in units of Fermi time $t_F = \hbar/\varepsilon_F$.

All simulations show that in the long-time regime impurities separate and each one diffuses according to the dynamics described by Eq. (2.70), i.e. two separate single-impurity Brownian motions are present. In Fig. 2.4 two typical trajectories are shown: in panel a) the distance between impurities is comparable to r_b throughout the simulation time shown, while in panel b) the dissociation process and the beginning of the two independent Brownian motions are shown.

The lifetime τ of the bound state is calculated as the average of dissociation times. In the low temperature regime, i.e. when the dissociation is a thermally activated process, Kramer's theory [50] can be used to compute τ:

$$\tau = 2\pi \sqrt{\frac{K}{K_a}} \frac{2m_I e^{\beta U}}{\sqrt{\gamma^2 + 4K m_I} - \gamma}, \tag{2.124}$$

where K and K_a are the curvature of the potential at the top and bottom of the barrier, U is the energy barrier that separates bound state and free continuum and the friction coefficient γ is taken from Eq. (2.92). Note that in this case the energy barrier is determined as $U = \max V(s) - V(r_b)$, and can be inferred directly from Fig. 2.3 a), because $\max V(s) \sim V(k_F s = 2.4)$. As one could expect, a larger scattering length will determine a larger U and a larger temperature a lower U.

The lifetime can also be inferred directly from numerical simulations, indeed the bound state is considered dissociated when $k_F s > 2.5$, since at this inter-impurity distance the slope of $V(s)$ changes. A typical evolution of the inter-impurity distance is shown if Fig. 2.5 a) for $k_F a = 0.19$ and $T/T_F = 0.2$ (dotted-dashed green line), $T/T_F = 0.1$ (dashed red line) and $T/T_F = 0.05$ (blue line). For the latter the dissociation occurs at $t > 350 t_F$, while for the others the beginning of the dissociation process is visible. Lifetime τ, shown in Fig. 2.5 b) for different
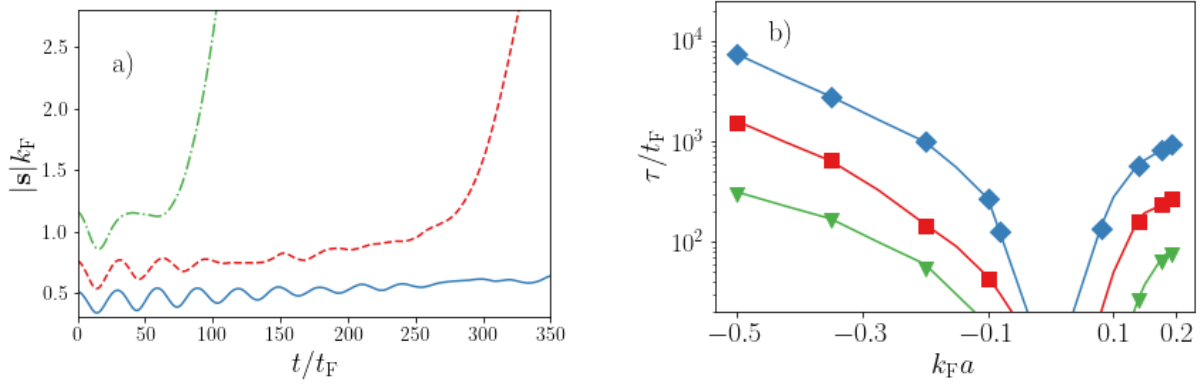
Figure 2.5.   Panel a): single shot time evolution of $s = |\mathbf{s}|$ at $k_\mathrm{F}a = 0.19$ for different temperatures: solid blue line is $T/T_\mathrm{F} = 0.05$, dashed red line is $T/T_\mathrm{F} = 0.1$ and green dotted-dashed line is $T/T_\mathrm{F} = 0.2$. The dissociation of the bound state is visible for $T/T_\mathrm{F} = 0.1$ and $T/T_\mathrm{F} = 0.2$. Panel b): Numerically observed lifetimes τ as filled symbols at different T/T_F and $k_\mathrm{F}a$, solid lines are theoretical predictions of Eq. (2.124). Statistical uncertainties are smaller than the size of the symbols.

$k_\mathrm{F}a$, is obtained averaging all the simulated trajectories. Numerical results (filled symbols) perfectly agree with the predictions of Kramer's theory, see Eq. (2.124), shown as solid lines in Fig. 2.5. The implication is that at the temperatures considered the dissociation is a thermally activated event. The considered range of temperatures is experimentally accessible. Moreover, typical Fermi time in recent experiments, see e.g. [4], is of order 10^{-2} ms, and therefore it should be possible to detect experimentally a dissociation time between 100 and 1000 t_F. An agreement between an experimental dissociation time and Kramer's theory would be a confirmation of the classical approach adopted here.

An interesting feature that can be inferred from simulated trajectories with long lived bound states is that the relative motion of the impurities tends to become quasi one-dimensional before dissociating. To analyze this feature, the evolution of the modulus L_orb of the internal orbital angular momentum $\mathbf{L}_\mathrm{orb} = m_\mathrm{I}\mathbf{s} \times \dot{\mathbf{s}}$ is studied. As shown in Fig. 2.6 for a typical trajectory, after an initial transient time L_orb tends to oscillate around a plateau value $L_\mathrm{p,s}$ and then it drops around the dissociation time. Since in the same time interval the values of $|\mathbf{s}|$ and $|\dot{\mathbf{s}}|$ are almost constant, the drop in internal orbital angular momentum indicates a more one-dimensional motion. The relative loss of L_orb for the single trajectory is calculated as $\Delta L_\mathrm{s}/L_\mathrm{p,s} = (L_\mathrm{orb}(t = \tau_\mathrm{s}) - L_\mathrm{p,s})/L_\mathrm{p,s}$ and $L_\mathrm{orb}(t = \tau_\mathrm{s})$ is the modulus of L_orb at dissociation time of the single trajectory τ_s, see Fig 2.6. For short time after dissociation L_orb increases rapidly due to the last momentum kick that causes the dissociation of the bound state. Finally, the averaged relative angular momentum loss $\Delta L/L_\mathrm{p}$ is calculated by averaging over all the trajectories with the same scattering length and is shown in the inset of Fig 2.6.

2.5   Effective mass

In the whole description of this system of impurities in a bath, a typical property of polaronic systems is absent: the effective mass. It is indeed well known [51] that when a full quantum mechanical description of a system made of an impurity in an environment is adopted, the bare mass of the impurity is dressed by the interactions with the environment. A similar result can be obtained also in this formalism, performing a second order expansion in frequency as it will be shown below. The net effect is that now in the influence functional terms proportional to $\dot{\mathbf{q}}^2$ and $\ddot{\mathbf{q}}$ are present, leading to a modification of the bare impurity mass m_I. A drawback of this
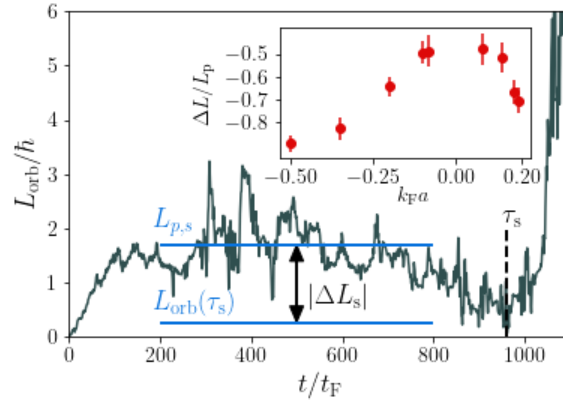
Figure 2.6. Time evolution of the modulus L_{orb} of the internal orbital angular momentum with $k_{\mathrm{F}}a = 0.19$ and $T/T_{\mathrm{F}} = 0.05$ along a typical trajectory. Solid blue lines indicates the value at the dissociation time $L_{\mathrm{orb}}(\tau_{\mathrm{s}})$ and the plateau value $L_{\mathrm{p,s}}$, while the vertical dashed line indicates the dissociation time τ_{s}. Also the absolute value $|\Delta L_{\mathrm{s}}|$ of momentum loss is shown. Inset: relative momentum loss averaged over all the trajectories with the same scattering length.

expansion is that it will be no longer possible to describe the system through a GLE: thus, the focus of this section is only the derivation of this mass dressing effect and the form of a new equation of motion will not be considered.

The new form of the small frequency expansion already performed in Section 2.2 is now

$$\Delta_{ab}(t, \mathbf{x}) = F_{ab}^{(0)}(\mathbf{x})\delta(t) + iF_{ab}^{(1)}(\mathbf{x})\frac{d}{dt}\delta(t) - \frac{1}{2}F_{ab}^{(2)}(\mathbf{x})\frac{d^2}{dt^2}\delta(t) + \dots, \tag{2.125}$$

with

$$F_{ab}^{(2)}(\mathbf{x} - \mathbf{y}) = \lim_{\omega \to 0} \frac{d^2}{d\omega^2}\Delta_{ab}(\omega, \mathbf{x} - \mathbf{y}). \tag{2.126}$$

The influence functional can be written as $\Phi = \Phi^{(0)} + \Phi^{(1)} + \Phi^{(2)}$, where $\Phi^{(i)}$ denotes the term of Φ that contains $F_{ab}^{(i)}$. The sum $\Phi^{(0)} + \Phi^{(1)}$ was derived before and gives Eq. (2.42), so only $\Phi^{(2)}$ has to be discussed here. The procedure is analogous to what has been done before

$$\Phi^{(2)}(\mathbf{Q}', \mathbf{Q}'') = \frac{i}{2}\sum_{a,b=\pm} I^{(2)}(\mathbf{Q}', \mathbf{Q}'') \tag{2.127}$$

$$I^{(2)}(\mathbf{Q}', \mathbf{Q}'') = -\frac{1}{2}\iint_0^t dt'dt'' \iint d\mathbf{x}d\mathbf{y}\; \rho_a(t', \mathbf{x})F_{ab}^{(2)}(\mathbf{x} - \mathbf{y})\left(\frac{d^2}{d(t'-t'')^2}\delta(t'-t'')\right)\rho_b(t'', \mathbf{y}) =$$

$$= -\frac{1}{2}\int_0^t du \int_{u-t}^u ds \iint d\mathbf{x}d\mathbf{y}\; \rho_a(u, \mathbf{x})F_{ab}^{(2)}(\mathbf{x} - \mathbf{y})\left(\frac{d^2}{ds^2}\delta(s)\right)\rho_b(u-s, \mathbf{y}) \tag{2.128}$$

First, consider the integral over time s. After an integration by parts the integral becomes

$$\int_{u-t}^{u} ds\, \rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \left(\frac{d^2}{ds^2}\delta(s)\right) \rho_b(u-s,\mathbf{y}) =$$

$$= C_0 + \frac{1}{2}\int_{u-t}^{u} ds\, \rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \frac{d}{ds}\delta(s)\frac{d}{ds}\rho_b(u-s,\mathbf{y}) =$$

$$= C_0 - \frac{1}{2}\int_{u-t}^{u} ds\, \rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \frac{d}{ds}\delta(s)\frac{d}{du}\rho_b(u-s,\mathbf{y}) =$$

$$= C_0 + C_1 + \frac{1}{2}\int_{u-t}^{u} ds\, \rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \delta(s)\frac{d^2}{ds\,du}\rho_B(u-s,\mathbf{y}) =$$

$$= C_0 + C_1 - \frac{1}{2}\int_{u-t}^{u} ds\, \rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \delta(s)\frac{d^2}{du^2}\rho_B(u-s,\mathbf{y}) =$$

$$= C_0 + C_1 - \frac{1}{2}\rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \frac{d^2}{du^2}\rho_b(u,\mathbf{y}), \tag{2.129}$$

where C_0 and C_1 are obtained after the two needed integration by parts

$$C_0 = -\frac{1}{2}\rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \frac{d}{du}\delta(u)\rho_b(u,\mathbf{y}) + \frac{1}{2}\rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \frac{d}{d(u-t)}\delta(u-t)\rho_b(t,\mathbf{y}) \tag{2.130}$$

$$C_1 = -\frac{1}{2}\rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \delta(u)\frac{d}{du}\rho_b(u,\mathbf{y}) + \frac{1}{2}\rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \delta(u-t)\frac{d}{du}\rho_b(t,\mathbf{y}). \tag{2.131}$$

It can be easily proved that

$$\int_0^t du\, (C_0 + C_1) = \frac{1}{2} F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \left[\dot\rho_a(0,\mathbf{x})\rho_b(0,\mathbf{y}) - \rho_a(0,\mathbf{x})\dot\rho_b(0,\mathbf{y}) \right.$$

$$\left. -\dot\rho_a(t,\mathbf{x})\rho_b(t,\mathbf{y}) + \rho_a(t,\mathbf{x})\dot\rho_b(t,\mathbf{y})\right] \tag{2.132}$$

and that

$$F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) = F_{ab}^{(2)}(\mathbf{y}-\mathbf{x}) \tag{2.133}$$

using the same procedure of Eq. (2.32). Combining Eq. (2.132) and Eq. (2.133) it follows immediately that

$$\sum_{a,b=\pm}\int_0^t du\, (C_0 + C_1) = 0, \tag{2.134}$$

and so these two terms do not contribute to $\Phi^{(2)}$, that can bow be written as

$$\Phi^{(2)}(\mathbf{Q}',\mathbf{Q}'') = -\frac{i}{4}\sum_{a,b=\pm}\int_0^t du \iint d\mathbf{x}d\mathbf{y}\, \rho_a(u,\mathbf{x}) F_{ab}^{(2)}(\mathbf{x}-\mathbf{y}) \ddot\rho_b(u,\mathbf{y}). \tag{2.135}$$

To proceed further, as done before the explicit form of ρ is used and the following relation for the total second derivative is used

$$\frac{d^2}{du^2}\rho_b(u,\mathbf{y}) = g\sum_{j=1}^{N}\left(\dot{\mathbf{q}}_{j,b}^2 \frac{\partial^2}{\partial y^2}\delta(\mathbf{q}_{j,b}(u)-y) - \ddot{\mathbf{q}}_{j,b}\frac{\partial}{\partial y}\delta(\mathbf{q}_{j,b}(u)-y)\right). \tag{2.136}$$

With this expression is possible to write, after the integration over $\mathbf{x}$ and $\mathbf{y}$ (now the sum over a,b is understood)

$$\Phi^{(2)}(\mathbf{Q}',\mathbf{Q}'') = -\frac{ig^2}{4}\sum_{i,j=1}^{N}\sum_{a,b=\pm}\int_0^t du \left[\dot{\mathbf{q}}_{jb}^2\frac{\partial^2}{\partial q_{jb}^2}F_{ab}^{(2)}(\mathbf{q}_{ia}-\mathbf{q}_{jb}) + \ddot{\mathbf{q}}_{jb}\frac{\partial}{\partial q_{jb}}F_{ab}^{(2)}(\mathbf{q}_{ia}-\mathbf{q}_{jb})\right]. \tag{2.137}$$
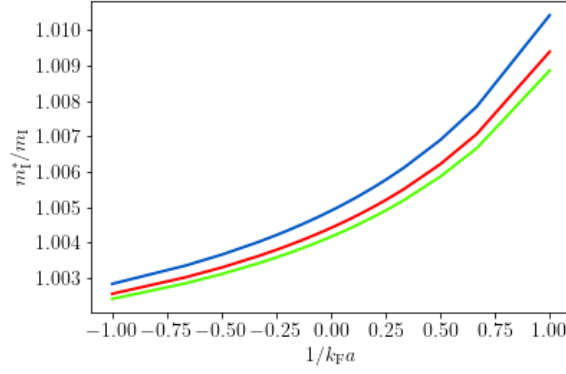
Figure 2.7. Effective mass $m_{\mathrm{I}}^*/m_{\mathrm{I}}$ for $T/T_{\mathrm{F}} = 0.05$, (blue), $T/T_{\mathrm{F}} = 0.1$ (red) and $T/T_{\mathrm{F}} = 0.2$ (green). Bare mass of the impurity is $m_{\mathrm{I}} = 30\,m$.

Next, properties of $F_{ab}^{(2)}$ have to be investigated. The same procedure of Sec 2.2.1 is used to obtain, with $\mathrm{Re}\widetilde{\Delta}_{\mathrm{R}}(\omega, \mathbf{k}) = \omega B^{\mathrm{R}}(\mathbf{k}) + \omega^3 C^{\mathrm{R}}(\mathbf{k})/6$

$$F_<^{(2)}(\mathbf{x}) = F_>^{(2)}(\mathbf{x}) \tag{2.138}$$

$$F_F^{(2)}(\mathbf{x}) = F_{\tilde{F}}^{(2)}(\mathbf{x})^* \tag{2.139}$$

$$F_<^{(2)}(\mathbf{k}) = \frac{\beta}{3}B^{\mathrm{R}}(\mathbf{k}) + \frac{2}{3\beta}C^{\mathrm{R}}(\mathbf{k}) \tag{2.140}$$

$$F_{\mathrm{T}}^{(2)}(\mathbf{k}) = \frac{\beta}{3}B^{\mathrm{R}}(\mathbf{k}) + \frac{2}{3\beta}C^{\mathrm{R}}(\mathbf{k}) + iV^{(2)}(\mathbf{k}) \tag{2.141}$$

$$V^{(2)}(\mathbf{k}) = \lim_{\omega \to 0} \frac{d^2}{d\omega^2}\mathrm{Re}D^{\mathrm{R}}(\omega, \mathbf{k}). \tag{2.142}$$

Until now, the focus was on the second order frequency expansion term $\Phi^{(2)}$ and on the properties of $F_{ab}^{(2)}$, but the relevant terms for the effective mass correction were not discussed. Indeed, an effective mass correction is expected from real terms that can be absorbed into the sum of the actions $iS_0 + i\Phi^{(2)}$: the only candidate for a real correction to the mass is the term $V^{(2)}$ that is present in $F_{\mathrm{T}}^{(2)}$ and $F_{\tilde{\mathrm{T}}}^{(2)}$, while $F_<^{(2)}$ only gives imaginary corrections that affect the friction tensor.

If more than one impurity is present in the system, some contributions to the effective mass that depend on the inter-impurity distance are present. However, also a single-impurity contribution has to be present in the system, analogously to the viscosity tensor. Therefore, only the single impurity case will be considered for simplicity to discuss mass dressing effects.

Consistently to what is done in Sec 2.2.2 and Appendix A, the classical limit and the expansion of $\Phi^{(2)}$ to second order in $\mathbf{y}$ are performed. The result of these operations is that now one has that

$$i(S_0 + \Phi^{(2)}) = -i\int_0^t du \left(m_{\mathrm{I}} + \frac{g^2}{2}\mathcal{H}_{V^{(2)}}(0)\right)\ddot{\mathbf{r}} \cdot \mathbf{y}, \tag{2.143}$$

where $\mathcal{H}_{V^{(2)}}$ is the Hessian of $V^{(2)}$ defined in Eq. (2.142). The effective mass of the impurity m_{I}^* is then defined as the prefactor of $\ddot{\mathbf{r}} \cdot \mathbf{y}$. With this definition the ratio between effective and bare mass is

$$\frac{m_{\mathrm{I}}^*}{m_{\mathrm{I}}} = 1 + \frac{g^2}{2m_{\mathrm{I}}}\mathcal{H}_{V^{(2)}}(0). \tag{2.144}$$

Considering the mass ratio $m_I/m = 30$ as done before, an estimate of the effective-bare mass ratio for different temperatures in function of the inverse scattering length $1/k_F a$ is shown in Fig. 2.7. In the BCS side, i.e. for $1/k_F a < 0$, the dressing effect is very small with a value about 10% of the mass of one particle of the bath, while on the BEC side, i.e. $1/k_F a > 0$, the effective mass increases. The increase of m_I^*/m_I from the BCS to the BEC side is in agreement with previous results [52]. Finally, the expected transition from polaron to molecules in the BEC side [51], that happens at $1/k_F a$ values closer to 0 for increasing impurity-bath particle mass ratio [53], is not present. Indeed, in the present semiclassical description it is not possible to capture the formation of the molecular state, that is a purely quantum effect.

2.6   Conclusions

The goal of this Chapter was to describe the dynamics of N heavy impurities in a fermionic bath and see how the bath influences the impurities. Some approximations were performed in order to trace out the degrees of freedom of the bath and describe the dynamics of the impurities with a semiclassical generalized Langevin equation Eq. (2.67). The label "semiclassical" is used for this equation because the quantum nature of the system is encoded in the induced force and viscosity terms, while the equation is itself classical. The main approximations are the low impurity density and heavy impurities: thanks to the first one an effective action at second order in the coupling constant g, defined in Eq. (2.4), is derived, and thanks to the second approximation the timescales of bath and impurities dynamics are separable.

The main focus was on system consisting of two impurities and on its dynamics. In the short-time regime it is found that the interplay between the induced interaction and the thermal fluctuations leads to the formation of a bound state characterized by a radius r_b and a lifetime τ.

A way to include further dressing effects in this treatment in order to describe the appearance of the effective mass is also described. This is relevant because effective mass is a typical feature of polaronic systems [51]. For this discussion, only the single-impurity scenario has been considered, and it is proven that in the heavy impurity approximation considered here the dressing of the bare impurity mass small effect, as expected considering previous work in literature on the effective mass of heavy particles [52]. Moreover, if the dressing of the mass is consistently included in the model it is no longer possible to derive a generalized Langevin equation for the impurities. On the other hand, since the dressing of the mass is small in the limits considered, a possible phenomenological extension of the model presented here is the substitution of m_I with m_I^* inside the GLE. This extension is also reasonable because the presence of other impurities is expected to have a weak effect on the effective mass.

The more promising experimental platforms on which these predictions can be tested are Bose-Fermi mixtures, which have been experimentally widely studied in past years for mixtures such as ^{40}K-^{23}Na [54], ^{41}K-^{6}Li [55, 56], ^{40}K-^{87}Rb [57] among many others. In recent years, two experimental realizations of a mixture of Bose-Einstein condensates of heavy impurities and Fermi gases of light particles designed to study the induced interaction between bosonic impurities have been achieved with a mixture of ^{87}Rb and ^{40}K atoms [58] and with a mixture of ^{133}Cs and ^{6}Li atoms [59]. However, in these systems the density of impurities is relatively high and therefore this description in terms of impurities independently diffusing may not be accurate enough to compare predictions made here and experimental results.

It is worth remembering that the same technique used here has been applied to the dynamics of heavy quarks diffusing in an ultra-relativistic quark-gluon plasma [32]. In this work, an effective model of quantum chromodynamics was employed, in which an effective finite temperature Abelian field theory is used to describe the dynamics of the deconfined plasma. In that approach,

heavy quarks and anti-quarks are two distinct types of impurities, while light quarks and anti-quarks play the role of the bath. All quarks in the system are coupled through a Debye screened Coulomb-type interaction. As a consequence, the sign of Γ_{12} is different from that of the present Fermi system. Therefore, the relative internal motion of the quark-antiquark pair is overdamped, while the motion of the center of mass experiences a reduced effective friction. It should be interesting, as an outlook, to mimic this situation in a cold gases experiment, using two atomic species or two properly selected different hyperfine levels that couple with opposite sign to the particles of the Fermi bath.

The extension of the present simulation strategy to a superfluid fermionic bath and to many-body systems of impurities would also be extremely valuable to understand the properties of the outer layers of neutron stars, such as modifications to transport properties of the crust like the thermal conductivity [60, 61], the neutrino opacity [62, 63, 64] and entrainment effects caused by the presence of the medium [65].

A final comment about the statistics of the impurities is also useful. Throughout all the Chapter, classical impurities were considered and this can directly impact the induced interaction, that is found to be always attractive. An interesting question is what would happen if the statistics of impurities is considered. If this is the case, the character of the induced interaction depends on the statistics of the impurities, and can be derived within Fermi liquid theory [66, 67, 68]. Within this framework, it has been proved [69] that the induced interaction is always attractive for bosonic impurities and always repulsive when the impurities are fermions. This result can be considered in agreement with the semiclassical derivation here adopted, that neglects the quantum statistics of the impurities: indeed, since fermions have no classical counterparts, induced interaction between classical impurities must have the same character of the bosonic induced interaction. A possible way to go beyond the limit of classical impurities is to consider also impurities in second quantization and derive a kinetic equation, similar to what will be done in the next Chapter for a different system. Another possibility is to derive a Lindblad-like quantum master equation for the density matrix of impurities, for which the limit of classical impurities is in principle not required [70]. In either case, it is not possible, however, to obtain equations of motion that have the simple form of coupled GLEs if the quantum statistics of impurities is retained.

Chapter 3

Fermi polarons and Rabi oscillations

3.1 Theoretical and experimental setup

3.1.1 Introduction to polarons

In quantum physics the problem of impurities in a complex environment spreads through several fields, spanning energies from liquid helium [71] and ultracold atoms to nuclear matter and quark-gluon plasma. This problem consists in the description of the properties of some particles when also a large bath is considered, and in seminal works on conduction electron in dielectric mediums Landau and Pekar [72, 73] introduced the concept of *polarons*, i.e. quasiparticles resulting from the dressing of electrons with collective excitations of the material.

The very same idea of impurities dressed by the interaction with the medium has been experimentally realized in the context of ultracold atoms with imbalanced mixtures made of different atomic species or using atoms of the same species in different hyperfine levels. In these mixtures, the atoms of the majority component act like a bath, while the atoms of the minority component play the role of impurities that will form the polarons after the dressing. As one could imagine, physical properties of the polarons are strongly dependent on bosonic or fermionic nature of the bath, therefore polarons are usually defined as Bose or Fermi polarons reflecting the underlying statistic of the bath. Moreover, also the physical process behind the dressing is different: for Bose polarons the excitations are single-particle for a thermal gas or Boguliobov-type for a condensate [74, 75, 76, 77, 78], while for Fermi polarons excitations come from particle-hole mechanism [52, 79].

Using cold atoms in the realization of polarons has some advantages both in theoretical description and in experimental realization. First of all, on the theoretical side, as result of low temperatures and short-range interatomic potentials, only s-wave scattering gives a non-negligible contribution. Second, in a large range of bath-impurity mass ratio m_B/m_I three-body effects can be neglected and the bare interaction can be considered as a contact interaction solely characterized by the s-wave scattering length a [80, 81]. Finally, it is often possible to experimentally tune the interaction between impurities and the bath using the mechanism of Feshbach resonance [43, 82], i.e. tuning an external magnetic field in order to change the scattering length in a very controlled way. With the help of Feshbach resonances it is possible to investigate both weakly and strongly interacting regimes for the polarons for the same system.

For polarons, some relevant physical properties (that will be characterized mathematically later in the Chapter) are usually defined:

1. Effective mass m_*

2. Polaron energy E_{pol}

3. Quasiparticle residue Z.

4. Decay rate Γ

The effective mass is a quite intuitive quantity and it was already mentioned in Section 2.5: as soon as the impurity starts to interact with the medium, it is dressed by the interaction with the other particles. One of the effect of this interaction is that the bare mass m_I is modified and an effective mass m_* has to be considered. For the same reason, also the ground state of the impurity is now different. Therefore, the energy spectrum is different from the non-interacting one and it is labelled as E_{pol}. The quasiparticle residue Z represents the overlap between the bare and quasiparticles states. The quasiparticle residue has values between 0 and 1, and $Z = 1$ refers to a perfectly defined quasiparticle while $Z = 0$ refers to the fact that a quasiparticle can not be created in the system under examination at the present conditions and the quasiparticle description is no longer valid. The quasiparticle residue can then be seen as a measure of how much the polaron is similar to the bare particle [83]. Finally, the decay rate is related to the lifetime of the polaron. For well defined quasiparticles, this decay rate has to be much smaller than the polaron energy.

The take-home message of this small introduction is that when polarons are involved, they have to be characterized via their relevant properties m_*, E_{pol}, Z and Γ. In literature, these properties have been investigated for both Fermi and Bose polarons in a variety of papers, experimentally [84, 85, 86, 87, 88] and theoretically with analytical methods or MonteCarlo calculations [89, 90, 91, 79]. The characterization of polaron properties is of central importance also when the dynamics is considered and therefore it will be treated properly in the theory herein developed.

After this short introduction on polarons, the focus is moved on a specific system where polarons are present. As a final remark, it is important to point out that while the method derived in this section will be compared with experimental results, the theory is general and it is not specifically designed to address a specific experiment.

3.1.2 Description of the system

The system under examination is the one experimentally realized in Ref. [4]: atoms of ^{6}Li are used to produce an imbalanced population mixture in the two lowest Zeeman states, that are labelled as $|1\rangle$ and $|2\rangle$. Atoms in $|1\rangle$ will form the bath, while atoms in $|2\rangle$ will act as impurities and an impurity-bath interaction between these levels is present. Also the third Zeeman level $|3\rangle$ is used for a specific reason: indeed, it is possible to tune the $3 \leftrightarrow 1$ interaction making it much stronger than the $2 \leftrightarrow 1$ interaction. In this way, $|2\rangle$ can be treated as a free level and polarons are thus formed only in $|3\rangle$ as a result of the interaction with $|1\rangle$. A Rabi coupling between $|2\rangle$ and $|3\rangle$ is then added and so an exchange channel between interacting and non-interacting impurity levels is opened. In the experimental procedure, the number of atoms in $|2\rangle$ and $|3\rangle$ is probed through separate in-situ absorption images at different times. In this way, it is possible to monitor the time evolution of the populations of the free level $|2\rangle$ and the interacting level $|3\rangle$. Note also that the atoms considered are fermions, therefore the polarons discussed are Fermi polarons. The goal of the theory derived here is therefore to obtain a theoretical description for the time evolution of atomic populations in different levels.

The system is modeled with the following Hamiltonian (in $\hbar = 1$ units)

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_\Omega + \hat{H}_{\text{int}}, \tag{3.1}$$

where $\hat{H}_i$ are the free Hamiltonians of the levels

$$\hat{H}_i = \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2m} \hat{f}^\dagger_{\mathbf{k},i} \hat{f}_{\mathbf{k},i}, . \tag{3.2}$$
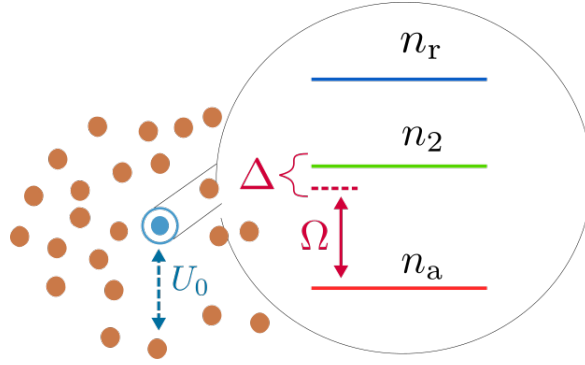
Figure 3.1.   A highly imbalanced mixture of atoms in state $|1\rangle$ (majority, orange) and $|2\rangle$ (minority, cyan dot in a circle) is held at temperature T with zero interaction between these levels. The Rabi coupling drives the transitions between states $|2\rangle$ and $|3\rangle$. In the latter, minority atoms occupy repulsive and attractive polaron branches, formed due to the interaction with the majority component (with coupling strength U_0), while Δ is the detuning applied to the non-interacting level.

where $\hat{f}_{\mathbf{k},i}^{\dagger}$ ($\hat{f}_{\mathbf{k},i}$) are the creation (annihilation) operator for an atom in level $|i\rangle$ with momentum $\mathbf{k}$ and m is the bare mass of the atoms. $\hat{H}_{\Omega}$ and $\hat{H}_{\text{int}}$ are respectively the Rabi and interaction Hamiltonians, that in the rotating wave approximation are:

$$\hat{H}_{\Omega} = \sum_{\mathbf{k}} \left[\frac{\Omega}{2}(\hat{f}_{\mathbf{k},3}^{\dagger}\hat{f}_{\mathbf{k},2} + \hat{f}_{\mathbf{k},2}^{\dagger}\hat{f}_{\mathbf{k},3}) + \Delta \hat{f}_{\mathbf{k},2}^{\dagger}\hat{f}_{\mathbf{k},2} \right] \tag{3.3}$$

$$\hat{H}_{\text{int}} = \frac{U_0}{V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{f}_{\mathbf{k}'-\mathbf{q},1}^{\dagger}\hat{f}_{\mathbf{k}+\mathbf{q},3}^{\dagger}\hat{f}_{\mathbf{k},3}\hat{f}_{\mathbf{k}',1}, \tag{3.4}$$

where Ω is the bare Rabi frequency and Δ is the bare detuning from the transition between $|2\rangle$ and $|3\rangle$. In $\hat{H}_{\text{int}}$ a contact interaction with strength U_0, renormalized over the volume V, is assumed. A pictorial representation of the system is given in Fig. 3.1.

As said before, the goal of this chapter is the derivation of an equation that describes the dynamics of impurities in the free and in the interacting levels. To do this, the total Hamiltonian Eq. (3.1) has to be written in second quantization on the Keldysh contour as introduced in Sec. 1.3. The second quantized total action S, where the fermionic creation and annihilation operators $f_{\mathbf{k},i}^{\dagger}$, $f_{\mathbf{k},i}$ are replaced with the fields $\bar{\psi}_i(\mathbf{k},t)$, $\psi_i(\mathbf{k},t)$, is

$$S = \sum_{i=1}^{3} S_i + S_{\Omega} + S_{\text{int}}, \tag{3.5}$$

with

$$S_i = \sum_{\mathbf{k}} \int_{-\infty}^{\infty} dt \, \bar{\psi}_i(\mathbf{k},t)(i\partial_t - \varepsilon_i(\mathbf{k}))\psi_i(\mathbf{k},t) \tag{3.6}$$

$$S_{\Omega} = \sum_{\mathbf{k}} \int_{-\infty}^{\infty} dt \, \frac{\Omega}{2}(\bar{\psi}_3(\mathbf{k},t)\psi_2(\mathbf{k},t) + \bar{\psi}_2(\mathbf{k},t)\psi_3(\mathbf{k},t)) + \Delta\bar{\psi}_2(\mathbf{k},t)\psi_2(\mathbf{k},t) \tag{3.7}$$

$$S_{\text{int}} = -U_0 \int d\mathbf{r} \int_{-\infty}^{\infty} dt \, \bar{\psi}_1(\mathbf{r},t)\bar{\psi}_3(\mathbf{r},t)\psi_3(\mathbf{r},t)\psi_1(\mathbf{r},t), \tag{3.8}$$

and ε_i is the energy dispersion relation of level $|i\rangle$. S_{int} is written in position space to highlight the contact nature of the interaction.

After the introduction of the Keldysh contour and the Keldysh rotation procedure for the fermionic case, Eqs.((1.196),1.197), the total action is written in position space with the 4D coordinate $x = (t, \mathbf{x})$. For sake of clarity, the terms of the total action S are written separately and moreover the field Ψ_1 is re-labelled as ϕ to better distinguish between the bath and impurity fields. Thus, $S_1 \equiv S_\phi$ has the following expression

$$S_\phi = \iint dx \, dx' \, (\bar{\phi}_1(x), \bar{\phi}_2(x)) \begin{pmatrix} G_{0,\phi}^{-1\,\mathrm{R}}(x, x') & G_{0,\phi}^{-1\,\mathrm{K}}(x, x') \\ 0 & G_{0,\phi}^{-1\,\mathrm{A}}(x, x') \end{pmatrix} \begin{pmatrix} \phi_1(x') \\ \phi_2(x') \end{pmatrix}, \tag{3.9}$$

where the bare inverse retarded and advanced GFs in position space are

$$G_{0,\phi}^{-1\,\mathrm{R(A)}}(x, x') = \delta(x - x') \left(i\partial_{t'} + \frac{1}{2m} \nabla_{\mathbf{r}'}^2 \pm i0 \right), \tag{3.10}$$

and the inverse Keldysh component is a pure regularization factor. The focus is now on S_{int}, because it is possible to derive an effective action with the introduction of a new field via a Hubbard-Stratonovich (HS) transformation. First, S_{int} is written as

$$S_{\mathrm{int}} = U_0 \int_C dx \, \bar{\chi}\chi, \tag{3.11}$$

with $\chi = \phi\psi_3$ and $\bar{\chi} = \bar{\psi}_3\bar{\phi}$. Then an auxiliary field η with bosonic statistics is introduced and the HS transformation is performed

$$\exp(iS_{\mathrm{int}}) = \exp\left(-iU_0 \int_C dx \, \bar{\chi}\chi \right) = \int D[\bar{\eta}, \eta] \exp\left(i(S_\eta + S_{\eta\chi}) \right). \tag{3.12}$$

The auxiliary field η is usually referred to as the molecular field [92, 91] because it accounts for the formation of a bound state between impurities and particles of the bath. This is inferred directly from the structure of the free molecular action S_η and the $\chi - \eta$ coupling action $S_{\eta\chi}$

$$S_\eta = \int_{\mathbb{c}} dx \, \bar{\eta}\frac{1}{U_0}\eta \tag{3.13}$$

$$S_{\eta\chi} = -\int_{\mathbb{c}} dx \, \bar{\chi}\eta + \bar{\eta}\chi. \tag{3.14}$$

Indeed, the first term inside $S_{\eta\chi}$ shows that when a particle η is annihilated an impurity and a particle of the bath are created, while the second term of this action is the conjugate process. After an explicit Keldysh rotation, these new two action terms become

$$S_\eta = \int dx \, \bar{\eta}_\alpha G_{0,\eta}^{-1\,\alpha\beta}\eta_\beta \tag{3.15}$$

$$S_{\eta\chi} = -\int dx \, \bar{\phi}_a\zeta_a + \bar{\zeta}_a\phi_a. \tag{3.16}$$

In Eq. (3.15) subscript α, β labels the classical or quantum component of the bosonic field η (as defined in Sec. 1.3), while $G_{0,\eta}^{-1}$ is the inverse bare GF for the molecules

$$G_{0,\eta}^{-1}(x, x') = \delta(x, x') \begin{pmatrix} 0 & G_{0,\Delta}^{-1\,\mathrm{A}} \\ G_{0,\Delta}^{-1\,\mathrm{R}} & G_{0,\Delta}^{-1\,\mathrm{K}} \end{pmatrix} = \begin{pmatrix} 0 & 1/U_0 - i0 \\ 1/U_0 + i0 & i0 \end{pmatrix}, \tag{3.17}$$

where the inverse Keldysh component is a pure regularization factor. The fermionic field ζ has been introduced for convenience in Eq. (3.16) to separate the bath field ϕ from all the other fields. The Keldysh rotation of the ζ field is defined as

$$\begin{aligned} \zeta_1 &= \frac{\bar{\psi}_{3,1}\eta_\mathrm{q} + \bar{\psi}_{3,2}\eta_\mathrm{cl}}{\sqrt{2}} & \zeta_2 &= \frac{\bar{\psi}_{3,1}\eta_\mathrm{cl} + \bar{\psi}_{3,2}\eta_\mathrm{q}}{\sqrt{2}} \\ \bar{\zeta}_1 &= \frac{\bar{\eta}_\mathrm{cl}\psi_{3,2} + \bar{\eta}_\mathrm{q}\psi_{3,1}}{\sqrt{2}} & \bar{\zeta}_2 &= \frac{\bar{\eta}_\mathrm{cl}\psi_{3,1} + \bar{\eta}_\mathrm{q}\psi_{3,2}}{\sqrt{2}}. \end{aligned} \tag{3.18}$$
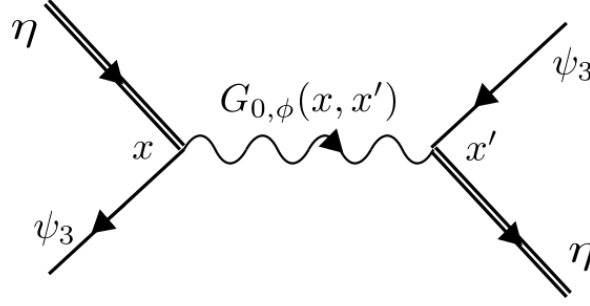
Figure 3.2.   Graphic representation of the interaction vertex of the theory. Double solid lines are molecular fields, solid lines are fields of level $|3\rangle$ and wavy line is the Greene function of the bath.

After the introduction of ζ, it is straightforward to integrate over the bath field ϕ, i.e. integrate out the bath degrees of freedom, and derive an effective action $S_{\eta 3}$ that describes the interaction between impurities and the bath. Note that the integral over bath fields is a standard Gaussian integral

$$S_{\eta 3} = -\iint dx \ dx' \ \bar{\zeta}_a(x) G_{0,\phi}^{ab}(x,x')\zeta_b(x') \tag{3.19}$$

that can also be written, after a normal ordering procedure, in position and momentum space as (sum over bosonic and fermionic Keldysh indices understood)

$$S_{\eta 3} = \frac{1}{2}\iint dx \ dx' \ \bar{\eta}_\alpha(x)\bar{\psi}_{3d}(x')\Gamma^\alpha_{ac} G_{0,\phi}^{ab}(x,x')\Gamma^\beta_{bd}\psi_{3c}(x)\eta_\beta(x') \tag{3.20}$$

$$S_{\eta 3} = \frac{1}{2V}\sum_{p_1,p_2,p_3,p_4} \bar{\eta}_\alpha(p_1)\bar{\psi}_{3d}(p_3)\Gamma^\alpha_{ac} G_{0,\phi}^{ab}(p_1-p_4,p_2-p_3)\Gamma^\beta_{bd}\psi_{3c}(p_4)\eta_\beta(p_2). \tag{3.21}$$

In the last expressions the two matrices Γ^q and Γ^{cl} are for convenience defined as

$$\Gamma^q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \Gamma^{cl} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{3.22}$$

and are used to write a shorter expression for $S_{\eta 3}$ in both position and momentum space. In Eq. (3.20) it is clear how the interaction is now described: through the scattering of molecules η and impurities in $|3\rangle$ mediated by a fermion of the bath ϕ. A pictorial representation of the vertex in position space is given in Fig 3.2.

Finally, the Rabi action S_Ω and the actions in the impurity levels S_2 and S_3 are considered. It is indeed convenient to write the together on the compact notation $S_2 + S_3 + S_\Omega = \tilde{S}_0$

$$\tilde{S}_0 = \sum_{i,i'=2,3}\iint dxdx' \ \bar{\psi}_{ia}(x)G_{0ii',ab}^{-1}(x,x')\psi_{i'b}(x'), \tag{3.23}$$

with bare retarded and advanced GFs

$$G_{0,ii'}^{-1\,\mathrm{R(A)}}(x_1,x_2) = \delta(x_1-x_2)\left[\left(i\partial_{t_2} + \frac{1}{2m}\nabla^2_{\mathbf{r}_2}\right)\mathbb{1}_2 - \mathbf{H}\cdot\hat{s}_{ii'} \pm i0\right], \tag{3.24}$$

while the Keldysh component is again a pure regularization factor. In the above equation, $\mathbb{1}_2$ is the 2×2 identity matrix, $\hat{s}$ is the vector of Pauli matrices and $\mathbf{H} = (\Omega/2, 0, \Delta/2)$. Therefore, all the bare GFs are now contained in $\tilde{S}_0$, while the interaction is encoded in $S_{\eta 3}$. As usual, the system is fully characterized by the total action on the Keldysh contour and all the relevant physical quantities and their dynamics can be derived via the partition function Z. However, this task is non trivial and a different strategy, involving Dyson equation and its solution, has to be used.
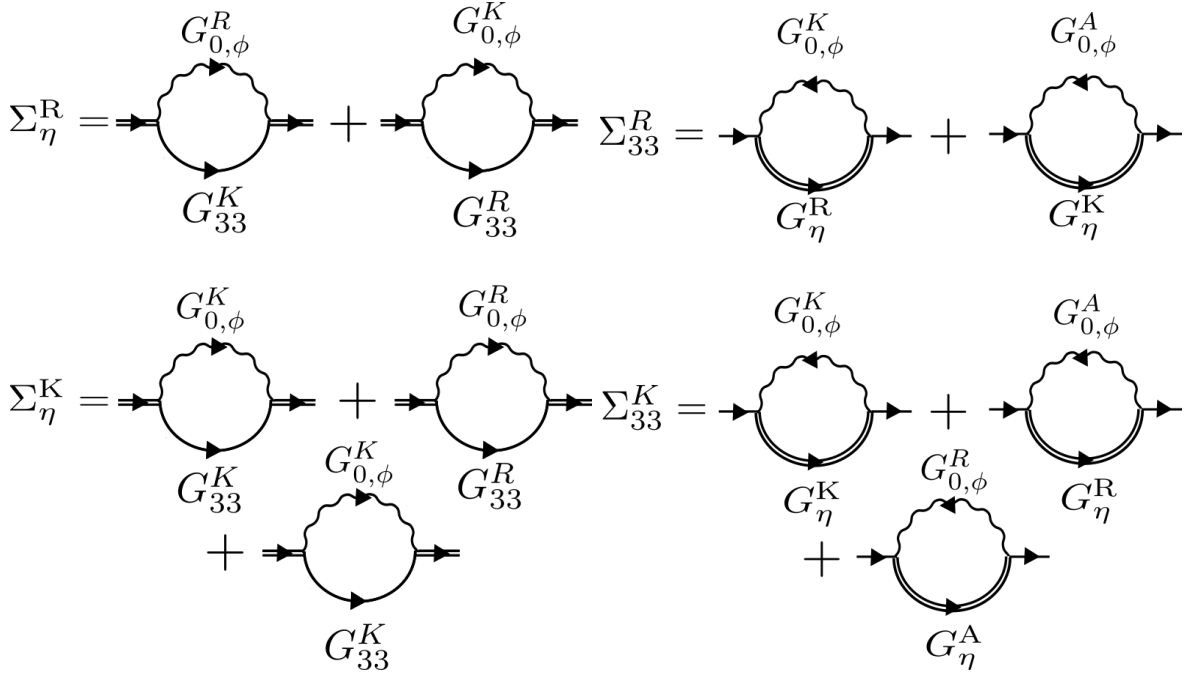
Figure 3.3. Pictorial representation of the molecular and impurity self-energies, Σ_η and Σ_{33}, defined in Eqs. (3.28)-(3.31). Wiggly lines denote $G_{0,\phi}$, solid lines G_{33} and double solid lines G_η, while the labels R, A, K denote the components of the propagators inside the loop.

3.2 Quantum kinetic equation and collisional integral

3.2.1 Dyson equation and self-energy

A description of the dynamics of the system under investigation requires the knowledge of the dressed (or full) GFs for both the molecular and impurity fields. As known from standard textbooks [23, 24] the dressed GF G can be calculated solving the Dyson equation (DE). In the Keldysh formalism the DE has the form

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \circ \hat{\Sigma} \circ \hat{G}, \tag{3.25}$$

where the hat accent is used to highlight the matrix structure of GFs and self-energy Σ and the symbol $\circ$ labels a matrix multiplication together with a convolution of the x coordinates.

In the system under investigation, two different coupled DE have to be solved: one for G_η and one for $G_{ii'}$. They can be written as

$$(\hat{G}_{0\eta}^{-1} - \hat{\Sigma}_\eta) \circ \hat{G}_\eta = \mathbb{1} \tag{3.26}$$

$$(\hat{G}_{0,ii'}^{-1} - \hat{\Sigma}_{ii'}) \circ \hat{G}_{ii'} = \mathbb{1}, \tag{3.27}$$

with the proper identity matrices. The different components of $\hat{\Sigma}_\eta$ and $\hat{\Sigma}_{ii'}$ are calculated at 1-loop contracting the vertex of $S_{\eta3}$ with the proper GF and summing over the Keldysh indices. The result is

$$\Sigma_\eta^{\mathrm{R}}(x,p) = \frac{i}{2V} \sum_q \left(G_{0,\phi}^{\mathrm{R}}(p-q) G_{33}^{\mathrm{K}}(x,q) + G_{0,\phi}^{\mathrm{K}}(p-q) G_{33}^{\mathrm{R}}(x,q) \right) \tag{3.28}$$

$$\Sigma_\eta^{\mathrm{K}}(x,p) = \frac{i}{2V} \sum_q \left\{ G_{0,\phi}^{\mathrm{K}}(p-q) G_{33}^{\mathrm{K}}(x,q) + [G_{0,\phi}^{\mathrm{R}}(p-q) - G_{0,\phi}^{\mathrm{A}}(p-q)][G_{33}^{\mathrm{R}}(x,q) - G_{33}^{\mathrm{A}}(x,q)] \right\}$$
$$\tag{3.29}$$

$$\Sigma_{33}^{\mathrm{R}}(x,p) = -\frac{i}{2V} \sum_q \left(G_{0,\phi}^{\mathrm{K}}(q) G_\eta^{\mathrm{R}}(x,p+q) + G_{0,\phi}^{\mathrm{A}}(q) G_\eta^{\mathrm{K}}(x,p+q) \right) \tag{3.30}$$

$$\Sigma_{33}^{\mathrm{K}}(x,p) = -\frac{i}{2V} \sum_q \left(G_{0,\phi}^{\mathrm{K}}(q) G_\eta^{\mathrm{K}}(x,p+q) + G_{0,\phi}^{\mathrm{A}}(q) G_\eta^{\mathrm{R}}(x,p+q) + G_{0,\phi}^{\mathrm{R}}(q) G_\eta^{\mathrm{A}}(x,p+q) \right), \tag{3.31}$$

with $x = (x_1 + x_2)/2$ and $p = (\omega, \mathbf{p})$ is the relative momentum, i.e. the conjugate coordinate of $x_1 - x_2$. Note that $\hat{\Sigma}_{33}$ is the only component of $\hat{\Sigma}_{ii'}$ different from zero, since $\hat{G}_{33}$ is the only impurity propagators that enters the interaction vertex. A pictorial representation of the self-energies is given in Fig. 3.3

In the Keldysh formalism, the DE is composed of three coupled equations for the retarded, advanced and Keldysh dressed GF respectively. The equations for the retarded and Keldysh component are separately discussed in the remaining part of this Section.

3.2.2   Retarded Green function

The first component of the DE considered is the retarded one, and the first dressed propagator studied is the retarded molecular one, G_η^{R}. From the matrix structure of Eq. (3.26) it follows that

$$(G_{0\eta}^{-1\,\mathrm{R}} - \Sigma_\eta^{\mathrm{R}}) \circ G_\eta^{\mathrm{R}} = 1, \tag{3.32}$$

that immediately leads to

$$G_\eta^{\mathrm{R}}(x,p) = \frac{1}{U_0^{-1} - \Sigma_\eta^{\mathrm{R}}(x,p)}. \tag{3.33}$$

Now, when the bath is considered at equilibrium it follows that $F_\phi(\mathbf{k}) = 1 - 2n_\phi^{\mathrm{eq}}(\mathbf{k})$ with $n_\phi^{\mathrm{eq}}(\mathbf{k})$ the Fermi-Dirac distribution at temperature T. When the impurity limit is considered, i.e. $N_3 \ll N_1$, the approximation $F_{33} \simeq 1$ can be used for the distribution function of level $|3\rangle$ (see Sec. 1.3.2 where the distribution function is introduced). An immediate consequence of this impurity limit is also that the x dependence of Σ_η^{R} and G_η^{R} vanishes and, employing this limit into the Eq. (3.28), together with the relation between the s-wave scattering length a_{13} and U_0 given by the Lippmann-Schwinger equation [93] $U_0^{-1} = m/4\pi a_{13} + \sum_{\mathbf{q}} m/\mathbf{q}^2$ the following result for G_η^{R} is found

$$G_\eta^{\mathrm{R}}(\omega, \mathbf{k}) = \left(\frac{m}{4\pi a_{13}} - \frac{1}{V} \sum_{\mathbf{q}} \frac{1 - n_1^{\mathrm{eq}}(\mathbf{k} - \mathbf{q})}{\omega - \varepsilon_3(\mathbf{q}) - \varepsilon_1(\mathbf{k} - \mathbf{q}) + i0^+} + \frac{m}{\mathbf{q}^2} \right)^{-1}. \tag{3.34}$$

The next GF of interest in $G_{ii'}^{\mathrm{R}}$, that is directly obtained from Eq. (3.27) in matrix form

$$\begin{pmatrix} G_{0,22}^{-1\,\mathrm{R}} \circ G_{22}^{-1\,\mathrm{R}} + G_{0,23}^{-1\,\mathrm{R}} \circ G_{32}^{-1\,\mathrm{R}} & G_{0,22}^{-1\,\mathrm{R}} \circ G_{23}^{-1\,\mathrm{R}} + G_{0,23}^{-1\,\mathrm{R}} \circ G_{33}^{-1\,\mathrm{R}} \\ G_{0,32}^{-1\,\mathrm{R}} \circ G_{22}^{-1\,\mathrm{R}} + (G_{0,33}^{-1\,\mathrm{R}} - \Sigma_{33}^{\mathrm{R}}) \circ G_{32}^{-1\,\mathrm{R}} & G_{0,32}^{-1\,\mathrm{R}} \circ G_{23}^{-1\,\mathrm{R}} + (G_{0,33}^{-1\,\mathrm{R}} - \Sigma_{33}^{\mathrm{R}}) \circ G_{33}^{-1\,\mathrm{R}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.35}$$

It is straightforward to obtain the following results for the dressed retarded propagators

$$(G_{0,33}^{-1\,\mathrm{R}} - \Sigma_{33}^{\mathrm{R}} - G_{0,32}^{-1\,\mathrm{R}} \circ G_{0,22}^{\mathrm{R}} \circ G_{0,23}^{-1\,\mathrm{R}}) \circ G_{33}^{\mathrm{R}} = 1 \tag{3.36}$$

$$(G_{0,22}^{-1\,\mathrm{R}} - G_{0,23}^{-1\,\mathrm{R}} \circ (G_{0,33}^{-1\,\mathrm{R}} - \Sigma_{33}^{\mathrm{R}})^{-1} \circ G_{0,32}^{-1\,\mathrm{R}}) \circ G_{22}^{\mathrm{R}} = 1 \tag{3.37}$$

$$G_{23}^{\mathrm{R}} = -G_{0,22}^{\mathrm{R}} \circ G_{0,23}^{-1\,\mathrm{R}} \circ G_{33}^{\mathrm{R}} \tag{3.38}$$

$$G_{32}^{\mathrm{R}} = -G_{33}^{\mathrm{R}} \circ G_{0,32}^{-1\,\mathrm{R}} \circ G_{22}^{\mathrm{R}}. \tag{3.39}$$

The meaning of these GFs is clear: G_{22}^{R} and G_{33}^{R} describe particles in levels $|2\rangle$ and $|3\rangle$ respectively, while G_{23}^{R} and G_{32}^{R} describes the coherences between these levels. Indeed, it follows directly from Eq. (3.24) that

$$G_{0,23}^{-1\,\mathrm{R}}(t) = G_{0,32}^{-1\,\mathrm{R}}(t) = -\Omega(t)/2. \tag{3.40}$$

In this expression it is made explicit that in general the Rabi coupling is time dependent. To describe the experimental condition under examination the Rabi coupling is modeled as $\Omega(t) = \Omega\theta(t)$ and further implications of this assumption will be discussed later. In the following, Ω is always considered as the time-dependent version, but with the time dependence is understood for sake of brevity.

Inserting into Eq. (3.36) the explicit form of the bare GFs the following expression for the dressed propagator in the interacting level is obtained

$$G_{33}^{\mathrm{R}}(x,p) = \left(\omega - \varepsilon_3(\mathbf{k}) - \Sigma_{33}^{\mathrm{R}}(x,p) - \frac{\Omega^2/4}{\omega - \varepsilon_2(\mathbf{k}) + \Delta + i0} \right)^{-1}, \tag{3.41}$$

where the last term is a consequence of the presence of the Rabi coupling between levels $|2\rangle$ and $|3\rangle$ and the poles of this GF are the spectrum of the polaron. As known from literature, for a positive scattering length two different types of polarons are possible, one at negative and one at positive energy. Respectively, they are defined *attractive* [88] and *repulsive* [94, 95]. In Eq. (3.41), a new feature is added: now each polaron branch is split in two new branches as an effect of the presence of the Rabi coupling Ω. The polaron dispersion relation in this system is

$$\varepsilon_{\alpha\,1,2}(\mathbf{k}) = \varepsilon_3(\mathbf{k}) + \frac{\mathrm{Re}\Sigma_{33}^{\mathrm{R}}(\varepsilon_{\alpha\,1,2}(\mathbf{k}),\mathbf{k}) - \Delta}{2} \pm \frac{1}{2}\sqrt{(\mathrm{Re}\Sigma_{33}^{\mathrm{R}}(\varepsilon_{\alpha\,1,2}(\mathbf{k}),\mathbf{k}) + \Delta)^2 + \Omega^2}, \tag{3.42}$$

and the subscript $\alpha = a, r$ labels the attractive (repulsive) branch that is split. In the description of the dynamics that follows, the dressing effect of Ω will not be considered and therefore the usual relation (with only attractive and repulsive branch) for the polaron energy is recovered

$$\varepsilon_\alpha(\mathbf{k}) = \varepsilon_3(\mathbf{k}) + \mathrm{Re}\Sigma_{33}^{\mathrm{R}}(\varepsilon_\alpha(\mathbf{k}),\mathbf{k}). \tag{3.43}$$

However, the effect of the Rabi coupling on polaron dispersion relation is discussed in Sec. 3.3.2 where it is also shown that the approximation of neglecting it is not a brutal one for this system. When the impurity limit is considered, the polaron dispersion relation in Eq. (3.43) is computed within the non self-consistent T-matrix (ladder) approximation, that is used to derive $\mathrm{Re}\Sigma_{33}^{\mathrm{R}}$ [52]. Indeed, it is straightforward to prove that the expression of G_η^{R} in the impurity limit, Eq. 3.34, is equal to the desired non self-consistent T-matrix.

Finally, also the quasiparticle residues Z_α and effective mass m_*^α for each branch will be computed within the non self-consistent T-matrix approximation. The non self-consistent T-matrix approximation is employed also because it is known from literature that theoretical predictions are in good agreement with experimental results and Quantum Monte-Carlo predictions [88, 51, 84, 91].

Advanced dressed GFs are obtained as complex conjugate of the retarded GFs and discussing them explicitly is not necessary. The detailed description of the other retarded dressed GFs, Eqs. (3.37-3.39), is not given here because these GFs do not affect the form of the equations for the dynamics of the system but only the parameters inside them. Anyway, a sketched of them version can be found in Appendix B.

3.2.3   Dynamics of the molecules and Keldysh Green function

It is useful to remember that, as pointed out in Chapter 1, the Keldysh component of the GF matrix is related to the distribution function F via the general expression $G^K = G^R \circ F - F \circ G^A$. The starting point for the discussion of the Keldysh GFs involved is the molecular one, whose DE is

$$G_\eta^{-1\,\mathrm{R}} \circ G_\eta^K \circ G_\eta^{-1\,\mathrm{A}} = \Sigma_\eta^K - G_{0,\eta}^{-1\,\mathrm{K}}, \tag{3.44}$$

that, thanks to $G_\eta^K = G_\eta^R \circ F_\eta - F_\eta \circ G_\eta^A$ can be written as

$$F_\eta \circ G_\eta^{-1\,\mathrm{A}} - G_\eta^{-1\,\mathrm{R}} \circ F_\eta = \Sigma_\eta^K - G_{0,\eta}^{-1\,\mathrm{K}}, \tag{3.45}$$

and from now on one neglects $G_{0,\eta}^{-1\,\mathrm{K}}$ because it is a pure regularization factor. Now the equation is no longer for G_η^K but for F_η, and dealing with convolutions, a task that could be very complicated, is necessary in order to solve it. For this reason, the so-called Wigner transformation (WT) is performed to remove convolutions from the equations (see Appendix B for details). The WT transforms F as

$$F(x_1, x_2) \xrightarrow{\mathrm{WT}} F(x, p), \tag{3.46}$$

with $x = (x_1 + x_2)/2$ and p the conjugate coordinate of the relative distance $x_1 - x_2$. It can be proved that the following approximations at linear order in gradients hold for the WT

$$A \circ B \xrightarrow{\mathrm{WT}} AB + \frac{i}{2}\{A, B\} \tag{3.47}$$

$$A \circ B - B \circ A \xrightarrow{\mathrm{WT}} = i\{A, B\} \tag{3.48}$$

$$AB \xrightarrow{\mathrm{WT}} = \sum_q A(x, p - q)B(x, q), \tag{3.49}$$

where the curly brackets are defined as

$$\{A, B\} = \partial_x A \partial_p B - \partial_p A \partial_x B$$
$$= \nabla_{\mathbf{r}} A \nabla_{\mathbf{p}} B - \partial_t A \partial_\omega B - \nabla_{\mathbf{p}} A \nabla_{\mathbf{r}} + \partial_\omega A \partial_t B. \tag{3.50}$$

The WT is then applied to Eq. (3.45) and at zeroth order in gradients the result is

$$2iF_\eta(x, p)\mathrm{Im}\Sigma_\eta^{\mathrm{R}}(x, p) = \Sigma_\eta^K(x, p), \tag{3.51}$$

and from now on, all the (x, p) dependence in the Wigner-transformed equation will be understood for sake of brevity. The assumption of the zeroth order expansion for the molecular dynamics means that the dynamics of the molecules is considered subordinated to the dynamics of impurities.

In this approximation for the dynamics of the molecules, it is possible to prove that the following equalities hold

$$F_\eta(G_\eta^{\mathrm{R}} - G_\eta^{\mathrm{A}}) = |G_\eta^{\mathrm{R}}|^2 \Sigma_\eta^K \tag{3.52}$$

$$F_\eta \mathcal{A}_\eta = |G_\eta^{\mathrm{R}}|^2 i\Sigma_\eta^K \tag{3.53}$$

$$\mathcal{A}_\eta = -2|G_\eta^{\mathrm{R}}|^2 \mathrm{Im}\Sigma_\eta^{\mathrm{R}}, \tag{3.54}$$

where $\mathcal{A}_\eta = -2\mathrm{Im}G_\eta^{\mathrm{R}}$ is the usual spectral function of the molecules. The above expressions are the final result for the dynamics of the molecules, since they involve molecular distribution function F_η. They will be used later also in the dynamics of the impurities [96].

3.2.4   Dynamics of the impurities and Keldysh Green functions

Finally, all the ingredients necessary to describe the dynamics of the impurities and of the coherences are present. The final result for the dynamics of the impurities will be a set of kinematic equations. Before proceeding, it is important to mention that while the polaron properties calculated with G_{33}^{R} have been derived with the help of $\mathrm{Re}\Sigma_{33}^{\mathrm{R}}$ in the impurity limit, the kinematic equations are obtained beyond the impurity limit, i.e. the assumption $F_{33} \simeq 1$ will be no longer valid. Going beyond the impurity limit also for the calculation of ε_α, Z_α and m_*^α is beyond the scope of this work and therefore will not be discussed.

As a first step, note that of the 4 equations included in the DE for the Keldysh components of $G_{ii'}$, only 3 of them are independent, because $F_{23} = F_{32}^*$. It is also useful to introduce the definition

$$\tilde{G}_{0,ii'}^{-1\,\mathrm{R(A)}}(x_1, x_2) = \delta(x_1 - x_2)\left[\left(i\partial_{t_2} + \frac{1}{2m}\nabla_{\mathbf{r}_2}^2 \pm i0\right)\mathbb{1}_2\right], \tag{3.55}$$

so that $G_{0,ii}^{-1\,\mathrm{R(A)}} = \tilde{G}_{0,ii}^{-1\,\mathrm{R(A)}} - \mathbf{H}\cdot\hat{s}_{ii}$. The DE for the impurities can then be written as

$$\hat{F}\circ\hat{G}^{-1\,\mathrm{A}} - \hat{G}^{-1\,\mathrm{R}}\circ\hat{F} = \hat{\Sigma}^{\mathrm{K}} - \hat{G}_0^{-1\,\mathrm{K}}, \tag{3.56}$$

with

$$\hat{F} = \begin{pmatrix} F_{22} & F_{23} \\ F_{32} & F_{33} \end{pmatrix}. \tag{3.57}$$

After the matrix multiplication is explicitly carried on, one obtains this set of coupled equations

$$F_{22}\circ\tilde{G}_{0,22}^{-1\,\mathrm{A}} - \tilde{G}_{0,22}^{-1\,\mathrm{R}}\circ F_{22} + \frac{\Omega}{2}\circ F_{23}^* - F_{23}\circ\frac{\Omega}{2} = 0 \tag{3.58}$$

$$F_{33}\circ\tilde{G}_{0,33}^{-1\,\mathrm{A}} - \tilde{G}_{0,33}^{-1\,\mathrm{R}}\circ F_{33} + \frac{\Omega}{2}\circ F_{23} - F_{23}^*\circ\frac{\Omega}{2} + \Sigma_{33}^{\mathrm{R}}\circ F_{33} - F_{33}\circ\Sigma_{33}^{\mathrm{A}} = \Sigma_{33}^{\mathrm{K}} \tag{3.59}$$

$$F_{23}\circ\tilde{G}_{0,33}^{-1\,\mathrm{A}} - \tilde{G}_{0,22}^{-1\,\mathrm{R}}\circ F_{23} + \frac{\Omega}{2}\circ F_{33} - F_{22}\circ\frac{\Omega}{2} + \Delta F_{23} = F_{23}\circ\Sigma_{33}^{\mathrm{A}}. \tag{3.60}$$

After a WT on these three equation and an approximation to linear order in gradient, according to Eqs. (3.47, 3.48) the kinetic equations for the distributions functions are obtained (using that $\varepsilon_2 = \varepsilon_3$)

$$\{\omega - \varepsilon_2(\mathbf{p}),\, F_{22}\} - i\frac{\Omega}{2}(F_{23} - F_{23}^*) - \frac{1}{2}\left\{\frac{\Omega}{2}, F_{23} + F_{23}^*\right\} = 0 \tag{3.61}$$

$$\{\omega - \varepsilon_3(\mathbf{p}) - \mathrm{Re}\Sigma_{33}^{\mathrm{R}},\, F_{33}\} + i\frac{\Omega}{2}(F_{23} - F_{23}^*) - \frac{1}{2}\left\{\frac{\Omega}{2}, F_{23} + F_{23}^*\right\} = i\Sigma_{33}^{\mathrm{K}} +$$
$$+ 2\mathrm{Im}\Sigma_{33}^{\mathrm{R}}F_{33} \tag{3.62}$$

$$\left\{\omega - \varepsilon_3(\mathbf{p}) - \frac{1}{2}\mathrm{Re}\Sigma_{33}^{\mathrm{R}},\, F_{23}\right\} - i(\mathrm{Re}\Sigma_{33}^{\mathrm{R}} - \Delta)F_{23} - i\frac{\Omega}{2}(F_{22} - F_{33}) +$$
$$- \frac{1}{2}\left\{\frac{\Omega}{2}, F_{22} + F_{33}\right\} + \frac{i}{2}\{\mathrm{Im}\Sigma_{33}^{R}, F_{23}\} = \mathrm{Im}\Sigma_{33}^{\mathrm{R}}F_{23}. \tag{3.63}$$

In the right-hand side of Eq. (3.62) the *collisional integral* is defined

$$\tilde{I}_{\mathrm{coll}} = i\Sigma_{33}^{\mathrm{K}} + 2\mathrm{Im}\Sigma_{33}^{\mathrm{R}}F_{33}, \tag{3.64}$$

and this quantity accounts for the collisions between impurities and particles of the bath. A central role in these collisions belongs to Σ_{33}^{K}, and if this Keldysh component is not present a collisional integral can not be defined. Therefore, in the right-hand side of Eq. (3.63), where

only the imaginary part of the self energy is present, the *decoherence rate* $\tilde{\Gamma}^{\text{dec}}$ can be defined as

$$-\frac{\tilde{\Gamma}^{\text{dec}}}{2} = \text{Im}\Sigma_{33}^{\text{R}}. \tag{3.65}$$

After the Wigner transformation, convolutions are no longer present and all the functions in principle depend on two four dimensional variables $x = (\mathbf{r}, t)$ and $p = (\omega, \mathbf{p})$. A more suitable form for the kinetic equations is obtained through the explicit form of the Poisson brackets. Note that, since Σ_{33}^{R} is calculated in the non self-consistent T-matrix approximation, it does not depend on time. Moreover, the system is spatially homogeneous and thus all the functions do not depend on $\mathbf{r}$.

Kinetic equations for the distribution functions $F_{ij}(t, \omega, \mathbf{p})$ are, with $\Sigma_{33}^{\text{R}}(\mathbf{p}, \omega)$

$$\partial_t F_{22} - i\frac{\Omega}{2}(F_{23} - F_{32}^*) + \frac{1}{2}\partial_t \Omega \partial_\omega (F_{23} + F_{23}^*) = 0 \tag{3.66}$$

$$(1 - \partial_\omega \text{Re}\Sigma_{33}^{\text{R}})\partial_t F_{33} + i\frac{\Omega}{2}(F_{23} - F_{23}^*) + \frac{1}{2}\partial_t \Omega \partial_\omega (F_{23} + F_{23}^*) = \tilde{I}_{\text{coll}} \tag{3.67}$$

$$\left(1 - \frac{1}{2}\partial_\omega \text{Re}\Sigma_{33}^{\text{R}}\right)\partial_t F_{23} - i(\text{Re}\Sigma_{33}^{\text{R}} - \Delta)F_{23} - i\frac{\Omega}{2}(F_{22} - F_{33}) +$$

$$+ \frac{1}{2}\partial_t \Omega \partial_\omega (F_{22} + F_{33}) + \frac{i}{2}\partial_\omega \text{Im}\Sigma_{33}^{\text{R}}\partial_t F_{23} = -\frac{\tilde{\Gamma}^{\text{dec}}}{2}F_{23}. \tag{3.68}$$

Notice that since $\Omega(t) = \delta(t)\Omega$, this time dependence will be neglected from now on[1]. The above equations are for the distribution functions F_{ij} at any ω and not for the populations. In systems with a Rabi coupling, the connection between F_{ij} and the populations of the levels is not trivial to find, as opposed to the common situation in literature [2, 97, 98].

A way to find this connection is to work with the Kadanoff-Baym equation [21] for the Keldysh component of the GF. This equation is, in matrix form

$$D_0 G^{\text{K}} - G^{\text{K}} D_0 + \frac{i}{2}(\Gamma G^{\text{K}} + G^{\text{K}}\Gamma) + \frac{i}{2}\left[\{D_0, G^{\text{K}}\} - \{G^{\text{K}}, D_0\}\right] - \frac{1}{4}\left[\{\Gamma, G^{\text{K}}\} + \{G^{\text{K}}, \Gamma\}\right] =$$

$$= \Sigma^{\text{K}}G^{\text{A}} - G^{\text{R}}\Sigma^{\text{K}} + \frac{i}{2}\left[\{\Sigma^{\text{K}}, G^{\text{A}} - \{G^{\text{R}}, \Sigma^{\text{K}}\}\}\right], \tag{3.69}$$

where

$$D_0 = \begin{pmatrix} \omega - \varepsilon_{2,\mathbf{p}} & -\Omega/2 \\ -\omega/2 & \omega - \varepsilon_{3,\mathbf{p}} - \text{Re}\Sigma_{33}^{\text{R}} + \Delta \end{pmatrix} \tag{3.70}$$

$$\Gamma = \begin{pmatrix} 0 & 0 \\ 0 & -2\text{Im}\Sigma_{33}^{\text{R}} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \Gamma_{33} \end{pmatrix}. \tag{3.71}$$

When written in components, Kadanoff-Baym equation leads to equation that are similar to the ones for the distribution functions

$$\partial_t G_{22}^{\text{K}} + i\frac{\Omega}{2}(G_{23}^{\text{K}} - G_{32}^{\text{K}}) = 0 \tag{3.72}$$

$$(1 - \partial_\omega \text{Re}\Sigma_{33}^{\text{R}})\partial_t G_{33}^{\text{K}} - i\frac{\Omega}{2}(G_{23}^{\text{K}} - G_{23}^{\text{K}}) = i\Sigma_{33}^{\text{K}}(G_{33}^{\text{R}} - G_{33}^{\text{A}}) \tag{3.73}$$

$$\left(1 - \frac{1}{2}\partial_\omega \text{Re}\Sigma_{33}^{\text{R}}\right)\partial_t G_{23}^{\text{K}} - i(\text{Re}\Sigma_{33}^{\text{R}} - \Delta)G_{23}^{\text{K}} + i\frac{\Omega}{2}(G_{22}^{\text{K}} - G_{33}^{\text{K}}) +$$

$$+ \frac{i}{2}\partial_\omega \text{Im}\Sigma_{33}^{\text{R}}\partial_t G_{23}^{\text{K}} = -\frac{\Gamma_{33}}{2}G_{23}^{\text{K}} + iG_{23}^{\text{R}}\Sigma_{33}^{\text{K}}. \tag{3.74}$$

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[1]Even if this time dependence is included, it does not change the final kinetic equations because it will be removed by the procedure adopted.

At linear order in gradients of the WT, the matrix $\hat{G}^{\mathrm{K}}$ can be parametrized as

$$\hat{G}^{\mathrm{K}} = -\frac{i}{2}(\hat{\mathcal{A}}\hat{F} - \hat{F}\hat{\mathcal{A}}), \tag{3.75}$$

where $\hat{\mathcal{A}}$ is the matrix of spectral functions. In the limit of small Ω, i.e. when the Rabi coupling is a probe, the energies of levels $|2\rangle$ and $|3\rangle$ are not modified and the components of $\hat{G}^{\mathrm{K}}$ are

$$G_{22}^{\mathrm{K}} = -i\mathcal{A}_{22}F_{22} \tag{3.76}$$

$$G_{23}^{\mathrm{K}} = -\frac{i}{2}(\mathcal{A}_{22} + \mathcal{A}_{33})F_{23} \tag{3.77}$$

$$G_{32}^{\mathrm{K}} = -\frac{i}{2}(\mathcal{A}_{22} + \mathcal{A}_{33})F_{32} \tag{3.78}$$

$$G_{33}^{\mathrm{K}} = -i\mathcal{A}_{33}F_{33}, \tag{3.79}$$

and in the same limit the spectral functions are

$$\mathcal{A}_{22} = 2\pi\delta(\omega - \varepsilon_2(\mathbf{p})) \tag{3.80}$$

$$\mathcal{A}_{33} = \sum_{\alpha=a,r} Z_\alpha 2\pi\delta(\omega - \varepsilon_\alpha(\mathbf{p})), \tag{3.81}$$

where ε_2 is the bare energy of level $|2\rangle$ and ε_α is given by the polaron energy not modified by the Rabi coupling, Eq. (3.43). With the above results for spectral functions and components of $\hat{G}^{\mathrm{K}}$, it is possible to perform and integration over ω and obtain the so-called on-shell equation for the distribution functions. The advantage of using the Kadanoff-Baym equation instead of the DE is that for the former the on-shell projection is naturally defined, because all the distribution functions that of the equations are multiplied by a spectral function. In the on-shell equations, also the term with $\partial_\omega \mathrm{Im}\Sigma_{33}^{\mathrm{R}}$ is neglected because small. The final result is

$$\partial_t F_{22}^{(2)} - i\frac{\Omega}{2}\left[\frac{1}{2}(F_{23}^{(2)} - F_{32}^{(2)}) + \frac{1}{2}\sum_\alpha Z_\alpha(F_{23}^{(\alpha)} - F_{32}^{(\alpha)})\right] \tag{3.82}$$

$$\sum_\alpha \partial_t F_{33}^{(\alpha)} + i\frac{\Omega}{2}\left[\frac{1}{2}(F_{23}^{(2)} - F_{32}^{(2)}) + \frac{1}{2}\sum_\alpha Z_\alpha(F_{23}^{(\alpha)} - F_{32}^{(\alpha)})\right] = \sum_\alpha(i\Sigma_{33}^{\mathrm{K}\,(\alpha)} + 2\mathrm{Im}\Sigma_{33}^{\mathrm{R}\,(\alpha)}F_{33}^{(\alpha)}) \tag{3.83}$$

$$\left(1 - \frac{1}{2}\partial_\omega\mathrm{Re}\Sigma_{33}^{\mathrm{R}\,(2)}\right)\frac{1}{2}\partial_t F_{23}^{(2)} + \sum_\alpha \tilde{Z}_\alpha^{-1}Z_\alpha\frac{1}{2}\partial_t F_{23}^{(\alpha)} - i\left[(\mathrm{Re}\Sigma_{33}^{\mathrm{R}\,(2)} - \Delta)\frac{1}{2}F_{23}^{(2)} + \sum_\alpha \times\right.$$

$$\left.\times(\mathrm{Re}\Sigma_{33}^{\mathrm{R}\,(\alpha)} - \Delta)\frac{1}{2}Z_\alpha F_{23}^{(\alpha)}\right] + i\frac{\Omega}{2}(\sum_\alpha Z_\alpha F_{33}^{(\alpha)} - F_{22}^{(2)}) = \frac{1}{2}\left(\mathrm{Im}\Sigma_{33}^{(R)\,(2)}F_{23}^{(2)} + \sum_\alpha Z_\alpha\mathrm{Im}\Sigma_{33}^{(R)\,(\alpha)}F_{23}^{(\alpha)}\right), \tag{3.84}$$

where in the last equation the term $iG_{23}^{\mathrm{R}}\Sigma_{33}^{\mathrm{K}}$ vanishes on shell. The notation

$$F_{ij}^{(n)} \equiv F_{ij}(\omega = \varepsilon_n) \tag{3.85}$$

$$Z_\alpha = (1 - \partial_\omega\mathrm{Re}\Sigma_{33}^{\mathrm{R}}|_{\omega=\varepsilon_\alpha})^{-1} \tag{3.86}$$

$$\tilde{Z}_\alpha = \left(1 - \frac{1}{2}\partial_\omega\mathrm{Re}\Sigma_{33}^{\mathrm{R}}|_{\omega=\varepsilon_\alpha}\right)^{-1}, \tag{3.87}$$

has been used. Now, from the above equations for the on-shell distribution functions it is possible

to obtain the ones for the populations. Indeed, in general one has that

$$i \int_\omega G_{22}^K \equiv 1 - 2n_{22}^{(2)} = F_{22}^{(2)} \tag{3.88}$$

$$i \int_\omega G_{33}^K \equiv \sum_\alpha 1 - 2n_{33}^{(\alpha)} = \sum_\alpha Z_\alpha F_{33}^{(\alpha)} \tag{3.89}$$

$$i \int_\omega G_{23}^K \equiv f_{23}^{(2)} + \sum_\alpha f_{23}^{(\alpha)} = f_{23} = \frac{1}{2}(F_{23}^{(2)} + \sum_\alpha Z_\alpha F_{23}^{(\alpha)}) \tag{3.90}$$

With the above definition, the equations for the populations in $|2\rangle$ and $|3\rangle$ are easily obtained

$$\partial_t n_{22}^{(2)} + i\frac{\Omega}{2}(f_{23} - f_{23}^*) = 0 \tag{3.91}$$

$$\sum_\alpha \frac{1}{Z_\alpha} \partial_t n_{33}^{(\alpha)} - i\frac{\Omega}{2}(f_{23} - f_{23}^*) = \sum_\alpha I_{\text{coll}}^\alpha. \tag{3.92}$$

From the above equations, the conservation of coherent particles is obtained, i.e.

$$\partial_t(N_2 + N_3) = \int_{\mathbf{p}} \partial_t n_{22}^{(2)} + \sum_\alpha \frac{1}{Z_\alpha} \partial_t n_{33}^{(\alpha)} = 0. \tag{3.93}$$

The conservation of coherent particles inside the kinetic equations is a consequence of the assumption made on $\mathcal{A}_{33}$, Eq. (3.81), where the non-coherent part of the spectral function is totally neglected. Finally, in order to close the kinetic equations, only a single polaron branch has to be considered. In this case, both n_{ii} and f_{23} are projected on the same energy up to an effective mass correction and the kinetic equations become

$$\partial n_2 + i\frac{\Omega}{2}(f_{23} - f_{23}^*) = 0 \tag{3.94}$$

$$\partial n_\alpha - iZ_\alpha \frac{\Omega}{2}(f_{23} - f_{23}^*) = I_{\text{coll}}^\alpha \tag{3.95}$$

$$\partial f_{23} + i\tilde{Z}_\alpha \delta_\alpha f_{23} + i\frac{\Omega}{2}(n_\alpha - n_2) = -\frac{\Gamma_\alpha^{\text{dec}}}{2} f_{23}, \tag{3.96}$$

with $n_\alpha = n_{33}^{(\alpha)}$, $\delta_\alpha(\mathbf{p}) = \varepsilon_\alpha(\mathbf{p}) - \varepsilon_2(\mathbf{p}) - \Delta$ and $\Gamma_\alpha^{\text{dec}}$ is the decoherence rate. The absence of the tilde accent over collisional integral and decoherence rate indicates that they are written in terms of populations and not of distribution functions. Moreover, if $\delta_\alpha = 0$ and the terms on the right-hand side are neglected, it is possible to show explicitly that the Rabi frequency is renormalized as $\sqrt{Z_\alpha}\Omega$, in agreement with results obtained with variational Ansätz [84, 4]. This agreement is also an indication that the derived kinetic equations are a good model for the system. On the other hand, if only the decoherence rate is present, the renormalized Rabi frequency Ω_{ren} is given by

$$\Omega_{\text{ren}} = \sqrt{Z_\alpha \Omega^2 - (\Gamma_\alpha^{\text{dec}})^2}, \tag{3.97}$$

when only a single polaronic species is present in the system. For attractive polarons $\Gamma_a^{\text{dec}} \sim 0$ and the limit $\sqrt{Z_a}\Omega$ is recovered. Note that also this result for the renormalized Rabi frequency can also be obtained with a time dependent variational Ansätz [99].

The main result of the theoretical derivation are the kinetic equations for the single polaron species, Eqs. (3.94-3.96). Interestingly, they can also be derived starting from the DE for the Keldysh component, but the procedure to project on-shell and remove the ω dependence is better defined starting from the Kadanoff-Baym equation.

To better understand the kinetic equations, it is necessary to derive the explicit form of the collisional integral and of the decoherence rate. The strategy is the following: one starts from

the definitions, uses the kinetic equation for the dynamics of the molecules, projects on the polaron energy and then write everything in terms of the populations.

Starting from the definition of the collisional integral $\tilde{I}_{coll}$ given in Eq. 3.64, where Eqs. (3.52-3.54) and the definitions of self-energies, Eqs. (3.28-3.31) are used

$$
\begin{aligned}
\tilde{I}_{coll} = {}& i\Sigma_{33}^K + 2\mathrm{Im}\Sigma_{33}^R F_{33} = \\
= {}& \frac{2}{V}\sum_q \mathrm{Im}G_{0\phi}^R(q)\mathrm{Im}G_\eta^R(p+q)[F_{33}(p)(F_\phi(q) - F_\eta(p+q)) + 1 - F_\phi(q)F_\eta(p+q)] = \\
= {}& -\frac{1}{2V}\sum_q |G_\eta^R(p+q)|^2 \mathcal{A}_\phi(q)[i\Sigma_\eta^K(p+q)(F_{33}(p) + F_\phi(q)) + 2\mathrm{Im}\Sigma_\eta^R(p+q)(1 + F_{33}(p)F_\phi(q))] = \\
= {}& \left(\frac{1}{2V}\right)^2 \sum_{q,q'} |G_\eta^R(q)|^2 \mathcal{A}_\phi(q-p)\mathcal{A}_\phi(q-q')\mathcal{A}_{33}(q')\times \\
& \times [(F_{33}(p) + F_\phi(q-p))(1 + F_\phi(q-q')F_{33}(q')) - (1 + F_{33}(p)F_\phi(q-p))(F_{33}(q') + F_\phi(q-q'))],
\end{aligned}
$$
(3.98)

where in the last step the momentum $q = (\varepsilon, \mathbf{q})$ have been shifted. The integration over the energies ε and ε' contained in Eq. (3.98) can be performed, indeed

$$
\begin{aligned}
& \iint \frac{d\varepsilon d\varepsilon'}{(2\pi)^2} \, \mathcal{A}_\phi(q-p)\mathcal{A}(q-q')\mathcal{A}_{33}(q') = \\
& \iint d\varepsilon d\varepsilon' \, \delta(\varepsilon - \omega - \varepsilon_\phi(\mathbf{q}-\mathbf{p}))\delta(\varepsilon - \varepsilon' - \varepsilon_\phi(\mathbf{q}-\mathbf{q}')\mathcal{A}_{33}(q')) = \\
& = \mathcal{A}_{33}(\omega + \varepsilon_\phi(\mathbf{q}-\mathbf{p}) - \varepsilon_\phi(\mathbf{q}-\mathbf{q}'), \mathbf{q}').
\end{aligned}
$$
(3.99)

A hypothesis on $\mathcal{A}_{33}$ is needed to proceed further with the calculations. Indeed, it is assumed that the spectral function of the impurities in level $|3\rangle$ is peaked around polaron energies, so that it is possible to write that

$$
\mathcal{A}_{33}(q') = \sum_{\beta=a,r} 2\pi Z_\beta(\mathbf{q}')\delta(\varepsilon' - \varepsilon_\beta(\mathbf{q}')),
$$
(3.100)

and this assumption is consistent with the relation between distribution functions and populations. Finally, the collisional integral can be written as

$$
\begin{aligned}
\tilde{I}_{coll} = {}& \frac{2\pi}{(2V)^2}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\beta=a,r}|G_\eta^R(\omega + \varepsilon_\phi(\mathbf{q}-\mathbf{p}), \mathbf{q})|^2 Z_\beta(\mathbf{q}')\delta(\omega + \varepsilon_\phi(\mathbf{q}-\mathbf{p}) - \varepsilon_\beta(\mathbf{q}') - \varepsilon_\phi(\mathbf{q}-\mathbf{q}'))\times \\
& \times [(F_{33}(p) + F_\phi(\mathbf{q}-\mathbf{p}))(1 + F_\phi(\mathbf{q}-\mathbf{q}')F_{33}^\beta(\mathbf{q}')) - (1 + F_{33}(p)F_\phi(\mathbf{q}-\mathbf{p}))(F_{33}^\beta(\mathbf{q}') + F_\phi(\mathbf{q}-\mathbf{q}'))].
\end{aligned}
$$
(3.101)

As said before, the full G_η^R is equivalent to the T-matrix, so the notation $G_\eta^R = T_{sc}$ is used from now on. After the on-shell projection, the term inside $\sum_\alpha$ in the right-hand side of Eq. (3.83) becomes

$$
\begin{aligned}
\tilde{I}_{coll}^\alpha = {}& \frac{2\pi}{(2V)^2}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\beta=a,r}|T_{sc}(\varepsilon_\alpha(\mathbf{p}) + \varepsilon_\phi(\mathbf{q}-\mathbf{p}), \mathbf{q})|^2 Z_\beta(\mathbf{q}')\delta(\varepsilon_\alpha(\mathbf{p}) + \varepsilon_\phi(\mathbf{q}-\mathbf{p}) - \varepsilon_\beta(\mathbf{q}') - \varepsilon_\phi(\mathbf{q}-\mathbf{q}'))\times \\
& \times [(F_{33}^\alpha(\mathbf{p}) + F_\phi(\mathbf{q}-\mathbf{p}))(1 + F_\phi(\mathbf{q}-\mathbf{q}')F_{33}^\beta(\mathbf{q}')) - (1 + F_{33}^\alpha(\mathbf{p})F_\phi(\mathbf{q}-\mathbf{p}))(F_{33}^\beta(\mathbf{q}') + F_\phi(\mathbf{q}-\mathbf{q}'))].
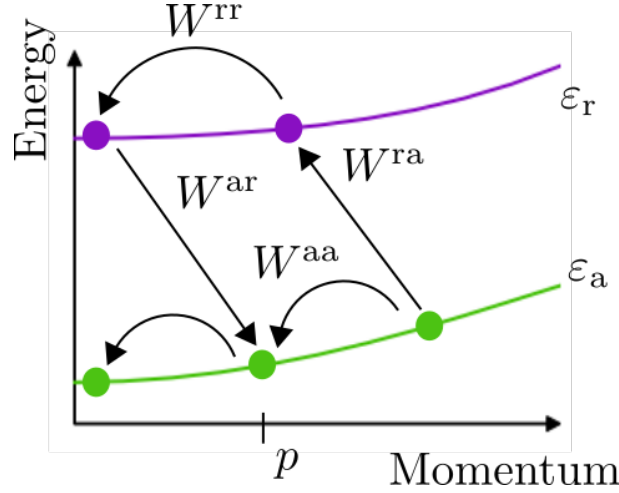\end{aligned}
$$
(3.102)

Figure 3.4. Pictorial representation of the scattering processes described by the collisional integral I_α in Eq. (3.62). In the rates $W^{\alpha\beta}$ and in the energies ε_α the labels a, r indicate attractive and repulsive polarons respectively.

The last step is to rewrite everything using the populations and to do this a bit of algebra is needed. The square bracket in the above equation can be written in a more suitable form as

$$8[n_\phi(\mathbf{q} - \mathbf{q}')n_\beta(\mathbf{q}') - n_\phi(\mathbf{q} - \mathbf{p})n_\alpha(\mathbf{p}) - n_\alpha(\mathbf{p})n_\phi(\mathbf{q} - \mathbf{q}')n_\beta(\mathbf{q}') + n_\alpha(\mathbf{p})n_\phi(\mathbf{q} - \mathbf{p})n_\beta(\mathbf{q}')+$$
$$+ n_\alpha(\mathbf{p})n_\phi(\mathbf{q} - \mathbf{p})n_\phi(\mathbf{q} - \mathbf{q}') - n_\phi(\mathbf{q} - \mathbf{p})n_\phi(\mathbf{q} - \mathbf{q}')n_\beta(\mathbf{q}')] =$$
$$= -8[(1 - n_\alpha(\mathbf{p}))(1 - n_\phi(\mathbf{q} - \mathbf{p}))n_\phi(\mathbf{q} - \mathbf{q}')n_\beta(\mathbf{q}') - n_\alpha(\mathbf{p})n_\phi(\mathbf{q} - \mathbf{p})(1 - n_\phi(\mathbf{q} - \mathbf{q}'))(1 - n_\beta(\mathbf{q}'))].$$
$$(3.103)$$

Now, all the ingredients necessary for writing I_{coll}^α are present. The first step is to substitute F_{ij} in the left-hand side of Eq. (3.83) with the expression for the populations and move Z_α^{-1} from the left-hand side to the right-hand side. Then, the collisional integral is written is his final form as

$$I_{\text{coll}}^\alpha = \sum_\beta I_{\alpha\beta}, \tag{3.104}$$

where $\sum_\beta I_{\alpha\beta}$ describes a scattering process between polarons in α and β. $I_{\alpha\beta}$ can be written as

$$I_{\beta\alpha}(\mathbf{p}) = \frac{1}{V}\sum_{\mathbf{q}'}\left\{W_{\mathbf{p}\mathbf{q}'}^{\alpha\beta}[1 - n_\alpha(\mathbf{p})]n_\beta(\mathbf{q}') - W_{\mathbf{q}'\mathbf{p}}^{\beta\alpha}[1 - n_\beta(\mathbf{p}')]n_\alpha(\mathbf{q})\right\}. \tag{3.105}$$

In this form, the collisional integral is expressed in terms of the transition rate $W_{\mathbf{q}'\mathbf{p}}^{\beta\alpha}$ (from the α polaron with momentum $\mathbf{p}$ to the β polaron with momentum $\mathbf{q}'$) and of its complementary process. The transition rates follow the Fermi golden rule and are given by

$$W_{\mathbf{p}\mathbf{q}'}^{\alpha\beta} = \frac{2\pi}{V}\sum_{\mathbf{q}}|T_{\text{sc}}(\varepsilon_\beta(\mathbf{q}') + \varepsilon_\phi(\mathbf{q} - \mathbf{q}'), \mathbf{q})|^2 Z_\alpha(\mathbf{q})Z_\beta(\mathbf{q}') \times \delta(\varepsilon_\alpha(\mathbf{p}) + \varepsilon_\phi(\mathbf{q} - \mathbf{p}) - \varepsilon_\phi(\mathbf{q} - \mathbf{q}') - \varepsilon_\beta(\mathbf{q}'))$$
$$\times n_\phi^{\text{eq}}(\mathbf{q} - \mathbf{q}')[1 - n_\phi^{\text{eq}}(\mathbf{q} - \mathbf{p})], \tag{3.106}$$

where it is now explicit that the population of the bath is at equilibrium, and therefore it is possible to use

$$n_\phi^{\text{eq}}(\mathbf{p}) = (1 + e^{\beta(\varepsilon_\phi(\mathbf{p}-\mu))})^{-1}, \tag{3.107}$$

with $\beta = 1/k_B T$ and μ is the chemical potential of the bath.

An illustration of the scattering processes involved in the collisional integral with the corresponding transition rates is given in Fig. 3.4. The term $|T_{\text{sc}}|^2$ is a cross-section for the scattering
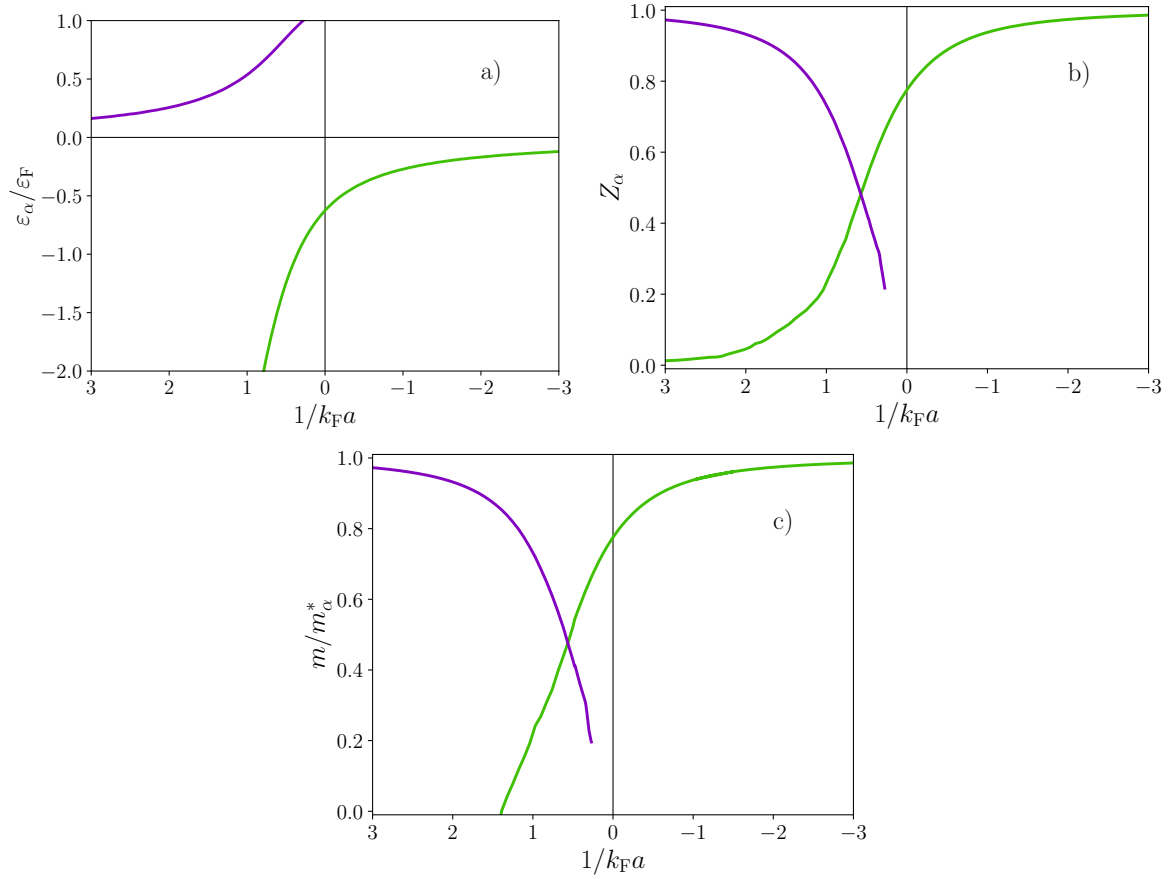
Figure 3.5. Panel a): 0-momentum energy ε_α at for the attractive (green) and repulsive (violet) polaron in the non self-consistent T-matrix approximation. Panel b): 0-momentum quasiparticle residue Z_α for repulsive and attractive polaron, same color code. Panel c): effective mass at 0-momentum for the attractive and the repulsive polaron, same color code.

process, the Dirac δ in Eq. (3.106) ensures the conservation of energy in the scattering process, the presence of the quasiparticle residues Z_α and Z_β is due to the fact that the process is happening between the polaron branches and thanks to $\sum_\beta$ both the relaxation processes on the same branch (W^{aa} and W^{rr}) and the conversion processes (W^{ar} and W^{ra}) are considered. Finally, also the meaning of the populations is clear: the first term in the curly brackets in Eq. (3.105) is for the *in* process, i.e. when a β polaron collides with an atom of the bath and the final product is an α polaron, while the second term describes the reverse *out* process.

A very similar procedure to what has been done for the collisional integral can be applied also to the decoherence rate, Eq. (3.65). The same procedure described for the collisional integral is applied

$$\tilde{\Gamma}_{33}^{\text{dec}} = \frac{2\pi}{V^2} \sum_{\mathbf{q},\mathbf{q}'} \sum_{\beta=a,r} |T_{\text{sc}}(\varepsilon_\beta(\mathbf{q}') + \varepsilon_\phi(\mathbf{q} - \mathbf{q}'), \mathbf{q})|^2 Z_\beta(\mathbf{q}') \delta(\omega + \varepsilon_\phi(\mathbf{q} - \mathbf{p}) - \varepsilon_\phi(\mathbf{q} - \mathbf{q}') - \varepsilon_\beta(\mathbf{q}'))$$
$$\times [(1 - n_\phi^{\text{eq}}(\mathbf{q} - \mathbf{q}'))(1 - n_\beta(\mathbf{q}'))n_\phi^{\text{eq}}(\mathbf{q} - \mathbf{p}) + (1 - n_\phi^{\text{eq}}(\mathbf{q} - \mathbf{p}))n_\phi^{\text{eq}}(\mathbf{q} - \mathbf{q}')n_\beta(\mathbf{q}')]. \quad (3.108)$$

After the projection on polaron energies and the substitution of distribution functions with population it is straightforward to obtain the final form of the decoherence rate

$$\Gamma_\alpha^{\text{dec}} = \frac{\tilde{Z}_\alpha(\mathbf{p})}{Z_\alpha(\mathbf{p})} \frac{1}{V} \sum_{\mathbf{q}'} \sum_{\beta=a,r} W_{\mathbf{p}\mathbf{q}'}^{\alpha\beta} n_\beta(\mathbf{q}') + W_{\mathbf{q}'\mathbf{p}}^{\beta\alpha}(1 - n_\beta(\mathbf{q}')), \quad (3.109)$$
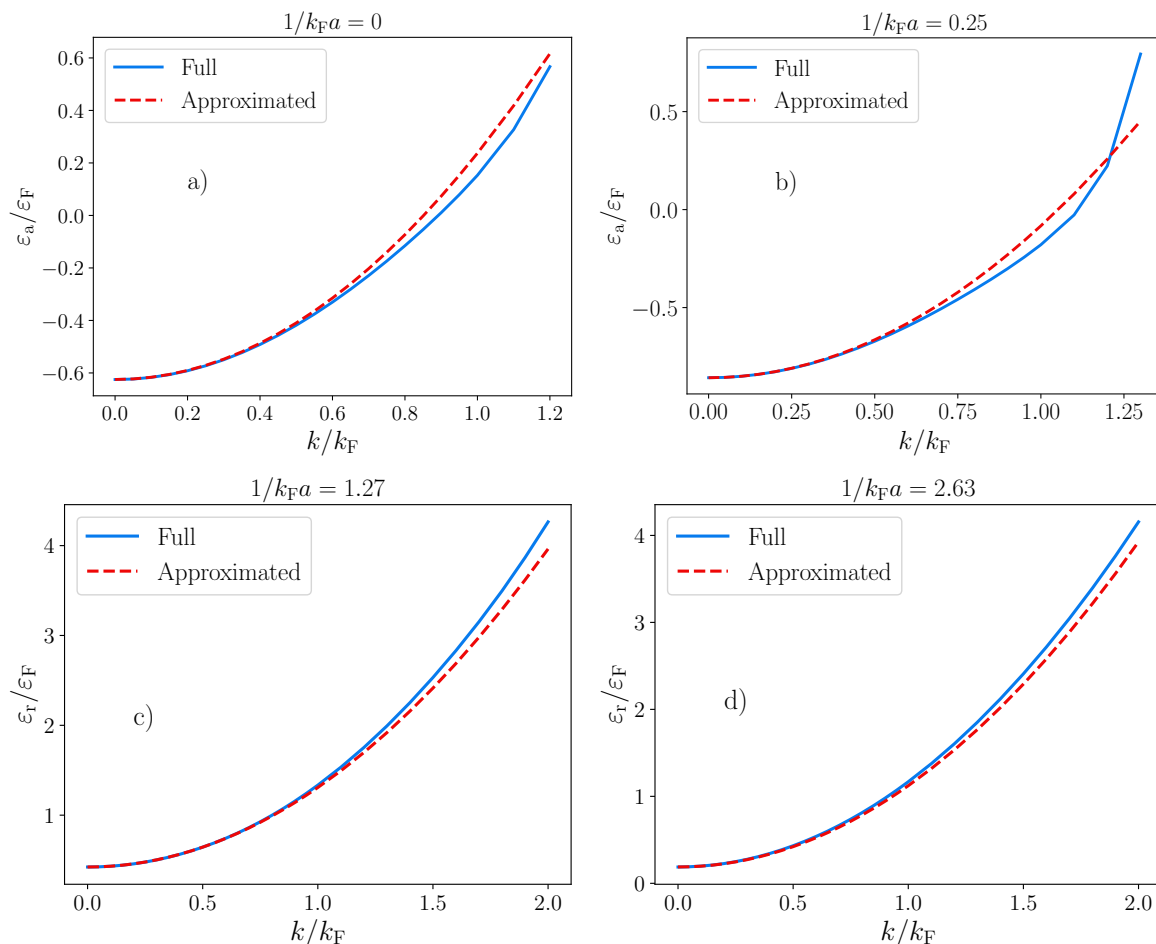
Figure 3.6. Comparison between the non self-consistent T-matrix dispersion relation, Eq. (3.43), and the approximated polaron dispersion relation, Eq. (3.113). Panel a) and b): attractive polaron Panel c) and d): repulsive polaron.

where the transition rates defined in Eq. (3.106) have been used. In this expression, the first term is related to the in processes, while the second is related to the out ones. Note that while both of them are originating from collisions of the impurity atom with the bath, collisional integral and decoherence rate are different in nature. The first one is indeed related to the imbalance of populations at different momenta and eventually at different branch, the second one affects coherences. In the long time, the collisional integral drives the population of minority atoms in thermal equilibrium with the bath.

The discussion on the kinetic equations for the system, Eqs. (3.61-3.63), is now completed, and the focus can move on. In the next section the numerical results obtained for the polaron properties and for the dynamics will indeed be discussed. It is also important to remember that even if the theoretical results might look as very specific for the system considered, an extension to different system can be easily made to obtain their kinematic equations.

3.3   Numerical results and comparison with experiment

In this section the focus is moved on the results for the static polaron properties and on the dynamics of the populations in level $|2\rangle$ and $|3\rangle$. The results will be computed using experimental parameters of Ref [4] that are:

- Temperature $T = 0.135T_F$, with T_F the Fermi temperature

- Rabi frequency $\Omega = 0.68\varepsilon_{\mathrm{F}}$

- Inverse scattering length $1/k_{\mathrm{F}}a = 0$, 0.25, 1.27, 2.63

- Impurity concentration in the non interacting level $\rho_2/\rho_\phi = 0.15$, with chemical potential of the impurities adjusted consequently

3.3.1 Static polaron properties

Until now, no quantitative analysis has been made on static polaron properties. An evaluation of the self-energy is necessary to do that, and this can be done only numerically with standard techniques for numerical integration.

All the properties are evaluated in the non self-consistent T-matrix approximation, where the retarded self-energy Σ_{33}^{R} is written as

$$\Sigma_{33}^{\mathrm{R}}(\omega, \mathbf{k}) = \sum_{\mathbf{q}} \frac{f_{\mathrm{FD}}(\xi_\phi(\mathbf{q}))}{\frac{m_{\mathrm{r}}}{2\pi a} - \sum_{\mathbf{p}} \left[\frac{1 - f_{\mathrm{FD}}(\xi_\phi(\mathbf{p}))}{\omega - \varepsilon_3(\mathbf{k}+\mathbf{q}-\mathbf{p}) - \varepsilon_\phi(\mathbf{p}) + \varepsilon_\phi(\mathbf{q}) + i0^+} + \frac{m}{p^2} \right]} , \tag{3.110}$$

with $\xi_i(\mathbf{q}) = \varepsilon_i(\mathbf{q}) - \mu_i$ and f_{FD} the Fermi-Dirac distribution at temperature T. With the experimental parameters and using Eq. (3.43) the results for the 0-momentum polaron energy at different scattering length are shown in Fig. 3.5 a) for the attractive and repulsive branch. The quasiparticle residue Z_α is defined as

$$Z_\alpha(\mathbf{p}) = \frac{1}{1 - \partial_\omega \mathrm{Re}\Sigma_{33}^{\mathrm{R}}(\omega, \mathbf{p})|_{\omega = \varepsilon_\alpha(\mathbf{p})}} , \tag{3.111}$$

and the 0-momentum results are shown in Fig 3.5 b). Finally, the effective mass is obtained as

$$m_\alpha^*(\mathbf{p}) = \frac{m/Z_\alpha(\mathbf{p})}{1 + \partial_{\varepsilon_3(\mathbf{p})}\mathrm{Re}\Sigma_{33}^{\mathrm{R}}(\mathbf{p}, \varepsilon_\alpha(\mathbf{p}))} , \tag{3.112}$$

and is shown in Fig. 3.5 c). With the results obtained for the effective mass and for the 0-momentum energy is possible to make a comparison between the polaron energy ε_α obtained with the non self-consistent T-matrix self-energy and the approximated form

$$\varepsilon_\alpha(\mathbf{p}) \approx \varepsilon_\alpha(0) + \frac{\mathbf{p}^2}{2m_\alpha^*(0)} . \tag{3.113}$$

The comparisons between the two dispersion relation for the polaron parameters in Table 3.1 and 3.2 are shown in Fig 3.6

$1/k_{\mathrm{F}}a$	$E_0/\varepsilon_{\mathrm{F}}$	m_*/m	$Z_{\mathrm{a}}(0)$
0	-0.625	1.16	0.775
0.25	-0.858	1.29	0.673

Table 3.1. Attractive polaron parameters at $T = 0.135T_F$.

$1/k_{\mathrm{F}}a$	$E_0/\varepsilon_{\mathrm{F}}$	m_*/m	$Z_{\mathrm{r}}(0)$
1.27	0.423	1.13	0.823
2.63	0.188	1.07	0.963

Table 3.2. Repulsive polaron parameters at $T = 0.135T_F$

3.3.2 Rabi coupling and polaron energy

As shown in Eq. (3.42), the presence of the Rabi coupling modifies the energy of the polarons. However, this fact has been neglected throughout the theoretical derivation made so far, e.g. when the projection over energies was made in the kinetic equations, the polaron energy was
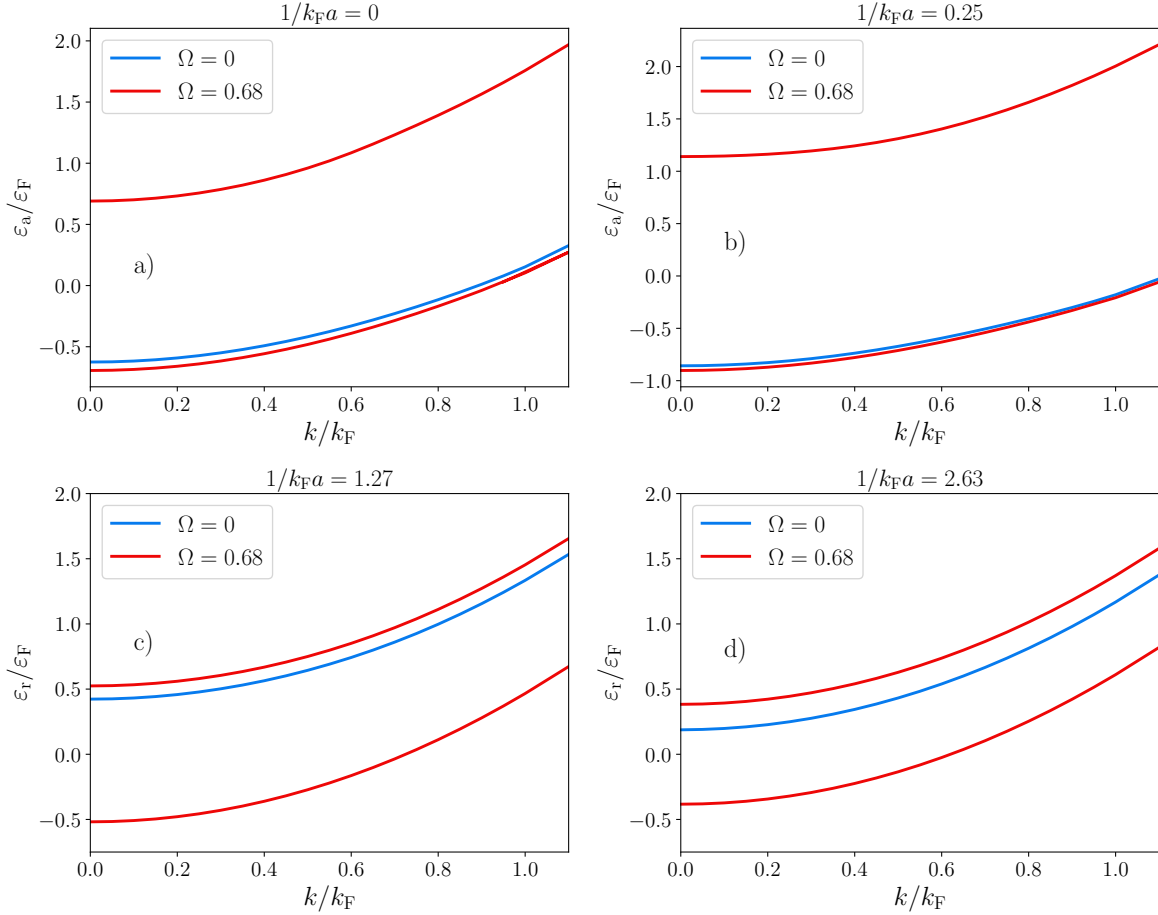
Figure 3.7. Comparison between exact polaron dispersion relation with and without Rabi frequency Ω for attractive, panel a) and b), and repulsive, panel c) and d), polarons at scattering lengths used in the experiment.

considered without the contribution from the Rabi coupling. The physical intuition behind this assumption is that, apart from Rabi coupling of great strength, the polaron is still a well-defined quasiparticle even in the presence of Ω. Conversely, when Ω is too large the polaron is not a well-defined quasiparticle and the system is more conveniently described with a superposition of states of levels $|2\rangle$ and $|3\rangle$.

The modified polaron energy can be calculated once the detuning Δ is fixed. To match experimental conditions, the detuning is set on resonance with the bare attractive and repulsive polaron at zero momentum, Eq. (3.43). The Rabi coupling split the bare attractive and repulsive branches both into two branches. For the experimental range of parameters considered, the results obtained are shown in Fig. 3.7. One of the new two branches is close to the bare one and the gap between the two branches is of order ε_F in any case, therefore the approximation of neglecting the splitting effect of the Rabi coupling in the projection over energies is justified by the large energy gap. Moreover, this approximation is based also on physical intuition: the Rabi coupling is indeed a probe in the experimental setup, so it is not expected to modify strongly the static properties. Otherwise, the polaron itself would be ill-defined in the theoretical framework and this will not match experimental conditions. Therefore, as long as the polaron formation process is fast and Ω is an adiabatic perturbation in the dynamics, the bare polaron energies ε_α can be considered as done here. In the opposite limit, where Ω is extremely fast, the polaron is not formed at all and the standard two level Rabi system is reproduced.
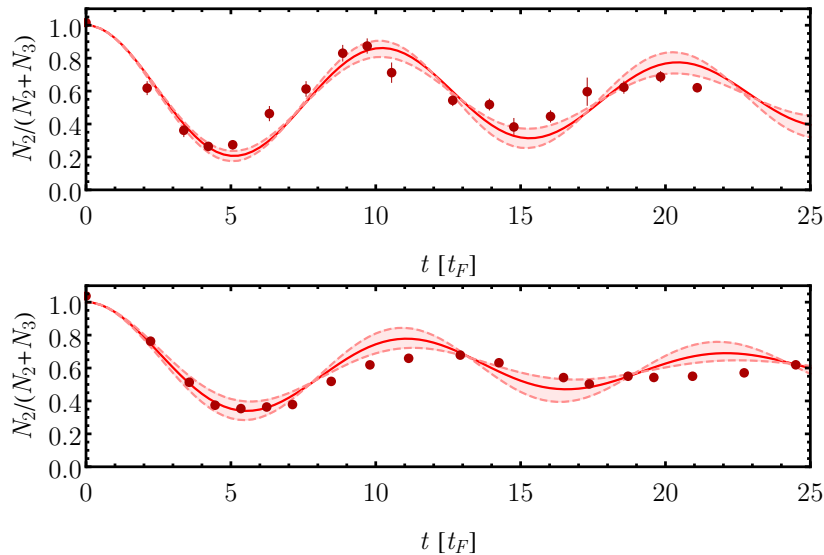
Figure 3.8. Rabi oscillations of the impurity populations for $1/(k_\mathrm{F}a) = 0, 0.25$ from top to bottom. Red dots are experimental results [4] and solid lines are the solutions of Eqs. (3.94-3.96). The shaded region indicates the confidence interval of 20% for the temperature.

3.3.3 Dynamics

Attractive polaron dynamics

Dynamics can be investigated by solving numerically Eqs. (3.94- 3.96). Initially, all the atoms are in state $|2\rangle$ and on resonance with the bare-to-polaron transition at 0 momentum, i.e. $\delta_\mathrm{a}(\mathbf{k} = 0) = 0$. The parameters used in simulations are the ones listed in Tab 3.1 and, due to significant detuning and small Z_r, the repulsive branch is assumed to be not populated. As shown by Eq. (3.93), the number of coherent particles in conserved by kinetic equations. Nonetheless, in the experimental procedure [4] also the incoherent particles are probed, and therefore to compare theoretical predictions and experimental result the number of particle has to be defined as

$$N_2 = \frac{1}{V} \sum_{\mathbf{k}} [Z_\mathrm{a} n_2 + (1 - Z_\mathrm{a}) n_2(t = 0)] \tag{3.114}$$

$$N_3 = \frac{1}{V} \sum_{\mathbf{k}} (n_\mathrm{a}). \tag{3.115}$$

In the last term in N_2 the density in state 2 that couples neither to the repulsive nor to the attractive (and it is therefore conserved) is considered. In Fig. 3.8 the results are shown for $1/k_\mathrm{F}a = 0, 0.25$ and $T = 0.135\, T_\mathrm{F}$ within a range of $\pm 20\%$.

The non self-consistent T-matrix approximation provides a reasonable agreement between experimental and numerical data for the considered scattering lengths.

Repulsive polaron dynamics

Dynamics of the repulsive branch is investigated in the same way of the attractive one. In this case, the initial condition on the detuning is $\delta_\mathrm{r}(\mathbf{k} = 0) = 0$. For $1/k_\mathrm{F}a = 1.27, 2.63$ and experimental parameters listed in Tab. 3.2 the detuning between the polaron branches is large and therefore also here it is assumed that the attractive branch is not populated. The particle number is defined in the same way of Eqs. (3.114-3.115), with the exchange of Z_a, n_a with Z_r, n_r. The uncertainty in temperature is almost not visible and the agreement with experimental
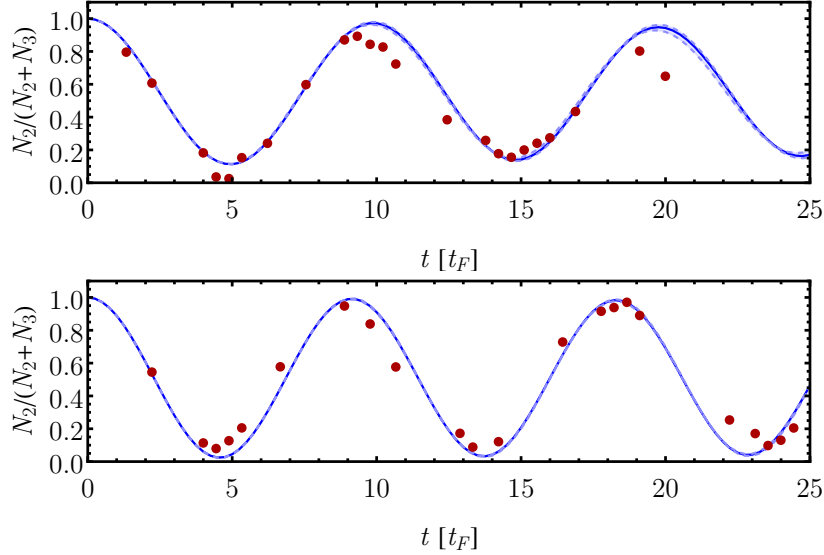
Figure 3.9. Rabi oscillations for $1/(k_{\mathrm{F}}a) = 1.27, 2.63$ from top to bottom. The shaded region that indicates the temperature confidence interval is barely visible.

data is good, see Fig. 3.9, if decay on the polaron branch is neglected in both the decay rate and the collisional integral. This assumption is necessary because on the timescale considered the decoherence of the repulsive polaron is not observable.

Interestingly, neglecting the collisional integral provides a good approximation for both the attractive and the repulsive dynamics. This means that the dynamics is dominated by the coherent transfer between the levels and decoherence rate $\Gamma_\alpha^{\mathrm{dec}}$ and that the thermalization of impurities is a slow process. Moreover, the observed Rabi oscillations are renormalized by $\sqrt{\alpha}$ for both branches as expected.

3.4 Conclusions

In this Chapter, a method to derive a set of kinetic equations for polarons coherently driven between two internal levels was derived. While the derivation of this kinetic equation is based on textbook definitions, the extension to the polaron case is surprisingly non trivial. Indeed, the approximations needed to obtain the physically intuitive kinetic equations Eqs. (3.94-3.96) are deeply connected to the physical properties of the system and not always trivial to perform. While the formalism used is a bit involved, thanks to it introducing *ad hoc* parameters is not necessary in the kinetic equations: indeed, they all arise naturally and are formally exact.

The coupling with the bath induces redistribution of momenta through the collisional integral and provides a decoherence rate which on the other hand preserves particles' momenta. The parameters in the kinetic equations are derived within the non self-consistent T-matrix approximation, which gives reliable results for equilibrium properties. It is important to stress out that simply going beyond this approximation for the T matrix it is not obvious that better results are immediately obtained for the dynamics. Indeed, this improvement has to be tuned with the other approximations made in the derivation of the collisional integral.

The theory provided here is therefore able to describe both attractive and repulsive polaron without external fitting parameters, contrary to what is needed when the dynamics is studied with a variational Ansätz [99]. Moreover, the theory is in general able to describe out-of-equilibrium effects related to quasiparticle properties such as repulsive-attractive polaron coherence, generation of quasiparticles in presence of strong Rabi coupling, impurity thermalization and others.

These effects are not described here but their study is an interesting future perspective.

Chapter 4

Conclusions

In this thesis, we introduced the general concept of open quantum systems and highlighted that it is relevant for different applications in the field of ultracold atoms.

In the first part, we discussed two different approaches for the dynamics of open quantum systems: the first one is based on master equations for the reduced density matrix and the second one is based on the so-called Keldysh field theory. While some introductory examples, e.g. quantum Brownian motion, are illustrated for the first approach, it is the second that is used in the rest of the thesis. The reason why the second approach was used is clear by looking at the aforementioned examples for the first one: when the number of degrees of freedom involved is large, a master equation approach is increasingly difficult both theoretically and numerically. On the other hand, an approach that relies on quantum field theory techniques possesses a large toolbox for dealing with such problem. The choice of Keldysh field theory is made because this formulation of quantum filed theory is designed for non-equilibrium scenarios for the dynamics.

In the second part, a paradigmatic system is treated: impurities interacting with a bath of free fermions. It is well known that induced inter-impurity interactions are hard to probe experimentally and to describe theoretically at the full quantum level, so we rely on Keldysh field theory to derive an effective semiclassical equation of motion, the so-called generalized Langevin equation (GLE), for the dynamics of impurities where induced inter-impurity interactions are present. The underlying quantum nature of the system is not lost but it is encoded in the coefficients of the GLE, where an induced attractive force (that is a finite temperature version of the RKKY interaction) between impurities and a configuration dependent friction matrix are present. Note that an induced force that is described as density ribbles is the result one would intuitively expect when the only interactions present are density-density interactions between impurities and bath particles. Interestingly, when also direct inter-impurity interactions are present in the system, the induced force is expected to be present at the level of the generalized Langevin equation as a correction to the direct interaction. On the other hand, the friction matrix structure is in agreement with classical results for incompressible fluids and it is given by a constant term and an inter-impurity distance-dependent one: the former is specifically related to the equilibrium properties of the bath and to its temperature, while the latter is a measure of how much each impurity changes the polarization of the bath in the vicinity of other impurities. The interplay between temperature and induced interactions can lead to the formation of bound states, whose lifetime can be predicted with Kramer's theory, finding excellent agreement with numerical simulations. We also suggest that, while at the moment experiments are lacking, our model should be experimentally accessible within the current technology. Finally, a discussion on the effective mass, absent in the generalized Langevin equation, is made, showing that in the limit of heavy impurities the renormalization of the mass is a small effect, in agreement with previous results for Fermi polarons in the heavy impurity limit. If anyway the effective mass has

to be included in this model, a possible phenomenological way would be the direct substitution of the bare impurity mass with the renormalized one: indeed, distance-dependent terms for the effective mass are expected to be small and negligible in our parameter regime.

In the last part, a two-level system is studied, of which one is non-interacting and in one polarons are present as consequence of the interaction with a bath, with Rabi coupling between them. This system has been investigated experimentally and our aim is to derive a general theory without external fitting parameters that is consistent with observed results and able to provide predictions.

With a slightly different implementation of Keldysh formalism, we obtain a set of coupled kinetic equations for the populations on the levels and for their coherences. The form of these equations is simple and physically intuitive, but their derivation is not possible with a variational Ansätz. They reproduce some well known results such as the renormalization of the Rabi frequency due to the quasiparticle residue, and provide a clear insight on the role of interactions, that is embedded in the explicit form of the collisional integral and of the decoherence rate: the former is responsible for population redistribution and transition between different branches, while the latter is responsible for loss of coherence between the free and interacting level. Another useful result of this theory is that the precise form of the collisional integral and of the decoherence rate is directly obtained without any *a priori* hypothesis on their possible form,.

The great advantage of this approach is that all the parameters that enters the kinetic equations arise naturally and are formally exact, so any further refinement of the approximations made is possible without a dramatic change in the underlying theory. As a proof of our results, the comparison between this theory and the experimental data is shown and there is a good agreement for both the repulsive and attractive polaron dynamics without any external fitting parameter. Moreover, even if not shown here, this formalism is able to deal with others non-equilibrium problems related to quasiparticles such as impurity thermalization, which would be very interesting to treat in future work.

Appendices

Appendix A

Derivation of transition probability

In this appendix, the analytic derivation that is needed to obtain Eq. (2.63) from Eq. (2.58) is illustrated. Fro convenience, Eq. (2.58) is reported here

$$\Phi(\mathbf{Q}', \mathbf{Q}'') = \frac{g^2}{2} \sum_{i,j=1}^{N} \int_0^t du \left\{ \mathcal{V}^*(\mathbf{q}_{i,2} - \mathbf{q}_{j,2}) - \mathcal{V}(\mathbf{q}_{i,1} - \mathbf{q}_{j,1}) + 2iW(\mathbf{q}_{i,1} - \mathbf{q}_{j,2}) + \right.$$

$$\left. + \frac{\beta}{2}(\dot{\mathbf{q}}_{i,1} + \dot{\mathbf{q}}_{j,2}) \frac{\partial}{\partial \mathbf{q}_{j,2}} W(\mathbf{q}_{i,1} - \mathbf{q}_{j,2}) \right\}. \quad (A.1)$$

As explained in Sec. 2.2.2, the first step is inserting the coordinates

$$\mathbf{r}_i = \frac{1}{2}(\mathbf{q}_{i,1} + \mathbf{q}_{i,2}) \qquad \mathbf{y}_i = \mathbf{q}_{i,1} - \mathbf{q}_{i,2}, \quad (A.2)$$

inside Eq. (2.58). The whole exponent of the transition probability

$$P(\mathbf{R}_f, t | \mathbf{R}_i, 0) = \int_{\mathbf{R}_i}^{\mathbf{R}_f} \mathcal{D}\mathbf{R} \int_0^0 \mathcal{D}\mathbf{Y} \ e^{iS_0[\mathbf{R},\mathbf{Y}] + \frac{i}{\hbar}\Phi[\mathbf{R},\mathbf{Y}]}, \quad (A.3)$$

is given by

$$iS_0[\mathbf{R}, \mathbf{Y}] = -\frac{im_\mathrm{I}}{\hbar} \sum_{i=1}^{N} \int_0^t du \ \ddot{\mathbf{r}}_i \cdot \mathbf{y}_i, \quad (A.4)$$

$$i\Phi[\mathbf{R}, \mathbf{Y}] = \frac{ig^2}{2} \sum_{i,j=1}^{N} \int_0^t du \left\{ \mathcal{V}^* \left(\mathbf{r}_i - \mathbf{r}_j + \frac{\mathbf{y}_j}{2} - \frac{\mathbf{y}_i}{2} \right) - \mathcal{V} \left(\mathbf{r}_i - \mathbf{r}_j + \frac{\mathbf{y}_i}{2} - \frac{\mathbf{y}_j}{2} \right) + \right.$$

$$2iW \left(\mathbf{r}_i - \mathbf{r}_j + \frac{\mathbf{y}_i}{2} + \frac{\mathbf{y}_j}{2} \right) + \frac{\beta}{2} \left(\dot{\mathbf{r}}_i + \dot{\mathbf{r}}_j + \frac{\dot{\mathbf{y}}_i}{2} - \frac{\dot{\mathbf{y}}_j}{2} \right)^T \times$$

$$\left. \times \left(\frac{\partial}{2\partial \mathbf{r}_j} - \frac{\partial}{\partial \mathbf{y}_j} \right) W \left(\mathbf{r}_i - \mathbf{r}_j + \frac{\mathbf{y}_i}{2} + \frac{\mathbf{y}_j}{2} \right) \right\}. \quad (A.5)$$

All the terms inside the integral in Eq. (A.5) have to be treated separately. The expansion of a function $f(\mathbf{x})$ where the argument is a vector is

$$f(\mathbf{x}) = f(\mathbf{a}) + (\mathbf{x} - \mathbf{a})^T \nabla f(\mathbf{a}) + \frac{1}{2}(\mathbf{x} - \mathbf{a})^T \mathcal{H}(\mathbf{a})(\mathbf{x} - \mathbf{a}) + \mathcal{O}(|\mathbf{x} - \mathbf{a}|^3), \quad (A.6)$$

Considering the first three terms of the influence functional, i.e. the ones where the derivative is not present, their expansions are given by

$$\mathcal{V}\left(\mathbf{r}_i - \mathbf{r}_j + \frac{1}{2}(\mathbf{y}_i - \mathbf{y}_j)\right) = \mathcal{V}(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{2}(\mathbf{y}_i - \mathbf{y}_j)^T \nabla \mathcal{V}(\mathbf{r}_i - \mathbf{r}_j) +$$

$$+ \frac{1}{8}(\mathbf{y}_i - \mathbf{y}_j)^T \mathcal{H}_\mathcal{V} \mathcal{V}(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i - \mathbf{y}_j), \tag{A.7}$$

$$\mathcal{V}^*\left(\mathbf{r}_i - \mathbf{r}_j - \frac{1}{2}(\mathbf{y}_i - \mathbf{y}_j)\right) = \mathcal{V}^*(\mathbf{r}_i - \mathbf{r}_j) - \frac{1}{2}(\mathbf{y}_i - \mathbf{y}_j)^T \nabla \mathcal{V}^*(\mathbf{r}_i - \mathbf{r}_j) +$$

$$+ \frac{1}{8}(\mathbf{y}_i - \mathbf{y}_j)^T \mathcal{H}_{\mathcal{V}^*} \mathcal{V}(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i - \mathbf{y}_j), \tag{A.8}$$

$$W\left(\mathbf{r}_i - \mathbf{r}_j + \frac{1}{2}(\mathbf{y}_i + \mathbf{y}_j)\right) = W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{2}(\mathbf{y}_i + \mathbf{y}_j)^T \nabla W(\mathbf{r}_i - \mathbf{r}_j) +$$

$$+ \frac{1}{8}(\mathbf{y}_i + \mathbf{y}_j)^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i + \mathbf{y}_j). \tag{A.9}$$

With these expansions, the term $\mathcal{V}^* - \mathcal{V}$ becomes

$$\sum_{i,j=1}^{N} \mathcal{V}^* - \mathcal{V} = \sum_{i,j=1}^{N} \mathcal{V}^*(\mathbf{r}_i - \mathbf{r}_j) - \mathcal{V}(\mathbf{r}_i - \mathbf{r}_j) - \frac{1}{2}(\mathbf{y}_i - \mathbf{y}_j)^T(\nabla \mathcal{V}^*(\mathbf{r}_i - \mathbf{r}_j) + \nabla \mathcal{V}(\mathbf{r}_i - \mathbf{r}_j)) +$$

$$+ \frac{1}{8}(\mathbf{y}_i - \mathbf{y}_j)^T[\mathcal{H}_\mathcal{V}(\mathbf{r}_i - \mathbf{r}_j) - \mathcal{H}_{\mathcal{V}^*}(\mathbf{r}_i - \mathbf{r}_j)](\mathbf{y}_i - \mathbf{y}_j) =$$

$$= \sum_{i,j=1}^{N} -2iW(\mathbf{r}_i - \mathbf{r}_j) - (\mathbf{y}_i - \mathbf{y}_j)^T \nabla V(\mathbf{r}_i - \mathbf{r}_j) - \frac{i}{4}(\mathbf{y}_i - \mathbf{y}_j)^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i - \mathbf{y}_j) =$$

$$= \sum_{i,j=1}^{N} -2iW(\mathbf{r}_i - \mathbf{r}_j) - (\mathbf{y}_i - \mathbf{y}_j)^T \nabla V(\mathbf{r}_i - \mathbf{r}_j) + \frac{i}{2}\mathbf{y}_j^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i - \mathbf{y}_j), \tag{A.10}$$

where the last equality is a consequence of the fact that $\mathcal{H}_\mathcal{V}(\mathbf{r}_i - \mathbf{r}_j) = \mathcal{H}_\mathcal{V}(\mathbf{r}_j - \mathbf{r}_i)$ and $\nabla \mathcal{V}(\mathbf{r}_i - \mathbf{r}_j) = -\nabla \mathcal{V}(\mathbf{r}_j - \mathbf{r}_i)$ because $\mathcal{V}(\mathbf{r}_i - \mathbf{r}_j) = \mathcal{V}(\mathbf{r}_j - \mathbf{r}_i)$. Another consequence is that

$$\sum_{i,j=1}^{N} (\mathbf{y}_i + \mathbf{y}_j)^T \nabla W(\mathbf{r}_i - \mathbf{r}_j) = \sum_{i,j=1}^{N} \mathbf{y}_i^T \nabla W(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i,j=1}^{N} \mathbf{y}_j^T \nabla W(\mathbf{r}_i - \mathbf{r}_j) =$$

$$= \sum_{i,j=1}^{N} \mathbf{y}_i^T \nabla W(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i,j=1}^{N} \mathbf{y}_i^T \nabla W(\mathbf{r}_j - \mathbf{r}_i) = 0, \tag{A.11}$$

and so the $2iW$ terms is

$$2i \sum_{i,j=1}^{N} W\left(\mathbf{r}_i - \mathbf{r}_j + \frac{1}{2}(\mathbf{y}_i + \mathbf{y}_j)\right) = 2i \sum_{i,j=1}^{N} W(\mathbf{r}_i - \mathbf{r}_j) + \frac{i}{2}\left(\mathbf{y}_i^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)\mathbf{y}_i + \mathbf{y}_i^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)\mathbf{y}_j\right)$$

$$\tag{A.12}$$

Eq. (A.10) and Eq. (A.12) can now be summed, and the result is

$$\sum_{i,j=1}^{N} -2iW(\mathbf{r}_i - \mathbf{r}_j) - (\mathbf{y}_i - \mathbf{y}_j)^T \nabla V(\mathbf{r}_i - \mathbf{r}_j) + \frac{i}{2}\mathbf{y}_j^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i - \mathbf{y}_j)+$$

$$+ 2iW(\mathbf{r}_i - \mathbf{r}_j) + \frac{i}{2}\mathbf{y}_i \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i + \mathbf{y}_j) =$$

$$= \sum_{i,j=1}^{N} -(\mathbf{y}_i - \mathbf{y}_j)^T \nabla V(\mathbf{r}_i - \mathbf{r}_j) + \frac{i}{2}(\mathbf{y}_j^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)\mathbf{y}_i - \mathbf{y}_j^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)\mathbf{y}_j+$$

$$+ \mathbf{y}_i^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)\mathbf{y}_i + \mathbf{y}_i^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)\mathbf{y}_j) =$$

$$= \sum_{i,j=1}^{N} 2\mathbf{y}_j^T \nabla V(\mathbf{r}_i - \mathbf{r}_j) + i\mathbf{y}_j^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)\mathbf{y}_i. \tag{A.13}$$

Now that the sum of the first three terms has been investigated, the focus is moved on the last term of the integrand. For this term, it is convenient to treat separately the cases $i \neq j$ and $i = j$:

$$i \neq j \quad \frac{\beta}{2}\left(\dot{\mathbf{r}}_i + \dot{\mathbf{r}}_j + \frac{\dot{\mathbf{y}}_i}{2} - \frac{\dot{\mathbf{y}}_j}{2}\right)^T \frac{\partial}{\partial \mathbf{r}_j}W\left(\mathbf{r}_i - \mathbf{r}_j + \frac{\mathbf{y}_i}{2} + \frac{\mathbf{y}_j}{2}\right) \tag{A.14}$$

$$i = j \quad -\beta\dot{\mathbf{r}}_i \frac{\partial}{\partial \mathbf{y}_i}W(\mathbf{y}_i). \tag{A.15}$$

In the case $i = j$ the insertion of the expansion for w leads to

$$\sum_{i=1}^{N} -\beta\dot{\mathbf{r}}_i^T \frac{\partial}{\partial \mathbf{y}_i}\left(W(0) + \mathbf{y}_i^T \nabla W(0) + \frac{1}{2}\mathbf{y}_i^T \mathcal{H}_W(0)\mathbf{y}_i\right) = \sum_{i=1}^{N} -\beta\dot{\mathbf{r}}_i^T \mathcal{H}_W(0)\mathbf{y}_i. \tag{A.16}$$

For the term $i \neq j$, the products that involve $\dot{\mathbf{r}}_i + \dot{\mathbf{r}}_j$ and $(\dot{\mathbf{y}}_i + \dot{\mathbf{y}}_j)/2$ in Eq. (A.14) are considered separately inside the sum over i, j. The term with the first of these products is

$$\frac{\beta}{2}\sum_{i \neq j}(\dot{\mathbf{r}}_i + \dot{\mathbf{r}}_j)\frac{\partial}{\partial \mathbf{r}_j}\left(W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{2}(\mathbf{y}_i + \mathbf{y}_j)^T \nabla W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{8}(\mathbf{y}_i + \mathbf{y}_j)^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i + \mathbf{y}_j)\right) =$$

$$= \frac{\beta}{2}\sum_{i \neq j}(\dot{\mathbf{r}}_i + \dot{\mathbf{r}}_j)\left(-\nabla W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{2}(\mathbf{y}_i + \mathbf{y}_j)^T \frac{\partial}{\partial \mathbf{r}_j}\nabla W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{8}(\mathbf{y}_i + \mathbf{y}_j)^T \frac{\partial}{\partial \mathbf{r}_j}\mathcal{H}_W\mathbf{r}_i - \mathbf{r}_j(\mathbf{y}_i + \mathbf{y}_j)\right) =$$

$$= \frac{\beta}{2}\sum_{i \neq j}\dot{\mathbf{r}}_j^T(\mathbf{y}_i + \mathbf{y}_j)^T \frac{\partial}{\partial \mathbf{r}_j}\nabla W(\mathbf{r}_i - \mathbf{r}_j) = \frac{\beta}{2}\sum_{i \neq j}\mathbf{y}_j^T\left(\dot{\mathbf{r}}_j\frac{\partial}{\partial \mathbf{r}_j} - \dot{\mathbf{r}}_i\frac{\partial}{\partial \mathbf{r}_i}\right)\nabla W(\mathbf{r}_i - \mathbf{r}_j), \tag{A.17}$$

while the second is

$$\frac{\beta}{4}\sum_{i \neq j}(\dot{\mathbf{y}}_i - \dot{\mathbf{y}}_j)\frac{\partial}{\partial \mathbf{r}_j}\left(W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{2}(\mathbf{y}_i + \mathbf{y}_j)^T \nabla W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{8}(\mathbf{y}_i + \mathbf{y}_j)^T \mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i + \mathbf{y}_j)\right) =$$

$$= \frac{\beta}{4}\sum_{i \neq j}(\dot{\mathbf{y}}_i - \dot{\mathbf{y}}_j)\left(-\nabla W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{2}(\mathbf{y}_i + \mathbf{y}_j)^T \frac{\partial}{\partial \mathbf{r}_j}\nabla W(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{8}(\mathbf{y}_i + \mathbf{y}_j)^T \frac{\partial}{\partial \mathbf{r}_j}\mathcal{H}_W\mathbf{r}_i - \mathbf{r}_j(\mathbf{y}_i + \mathbf{y}_j)\right) =$$

$$= \frac{\beta}{2}\sum_{i \neq j}\dot{\mathbf{y}}_j^T \frac{\partial}{\partial \mathbf{r}_i}W(\mathbf{r}_i - \mathbf{r}_j) + \frac{\beta}{16}\sum_{i \neq j}\dot{\mathbf{y}}_i^T(\mathbf{y}_i + \mathbf{y}_j)^T \frac{\partial}{\partial \mathbf{r}_j}\mathcal{H}_W(\mathbf{r}_i - \mathbf{r}_j)(\mathbf{y}_i + \mathbf{y}_j), \tag{A.18}$$

where in the last step of Eq.(A.17,A.18) symmetry properties of W have been used. The term proportional to $\beta/16$ is of order y^3 and can be neglected the expansion up to order y^2 used in

the derivation of the generalized Langevin equation. In the whole exponent the $i = j$ term is

$$i\sum_{j=1}^{N}\int_{0}^{t}du\left\{-\frac{m_{\mathrm{I}}}{\hbar}\ddot{\mathbf{r}}_{j}^{T}\mathbf{y}_{j}+\frac{g^{2}}{2}\left[i\mathbf{y}_{j}\mathcal{H}_{W}(0)\mathbf{y}_{i}-\beta\dot{\mathbf{r}}_{j}\mathcal{H}_{W}(0)\mathbf{y}_{j}\right]\right\}=$$

$$=i\sum_{j=1}^{N}\int_{0}^{t}du\left\{\mathbf{y}_{j}^{T}\left[-\frac{m_{\mathrm{I}}}{\hbar}\ddot{\mathbf{r}}_{j}-\frac{\beta g^{2}}{2}\mathcal{H}_{W}(0)\dot{\mathbf{r}}_{j}\right]+i\frac{g^{2}}{2}\mathbf{y}_{j}^{T}\mathcal{H}_{W}(0)\mathbf{y}_{j}\right\},\qquad\text{(A.19)}$$

while the $i \neq j$ term is

$$\frac{ig^{2}}{2}\sum_{i\neq j}^{N}\int_{0}^{t}du\left\{2\mathbf{y}_{j}^{T}\nabla V(\mathbf{r}_{i}-\mathbf{r}_{j})+i\mathbf{y}_{j}^{T}\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})\mathbf{y}_{i}+\frac{\beta}{2}\left[\mathbf{y}_{j}^{T}\left(\dot{\mathbf{r}}_{j}\frac{\partial}{\partial\mathbf{r}_{j}}-\dot{\mathbf{r}}_{i}\frac{\partial}{\partial\mathbf{r}_{i}}\right)+\dot{\mathbf{y}}_{j}^{T}\right]\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j})\right\}=$$

$$=\frac{ig^{2}}{2}\sum_{i\neq j}^{N}\int_{0}^{t}du\,\mathbf{y}_{j}^{T}\left[\nabla V(\mathbf{r}_{i}-\mathbf{r}_{j})+i\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})\mathbf{y}_{i}+\frac{\beta}{2}\left(\dot{\mathbf{r}}_{j}\frac{\partial}{\partial\mathbf{r}_{j}}-\dot{\mathbf{r}}_{i}\frac{\partial}{\partial\mathbf{r}_{i}}-\frac{d}{du}\right)\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j})\right],$$

$$\text{(A.20)}$$

where an integration by parts to remove the $\dot{\mathbf{y}}$ has been performed. Now the exponent is

$$i\sum_{j}\int_{0}^{t}du\,\mathbf{y}_{j}^{T}\left\{-\frac{m_{\mathrm{I}}}{\hbar}\ddot{\mathbf{r}}_{j}-\frac{\beta g^{2}}{2}\mathcal{H}_{W}(0)\dot{\mathbf{r}}_{j}+\frac{ig^{2}}{2}\mathcal{H}_{W}(0)\mathbf{y}_{j}+\right.$$

$$\left.+\frac{g^{2}}{2}\sum_{i\neq j}\left[2\nabla V(\mathbf{r}_{i}-\mathbf{r}_{j})+\frac{\beta}{2}\left(\dot{\mathbf{r}}_{j}\frac{\partial}{\partial\mathbf{r}_{j}}-\dot{\mathbf{r}}_{i}\frac{\partial}{\partial\mathbf{r}_{i}}-\frac{d}{du}\right)\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j})+i\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})\mathbf{y}_{i}\right]\right\}=$$

$$=i\int_{0}^{t}du\,\sum_{j}\left[\mathbf{y}_{j}^{T}\mathbf{v}_{j}+\frac{ig^{2}}{2}\sum_{\mathrm{I}}\mathbf{y}_{j}^{T}\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})\mathbf{y}_{i}\right].$$

where $\mathbf{v}_{j}$ is defined as

$$\mathbf{v}_{j}=-\frac{m_{\mathrm{I}}}{\hbar}\ddot{\mathbf{r}}_{j}-\frac{\beta g^{2}}{2}\mathcal{H}_{W}(0)\dot{\mathbf{r}}_{j}+\frac{g^{2}}{2}\sum_{i\neq j}2\nabla V(\mathbf{r}_{i}-\mathbf{r}_{j})+\frac{\beta}{2}\left(\dot{\mathbf{r}}_{j}\frac{\partial}{\partial\mathbf{r}_{j}}-\dot{\mathbf{r}}_{i}\frac{\partial}{\partial\mathbf{r}_{i}}-\frac{d}{du}\right)\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j}).$$

$$\text{(A.21)}$$

A rewriting of $\mathbf{v}_{j}$ is possible noticing that

$$\left(\dot{\mathbf{r}}_{j}\frac{\partial}{\partial\mathbf{r}_{j}}-\dot{\mathbf{r}}_{i}\frac{\partial}{\partial\mathbf{r}_{i}}\right)\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j})=$$

$$=\left(\dot{\mathbf{r}}_{j}\frac{\partial(\mathbf{r}_{i}-\mathbf{r}_{j})}{\partial\mathbf{r}_{j}}\frac{\partial}{\partial(\mathbf{r}_{i}-\mathbf{r}_{j})}-\dot{\mathbf{r}}_{i}\frac{\partial(\mathbf{r}_{i}-\mathbf{r}_{j})}{\partial\mathbf{r}_{i}}\frac{\partial}{\partial(\mathbf{r}_{i}-\mathbf{r}_{j})}\right)\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j})=-\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})(\dot{\mathbf{r}}_{i}+\dot{\mathbf{r}}_{j}),$$

$$\text{(A.22)}$$

$$-\frac{d}{du}\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j})=-\frac{d(\mathbf{r}_{i}-\mathbf{r}_{j})}{du}\frac{\partial}{\partial(\mathbf{r}_{i}-\mathbf{r}_{j})}\nabla W(\mathbf{r}_{i}-\mathbf{r}_{j})=-\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})(\dot{\mathbf{r}}_{i}-\dot{\mathbf{r}}_{j}),\qquad\text{(A.23)}$$

and this leads to

$$\mathbf{v}_{j}=-\frac{m_{\mathrm{I}}}{\hbar}\ddot{\mathbf{r}}_{j}-\frac{\beta g^{2}}{2}\mathcal{H}_{W}(0)\dot{\mathbf{r}}_{j}+g^{2}\sum_{i\neq j}\left(\nabla V(\mathbf{r}_{i}-\mathbf{r}_{j})-\frac{\beta}{2}\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})\dot{\mathbf{r}}_{i}\right).\qquad\text{(A.24)}$$

The final result for the exponent is

$$-\frac{i}{\hbar}\sum_{i,j=1}^{N}\int_{0}^{t}du\left\{\mathbf{y}_{j}^{T}\left[\frac{m_{\mathrm{I}}}{\hbar}\ddot{\mathbf{r}}_{j}+\frac{\beta g^{2}}{2}\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})\dot{\mathbf{r}}_{i}+g^{2}\nabla V(\mathbf{r}_{i}-\mathbf{r}_{j})\right]-i\frac{g^{2}}{2}\mathbf{y}_{j}^{T}\mathcal{H}_{W}(\mathbf{r}_{i}-\mathbf{r}_{j})\mathbf{y}_{i}\right\}.$$

$$\text{(A.25)}$$

From equation Eq. (A.25) it is immediate to obtain Eq. (2.63) after the introduction of the rescaled imaginary potential W_{R}, Eq. (2.62).

Appendix B

Wigner transformation

In this Appendix more details on the Wigner transformation (WT), on the projection on polaron energies and on the renormalized polaron distribution function used in Chapter 3 to derive the kinetic equations are given.

B.1   Wigner transformation

As discussed in the main text, in general one has to deal with distribution functions that depend on two space-time variables, $F(x_1, x_2)$. As first step, the function of interest is written with the change of variables x, x', with $x = (x_1 + x_2)/2$ and $x' = x_1 - x_2$. Then, a Fourier transform is performed on the relative variable x' to obtain the Wigner-transformed function $F(x, p)$

$$F(x, p) = \int dx' e^{-ipx'} F\left(x + \frac{x'}{2}, x - \frac{x'}{2}\right), \tag{B.1}$$

with $px' = \mathbf{p}\mathbf{x}' - \omega t$. The inverse WT takes the form

$$F(x_1, x_2) = \sum_{\mathbf{p}} \int \frac{d\omega}{2\pi} e^{ip(x_1 - x_2)} F\left(\frac{x_1 + x_2}{2}, p\right). \tag{B.2}$$

Before going on, a small comment on why the WT can be useful is needed. With the introduction of the forward and relative coordinate x and x' it is indeed possible to define without ambiguity the distribution function for non-equilibrium cases [98]. Indeed, in equilibrium the time dependence of the forward coordinate is no longer present and only the relative time coordinate is relevant, because distribution functions and correlation are invariant under time translation. Therefore, the new coordinates x and x' are a very convenient representation for non-equilibrium functions.

A function F defined as the convolution of two functions A and B is now considered

$$F(x_1, x_2) = A \circ B = \int dx_3 \ A(x_1, x_3) B(x_3, x_2) =$$

$$= \int dx_3 \sum_{p_1, p_2} e^{ip_1(x_1 - x_3) - ip_2(x_2 - x_3)} A\left(\frac{x_1 + x_3}{2}, p_1\right) B\left(\frac{x_2 + x_3}{2}, p_2\right), \tag{B.3}$$

where the definition of inverse WT in Eq. (B.2) has been used. The WT is then performed using

the usual coordinates x and x'

$$F(x,p) = \int dx' \, e^{-ipx'} \int dx_3 \sum_{p_1,p_2} e^{ip_1(x+x'/2-x_3)-ip_2(x-x'/2-x_3)} \times$$
$$A\left(\frac{x+x'/2+x_3}{2},p_1\right) B\left(\frac{x-x'/2+x_3}{2},p_2\right). \qquad (B.4)$$

New variables can be introduced to simplify the expression above. These variables are the coordinates $x_{a,b} = x_3 - x \pm x'/2$ and the shifted momenta $p_{a,b} = p_{1,2} - p$. With these variables the second exponent in the equation above reads

$$ip_1(x+x'/2-x_3) - ip_2(x-x'/2-x_3) = i(p_a+p)(-x_b) + i(p+p_b)x_a =$$
$$= i(p_b x_a - p_a x_b - p x_b + p x_a), \qquad (B.5)$$

and the last two terms cancel the first exponent. So, the WT can now be written as

$$F(x,p) = \iint dx_a dx_b \sum_{p_a,p_b} e^{i(p_b x_a - p_a x_b)} A\left(x+\frac{x_a}{2},p+p_a\right) B\left(x+\frac{x_b}{2},p+p_b\right). \qquad (B.6)$$

Finally, all the integrations have to be performed. As a first step, A and B are both expanded in terms of momenta $p_{a,b}$

$$A\left(x+\frac{x_a}{2},p+p_a\right) = A\left(x+\frac{x_a}{2},p\right) + p_a \partial_{p_a} A\left(x+\frac{x_a}{2},p+p_a\right)|_{p_a=0} + \ldots =$$
$$= A\left(x+\frac{x_a}{2},p\right) + p_a \partial_p A\left(x+\frac{x_a}{2},p\right) + \ldots = \sum_{n_a} p_a^{n_a} f_A^{(n_a)}\left(x+\frac{x_a}{2},p\right) \qquad (B.7)$$

$$B\left(x+\frac{x_b}{2},p+p_b\right) = B\left(x+\frac{x_b}{2},p\right) + p_b \partial_{p_b} B\left(x+\frac{x_b}{2},p+p_a\right)|_{p_b=0} + \ldots =$$
$$= B\left(x+\frac{x_b}{2},p\right) + p_b \partial_p B\left(x+\frac{x_b}{2},p\right) + \ldots = \sum_{n_b} p_b^{n_b} f_B^{(n_b)}\left(x+\frac{x_b}{2},p\right), \qquad (B.8)$$

with $f_A^{(n_a)}$ ($f_B^{(n_b)}$) the n_a-th (n_b-th) order derivative that enters the Taylor expansion for A (B). Using the above expansions

$$F(x,p) = \iint dx_a dx_b \sum_{p_a,p_b} e^{i(p_b x_a - p_a x_b)} \sum_{n_a,n_b} p_a^{n_a} p_b^{n_b} f_A^{(n_a)}\left(x+\frac{x_a}{2},p\right) f_B^{(n_b)}\left(x+\frac{x_b}{2},p\right), \qquad (B.9)$$

and thanks to the equalities

$$\sum_{p_a} e^{-ip_a x_b} p_a^{n_a} = i^{n_a} \delta^{(n_a)}(x_b) \qquad \sum_{p_b} e^{-ip_b x_a} p_b^{n_b} = (-i)^{n_b} \delta^{(n_b)}(x_a), \qquad (B.10)$$

the function $F(x,p)$ is written as

$$F(x,p) = \iint dx_a dx_b \sum_{n_a,n_b} (-i)^{n_b} i^{n_a} \delta^{(n_a)}(x_b) \delta^{(n_b)}(x_b) f_A^{(n_a)}\left(x+\frac{x_a}{2},p\right) f_B^{(n_b)}\left(x+\frac{x_b}{2},p\right) =$$
$$= T_{0,0} + T_{1,0} + T_{0,1} + \ldots \qquad (B.11)$$

where the term T_{n_a,n_b} labels the power of the δ function and the order of derivative considered

for n_a and n_b. The first three terms are

$$T_{0,0} = \iint dx_a dx_b \; \delta(x_a)\delta(x_b)A\left(x + \frac{x_a}{2}, p\right) B(x + \frac{x_b}{2}, p) = A(x,p)B(x,p) \tag{B.12}$$

$$T_{1,0} = \iint dx_a dx_b \; i\delta(x_a)\delta^{(1)}(x_b)B\left(x + \frac{x_b}{2}, p\right) \partial_p A\left(x + \frac{x_a}{2}, p\right) =$$

$$= -i\partial_p A(x,p)\partial_{x_b} B\left(x + \frac{x_b}{2}, p\right)|_{x_b=0} = -\frac{i}{2}\partial_p A(x,p)\partial_x B(x,p) \tag{B.13}$$

$$T_{0,1} = \iint dx_a dx_b \; (-i)\delta^{(1)}(x_a)\delta(x_b)A\left(x + \frac{x_a}{2}, p\right) \partial_p B\left(x + \frac{x_b}{2}, p\right) =$$

$$= i\partial_p B(x,p)\partial_{x_a} A\left(x + \frac{x_a}{2}, p\right)|_{x_a=0} = \frac{i}{2}\partial_x A(x,p)\partial_p B(x,p). \tag{B.14}$$

All the other T_{n_a,n_b} can be derived similarly, and the convolution can therefore be formally written as

$$F(x,p) = A(x,p)e^{\frac{i}{2}(\overleftarrow{\partial_x}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_x})}B(x,p) \tag{B.15}$$

where the arrows indicate the function the derivative is acting on and the product of the derivatives is defined in analogy with the product of p and x

$$\partial_x A \partial_p B = \nabla_{\mathbf{r}} A \nabla_{\mathbf{p}} B - \partial_t A \partial_\omega B. \tag{B.16}$$

If the exponential operator is expanded at first order in gradients, only the terms $T_{0,0}$, $T_{0,1}$ and $T_{1,0}$ are retained and Eqs. (3.47, 3.48) are immediately obtained

$$A \circ B = AB + \frac{i}{2}(\partial_x A \partial_p B - \partial_p A \partial_x B) \tag{B.17}$$

$$A \circ B - B \circ A = i(\partial_x A \partial_p B - \partial_p A \partial_x B) \tag{B.18}$$

Note that Eq. (B.15) is an exact result, while in the main text only the linear order expansion to gradients is used and this is done, because the exact form of the WT is still too complicated. The linear order expansion in gradients is justified as long as the forward evolution is slow if compared to the relative evolution. If this is the case, then the higher order terms in the expansion of Eq. (B.15) can be neglected. Finally, the derivation of the WT of

$$F(x_1, x_2) = A(x_1, x_2)B(x_1, x_2) \xrightarrow{\text{WT}} F(x,p) = \sum_q A(x, p-q)B(x,q) \tag{B.19}$$

is a direct consequence of the convolution theorem.

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