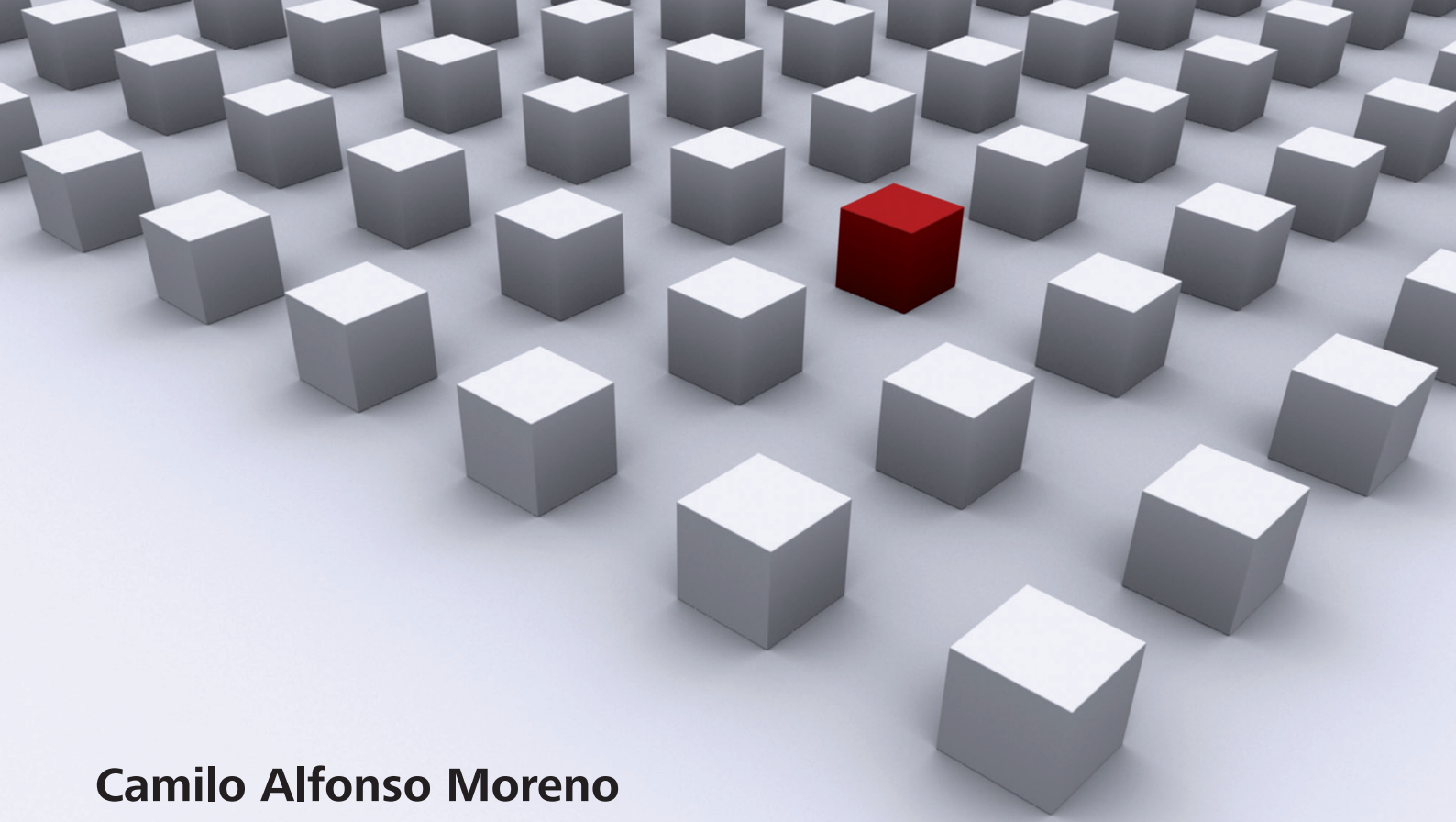

Camilo Alfonso Moreno Jaimes

# The semiclassical approach to open quantum systems beyond the weak coupling regime: quantum-classical transition and many-body interference

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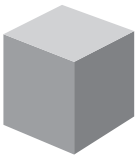
Camilo Alfonso Moreno Jaimes



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Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften (Dr. rer. nat.)
der Fakultät für Physik der Universität Regensburg
vorgelegt von

Camilo Alfonso Moreno Jaimes

aus Sogamoso
im November 2020

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# Contents

**List of publications:**

- C. Moreno and J.-D. Urbina, "Strong coupling and non-Markovian effects in the statistical notion of temperature", Phys. Rev. E **99**, 062135 (2019).
- C. Moreno and J.-D. Urbina, "Interplay between coherent and incoherent decay processes in chaotic systems: The role of quantum interference", Phys. Rev. E **103**, 052201 (2021).
- Davalos, D. and Moreno, C. and Urbina, J.-D. and Pineda, C., "Position representation of single-mode Gaussian channels beyond the Gaussian functional form", Journal of Physics A: Mathematical and Theoretical, 42 (2020).

# Introduction

*In the beginning was the Act.*
*Goethe. "Faust"*

There are some important principles that modern science assumes about the laws of nature [1]. One is the *universality* of these laws, meaning the laws we have discovered, we believe are valid at any time on any place in the Universe. They describe how things *change* or evolve in time. Moreover, we also believe that in order to describe how things interact with each other and change accordingly in the immediate future, we only need to take into account conditions in the immediate vicinity. The laws of motion are *local*. There is, however, one assumption that quantum theory has challenged, even though it took a long time after the formulation of this theory to be fully recognized [2]. This assumption is the presumption that the "legality" of an object, in other words, its properties, intrinsic laws, and all the conditions that defined them are *always* determined by inherent attributes of the object itself. It was believed that to fully comprehend the laws governing the behavior of an object one should try to isolate it from its surroundings. This approach was proven to be very fruitful at the beginning of modern science, when the Newtonian laws of motion were developed.
However, quantum theory has taught us that in many circumstances the legality of an object is indeed an *emergent attribute* of interacting systems. In other words, may the reader allow us to use philosophical jargon, in many situations the interaction of quantum objects has *an ontological status*, which may explain, for instance, the origin of "local ignorance" in physics, as discussed below. In this sense, the study of systems interacting with each other, and more explicitly, systems interacting with their surroundings (open systems), has gained enormous importance, for instance in the so-called quantum-to-classical transition problem: the question about how, if quantum theory is considered a fundamental theory of nature, may the classical realm, with so many distinctly different features from the quantum phenomena, "emerge" from the quantum substrate. One key concept regarding this question is *decoherence* [3–8]. As discussed in more detail in chapter 1, this is the phenomenon related to the delocalization of a system's quantum interference in virtue of its interaction with the environment. This quantum interaction produces *entanglement* between certain states of the system and its environment, selecting accordingly those states which we may observe within the classical domain. In this sense, classicality emerges from quantum interactions with large environments. In this picture, as will be discussed in chapter 4, the huge number of degrees of freedom within the, for all practical purposes, uncontrollable environment is vital to understand the emergence of effective irreversibility involving typical processes of open quantum systems, like dissipation of energy and decoherence.

There exists another picture in the context of the quantum-to-classical transition problem. This picture involves the study of a quantum system in the regime of high energy, large number of particles, or more precisely, large *actions* in terms of the quantum action unit $\hbar$, involved in the transition amplitude of a quantum process. These amplitudes can be visualized as *waves* able to merge themselves producing interference, where each of them comes with a specific phase that depends on the action. The *semiclassical approach* [9,10], studies the regime where rapidly oscillatory phases tend to cancel out each other, surviving only those superpositions where the *action is stationary*. In this regime, the stationary condition for the action actually gives rise to the *classical* equations of motion of the system, as discussed in detail in chapter 1. Thus, within this picture, the *principle of constructive interference* explains the emergence of classical trajectories.
Remarkably, the semiclassical methods rely on asymptotic analysis, the Saddle-Point-Analysis (SPA) techniques [11], which aim to look for certain configurations of the system that, in general, can not be reached by perturbation theory in $\hbar$. Indeed, the range of validity of the semiclassical methods is characterized by the typical action of the system, compared to $\hbar$, giving a dimensionless parameter, which we may call *effective* Planck's constant $\hbar_e$. This parameter enters in the quantum amplitude *non-analytically* $\sim \mathrm{e}^{i/\hbar_e}$, controlling accordingly the semiclassical limit $\hbar_e \to 0$. Another branch where asymptotic analysis has been successful is in high-energy physics, where the non-perturbative objects are known as solitons [12, 13], and in condensed matter theory, where SPA explains satisfactorily the existence of the superconducting gap in the BCS theory [11, 14], to mention only few examples.
The interplay between the open system approach, where a central system $\mathcal{A}$ is coupled to an environment modeled by harmonic oscillators $\mathcal{E}$, and the semiclassical limit, where large actions in the quantum propagator, and the corresponding SPA approximation, give rise to classical trajectories, is the main topic of this thesis. In particular, we will investigate how does the two main features related to open systems: dissipation of energy and decoherence, look like in the semiclassical limit. In the closed-system scenario, the semiclassical analysis of the quantum propagator assumes the form of a sum or superposition of classical trajectories with given boundary conditions. This form allows the possibility to observe interference effects between different classical paths. In short, the hallmark of semiclassical analysis for closed systems is the possibility to use classical information to see interference phenomena, which is a defining feature of quantum theory.
On the other hand, in the open system scenario, the coupling with the environment produces a rich variety of emergent dynamics, with dissipation and decoherence been the main hallmark. However, as will be seen throughout the thesis, it is precisely the complicated interplay between paths of the open system in the Feynman-Vernon approach, mediated by the environment, that makes the semiclassical limit fundamentally different in form from that of the closed setup. Especially, the search for a semiclassical configuration showing interference between different dissipative classical trajectories is a challenging and elusive task. We hope to shed some light on this direction in this work.
We close the introduction showing the relation between entanglement, decoherence, and the emergence of local ignorance in quantum systems, as a first but very important in-

stance of open systems that may help understand how certain physical phenomena have their origin through interaction between subsystems.

## Entanglement, decoherence and local ignorance

The foundations of quantum theory rest upon few principles, which except maybe for the *measurement postulate*, are regarded as uncontroversial [15]. The first one is the assumption that the state of a quantum system $\mathcal{A}$ is represented by a vector in its Hilbert space $\mathcal{H}_{\mathcal{A}}$. The second says that quantum evolution is *unitary*, namely, it is represented by a unitary operator which, in the non-relativistic case, fulfills the Schrödinger equation. An additional postulate is related to the fact that the universe is made up of many subsystems interacting with each other, and it says that states of a composite quantum system are represented by a vector in the tensor product of the Hilbert space of its components. The other postulates involve the quantum measurement process and Born's rule of the probability of outcomes, which are the only part of the core of postulates that are non-linear and non-unitary in nature [16]. They say that the measurement outcomes are limited to an orthonormal set of the eigenstates of the measured observable. The probability $p_k$ of an outcome $|\alpha_k\rangle$ in such measurement of a quantum system previously prepared in the state $|\phi\rangle$ is given by $|\langle\alpha_k|\phi\rangle|^2$. This sharp difference in nature between the measurement and the rest of the postulates has given rise to a vast literature and debate about the interpretation of quantum mechanics, and to efforts in trying to "derive" the measurement postulates from the other, non-controversial part of principles [2, 6, 7, 17–21].

The unitary and linear structure of quantum theory allow the existence of composite states which can not be written as a product of pure states of its components. They are called *entangled* states. To be more specific, let us suppose two subsystems with Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. If each subsystem is prepared in a *pure state* $|\phi\rangle_i$, where $i = 1, 2$, then the total composite state has the form

$$|\phi\rangle = |\phi\rangle_1 |\phi\rangle_2 . \tag{0.1}$$

In this case, any local measurement on system 1 does not affect the state 2 and vice-versa. Indeed, the *density matrix* corresponding to the state in Eq. (0.1) is given by

$$\hat{\rho} = |\phi_1\phi_2\rangle\langle\phi_1\phi_2| = \hat{\rho}_1 \otimes \hat{\rho}_2, \tag{0.2}$$

representing a situation in which the measurements in 1 and 2 are *uncorrelated*. However, linearity of quantum mechanics implies that superpositions of pure states are also possible, for instance

$$|\phi\rangle = \frac{1}{\sqrt{2}}\Big( |\psi_1\rangle |\psi_2\rangle + |\phi_1\rangle |\phi_2\rangle \Big), \tag{0.3}$$

which can not be written as a product of two pure states as in Eq. (0.1). In this case the density matrix

$$\hat{\rho} = |\phi\rangle\langle\phi| \neq \hat{\rho}_1 \otimes \hat{\rho}_2, \tag{0.4}$$

represents a situation in which the measurements in 1 and 2 are *correlated*. This is an entangled state, a quantum feature with no classical counterpart, showing the non-local character of quantum states. Even when the two subsystems 1 and 2 are far away from each other after the entanglement has taken place, a measurement of an observable in 1 will affect the result of an immediate measurement of an observable in 2.
The basic idea behind decoherence is the following: suppose an interaction Hamiltonian between a system $\mathcal{A}$ and its environment $\mathcal{E}$, $\mathcal{H}_{\mathcal{AE}}$, is such that certain states of the system, say $(|\uparrow\rangle, |\downarrow\rangle)$ do not get entangled in virtue of the interaction. These are called pointer states, and it is possible to show that these states, in order to survive entanglement with $\mathcal{E}$, have to be orthogonal [22, 23]. More detailed discussion and physical examples of this mechanism will be given in chapter 1. For now it is enough to consider the main idea. Suppose $\mathcal{A}$ starts in a superposition of the pointer states, and $\mathcal{E}$ in some initial state $|\epsilon_0\rangle$. Then, due to the interaction the composite initial state transforms into an entangled state

$$\big(\alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle\big)\,|\epsilon_0\rangle \xrightarrow{\mathcal{H}_{\mathcal{AE}}} \alpha\,|\uparrow\rangle\,|\epsilon_\uparrow\rangle + \beta\,|\downarrow\rangle\,|\epsilon_\downarrow\rangle = |\psi_{\mathcal{AE}}\rangle\,. \tag{0.5}$$

Thus, neither $\mathcal{A}$ nor $\mathcal{E}$ alone have a pure state after the interaction. Indeed, if the environmental states are orthogonal $\langle\epsilon_\uparrow|\epsilon_\downarrow\rangle = 0$, meaning the environment "distinguishes" perfectly between the two pointer states, then the *reduced density matrix*, $\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{E}}\hat{\rho}$, obtained after tracing out the degrees of freedom of the environment from the composite density matrix $\hat{\rho} = |\psi_{\mathcal{AE}}\rangle\langle\psi_{\mathcal{AE}}|$, is given by

$$\hat{\rho}_{\mathcal{A}} = |\alpha|^2\,|\uparrow\rangle\langle\uparrow| + |\beta|^2\,|\downarrow\rangle\langle\downarrow|\,, \tag{0.6}$$

yielding a *mixed state*. This represents a loss of purity of the system, whose initial state was completely known, and after entanglement with the environment, Eq. (0.6) denotes the surviving information about $\mathcal{A}$. This loss of purity due to environmental entanglement is the essence of decoherence.
Let us now consider the same situation as in Eq. (0.5) but analyzing only symmetries of the entanglement mechanism without employing the trace operation that gave rise to Eq. (0.6), which necessarily assumes the probability interpretation of Born's rule from the beginning. For those trying to derive consistently the measurement postulates from the first part of the quantum theory principles, avoiding a priory use of Born's rule is very important. For us, it is a way to see things from a different perspective.
In quantum theory phases between different states of a superposition produce interference patterns that can be measured. For example, consider the superposition state $|\rightarrow\rangle = \frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}$, and the phase shift operator $\mathbf{u}^{\varphi}_{\mathcal{A}} = |\uparrow\rangle\langle\uparrow| + \mathrm{e}^{i\varphi}\,|\downarrow\rangle\langle\downarrow|$. For instance, for $\varphi = \pi$ it transforms $|\rightarrow\rangle$ into its orthogonal counterpart $|\leftarrow\rangle = \frac{|\uparrow\rangle-|\downarrow\rangle}{\sqrt{2}}$. Thus, $\mathbf{u}^{\varphi}_{\mathcal{A}}$ may shift the interference pattern, which is *a measurable observable on* $\mathcal{A}$. However, when acting on the composite entangled state $|\psi_{\mathcal{AE}}\rangle$, the operator $\mathbf{u}^{\varphi}_{\mathcal{A}} \otimes \mathbf{1}_{\mathcal{E}}$ *can not have any effect on its local state* [15], because it can be undone by a counter-shift $\mathbf{u}^{-\varphi}_{\mathcal{E}} = |\epsilon_\uparrow\rangle\langle\epsilon_\uparrow| + \mathrm{e}^{-i\varphi}\,|\epsilon_\downarrow\rangle\langle\epsilon_\downarrow|$, acting on system $\mathcal{E}$ (possible faraway from $\mathcal{A}$). That is

$$\mathbf{u}^{-\varphi}_{\mathcal{E}}\big(\mathbf{u}^{\varphi}_{\mathcal{A}}\,|\psi_{\mathcal{AE}}\rangle\big) = \mathbf{u}^{-\varphi}_{\mathcal{E}}\big(\alpha\,|\uparrow\rangle\,|\epsilon_\uparrow\rangle + \mathrm{e}^{i\varphi}\beta\,|\downarrow\rangle\,|\epsilon_\downarrow\rangle\big) = |\psi_{\mathcal{AE}}\rangle\,, \tag{0.7}$$

assuming $\langle \epsilon_\uparrow | \epsilon_\downarrow \rangle = 0$[1]. Thus, since phases in $|\psi_{\mathcal{AE}}\rangle$ can be changed acting on $\mathcal{E}$, which may be decoupled and faraway from $\mathcal{A}$, they can no longer influence the *local state of* $\mathcal{A}$. In other words, local phases lose significance for $\mathcal{A}$ alone. They "delocalize", implying the loss of quantum phase coherence or *decoherence*. Information about $\mathcal{A}$ is lost, displaced into correlations between $\mathcal{A}$ and $\mathcal{E}$. This loss of information about local phases due to entanglement-invariance of the state $\mathcal{A}$ (a unitary phase-shift transformation on a local entangled state can be undone by a counter-shift on its partner) is the key to understand the origin of *local ignorance* in quantum theory. And indeed, it may be used as a starting point in trying to derive the probabilistic nature of quantum measurements, as Zurek has suggested [17].

In summary, the interaction between subsystems producing entanglement, which is a unique quantum feature, has the result that local information about phase correlations get lost into the whole entangled state. In this sense, the knowledge of the whole implies the ignorance of the part. This is in sharp contrast with classical physics, where knowledge about a system does not determine the system itself or its evolution. When an observer in classical physics has incomplete knowledge about a physical system, she usually makes use of *ensembles*: infinite copies of the same system reflecting her ignorance about microstates. However, the state of knowledge of the observer does not affect the individual physical system. In quantum theory, by contrast, the state of a system has a double role: an epistemic status reflecting the state of knowledge, and an ontological status reflecting what exists. Quantum states are "epiontic" [17]. The same ideas have been applied by Zurek in [15] in order to understand microcanonical equilibrium without the use of ensembles, only by considering symmetries of entangled states of a composite system.

[1] In chapter 1 we will see how the orthogonality of environmental states is in fact a dynamical property, coming from the huge number of degrees of freedom within $\mathcal{E}$.

# Outline of the thesis

The thesis is organized as follows:
Chapter 1 is devoted to review and introduce important concepts and tools related to open quantum systems. In particular, the van Vleck-Gutzwiller semiclassical propagator for closed systems is studied, showing how the stationary condition of the classical action at the path integral level gives rise to the classical equations of motion for the system. Then, the concept of decoherence is studied in detail. Namely, the loss of quantum coherence in a system coupled to an environment. We show a specific solvable model where the main features concerning decoherence can be analyzed in detail. Finally, the path integral approach to the Caldeira-Leggett model is introduced, consisting of a central system coupled to a bunch of harmonic oscillators playing the role of an environment. This model is widely used in the literature of open systems and is the main model we use throughout the thesis. We close the chapter analyzing the classical limit of this model, and the problems one faces when trying to derive a semiclassical treatment when compared to the closed-system scenario.
In chapter 2 the first of our main results is presented. We show that it is possible to obtain a meaningful notion of temperature for strongly coupled systems in the thermodynamic limit, starting from the fundamental microcanonical equilibrium and applying SPA techniques. We also show that this coupling-dependent temperature obeys consistent microcanonical thermodynamics, by applying the ideas to the Quantum Brownian Motion model. Finally, we introduce a generalized notion of ensemble equivalence for strongly coupled systems. The results were published in [24].
Chapter 3 is devoted to the semiclassical analysis of decoherence in a system with a classically chaotic limit. A quantum system inside a chaotic cavity is subject to decoherence in virtue of environmental coupling. The interplay between coherence effects from the open cavity and decoherence from the environment is studied in the semiclassical limit, yielding a decrement of the quantum survival probability due to environmental decoherence. We have published the main results of this topic in [25].
In chapter 4 we study the semiclassical limit of a Bose-Hubbard model with two sites, where one of them is coupled to a bosonic environment. We show how the key to understanding the irreversible nature of dissipation has its root in the uncontrollable nature of the environment. Further, we propose an approach that in principle may reveal, for the first time, interference between different dissipative classical trajectories in the semiclassical limit of the system.
Finally, in chapter 5 the aim is to apply semiclassical methods to the study of work in quantum systems, namely, a quantum system subject to an external force. The starting point is to use the path integral approach to the characteristic function of quantum work, in terms of the two-point measurement definition of quantum work, and develop a

semiclassical analysis based on the van Vleck-Gutzwiller propagator. The quantum-to-classical correspondence is studied, and similarly, the semiclassical analysis of work in a non-autonomous system coupled to an environment is discussed. The thesis finishes with general conclusions and an outlook for future research at the end.

# 1. Open quantum systems, semiclassical methods and the emergence of classicality

In this chapter, we discuss concepts and tools related to semiclassical methods on one hand, and open quantum systems on the other hand, both within the framework of the emergence of classicality. This discussion is not intended to cover all the extensive results of these fields, but only to introduce basic ideas behind this fascinating topic as an excuse to present important tools that will be used throughout the next chapters.

In section 1.1 we discuss the semiclassical van Vleck-Gutzwiller propagator in closed systems and investigate how we understand the emergence of classical equations of motion and trajectories in that context. Section 1.2 is devoted to open systems. We present the general framework of the role of decoherence in the quantum-to-classical transition problem, studying an environment of spins. Then we introduce the ubiquitous Caldeira-Leggett approach, which consists of an environment of continuous boson modes, making the model more suitable for semiclassical analysis, and we investigate in more detail its classical limit, which gives rise to a dissipative classical equation of motion of the central particle with environmental noise.

## 1.1. Closed systems

In this section, we will present briefly the van Vleck-Gutzwiller propagator, which is a semiclassical approximation to the propagator in quantum mechanics. The discussion will start, as usual, with the coordinate representation of the propagator of quantum states, the *amplitude* transition probability, and later we will discuss the evolution of *density matrices* in the semiclassical limit, which involves the product of two such propagators. We will show that these are two equivalent ways to represent a semiclassical description of the quantum evolution in *closed* systems, but there are many subtleties when one is facing the problem of open quantum systems.

### 1.1.1. Amplitudes and the van Vleck-Gutzwiller propagator

For simplicity let us present the discussion for a $d$-dimensional non-relativistic particle of mass $m$ with time-independent Hamiltonian (generalization to time-dependent Hamiltonians is straightforward)

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \hat{V}(\hat{\mathbf{q}}). \tag{1.1}$$

The time evolution of the particle is governed by the unitary operator $\hat{U}(t)$, acting on the Hilbert space $\mathcal{H}$ of the system, which fulfills the Schrödinger equation

$$i\hbar\,\partial_t\hat{U}(t) = \hat{H}\,\hat{U}(t), \tag{1.2}$$

with the initial condition $\hat{U}(0) = \hat{1}$, where $\hat{1}$ is the identity operator in $\mathcal{H}$. The solution of Eq. (1.2) is then given by

$$\hat{U}(t) = \mathrm{e}^{-\frac{i}{\hbar}\hat{H}t}. \tag{1.3}$$

The propagator is, in this context, the coordinate representation of the evolution operator, $K(\mathbf{q}_f, t; \mathbf{q}_i, 0) = \langle \mathbf{q}_f |\, \mathrm{e}^{-\frac{i}{\hbar}\hat{H}t}\, |\mathbf{q}_i\rangle$, which gives the transition amplitude to go from an initial position $\mathbf{q}_i$ at time $s = 0$ to a final position $\mathbf{q}_f$ at time $s = t$. An initial state $\psi(\mathbf{q}_i, 0) = \langle \mathbf{q}_i|\psi(0)\rangle$, will evolve unitarilly under $\hat{H}$ as

$$\psi(\mathbf{q}_f, t) = \int d\mathbf{q}_i\; K(\mathbf{q}_f, t; \mathbf{q}_i, 0)\psi(\mathbf{q}_i, 0), \tag{1.4}$$

where the propagator in coordinate representation can be written as a Feynman path integral [26, 27] (here in Hamiltonian form)

$$K(\mathbf{q}_f, t; \mathbf{q}_i, 0) = \int_{\mathbf{q}_i\to\mathbf{q}_f} \mathcal{D}[\mathbf{q}(s)]\mathcal{D}[\mathbf{p}(s)]\; \mathrm{e}^{\frac{i}{\hbar}S[\mathbf{q}(s),\mathbf{p}(s)]}, \tag{1.5}$$

with the action functional given by

$$S[\mathbf{q}(s), \mathbf{p}(s)] = \int_0^t ds\; \big(\mathbf{p}(s)\dot{\mathbf{q}}(s) - H(\mathbf{q}, \mathbf{p})\big). \tag{1.6}$$

The path integral representation of the propagator Eq. (1.5) involves a *superposition* of all paths $(\mathbf{q}(s), \mathbf{p}(s))$ connecting the initial point $\mathbf{q}(0) = \mathbf{q}_i$ with the final point $\mathbf{q}(t) = \mathbf{q}_f$, during the time interval $t$, with unconstrained momentum $\mathbf{p}$. This path integral can also be extended to a many-body system in other general quadratures, as we use it for the Bose-Hubbard model in chapter 4, and for non-autonomous systems, as applied in chapter 5 when we study the path integral representation of work and energy in quantum thermodynamics. But for the physical results we want to present here it is enough to work with Eq. (1.5).

For a Hamiltonian that is quadratic in momentum, like in Eq. (1.1), one can perform the integral with respect to $\mathbf{p}$ in Eq. (1.5), and obtain[1]

$$K(\mathbf{q}_f, t; \mathbf{q}_i, 0) = \int_{\mathbf{q}_i\to\mathbf{q}_f} \mathcal{D}[\mathbf{q}(s)]\; \mathrm{e}^{\frac{i}{\hbar}S[\mathbf{q}(s)]}, \tag{1.7}$$

with the action involving now the Lagrangian $\mathcal{L}$

$$S[\mathbf{q}(s)] = \int_0^t ds\; \mathcal{L}(\mathbf{q}(s), \dot{\mathbf{q}}(s)) = \int_0^t ds\; \left(\frac{m}{2}\dot{\mathbf{q}}^2 - V(\mathbf{q})\right). \tag{1.8}$$

[1] It is understood that a redefinition of $\mathcal{D}[\mathbf{q}(s)]$ is necessary to account for extra factors after the $\mathbf{p}$ integration.

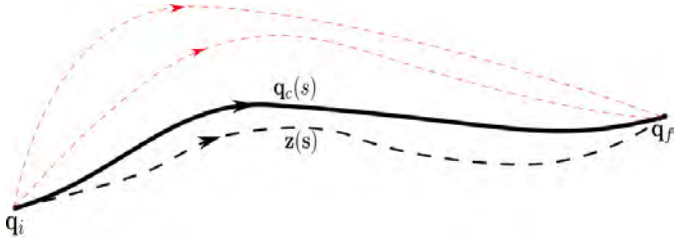


Figure 1.1: The figure shows possible paths connecting $\mathbf{q}_i$ with $\mathbf{q}_f$ in time $t$. In general, for large $S/\hbar$, a small variation along a given path gives rise to a large variation in its corresponding action (dotted red paths), except in a region where the action is stationary. There a small variation along the stationary path (thick black curve) gives rise to a tiny variation in the action.

The semiclassical approximation to the propagator in Eq. (1.7) comes when one notice that for actions $S$ much bigger than $\hbar$, the so-called semiclassical regime, Eq. (1.7) involves an integral over highly oscillatory contributions which tends to cancel out each other, except in the region where the action is *stationary*. Then to solve the path integral Eq. (1.7), for large $S$, the use of the Stationary Phase Approximation (SPA) [28] is justified.

Following the SPA we expand the action around the path $\mathbf{q}_c(s)$ which makes $S$ stationary (see Fig. 1.1),

$$\frac{\delta S}{\delta \mathbf{q}(s)}\Big|_{\mathbf{q}=\mathbf{q}_c} = 0. \tag{1.9}$$

That is, making $\mathbf{q}(s) = \mathbf{q}_c(s) + \eta \mathbf{z}(s)$, for small $\eta$, demanding the stationary path $\mathbf{q}_c(s)$ to fulfill the boundary conditions $\mathbf{q}_c(0) = \mathbf{q}_i$, $\mathbf{q}_c(t) = \mathbf{q}_f$, and the so-called *fluctuations* $\mathbf{z}(s)$ fulfilling $\mathbf{z}(0) = \mathbf{z}(t) = 0$, the expansion of the action reads

$$S[\mathbf{q}_c(s) + \eta \mathbf{z}(s)] = \sum_{k=0}^{\infty} \frac{\eta^k}{k!} \frac{\delta^k S[\mathbf{q}(s); \mathbf{z}(s)]}{\delta^k \mathbf{q}(s)}\Big|_{\mathbf{q}=\mathbf{q}_c}. \tag{1.10}$$

The zeroth-order contribution in Eq. (1.10) is just the action evaluated along the path $\mathbf{q}_c(s)$

$$\frac{\delta^0 S[\mathbf{q}(s); \mathbf{z}(s)]}{\delta^0 \mathbf{q}(s)}\Big|_{\mathbf{q}=\mathbf{q}_c} = S[\mathbf{q}_c(s)], \tag{1.11}$$

while the first-order contribution gives

$$\begin{aligned} \frac{\delta S[\mathbf{q}(s); \mathbf{z}(s)]}{\delta \mathbf{q}(s)}\Big|_{\mathbf{q}=\mathbf{q}_c} &= \int_0^t ds \left( \frac{\partial \mathcal{L}}{\partial \mathbf{q}(s)}\Big|_{\mathbf{q}_c} \mathbf{z}(s) + \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}(s)}\Big|_{\dot{\mathbf{q}}_c} \dot{\mathbf{z}}(s) \right) \\ &= \int_0^t ds \left( \frac{\partial \mathcal{L}}{\partial \mathbf{q_c}(s)} - \frac{d}{ds} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_c(s)} \right) \mathbf{z}(s) \stackrel{!}{=} 0. \end{aligned} \tag{1.12}$$

To obtain the second integral of the last equation a partial integration was performed.

The stationarity condition in Eq. (1.12) translates then into a condition for the path $\mathbf{q}_c(s)$ which has to satisfy the *classical* equations of motion

$$\frac{\partial \mathcal{L}}{\partial \mathbf{q}_c(s)} - \frac{d}{ds}\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_c(s)} = 0, \tag{1.13}$$

coming from the second line in Eq. (1.12), which is a term *linear* in the fluctuations $\mathbf{z}(s)$. Eq. (1.13) is of course the Euler-Lagrange equation [29]. Contrary to the case where *initial conditions* are specified, and accordingly a unique solution of Eq. (1.13) exists, in this case of *boundary conditions*, there are in general *many or none classical paths* $\mathbf{q}_c(s)$ (that is the reason for the subscript $c$), solutions to Eq. (1.13), satisfying $\mathbf{q}_c(0) = \mathbf{q}_i$, $\mathbf{q}_c(t) = \mathbf{q}_f$.

Further, the second-order term in the expansion reads

$$\begin{aligned}\frac{\delta^2 S[\mathbf{q}(s);\mathbf{z}(s)]}{\delta^2 \mathbf{q}(s)}\Big|_{\mathbf{q}=\mathbf{q}_c} = \int_0^t ds \Bigg( & \frac{\partial^2 \mathcal{L}}{\partial \mathbf{q}(s)^2}\Big|_{\mathbf{q}_c} \mathbf{z}(s)^2 \\ & + 2\frac{\partial^2 \mathcal{L}}{\partial \dot{\mathbf{q}}(s)\mathbf{q}(s)}\Big|_{\mathbf{q}_c,\dot{\mathbf{q}}_c} \dot{\mathbf{z}}(s)\mathbf{z}(s) + \frac{\partial^2 \mathcal{L}}{\partial \dot{\mathbf{q}}(s)^2}\Big|_{\dot{\mathbf{q}}_c} \dot{\mathbf{z}}(s)^2 \Bigg),\end{aligned} \tag{1.14}$$

and the action Eq. (1.8) becomes

$$\begin{aligned}S[\mathbf{q}_c(s);\mathbf{z}(s)] = & \int_0^t ds \left( \frac{m}{2}\dot{\mathbf{q}}_c(s)^2 - V(\mathbf{q}_c(s)) \right) \\ & + \int_0^t ds \left( \frac{m}{2}\dot{\mathbf{z}}(s)^2 - \frac{1}{2}V''(\mathbf{q}_c(s))\mathbf{z}(s)^2 \right) + ...,\end{aligned} \tag{1.15}$$

where $V''$ denotes second derivative with respect to $\mathbf{q}_c$. The first term in Eq. (1.15) corresponds to the classical action $S[\mathbf{q}_c]$, while the second term is the leading-order, quadratic, term in the fluctuations.

There will be in general higher order terms in the fluctuations contributing to Eq. (1.15), however, the *semiclassical approximation* consists in neglecting these higher terms, to construct the semiclassical action

$$S_{\rm sc}[\mathbf{q}(s)_c;\mathbf{z})(s)] = S[\mathbf{q}(s)_c] - \frac{1}{2}\int_0^t ds\, \mathbf{z}^T(s)\left( m\frac{d^2}{ds^2} + V''(\mathbf{q}_c(s)\right)\mathbf{z}(s), \tag{1.16}$$

obtained after a partial integration. The second term in Eq. (1.16) corresponds to a contribution quadratic in the fluctuations, and in order to contribute, it requires its squared magnitude to be of the order $\hbar$, $|\mathbf{z}(s)|^2 \lessapprox \mathcal{O}(\hbar)$. Thus the typical magnitude of fluctuations should be at most of order $\sqrt{\hbar}$. Moreover, the third-order term in the fluctuations is a magnitude of order $\sqrt{\hbar}$ smaller than the second order. And so, the semiclassical approximation is accurate up to corrections of $\mathcal{O}(\sqrt{\hbar})$.

After inserting the semiclassical action Eq. (1.16) in the propagator Eq. (1.7) one has to evaluate the path integral in the fluctuations which, being quadratic, yields a functional Gaussian integral with an exact solution. To evaluate the prefactor for this Gaussian integral it is necessary to determine the fluctuation determinant, $\det\left(m\frac{d^2}{ds^2}+V''(\mathbf{q}_c(s)\right)$, depending on each classical path. However, this can be done using the semi-group property of the quantum propagator as shown in detail, for example in [30]. In the end, we obtain the so-called semiclassical van Vleck-Gutzwiller propagator

$$K_{\rm sc}(\mathbf{q}_f,t;\mathbf{q}_i,0)=\sum_{\mathbf{q}_\gamma:\ \mathbf{q}_i\to\mathbf{q}_f}\frac{1}{(2\pi\hbar)^{d/2}}\left|\det\left[\frac{\partial^2 S[\mathbf{q}_\gamma]}{\partial\mathbf{q}_f\partial\mathbf{q}_i}\right]\right|^{1/2}\exp\left[\frac{i}{\hbar}S[\mathbf{q}_\gamma(s)]-i\left(\frac{\pi d}{4}+\nu_\gamma\frac{\pi}{2}\right)\right], \tag{1.17}$$

which is a sum over all classical paths $\mathbf{q}_\gamma(s)$ ,i.e. solutions of the equation of motion Eq. (1.13), connecting the initial point $\mathbf{q}_i$ with the final point $\mathbf{q}_f$ during time $t$. The Morse index $\nu_\gamma$ denotes the number of sign changes of the quantity $\det\left[\partial^2 S[\mathbf{q}_\gamma]/\partial\mathbf{q}_f\partial\mathbf{q}_i\right]$ [28]. Using the relation $\frac{\partial S}{\partial\mathbf{q}_i}=-\mathbf{p}_i$, the prefactor in Eq. (1.17) can be interpreted as

$$\left|\det\frac{\partial^2 S[\mathbf{q}_\gamma]}{\partial\mathbf{q}_f\partial\mathbf{q}_i}\right|^{-1}=\left|\det\frac{\partial\mathbf{p}_i^\gamma}{\partial\mathbf{q}_f}\right|^{-1}, \tag{1.18}$$

which relates the change of the final point of the path $\mathbf{q}_\gamma$ as a function of its initial momentum. Therefore, a divergence of the prefactor is a *conjugate point* where the final point is independent of the initial momentum. It is worth mentioning that the van Vleck propagator (1.17) fulfills the unitarity condition $\int d\mathbf{q}\ K_{\rm sc}(\mathbf{q}_f,t;\mathbf{q},0)K^*_{\rm sc}(\mathbf{q}_i,t;\mathbf{q},0)=\delta(\mathbf{q}_f-\mathbf{q}_i)$, evaluated in SPA, thus providing a consistent quantum propagator.

The van Vleck-Gutzwiller propagator represents a sum over classical paths of the form $\sum_\gamma A_\gamma \mathrm{e}^{\frac{i}{\hbar}S[\mathbf{q}_\gamma]}$, allowing the possibility to see *interference* effects between different trajectories. This is at the heart of semiclassical methods, and brings the possibility to use classical information (encoded in the classical action) to see interference phenomena, which is a fundamental quantum feature. The essential structure behind Eq. (1.17) can also be applied in other contexts where a quantum system does not have a classical analog, but what is called the classical limit there means the equations of motion coming from extremizing an action. For example, the time evolution of a lattice of bosons with hopping due to quantum tunneling (which of course does not have a classical counterpart), can be described, for a large number of bosons, by a semiclassical propagator whose stationary action results in the Gross-Pitaevskii mean-field equation of motion [31].

In summary, starting from the Schrödinger equation, whose linearity allows to build a superposition of many solutions, and thus to construct the Feynman path integral Eq. (1.7), the emergence of classicality in closed systems can be explained as an asymptotic approximation to the propagator, an approximation that is based on the non-analyticity of the phase $S[\mathbf{q}]/\hbar$ in $\hbar$. The principle of *constructive interference* allows us to keep, in the semiclassical limit of large $S$, only paths in the propagator coming from solutions of the stationarity condition of the action $\delta S/\delta\mathbf{q}=0$, which gives rise to the

classical equations of motion for the particle. It is remarkable, as noted in [32], that this general strategy to obtain "classical" equations of motion using the stationary action principle is applicable also for very general physical theories, as in quantum field theory.

### 1.1.2. Density matrix approach

Having at hand the semiclassical propagator Eq. (1.17) the time evolution of quantum observables, which involves a product of two propagators, can be evaluated. A semiclassical description of the time evolution of observables has been developed in [33], showing the emergence of the so-called truncated Wigner approximation as the consequence of the so-called diagonal approximation involving a pair of identical trajectories (see below). In a similar way here we consider the time evolution of the density matrix $\hat{\rho}$ of a closed system, evolving under a time-independent Hamilotian $\hat{H}$, in the semiclassical limit.

A general density matrix may describe a pure state $\hat{\rho} = |\psi\rangle\langle\psi|$, or a statistical mixture $\hat{\rho} = \sum_j p_j \, |\psi_j\rangle\langle\psi_j|$, with $\sum_j p_j = 1$, where the time evolution is given by

$$\hat{\rho}(t) = \mathrm{e}^{-\frac{i}{\hbar}\hat{H}t}\hat{\rho}(0)\mathrm{e}^{\frac{i}{\hbar}\hat{H}t}, \tag{1.19}$$

which in coordinate representation reads

$$\rho(\mathbf{q}_f, \mathbf{q}'_f, t) = \int d\mathbf{q}_i d\mathbf{q}'_i \; \rho(\mathbf{q}_i, \mathbf{q}'_i) K(\mathbf{q}_f, t; \mathbf{q}_i, 0) K^*(\mathbf{q}'_f, t; \mathbf{q}'_i, 0). \tag{1.20}$$

Inserting the semiclassical propagator Eq. (1.17) into Eq. (1.20) one arrives at

$$\rho^{\mathrm{sc}}(\mathbf{q}_f, \mathbf{q}'_f, t) = \int d\mathbf{q}_i d\mathbf{q}'_i \; \rho(\mathbf{q}_i, \mathbf{q}'_i) \frac{1}{(2\pi\hbar)^d} \sum_{\mathbf{q}_{\tilde{\gamma}}:\, \mathbf{q}_i \to \mathbf{q}_f} \sum_{\mathbf{q}_{\tilde{\gamma}'}:\, \mathbf{q}'_i \to \mathbf{q}'_f} A_{\tilde{\gamma}} A^*_{\tilde{\gamma}'} \; \mathrm{e}^{\frac{i}{\hbar}\left(S_{\tilde{\gamma}} - S_{\tilde{\gamma}'}\right)}, \tag{1.21}$$

where $A_{\tilde{\gamma}}$ contains all the remaining prefactors in Eq. (1.17). This is an equation which involves a double sum over classical trajectories $(\tilde{\gamma}, \tilde{\gamma}')$ coming from the two propagators in semiclassical approximation. The double sum can reveal *coherent* interference effects between correlated trajectories, a fact that is used extensively in systems with chaotic classical limit. The diagonal part of the density matrix $\mathbf{q}_f = \mathbf{q}'_f$ gives the probability to find the particle in position $\mathbf{q}_f$ after the evolution at time $t$, and the off-diagonal components $\mathbf{q}_f \neq \mathbf{q}'_f$ contains the *coherences* or interference between different position states. A system behaves more "classical" when its evolution is dominated by the diagonal part of the density matrix.

Taking into account that Eq. (1.17) is valid under the condition $S \gg \hbar$, the action difference $(S_{\tilde{\gamma}} - S_{\tilde{\gamma}'})/\hbar$ is in general a highly oscillatory quantity which tends to produce cancellations, for example, after an average over initial position, like in Eq. (1.21), unless the action difference is of order $\hbar$: $S_{\tilde{\gamma}} - S_{\tilde{\gamma}'} \sim \mathcal{O}(\hbar)$. So the non-vanishing contribution to Eq. (1.21) comes from pairs of trajectories close to each other in phase-space which lead to small action difference. Fig. 1.2 shows the construction of two such trajectories,

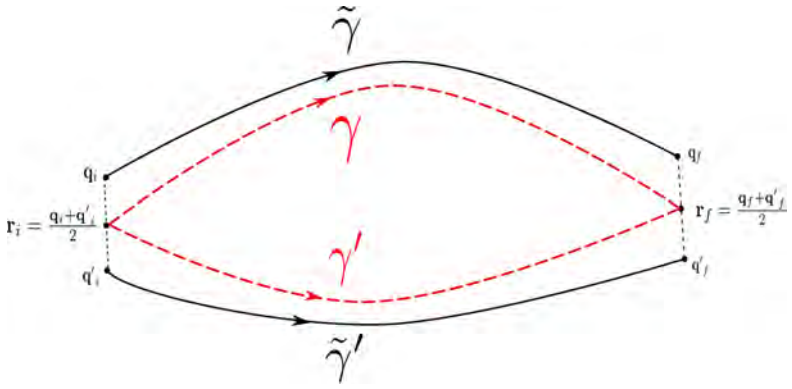


Figure 1.2: We select an initial and final point in center of mass coordinates $\mathbf{r} = (\mathbf{q} + \mathbf{q}')/2$, from which two near trajectories $\gamma$ and $\gamma'$ are constructed. In this way expanding $S_{\tilde{\gamma}}$ around $S_\gamma$, and $S_{\tilde{\gamma}'}$ around $S_{\gamma'}$, up to first-order in the relative coordinates $\mathbf{q} - \mathbf{q}'$, Eq. (1.23) is built as a double sum over such pair of close trajectories.

by selecting an initial point $\mathbf{r}_i \equiv (\mathbf{q}_i + \mathbf{q}'_i)/2$ and a final point at $\mathbf{r}_f \equiv (\mathbf{q}_f + \mathbf{q}'_f)/2$, from which two new trajectories $(\gamma, \gamma')$ are constructed close to each other.

Expanding the action $S_{\tilde{\gamma}}$ around the trajectory $\gamma$ up to first-order in the difference $\mathbf{y} \equiv \mathbf{q} - \mathbf{q}'$ (first-order in the off-diagonal components), using Eq. (1.10) we obtain

$$\begin{aligned} S_{\tilde{\gamma}}(\mathbf{q}_f, \mathbf{q}_i, t) &\approx S_\gamma(\mathbf{r}_f, \mathbf{r}_i, t) \\ &+ \int_0^t ds \left( \frac{\partial \mathcal{L}}{\partial \mathbf{q}_\gamma(s)} - \frac{d}{ds} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_\gamma(s)} \right) \frac{\mathbf{y}(s)}{2} + \frac{\mathbf{y}(t)}{2} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_\gamma(t)} - \frac{\mathbf{y}(0)}{2} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_\gamma(0)} \\ &= S_\gamma(\mathbf{r}_f, \mathbf{r}_i, t) - \frac{1}{2}\mathbf{p}_i^\gamma \cdot \mathbf{y}_i + \frac{1}{2}\mathbf{p}_f^\gamma \cdot \mathbf{y}_f, \end{aligned} \tag{1.22}$$

where $\mathbf{p}_{i(f)}^\gamma$ denotes the initial (final) momentum of the trajectory $\gamma$. When a similar expansion is carried out for $S_{\tilde{\gamma}'}$ around $\gamma'$, Eq. (1.21) becomes

$$\begin{aligned} \rho^{\text{sc}}(\mathbf{r}_f + \mathbf{y}_f/2, \mathbf{r}_f - \mathbf{y}_f/2, t) = \int d\mathbf{r}_i d\mathbf{y}_i \; \rho(\mathbf{r}_i + \mathbf{y}_i/2, \mathbf{r}_i - \mathbf{y}_i/2) \\ \frac{1}{(2\pi\hbar)^d} \sum_{\gamma:\, \mathbf{r}_i \to \mathbf{r}_f} \sum_{\gamma':\, \mathbf{r}_i \to \mathbf{r}_f} A_\gamma A^*_{\gamma'} \, \mathrm{e}^{\frac{i}{\hbar}\left(S_\gamma - S_{\gamma'}\right)} \, \mathrm{e}^{-\frac{i}{\hbar}(\mathbf{p}_i^\gamma + \mathbf{p}_i^{\gamma'}) \cdot \mathbf{y}_i/2} \, \mathrm{e}^{\frac{i}{\hbar}(\mathbf{p}_f^\gamma + \mathbf{p}_f^{\gamma'}) \cdot \mathbf{y}_f/2}. \end{aligned} \tag{1.23}$$

We further perform the integral over the $\mathbf{y}_i$ variable, from which we recognize

$$\mathcal{W}_0\Big(\mathbf{r}_i, (\mathbf{p}_i^\gamma + \mathbf{p}_i^{\gamma'})/2\Big) = \frac{1}{(2\pi\hbar)^d} \int d\mathbf{y}_i \; \rho(\mathbf{r}_i + \mathbf{y}_i/2, \mathbf{r}_i - \mathbf{y}_i/2) \mathrm{e}^{-\frac{i}{\hbar}(\mathbf{p}_i^\gamma + \mathbf{p}_i^{\gamma'}) \cdot \mathbf{y}_i/2}, \tag{1.24}$$

as the Wigner function of the initial density matrix evaluated at momentum $(\mathbf{p}_i^\gamma + \mathbf{p}_i^{\gamma'})/2$.

With this, Eq. (1.23) reads

$$\rho^{\rm sc}(\mathbf{r}_f+\mathbf{y}_f/2,\mathbf{r}_f-\mathbf{y}_f/2,t)=\int d\mathbf{r}_i \sum_{\gamma:\,\mathbf{r}_i\to\mathbf{r}_f}\sum_{\gamma':\,\mathbf{r}_i\to\mathbf{r}_f} A_\gamma A^*_{\gamma'} \times\mathcal{W}_0\big(\mathbf{r}_i,(\mathbf{p}_i^\gamma+\mathbf{p}_i^{\gamma'})/2\big)\,\mathrm{e}^{\frac{i}{\hbar}\left(S_\gamma-S_{\gamma'}\right)}\,\mathrm{e}^{\frac{i}{\hbar}(\mathbf{p}_f^\gamma+\mathbf{p}_f^{\gamma'})\cdot\mathbf{y}_f/2}. \tag{1.25}$$

Moreover, a full phase-space description is achieved if we multiply the last equation by $\mathrm{e}^{-\frac{i}{\hbar}\mathbf{p}_f\cdot\mathbf{y}_f}$, and integrate over $\mathbf{y}_f$. The left-hand side of Eq. (1.25) transforms into the Wigner function at time $t$ with momentum $\mathbf{p}_f$, and the right-hand side gives just a delta function. Thus we obtain the important result

$$\mathcal{W}_t^{\rm sc}\big(\mathbf{r}_f,\mathbf{p}_f\big)=\int d\mathbf{r}_i \sum_{\gamma:\,\mathbf{r}_i\to\mathbf{r}_f}\sum_{\gamma':\,\mathbf{r}_i\to\mathbf{r}_f} A_\gamma A^*_{\gamma'}\,\mathrm{e}^{\frac{i}{\hbar}\left(S_\gamma-S_{\gamma'}\right)} \times\mathcal{W}_0\Big(\mathbf{r}_i,(\mathbf{p}_i^\gamma+\mathbf{p}_i^{\gamma'})/2\Big)\,\delta\Big(\mathbf{p}_f-(\mathbf{p}_f^\gamma+\mathbf{p}_f^{\gamma'})/2\Big), \tag{1.26}$$

which involves a double sum over trajectories $(\gamma,\gamma')$ starting at $\mathbf{r}_i$ and ending at $\mathbf{r}_f$, during time $t$, with the constraint in the final momentum given by the delta function. This is how the Wigner function evolves semiclassically as a double sum over classical paths $(\gamma,\gamma')$ with small action difference.

From the double sum in Eq. (1.26) the most important contribution comes from pairs of identical trajectories $\gamma=\gamma'$. This is the *diagonal* ($dg$) approximation, which results in

$$\mathcal{W}_t^{dg}(\mathbf{r}_f,\mathbf{p}_f)=\int d\mathbf{r}_i \sum_{\gamma:\mathbf{r}_i\to\mathbf{r}_f}|A_\gamma|^2\,\mathcal{W}_0(\mathbf{r}_i,\mathbf{p}_i^\gamma)\,\delta(\mathbf{p}_f-\mathbf{p}_f^\gamma), \tag{1.27}$$

which, using $|A_\gamma|^2=\det\left|\frac{\partial\mathbf{p}_f^\gamma}{\partial\mathbf{r}_i}\right|$ as a Jacobian transformation from initial position to final momentum yields

$$\mathcal{W}_t^{\rm dg}(\mathbf{r}_f,\mathbf{p}_f)=\mathcal{W}_0\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{p}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{p}_f,t)\Big). \tag{1.28}$$

This equation gives the Wigner function at time $t$ in terms of the initial Wigner function, and *evaluated at points coming from the solution of the classical equations of motion* $(\mathbf{r}_f,\mathbf{p}_f)=(\mathbf{r}_f(\mathbf{r}_i,\mathbf{p}_i,t),\mathbf{p}_f(\mathbf{r}_i,\mathbf{p}_i,t))$, the so-called truncated Wigner approximation [33–35]. The diagonal approximation represents the classical evolution of the Winger function in phase-space, which becomes a good approximation to Eq. (1.26) after some average process has been taken place in order to wash out oscillatory terms. The average may be taken over a small time window such that $\langle\mathcal{W}_t^{\rm sc}\rangle=\frac{1}{\Delta t}\int_{t-\Delta t/2}^{t+\Delta t/2}dt'\,\mathcal{W}_{t'}^{\rm sc}$, with $\Delta t\ll t$. In this way, starting from quantum states in Hilbert spaces under unitary evolution, in the semiclassical limit we end up with classical evolution of *trajectories* in phase-space.

We remark here that the classical trajectories are solutions of the equations of motion obtained from the stationary condition applied to the *quantum propagator*, which leads to Eq. (1.17). We use information from the semiclassical propagator (amplitudes) to obtain the semiclassical evolution for the density matrix (probabilities). This point, which seems

obvious in closed systems, is dramatically different in open quantum systems, as we will show later.

The idea behind the diagonal approximation to Eq. (1.26) is that all the fluctuations (the off-diagonal components in Eq. (1.21)) tend to cancel out each other, or at least they are very small compared to the diagonal contribution. This "loss of information" about off-diagonal correlations, which is usually further justified after an average process has taken place (for example in a small time-window) [36], is at the heart of the emergence of classicality. However, to understand this emergence in a more fundamental way it is necessary to recognize that any macroscopic system is unavoidably coupled to many degrees of freedom of an environment, and that the practical impossibility to control all the environmental degrees of freedom is responsible for the loss of the system's quantum coherence, as it will be explored in the next sections.

The next order contributions to Eq. (1.26) come from pair of classical trajectories that are close to each other but not identical. These are genuinely quantum corrections coming from *interference* between pair of trajectories.

To construct these corrections beyond the diagonal approximation in a systematic way is a difficult task for integrable systems [37], which are systems with enough constants of motions in involution to confine its phase-space dynamics on a torus, see for example [38].

For a system with classic chaotic limit, on the other hand, Sieber and Richter [39] developed a systematic approach to constructing action correlations based on the ergodic and hyperbolic properties of chaotic dynamics. This will be seen in Chapter 3, where we use this approach to calculate quantum corrections of an open chaotic system subject to decoherence. And it is actually quite interesting that for a closed system with classically chaotic behavior all quantum corrections to Eq. (1.26) cancel out, meaning the diagonal approximation in the semiclassical regime represents already a very good approximation to the quantum dynamics of the system with chaotic classical limit, as will be discussed in more detail in chapter 3.

## 1.2. Open systems

In this section we will use the open system approach to study the emergence of classicality as a result of interaction between subsystems. This is based on the recognition that every system of the everyday-life, let us call it $\mathcal{A}$, interacts unavoidably with its environment. But, contrary to the spirit behind the construction of classical mechanics, in the quantum world this inevitability of subsystem interactions plays a decisive role in defining what we *observe*. In other words, only through interactions there is a meaningful definition of observation in quantum theory. More importantly to our discussion, when a system interacts with *many* degrees of freedom from other systems, the latter being considered as an *environment* $\mathcal{E}$, the correlations between the subsystems built up through the interaction implies that *local* correlations between states in $\mathcal{A}$ may get lost in correlations involving the global system $\mathcal{AE}$, making the subsystem $\mathcal{A}$ loose local coherence (decoherence) and then looking more "classical", as will be shown in the next subsections. The role of decoherence in the emergence of classicality, recognized by Joos

and Zeh [6], was used by Zurek [40] to develop a theory recognizing the coupling with the environment as responsible for selecting the special and robust classical states of the central system through entanglement between $\mathcal{A}$ and $\mathcal{E}$, a process which is called *environment-induced superselection* (einselection). In the next section, and as an introduction to the main features of decoherence, we will review a model which is exactly solvable and was used by Zurek [8] to study the main ideas behind einselection.

In section 1.2.2 we will introduce and study a model for system-plus-environment in the continuous position basis, which is more suitable for semiclassical analysis in the next chapters.

### 1.2.1. Spin environment and decoherence

In this subsection we will mostly follow the discussion in [2] and introduce a simple yet complete model for decoherence which allows us to study relevant features concerning our discussion of quantum-to-classical transition in open systems.

The model consists of a central two-level system $\mathcal{A}$ linearly coupled to $N$ other two-level systems playing the role of the environment $\mathcal{E}$. We may think about this model as spin systems with the two-level consisting of spin up and down along some $z$-axes, or as photons with two polarization states along some direction, to mention two examples. In the quantum computing community these two-level systems are called "qubits", representing states with basis $\{|0\rangle, |1\rangle\}$ [41].

One central assumption introduced here is that the interaction Hamiltonian dominates the whole dynamics. It means that we neglect any intrinsic dynamics associated with the central system $\mathcal{A}$ or the environment $\mathcal{E}$. This is the so-called quantum-measurement limit [2] and will allow us to focus on the formation of correlations between the subsystems, and the role of decoherence. For a study of this model with an internal dynamics see [42].

The global system $\mathcal{AE}$ will evolve under the interaction Hamiltonian which operates on the joint $\mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{E}$ Hilbert space, and is given by

$$\hat{H} = \frac{1}{2}\hat{\sigma}_z \otimes \sum_{k=1}^{N} g_k \hat{\sigma}_z^{(k)}, \tag{1.29}$$

where $\hat{\sigma}_z$, $\hat{\sigma}_z^{(k)}$ is the $z$-component of the Pauli operator acting on the central system and the $k$-th spin environment, respectively. This represents an interaction linear in the coupling, with strength $g_k$. Moreover, since the interaction Hamiltonian commutes with $\hat{\sigma}_z$, the populations of the central system is a conserved quantity, and thus, there is no exchange of energy between the system and the environment. This represents a model of decoherence without dissipation, which implies the environment can only influence the degree of coherence on the central system states.

Choosing the basis $\{|0\rangle, |1\rangle\}$ in $\mathcal{A}$, and $\{|0\rangle_k, |1\rangle_k\}$ in $\mathcal{E}$, with $k = 1, ..., N$, in which the interaction Hamiltonian $\hat{H}$ is diagonal, the energy eigenstates $|n\rangle$ of $\mathcal{E}$ are then given by products of the form

$$|n\rangle = |1\rangle_1 |0\rangle_2 ... |1\rangle_N, \tag{1.30}$$

with $0 \leq n \leq 2^N - 1$. The energy $\epsilon_n$ associated with the state $|n\rangle$ is given by

$$\epsilon_n = \sum_{k=1}^{N} (-1)^{n_k} g_k, \tag{1.31}$$

where $n_k = 1$ if the $k$-th environmental spin is in the "down" state $|0\rangle_k$, and $n_k = 0$ otherwise.

In this way *any* arbitrary pure state $|\Psi\rangle$ of the joint system $\mathcal{AE}$ can be written as a superposition of the form

$$|\Psi\rangle = \sum_{n=0}^{2^N-1} \Big( c_n |0\rangle |n\rangle + d_n |1\rangle |n\rangle \Big). \tag{1.32}$$

We now assume that at time $t = 0$ the initial state $|\Psi\rangle$ has no correlations between $\mathcal{A}$ and $\mathcal{E}$. So we write $|\Psi(0)\rangle$ as a product state

$$|\Psi(0)\rangle = (a |0\rangle + b |1\rangle) \sum_{n=0}^{2^N-1} c_n |n\rangle . \tag{1.33}$$

This means that before the interaction is turned on, there is no entanglement between the subsystems. The whole composite system $\mathcal{AE}$ evolves under the Hamiltonian Eq. (1.29) as

$$|\Psi(t)\rangle = \mathrm{e}^{-\hat{H}t} |\Psi(0)\rangle = a |0\rangle |\mathcal{E}_0(t)\rangle + b |1\rangle |\mathcal{E}_1(t)\rangle , \tag{1.34}$$

where

$$|\mathcal{E}_0(t)\rangle = |\mathcal{E}_1(-t)\rangle = \sum_{n=0}^{2^N-1} c_n \mathrm{e}^{-i\epsilon_n t/2} |n\rangle . \tag{1.35}$$

The structure in Eq. (1.34), which starts from an uncorrelated (factorized) state $|\Psi(0)\rangle$ and, through the interaction of the system with the environment, ends up with an entangled state, is the general structure behind the *einselection* process [7], in which an apparatus (the central system in this case) gets correlated through interactions with its surroundings (the environment $\mathcal{E}$), which acquires in this way information about the state of the system, selecting a privilege set of "pointer states" (see Fig.1.3 and the discussion below).

### Reduced dynamics

It is important to note that the global $\mathcal{AE}$ evolution is unitary and thus in principle an inverse unitary transformation exists such that the entanglement process can be reversed. However, the environment is made up of many degrees of freedom which usually are not *under control* of the observer, and in this way an inverse transformation is *for all practical purposes* out of reach. This observation is also important to understand the origin of irreversibility in the measurement process on one hand, and in dissipative systems on the other hand, as will be seen in more detail in chapter 4.

If we can only access information about the central system, meaning we can only measure local observables on $\mathcal{A}$, we need to calculate the reduced density matrix of the

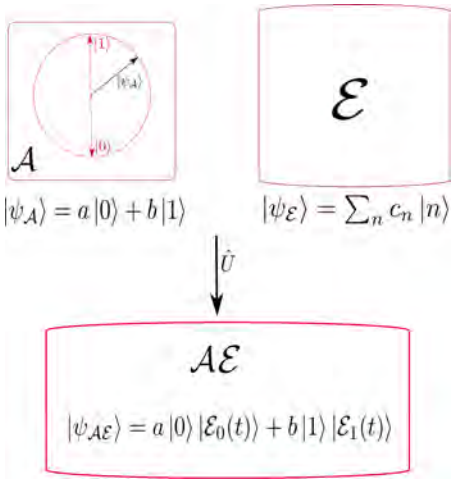


Figure 1.3: An initial uncorrelated state $(a\,|0\rangle + b\,|1\rangle)\sum_{n=0}^{2^N-1} c_n\,|n\rangle$ transforms into an entangled state $a\,|0\rangle\,|\mathcal{E}_0(t)\rangle + b\,|1\rangle\,|\mathcal{E}_1(t)\rangle$ through a unitary operation $\hat{U}$ given by the interaction Hamiltonian between system and environment. In this way, initial local correlations between states $\{|0\rangle, |1\rangle\}$ in $\mathcal{A}$ get delocalized onto the global $\mathcal{AE}$ system producing decoherence in $\mathcal{A}$, emerging $\{|0\rangle, |1\rangle\}$ as pointer (quasi-classical) states.

system. That is, from the pure state $\hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)|$ we trace out [2] the degrees of freedom of the environment

$$\begin{aligned}\hat{\rho}_{\mathcal{A}}(t) \equiv \mathrm{Tr}_{\mathcal{E}}\,\hat{\rho}(t) &= \mathrm{Tr}_{\mathcal{E}}\,|\Psi(t)\rangle\langle\Psi(t)| \\ &= |a|^2\,|0\rangle\langle 0| + |b|^2\,|1\rangle\langle 1| + ab^* r(t)\,|0\rangle\langle 1| + a^* b\,r^*(t)\,|1\rangle\langle 0|\,.\end{aligned} \tag{1.36}$$

Here we have defined the overlap between relative states of the environment as

$$r(t) \equiv \langle\mathcal{E}_1(t)|\mathcal{E}_0(t)\rangle = \sum_{n=0}^{2^N-1} |c_n|^2 \mathrm{e}^{-i\epsilon_n t}, \tag{1.37}$$

with $|c_n|^2 \leq 1$ and $\sum_{n=0}^{2^N-1} |c_n|^2 = 1$. The off-diagonal terms in Eq. (1.36) are controlled by the factor $r(t)$ in Eq. (1.37) involving the overlap of environmental states at time $t$. When these two relative states become distinguishable, $\langle\mathcal{E}_1(t)|\mathcal{E}_0(t)\rangle \sim 0$, the off-diagonal terms in Eq. (1.36) vanish, resulting in the diagonal reduced density matrix

$$\hat{\rho}_{\mathcal{A}}(t) = |a|^2\,|0\rangle\langle 0| + |b|^2\,|1\rangle\langle 1|\,, \tag{1.38}$$

which is an *incoherent mixture* of the system states $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$. This is the phenomenon of *decoherence*, the suppression of off-diagonal components (coherences) in a given basis resulting in a mixture state of the central system in that basis.

[2] Let $\{|\phi_i\rangle\}$ be any orthonormal basis of a system, the trace of an operator $\hat{A}$ is defined as $\mathrm{Tr}\left(\hat{A}\right) = \sum_i \langle\phi_i|\,\hat{A}\,|\phi_i\rangle$. The trace is a basis-independent operation.

Comparing the reduced density matrix, Eq. (1.38), with the density matrix in the closed-system scenario, Eq. (1.26), in the latter approach the vanishing of off-diagonal components was associated, in the semiclassical limit, with an average which washes out correlations between pairs of close classical trajectories. This implies a loss of information associated with the average. On the contrary, in Eq. (1.38) the vanishing of off-diagonal components is associated with correlations established between system and environment (see the entangled state in Eq. (1.34)). These global $\mathcal{AE}$ correlations *delocalize* local correlations between the states $\{|0\rangle, |1\rangle\}$ of the system onto the larger system-plus-environment state [6], and in this way coherences between states $\{|0\rangle, |1\rangle\}$ are no longer a property of the system alone. After tracing out the environmental degrees of freedom, decohrence is responsible for the wash-out of off-diagonal components in Eq. (1.36). Here, there is no loss of information, or in better words, the information has been displaced [8]. It is interesting though, that in the closed-system approach the wash-out of off-diagonal components is "more efficient" when the system has a classically chaotic limit.

Of course, in the context of this subsection, the states $\{|0\rangle, |1\rangle\}$ in Eq. (1.38) do not follow classical trajectories in phase-space, but the classicality is understood as the emergence, through environment-induced superselection, of robust states which survive entanglement with the environment and, in this way, superpositions of these states tend to vanish. These states are known as pointer-states in the context of quantum measurement, and this process is independent to whether it is even possible to take the semiclassical limit in the central system.

Coming back to Eq. (1.37), we find a is a sum over $2^N$ vectors of magnitude $\left|c_n\right|^2$ which rotate in the complex plane with different frequencies, each of value $\epsilon_n$ at time $t$. Actually, this is a two-dimensional random-walk problem, which was analyzed in [8, 42], finding an average step length (average magnitude of $\left|c_n\right|^2$) of order $2^{-N}$. In this way, the average squared length of the vector $r(t)$ in the complex plane scales as

$$\langle \left|r(t)\right|^2 \rangle \propto 2^{-N} = \mathrm{e}^{-N \log 2}, \tag{1.39}$$

showing that $r(t)$, known as the *decoherence factor*, becomes exponentially suppressed by increasing the number of particles in the environment. Moreover, for large $N$ and certain class of coupling distributions $g_k$, it was shown that $r(t)$ decays Gaussian in time [42]

$$r(t) \sim \mathrm{e}^{-\gamma t^2}, \tag{1.40}$$

with some constant $\gamma$ that depends on the initial state of the environment and the distribution of couplings. This shows that the time decay of $r(t)$ is a dynamical process involving a large number of particles of the environment. The loss of quantum coherence in the basis $\{|0\rangle, |1\rangle\}$ is due to a practical impossibility to control all the degrees of freedom of the environment, yielding an asymptotic time decay of coherence and, in this way, an irreversible decoherence process.

It is important to note, as nicely stated in [2], that Eq. (1.37), being a sum over periodic functions, means that for a *finite* number $N$ of particles in the environment there is always a finite *recurrence time* in which $r(t)$ returns to its initial value, this time

being a function of the coupling distribution $g_k$ and the initial state. For example, for a highly *non-random* initial state of the environment, such that

$$|\Psi(0)\rangle = \big(a\,|0\rangle + b\,|1\rangle\,\big)\prod_{k=1}^{N}\frac{1}{\sqrt{2}}\big(\,|0\rangle_k + |1\rangle_k\,\big), \tag{1.41}$$

and $g_k = g$ for all $k$, the decoherence factor gives

$$r(t) = \cos^N(gt), \tag{1.42}$$

which represents a periodic return to its initial value at times $\tau_{\text{return}} = \pi/g$, and thus a reverse of the decoherence process for possibly short times. Actually, when the initial state of the environment is an energy eigenstate $|n\rangle$, the decoherence factor $r(t)$ does not decay at all.

For a finite environment, information in the sense of correlations encoded in $r(t)$ can never disappear. Every periodic or quasi-periodic function has a recurrence time in which the function returns arbitrarily close to any value within their range. But as shown in [8], for macroscopic environments this time may be longer than the lifetime of the Universe.

Let us summarize what we have discussed in this subsection. The structure of quantum mechanics allows the possibility to construct superpositions of states within the Hilbert space of the system. This superposition principle is behind the interference phenomenon, which is a main cornerstone of quantum mechanics. But on the other hand, classical physics is characterized by localized states, and no general superposition of classical states seems possible: we observe in the classical realm a particle localized in a position state and not in a superposition of position states, for example. Assuming that quantum mechanics is a fundamental theory, how can these *classical* states emerge from the fundamental quantum substrate?

Einselection asserts that the unavoidable and uncontrollable interaction of a system with its surroundings is responsible for selecting, through the formation of correlations, certain robust "classical" states, which are more reticent to entanglement with the environment, while local superposition (coherences) of these states are lost. The pointer states selected in this manner depend on the specific form of the interaction Hamiltonian, as shown in Eq. (1.29), where the states of the system $\{|0\rangle, |1\rangle\}$, which diagonalize the Hamiltonian, are the selected pointer states in the quantum-measurement limit. In situations where one has to take into account the internal dynamics of the subsystems the selected pointer states may have a more complex structure.

Finally, it is important to mention that an understanding of the emergence of pointer states using semiclassical methods is still an open question. However, in the scenario where semiclassical limit and open systems meet, as shown in the next section, the role of the environment as analyzed here is illuminating.

### 1.2.2. The Caldeira-Leggett model

In the last section we discussed a model of environment as a bunch of two-level systems, but in many situations of interest it is convenient to model the environment as a continuum of delocalized bosonic modes which effectively yields an irreversible decoherence process. The canonical model for this type of environment is represented by a set of harmonic oscillators linearly coupled to the central system. This model produces as well an irreversible loss of energy on the central system.

An environment of harmonic oscillators linearly coupled to the central system has been shown to represent fairly general physical situations, for example in the pioneering works of Feynman and Vernon [43] and Caldeira and Leggett [44], including the spin-boson model [45]. In this section we introduce and study the so-called Caldeira-Leggett model in the path integral representation, which is suitable for semiclassical analysis.

The model consist of a central particle $\mathcal{A}$, for simplicity here moving in one spatial dimension, linearly coupled to $N$ non-interacting harmonic oscillators which play the role of an environment $\mathcal{E}$. We will consider the subsystems $\mathcal{A}$ and $\mathcal{E}$ have been coupled in their position basis. Here we follow the steps of the derivation in [46]. As usual, we decompose the total Hamiltonian $\hat{H}$ into three parts,

$$\hat{H} = \hat{H}_{\mathcal{A}} + \hat{H}_{\mathcal{E}} + \hat{H}_{\mathcal{AE}}, \tag{1.43}$$

where

$$\hat{H}_{\mathcal{A}} = \frac{\hat{P}^2}{2m} + \hat{V}(\hat{Q}), \tag{1.44}$$

is the self-Hamiltonian of the central particle with mass $m$, momentum $\hat{P}$ and position operator $\hat{Q}$. The self-Hamiltonian of $\mathcal{E}$ is

$$\hat{H}_{\mathcal{E}} = \sum_{k=1}^{N} \frac{1}{2}\Big(\hat{p}_k^2/m_k + m_k\omega_k^2\hat{q}_k^2\Big), \tag{1.45}$$

with $\hat{p}_k$, $\hat{q}_k$ momentum and position operator of each harmonic oscillator with natural frequency $\omega_k$ and mass $m_k$. The interaction Hamiltonian $\hat{H}_{\mathcal{AE}}$ couples linearly the position of the particle with each position oscillator with strength $g_k$,

$$\hat{H}_{\mathcal{AE}} = -\hat{Q} \otimes \sum_{k=1}^{N} g_k\hat{q}_k + \hat{Q}^2 \sum_{k=1}^{N} \frac{g_k^2}{2m_k\omega_k^2}. \tag{1.46}$$

The bilinear term $\hat{Q} \otimes \sum_{k=1}^{N} g_k\hat{q}_k$ describes a continuous monitoring of the position particle by the environment, as described in section 1.2.1. The last term in Eq. (1.46), which contains only an operator on the Hilbert space of $\mathcal{A}$ is introduced to cancel out a potential renormalization induced by the first term. This can be shown by considering the minimum of the classical Hamiltonian with respect to the system and environment coordinates (applying the Hellmann-Feynman theorem). First the equation

$$\frac{\partial H}{\partial q_k} = m_k\omega_k^2 q_k - g_k Q \stackrel{!}{=} 0 \tag{1.47}$$

implies $q_k = \frac{g_k}{m_k\omega_k^2}Q$. And with this the minimum condition of the Hamiltonian with respect to the particle coordinates reads

$$\frac{\partial H}{\partial Q} = \frac{\partial V}{\partial Q} - \sum_{k=1}^{N} g_k q_k + \sum_{k=1}^{N} \frac{g_k^2}{m_k\omega^2} = \frac{\partial V}{\partial Q}. \tag{1.48}$$

In this way the extra term in Eq. (1.46) assures that the minimum is given by the bare potential $V(Q)$. A general global state $\hat{\rho}_{\mathcal{AE}}$ evolves unitarilly under the Hamiltonian $\hat{H}$,

$$\hat{\rho}_{\mathcal{AE}}(t) = \mathrm{e}^{-i\hat{H}t/\hbar}\hat{\rho}_{\mathcal{AE}}(0)\mathrm{e}^{i\hat{H}t/\hbar}. \tag{1.49}$$

The global unitary dynamics however will induce a non-unitary dynamics on the reduced density matrix of the system $\mathcal{A}$. That is, if we are not interested, and often can not control, the degrees of freedom of the environment, we obtain the reduced dynamics after tracing out the environment. First we can write Eq. (1.49) in coordinate representation

$$\begin{aligned}\langle Q_f, \mathbf{q}_f|\, \hat{\rho}_{\mathcal{AE}}(t)\, |Q'_f, \mathbf{q}'_f\rangle = \int dQ_i dQ'_i d\mathbf{q}_i d\mathbf{q}'_i K(Q_f, \mathbf{q}_f, t; Q_i, \mathbf{q}_i, 0) \\ \times \langle Q_i, \mathbf{q}_i|\, \hat{\rho}_{\mathcal{AE}}(0)\, |Q'_i, \mathbf{q}'_i\rangle\, K^*(Q'_f, \mathbf{q}'_f, t; Q'_i, \mathbf{q}'_i, 0),\end{aligned} \tag{1.50}$$

where we have introduced the $N$-component vector $\mathbf{q} = (q_1, ..., q_N)$, and the coordinate representation of the time evolution operator,

$$K(Q_f, \mathbf{q}_f, t; Q_i, \mathbf{q}_i, 0) = \langle Q_f, \mathbf{q}_f|\, \mathrm{e}^{-i\hat{H}t/\hbar}\, |Q_i, \mathbf{q}_i\rangle\,. \tag{1.51}$$

The evolution operator in Eq. (1.51) can be written as a path integral, such that

$$K(Q_f, \mathbf{q}_f, t; Q_i, \mathbf{q}_i, 0) = \int \mathcal{D}Q\mathcal{D}\mathbf{q}\, \mathrm{e}^{iS[Q,\mathbf{q}]/\hbar}, \tag{1.52}$$

representing a path-integral over all paths with endpoints $Q(0) = Q_i, Q(t) = Q_f$ and $\mathbf{q}(0) = \mathbf{q}_i, \mathbf{q}(t) = \mathbf{q}_f$. The action $S = S_{\mathcal{A}} + S_{\mathcal{E}} + S_{\mathcal{AE}}$ is given by

$$S = \int_0^t dt' \Big( \mathcal{L}_{\mathcal{A}}(t') + \mathcal{L}_{\mathcal{E}}(t') + \mathcal{L}_{\mathcal{AE}}(t') \Big), \tag{1.53}$$

with the Lagrangians

$$\begin{aligned}\mathcal{L}_{\mathcal{A}} = \frac{1}{2}m\dot{Q}^2 - V[Q]; \quad \mathcal{L}_{\mathcal{E}} = \frac{1}{2}\sum_{k=1}^{N} m_k(\dot{q}_k^2 - \omega_k^2 q_k^2); \\ \mathcal{L}_{\mathcal{AE}} = \sum_{k=1}^{N}\left( g_k q_k Q - \frac{1}{2}\frac{g_k^2}{m_k\omega_k^2}Q^2 \right).\end{aligned} \tag{1.54}$$

To obtain the reduced dynamics for $\mathcal{A}$ we trace out the degrees of freedom of the environment in Eq. (1.50), $\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{E}}[\hat{\rho}_{\mathcal{AE}}]$, and get

$$\begin{aligned}\rho_{\mathcal{A}}(Q_f,Q'_f,t) &= \int d\mathbf{q}_f \,\langle Q_f,\mathbf{q}_f|\,\hat{\rho}_{\mathcal{AE}}(t)\,|Q'_f,\mathbf{q}_f\rangle \\ &= \int dQ_i dQ'_i d\mathbf{q}_i d\mathbf{q}'_i d\mathbf{q}_f K(Q_f,\mathbf{q}_f,t;Q_i,\mathbf{q}_i,0) \\ &\quad\times \langle Q_i,\mathbf{q}_i|\,\hat{\rho}_{\mathcal{AE}}(0)\,|Q'_i,\mathbf{q}'_i\rangle\, K^*(Q'_f,\mathbf{q}_f,t;Q'_i,\mathbf{q}'_i,0).\end{aligned} \tag{1.55}$$

Throughout the thesis we are mainly interested in a special kind of initial state where $\mathcal{A}$ and $\mathcal{E}$ are uncorrelated at time $t=0$. Even though this initial state may be hard to set up experimentally it will be helpful in order to understand the dynamical formation of correlations through the interaction between the subsystems. For a treatment involving more general initial states see [47].

We further assume then $\hat{\rho}_{\mathcal{AE}}(0)$ is in a factorized form, $\hat{\rho}_{\mathcal{A}}(0)\otimes\hat{\rho}_{\mathcal{E}}(0)$, and the initial state of $\mathcal{E}$ is a canonical thermal equilibrium state,

$$\hat{\rho}_{\mathcal{AE}}(0) = \hat{\rho}_{\mathcal{A}}(0)\otimes\frac{\mathrm{e}^{-\beta\hat{H}_{\mathcal{E}}}}{Z_{\mathcal{E}}}, \tag{1.56}$$

where $Z_{\mathcal{E}}$ is the partition function. This thermal state of the environment, which models a particle immerse in a *bath reservoir*, is called Quantum Brownian Motion (QBM), because the classical limit of the particle dynamics gives the so-called Langevin equation; an equation of motion which involves dissipation of energy and a fluctuating force acting on the particle (noise), as will be shown below.

It can be shown [47] that the central system will reach a stationary state for long times, and if the interaction with the bath is weak enough, the particle will acquire a canonical state at the same temperature of the bath. In next chapters we will go beyond this initial thermal state assumption to understand the emergence of temperature in a more fundamental way and the role of interference in dissipative systems.

Inserting Eq. (1.56) into (1.55) we obtain

$$\rho_{\mathcal{A}}(Q_f,Q'_f,t) = \int dQ_i dQ'_i\; \mathcal{J}(Q_f,Q'_f,t;Q_i,Q'_i,0)\rho_{\mathcal{A}}(Q_i,Q'_i,0), \tag{1.57}$$

where we introduce the *propagating function* $\mathcal{J}$, describing the time evolution of $\hat{\rho}_{\mathcal{A}}$ under the influence of the environment,

$$\mathcal{J}(Q_f,Q'_f,t;Q_i,Q'_i,0) = \int \mathcal{D}Q\mathcal{D}Q'\; \mathrm{e}^{i(S_{\mathcal{A}}[Q]-S_{\mathcal{A}}[Q'])/\hbar}\mathcal{F}[Q,Q'], \tag{1.58}$$

in terms of the so-called *Feynman-Vernon* influence functional [43]

$$\begin{aligned}\mathcal{F}[Q,Q'] &= \int d\mathbf{q}_f d\mathbf{q}_i d\mathbf{q}'_i\; \rho_{\mathcal{E}}(\mathbf{q}_i,\mathbf{q}'_i,0)\int_{(\mathbf{q}_i,\mathbf{q}'_i)\to\mathbf{q}_f}\mathcal{D}\mathbf{q}\mathcal{D}\mathbf{q}' \\ &\quad\times \mathrm{e}^{\frac{i}{\hbar}(S_{\mathcal{E}}[\mathbf{q}]+S_{\mathcal{AE}}[Q,\mathbf{q}]-S_{\mathcal{E}}[\mathbf{q}']-S_{\mathcal{AE}}[Q',\mathbf{q}'])} \\ &\equiv \int d\mathbf{q}_f d\mathbf{q}_i d\mathbf{q}'_i\; \rho_{\mathcal{E}}(\mathbf{q}_i,\mathbf{q}'_i,0)F(Q,\mathbf{q}_f,\mathbf{q}_i)F^*(Q',\mathbf{q}_f,\mathbf{q}'_i).\end{aligned} \tag{1.59}$$

While functional $F(Q,\mathbf{q}_f,\mathbf{q}_i) = \int \mathcal{D}\mathbf{q}\ \mathrm{e}^{i(S_{\mathcal{E}}[\mathbf{q}]+S_{\mathcal{AE}}[Q,\mathbf{q}])/\hbar}$, involves all paths $\mathbf{q}$ with endpoints $\mathbf{q}(0)=\mathbf{q}_i$ and $\mathbf{q}(t)=\mathbf{q}_f$. For the environment model ($N$ harmonic oscillators) given in Eq. (1.54) and the initial state Eq. (1.56), $\rho_{\mathcal{E}}(\mathbf{q}_i,\mathbf{q}_i',0)$ and $F(Q,\mathbf{q}_f,\mathbf{q}_i)$ can be written as a product over all the $N$ modes in $\mathcal{E}$,

$$\begin{aligned}\rho_{\mathcal{E}}(\mathbf{q}_i,\mathbf{q}_i',0) &= \prod_{k=1}^{N}\rho_{\mathcal{E}}^{k}(q_{i,k},q_{i,k}'),\\ F(Q,\mathbf{q}_f,\mathbf{q}_i) &= \prod_{k=1}^{N}F_k(Q,q_{f,k},q_{i,k}),\end{aligned} \tag{1.60}$$

where $\rho_{\mathcal{E}}^{k}(q_{i,k},q_{i,k}')$ is the coordinate representation of the canonical density matrix of the $k$-th harmonic oscillator, which reads

$$\begin{aligned}\rho_{\mathcal{E}}^{k}(q_{i,k},q_{i,k}') = &\Big(\frac{m_k\omega_k}{2\pi\hbar\sinh(\beta\hbar\omega_k)}\Big)^{1/2}2\sinh(\beta\hbar\omega_k/2)\\ &\times\exp\left(\frac{m_k\omega_k}{2\hbar\sinh(\beta\hbar\omega_k)}\Big[(q_{i,k}^2+q_{i,k}'^2)\cosh(\beta\hbar\omega_k)-2q_{i,k}q_{i,k}'\Big]\right).\end{aligned} \tag{1.61}$$

The action in the path functional $F(Q,\mathbf{q}_f,\mathbf{q}_i)$ involves quadratic terms in $\mathbf{q}$, and thus represents a Gaussian path integral for which an exact solution can be found [46], yielding

$$F(Q,\mathbf{q}_f,\mathbf{q}_i) = \Big(\frac{m_k\omega_k}{2\pi i\hbar\sin(\omega_k t)}\Big)^{1/2}\exp\Big(\frac{i}{\hbar}\phi_k[Q,q_{f,k},q_{i,k}]\Big), \tag{1.62}$$

where

$$\begin{aligned}\phi_k[Q,q_{f,k},q_{i,k}] =&\frac{m_k\omega_k}{2\sin(\omega_k t)}[(q_{i,k}^2+q_{f,k}^2)\cos(\omega_k t)-2q_{i,k}q_{f,k}]\\ &+\frac{q_{i,k}\ g_k}{2\sin(\omega_k t)}\int_0^t ds\sin(\omega_k(t-s))Q(s)\\ &+\frac{q_{f,k}\ g_k}{2\sin(\omega_k t)}\int_0^t ds\sin(\omega_k s)Q(s)-\frac{g_k^2}{2m_k\omega_k^2}\int_0^t ds\ Q^2(s)\\ &-\frac{g_k^2}{m_k\omega_k\sin(\omega_k t)}\int_0^t ds\int_0^s du\sin(\omega_k(t-s))\sin(\omega_k u)Q(s)q(u).\end{aligned} \tag{1.63}$$

With all these ingredients from Eqs. (1.61-1.63), the double path integral in Eq. (1.59), being Gaussian, can be solved exactly yielding finally an effective action for the system $\mathcal{A}$ under the influence of the bath. Using relative and center of mass coordinates, $y=Q-Q'$, $r=(Q+Q')/2$, the reduced density matrix finally reads

$$\begin{aligned}&\rho_{\mathcal{A}}(r_f+y_f/2,r_f-y_f/2,t) = \int dr_i dy_i\ \rho_{\mathcal{A}}(r_i+y_i/2,r_i-y_i/2,0)\\ &\int_{r_i\to r_f}\mathcal{D}r\int_{y_i\to y_f}\mathcal{D}y\times\mathrm{e}^{i\left(S_{\mathcal{A}}(r+y/2)-S_{\mathcal{A}}(r-y/2)-S^{F}[r,y]\right)/\hbar}\ \mathrm{e}^{-S^{\mathcal{N}}[y]/\hbar},\end{aligned} \tag{1.64}$$

where so-called noise action

$$S^{\mathcal{N}}[y] = \int_0^t ds \int_0^s du\ y(s)K(s-u)y(u), \tag{1.65}$$

involves only the off-diagonal variables $y$, and the friction action is given by

$$S^F[r,y] = m\int_0^t ds \int_0^s du\ y(s)\gamma(s-u)\dot{r}(u) + mr(0)\int_0^t ds\ \gamma(s)y(s). \tag{1.66}$$

The kernels in the integrals of Eqs. (1.65,1.66)

$$\begin{aligned} K(s) =& \frac{1}{\pi}\int_0^\infty d\omega\ J(\omega)\coth(\beta\hbar\omega/2)\cos(\omega s), \\ \frac{m}{2}\frac{d\gamma(s)}{ds} =& -\frac{1}{\pi}\int_0^\infty d\omega\ J(\omega)\sin(\omega s), \end{aligned} \tag{1.67}$$

depend on the *spectral density*, related with the bath coupling, defined as

$$J(\omega) = \pi\sum_{k=1}^{N}\frac{g_k^2}{2m_k\omega_k}\delta(\omega-\omega_k). \tag{1.68}$$

We will see in the next section that $S^F$ produces a contribution to the equations of motion which gives rise to a damping force $\int_0^s du\ \gamma(s-u)\dot{r}(u)$, acting on the diagonal path $r(s)$. On the other hand, the action $S^{\mathcal{N}}$ produces a decay of off-diagonal paths $y(s)$ due to the coupling with the thermal bath. To see this, let us assume a continuum of bath oscillators and choose a spectral density proportional to $\omega$. In this so-called *Ohmic* scenario, $J(\omega) = \gamma\omega$. Further, in the limit of high temperatures, $\beta \to 0$, the kernel $K$ transforms into $K(s-u) = \frac{2\gamma}{\hbar\beta}\delta(s-u)$, and if we consider two spatially localized waves with separation $Q - Q' \equiv y_0$, the noise action gives

$$S^{\mathcal{N}} = \frac{2\gamma}{\hbar\beta}\int_0^t ds\ y(s)^2 \sim \frac{2\gamma t}{\hbar\beta}y_0^2. \tag{1.69}$$

In this way inserting Eq. (1.69) into Eq. (1.64) we see that $S^{\mathcal{N}}$ is responsible for the extinction of quantum coherence (off-diagonal components of the density matrix) between paths $Q$ and $Q'$, given by $\mathrm{e}^{-t\frac{2\gamma}{\hbar\beta}y_0^2}$. We recognize here the *decoherence factor* $\gamma_{\mathrm{decoh}} = \frac{2\gamma}{\hbar\beta}y_0^2$, as the inverse time scale for decoherence of two states.

It can be shown, on the other hand, that the dissipative effects are characterized by the *damping rate* $\gamma_{\mathrm{damping}} = \frac{\gamma}{m}$. The ratio of this two quantities is given by

$$\gamma_{\mathrm{decoh}}/\gamma_{\mathrm{damping}} = y_0^2/\lambda_{\mathrm{th}}^2, \tag{1.70}$$

with the thermal wave length of the particle $\lambda_{\mathrm{th}} = \hbar/\sqrt{m\beta^{-1}}$. Finally, for a typical macroscopic scenario [46], the mass of the particle $m = 1\ g$, the temperature $T = 300\ K$ and $y_0 = 1\ mm$, the ratio Eq. (1.70) gives a value of $10^{38}$. We see then that for most typical macroscopic situations the decoherence time scale is astronomically faster than the time scale of dissipation.

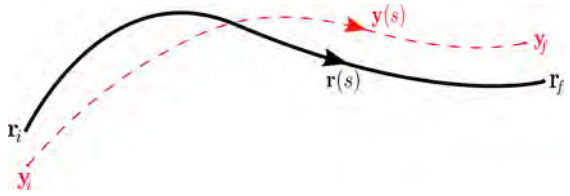


Figure 1.4: To construct the semiclassical approximation to Eq. (1.64) we follow paths along the diagonal $r(s)$ and expand the action accordingly around small path fluctuations $y(s)$. Notice the similarity with Fig .1.2 in the closed-system scenario, but here the classical equations of motion do not come from stationary condition of amplitudes. The arrows show the direction of time

### 1.2.3. Semiclassical approximation to the Caldeira-Legget model

So far Eq. (1.64) is exact and gives the reduced density matrix $\rho_{\mathcal{A}}$ evolved for a time $t$ from the initial reduced matrix, under the influence of the bath $\mathcal{E}$, encoded in the effective actions $S^{\mathcal{N}}$ and $S^{F}$. When the central system $\mathcal{A}$ represents a harmonic oscillator, all the actions in Eq. (1.64) involve quadratic terms in the coordinates $(r, y)$, and the integrals can be solved exactly, as shown for example in [47]. But for a more general system, to solve the path integral becomes a very difficult task, and an approximation to obtain the reduced dynamics is needed. In a similar spirit used in section 1.1.2 we will calculate the semiclassical approximation to Eq. (1.64), but an important difference here is that the classical equations of motion are *not coming* from the semiclassical amplitude, and thus the approximation does not have the form of Eq. (1.21) as a product of two semiclassical propagators. The reason behind this discrepancy from the closed-system scenario has its root in an intrinsic incompatibility of the action-based theory of physical processes between initial conditions and irreversible dynamics, and therefore, with dissipative and open systems. We will explore this issue in detail in chapter 4. We construct the semiclassical approximation to Eq. (1.64) going through the diagonal components, or in other words, through the center of mass coordinates $r(s)$, and treat accordingly the relative coordinates $y(s)$ as "fluctuations", as shown in Fig. 1.4. A similar idea is used in the closed-system scenario in Eq. (1.22), expanding the action around $r$, but this time keeping up to second-order in the relative coordinates (see also Fig. 1.2). With this in mind, we expand the bare action $S_{\mathcal{A}}$ around the center of mass and take the difference between the "forward" and "backward" paths in Eq. (1.64), assuming $y(s)$ small according to

$$S_{\mathcal{A}}\big[r + y/2\big] - S_{\mathcal{A}}\big[r - y/2\big] = \int_0^t ds \Bigg( y(s)\frac{\partial}{\partial r}\mathcal{L}_{\mathcal{A}}(r,\dot{r}) + \dot{y}(s)\frac{\partial}{\partial \dot{r}}\mathcal{L}_{\mathcal{A}}(r,\dot{r}) + \mathcal{O}(y^3, \dot{y}^3)\Bigg). \tag{1.71}$$

On the other hand, the effective actions $S^{\mathcal{N}}, S^{F}$ are at most quadratic in $y$, and with the last expansion, keeping terms up to second-order in $y$, Eq. (1.64) reads

$$\rho_{\mathcal{A}}(r_f+y_f/2,r_f-y_f/2,t)\approx\int dr_i dy_i\;\rho_{\mathcal{A}}(r_i+y_i/2,r_i-y_i/2,0)\int_{r_i\to r_f}\mathcal{D}r\int_{y_i\to y_f}\mathcal{D}y$$
$$\exp\frac{i}{\hbar}\Bigg[\left(y(s)\frac{\partial}{\partial\dot{r}}\mathcal{L}_{\mathcal{A}}(r,\dot{r})\right)\Bigg|_0^t-\int_0^t ds\;y(s)\Bigg(\frac{d}{ds}\frac{\partial}{\partial\dot{r}}\mathcal{L}_{\mathcal{A}}(r,\dot{r})-\frac{\partial}{\partial r}\mathcal{L}_{\mathcal{A}}(r,\dot{r})$$
$$+m\int_0^s du\;\gamma(s-u)\dot{r}(u)+mr_i\gamma(s)-i\int_0^s du\;K(s-u)y(u)\Bigg)\Bigg]. \tag{1.72}$$

The first term in the second line of Eq. (1.72) is a surface term coming from the usual integration by parts taken in Eq. (1.71).

Before proceeding further, from Eq. (1.72) we see that in the closed-system scenario, where the last line in Eq. (1.72) vanishes, we can integrate out the paths $y(s)$, and obtain

$$\rho_{\mathcal{A}}^{\text{closed}}(r_f+y_f/2,r_f-y_f/2,t)\sim\int dr_i dy_i\;\rho_{\mathcal{A}}(r_i+y_i/2,r_i-y_i/2,0)\int_{r_i\to r_f}\mathcal{D}r$$
$$\exp\frac{i}{\hbar}\left[\left(y(s)\frac{\partial}{\partial\dot{r}}\mathcal{L}_{\mathcal{A}}(r,\dot{r})\right)\Bigg|_0^t\right]\;\delta\left(\frac{d}{ds}\frac{\partial}{\partial\dot{r}}\mathcal{L}_{\mathcal{A}}(r,\dot{r})-\frac{\partial}{\partial r}\mathcal{L}_{\mathcal{A}}(r,\dot{r})\right), \tag{1.73}$$

which is a path integral over $r(s)$ following the classical equation of motion (Euler-Lagrange equation) imposed by the delta function. Moreover, if the initial and final fluctuations vanish $y_i=y_f=0$, the last equation gives just the *diagonal* approximation found in Eq. (1.27). Actually, variations of the action in Eq. (1.72) in the closed-system setup with respect to $r(s)$, calculated from Eq. (1.71), gives (neglecting higher order terms in $y$)

$$\begin{aligned}\frac{\delta}{\delta r}\Big(S_{\mathcal{A}}\big[r+y/2\big]-S_{\mathcal{A}}\big[r-y/2\big]\Big)&=\int_0^t ds\;\Bigg(\frac{\partial^2\mathcal{L}_{\mathcal{A}}}{\partial r^2}y(s)+\frac{\partial^2\mathcal{L}_{\mathcal{A}}}{\partial r\partial\dot{r}}\dot{y}(s)\\&\quad-\frac{d}{ds}\left(\frac{\partial^2\mathcal{L}_{\mathcal{A}}}{\partial r\partial\dot{r}}y(s)+\frac{\partial^2\mathcal{L}_{\mathcal{A}}}{\partial\dot{r}^2}\dot{y}(s)\right)\Bigg)\delta r(s)\\&=-\int_0^t ds\;\left(m\frac{d^2}{ds^2}+V''(r)\right)y(s)\delta r(s),\end{aligned} \tag{1.74}$$

where we have used the Lagrangian $\mathcal{L}_{\mathcal{A}}$ from Eq. (1.54) to obtain the last line. We recognize the last equation as the one in Eq. (1.16) which was obtained evaluating along classical paths coming from variations in the *amplitude*. This shows the consistency of the approximation in Eq. (1.72) in the closed-system scenario.

Coming back to open systems and the complete Eq. (1.72), let us see the action in

more detail. Eq. (1.72) can be written as

$$\rho_{\mathcal{A}}(r_f + y_f/2, r_f - y_f/2, t) \approx \int dr_i dy_i \; \rho_{\mathcal{A}}(r_i + y_i/2, r_i - y_i/2, 0) \int_{r_i \to r_f} \mathcal{D}r \int_{y_i \to y_f} \mathcal{D}y \; \mathrm{e}^{\frac{i}{\hbar}\Phi[r,y]}, \tag{1.75}$$

with the action given by

$$\Phi = \left( y(s) \frac{\partial}{\partial \dot{r}} \mathcal{L}_{\mathcal{A}}(r, \dot{r}) \right) \Bigg|_0^t - \int_0^t ds \; y(s) \Bigg( \frac{d}{ds} \frac{\partial}{\partial \dot{r}} \mathcal{L}_{\mathcal{A}}(r, \dot{r}) - \frac{\partial}{\partial r} \mathcal{L}_{\mathcal{A}}(r, \dot{r}) + m \int_0^s du \; \gamma(s-u) \dot{r}(u) + m r_i \gamma(s) - i \int_0^s du \; K(s-u) y(u) \Bigg). \tag{1.76}$$

We emphasize that, so far, the approximation in Eq. (1.75) is due to an expansion of the action along the diagonal $r(s)$ up to second-order terms in the fluctuation path $y(s)$, which leads to the action Eq. (1.76).

### Noise and damping kernel

The kernels $K(s)$ and $\gamma(s)$ appearing in Eq. (1.76) encode all the information concerning the influence of the bath on the central system. It is instructive to see how they are related with correlations of the bath modes and how they encode information about "memory" effects within the bath. To this end let us examine a central quantity in open systems which is the so-called environment self-correlation function which in this case, since the interaction Hamiltonian involves position operators, is given by

$$\mathcal{C}(\tau) = \sum_{ij} g_i g_j \left\langle \hat{q}_i(\tau) \hat{q}_j \right\rangle_{\hat{\rho}_{\mathcal{E}}} = \sum_i g_i^2 \left\langle \hat{q}_i(\tau) \hat{q}_i \right\rangle_{\hat{\rho}_{\mathcal{E}}(0)}, \tag{1.77}$$

where the average is taken over the initial thermal state of the environment $\hat{\rho}_{\mathcal{E}}(0)$, and the time-dependent environment position operator $\hat{q}(\tau)$ is described in the interaction picture. Due to the fact that the harmonic oscillators in $\mathcal{E}$ do not interact with each other they are uncorrelated, and so the sum in Eq. (1.77) vanishes for $i \neq j$.

The correlation function Eq. (1.77) is a quantity which gives a notion of how correlated is a measurement of the initial position of the environment with a later position measurement, due to the coupling with the central system. In other words, it tells about the degree of information retained by the environment over time due to its interaction with the system. In the following lines we sketch the derivation given in [2]. To compute Eq. (1.77) we switch to the representation of the harmonic position operator in terms of creation $\hat{a}^\dagger$ and annihilation $\hat{a}$ operators

$$\hat{q}_i = \sqrt{\frac{\hbar}{2 m_i \omega_i}} \left( \hat{a}_i^\dagger + \hat{a}_i \right), \tag{1.78}$$

and the time evolution of the position operator, in the interaction picture, is given by

$$\hat{q}_i(\tau) = \mathrm{e}^{i\hat{H}_{\mathcal{E}}\tau/\hbar}\hat{q}_i\mathrm{e}^{-i\hat{H}_{\mathcal{E}}\tau/\hbar} = \sqrt{\frac{\hbar}{2m_i\omega_i}}\Big(\mathrm{e}^{i\omega_i\tau}\hat{a}_i^\dagger + \mathrm{e}^{-i\omega_i\tau}\hat{a}_i\Big). \tag{1.79}$$

With this the thermal average becomes

$$\begin{aligned}\langle\hat{q}_i(\tau)\hat{q}_i\rangle_{\hat{\rho}_{\mathcal{E}}} =& \frac{\hbar}{2m_i\omega_i}\,\langle\hat{a}_i\hat{a}_i^\dagger\mathrm{e}^{-i\omega_i\tau} + \hat{a}_i^\dagger\hat{a}_i\mathrm{e}^{i\omega_i\tau}\rangle_{\hat{\rho}_{\mathcal{E}}} \\ =& \frac{\hbar}{2m_i\omega_i}\left(\,\langle\hat{a}_i\hat{a}_i^\dagger\rangle_{\hat{\rho}_{\mathcal{E}}}\,\mathrm{e}^{-i\omega_i\tau} + \langle\hat{a}_i^\dagger\hat{a}_i\rangle_{\hat{\rho}_{\mathcal{E}}}\,\mathrm{e}^{i\omega_i\tau}\right).\end{aligned} \tag{1.80}$$

On the other hand, the quantity $N_i = \langle\hat{a}_i^\dagger\hat{a}_i\rangle_{\hat{\rho}_{\mathcal{E}}}$ denotes the mean occupation number of the $i$-th oscillator in $\mathcal{E}$. Since the initial state of the environment is a thermal equilibrium state, the bosonic thermal distribution corresponds to

$$N_i \equiv N_i(T) = \frac{1}{\mathrm{e}^{\hbar\omega_i/k_BT} - 1}, \tag{1.81}$$

with $T$ the bath temperature and $k_B$ the Boltzmann constant. Finally, using the last expression and the commutation relation $[\hat{a}_i, \hat{a}_i^\dagger] = 1$ we obtain

$$\begin{aligned}\langle\hat{q}_i(\tau)\hat{q}_i\rangle_{\hat{\rho}_{\mathcal{E}}} =& \frac{\hbar}{2m_i\omega_i}\left((1 + N_i(T))\mathrm{e}^{-i\omega_i\tau} + N_i(T)\mathrm{e}^{i\omega_i\tau}\right) \\ =& \frac{\hbar}{2m_i\omega_i}\left(\,\coth\Big(\frac{\hbar\omega_i}{2k_BT}\Big)\cos(\omega_i\tau) - i\sin(\omega_i\tau)\right),\end{aligned} \tag{1.82}$$

where the last line was obtained with the help of the identity

$$\begin{aligned}1 + 2N_i(T) =& 1 + \frac{2}{\mathrm{e}^{\hbar\omega_i/k_BT} - 1} \\ =& \frac{\mathrm{e}^{\hbar\omega_i/k_BT} + 1}{\mathrm{e}^{\hbar\omega_i/k_BT} - 1} = \coth\Big(\frac{\hbar\omega_i}{2k_BT}\Big).\end{aligned} \tag{1.83}$$

With this Eq. (1.77) becomes

$$\mathcal{C}(\tau) = \hbar\sum_i \frac{g_i^2}{2m_i\omega_i}\left(\,\coth\Big(\frac{\hbar\omega_i}{2k_BT}\Big)\cos(\omega_i\tau) - i\sin(\omega_i\tau)\right), \tag{1.84}$$

which, with the help of Eq. (1.68), can finally be written as

$$\begin{aligned}\mathcal{C}(\tau) =& \hbar\int_0^\infty d\omega\;\frac{J(\omega)}{\pi}\left(\,\coth\Big(\frac{\hbar\omega_i}{2k_BT}\Big)\cos(\omega_i\tau) - i\sin(\omega_i\tau)\right) \\ =& \hbar\Big(K(\tau) + i\frac{m}{2}\frac{d}{d\tau}\gamma(\tau)\Big).\end{aligned} \tag{1.85}$$

In the last line of the above equation we have recognized the noise and damping kernels from Eq. (1.67). In this way we observe that the real part of the environment self-correlation function is related with the noise kernel responsible for decoherence, while the imaginary part gives the damping kernel, which we will see, is responsible for dissipation of energy, with a history-dependent damping kernel.

### Classical equations of motion

In order to obtain the classical equation of motion, we need to calculate the variations of the action Eq. (1.76) with respect to the paths $r(s), y(s)$. Variation of the action with respect to $y(s)$ yields

$$\begin{aligned}\frac{\delta\Phi}{\delta y(s)} = \frac{d}{ds}\frac{\partial}{\partial\dot{r}}\mathcal{L}_{\mathcal{A}}(r,\dot{r}) - \frac{\partial}{\partial r}\mathcal{L}_{\mathcal{A}}(r,\dot{r}) + m\int_0^s du\,\gamma(s-u)\dot{r}(u) + mr_i\gamma(s) \\ -i\int_0^t du\,K(s-u)y(u) \stackrel{!}{=} 0,\end{aligned} \tag{1.86}$$

yielding

$$m\ddot{r}(s) + V'(r(s)) + m\int_0^s du\,\gamma(s-u)\dot{r}(u) + mr_i\gamma(s) = i\int_0^t du\,K(s-u)y(u). \tag{1.87}$$

In the same way variation with respect to $r(s)$ gives

$$\frac{\delta\Phi}{\delta r(s)} = m\ddot{y}(s) + y(s)V''(r(s)) - m\int_s^t du\,\gamma(u-s)\dot{y}(u) + my_f\gamma(t-s) \stackrel{!}{=} 0. \tag{1.88}$$

These conditions give the equations of motion for the center of mass and relative coordinate of the central system.

Setting $y(s) = 0$ in Eq. (1.87), the resulting equation represents the *classical evolution* of the system, with a velocity-dependent, non-local term $m\int_0^s du\,\gamma(s-u)\dot{r}(u)$. While in general the memory-friction kernel $\gamma(s)$ involves retardation due to the heat reservoir, for the ohmic case (see section 1.2.2), the spectral density $J(\omega) = m\gamma\omega$ leads to $\gamma(s) = 2\delta(s)$, and so Eq. (1.87) becomes

$$m\ddot{r}(s) + V'(r(s)) + 2m\dot{r} = 0, \tag{1.89}$$

which yields a *deterministic damped* evolution.
It is important to note that Eq. (1.88) represents an equation of motion for the fluctuations which looks dissipative but time-reversed. That is, if we insert the time-reversed path $\tilde{y}(t-s)$ in Eq. (1.88) it transforms into the left-hand-side of Eq. (1.87). And even more important, within the open system scenario the interplay between forward $Q(s)$ and backward paths $Q'(s)$ is the vital feature to obtain a dissipative equation of motion for the diagonal (center of mass) part of the density matrix, as it will be explored in more detail in chapter 4. There we will show that precisely this interplay of forward and

backward paths is crucial to break the time-reversal symmetry implicit in the description of amplitudes for closed-systems. Finally, let us emphasize that being Eq. (1.88) a linear second-order differential equation, assuming vanishing initial and final fluctuations $y_i = y_f = 0$, then $y(s) = 0$ is the unique solution, and then Eq. (1.87) becomes

$$m\ddot{r}(s) + V'(r(s)) + m\int_0^s du\, \gamma(s-u)\dot{r}(u) + mr_i\gamma(s) = 0, \tag{1.90}$$

representing a deterministic damped-particle with memory-friction kernel. This equation is in general non-linear, and thus multiple solutions $r(s)$ with boundary conditions $r(0) = r_i, r(t) = r_f$ may exist.

Notice that the last term in the action Eq. (1.76), yields an exponential suppression of off-diagonal components, or decoherence (see Eq. (1.65) and the discussion thereafter), which acts as a Gaussian filter (noise). When this noise is integrated out in Eq. (1.75), which is a functional Gaussian integral, assuming $y_i = y_f = 0$, the density matrix becomes, omitting a normalization constant [46]

$$\rho_{\mathcal{A}}(r_f, t) \sim \int \mathcal{D}[r] \exp\Big[-\frac{1}{2\hbar}\int_0^t ds \int_0^t du\, \xi[r(s)]K^{-1}(s-u)\xi[r(u)]\Big], \tag{1.91}$$

where the functional $\xi[r(s)]$ is defined as

$$\xi[r(s)] = m\ddot{r}(s) + V'[r(s)] + m\int_0^s du\, \gamma(s-u)\dot{r}(u) + mr_i\gamma(s). \tag{1.92}$$

As shown in [46], it is possible to introduce a measure of path integration associated with $\xi(t)$, and make the transformation from paths $r$ to the path fluctuations $\xi$, with the Jacobian independent of the choice of the potential $V(r)$. In this way, $\xi$ can be considered as an independent stochastic variable, and thus Eq. (1.92) can be interpreted as a Langevin equation

$$m\ddot{r}(s) + V'(r(s)) + m\int_0^s du\, \gamma(s-u)\dot{r}(u) + mr_i\gamma(s) = \xi(t), \tag{1.93}$$

with a fluctuating force $\xi(t)$. With Eq. (1.91), we observe that $\xi$ undergoes a Gaussian stochastic process, with

$$\begin{aligned} \langle \xi(t) \rangle &= 0, \\ \mathrm{Re}\, \langle \xi(t)\xi(0) \rangle &= \hbar K(t), \end{aligned} \tag{1.94}$$

that remarkably also appears in Eq. (1.85).

Finally, if $r_{\mathrm{cl}}(s), y_{\mathrm{cl}}(s)$ are solutions to Eqs. (1.88, 1.87) with the given boundary conditions, inserting them in the action Eq. (1.76) gives

$$\begin{aligned} \Phi_{\mathrm{sc}}(r_i, r_f, y_i, y_f) =& m\Big(\dot{r}_{\mathrm{cl}}(t)y_f - \dot{r}_{\mathrm{cl}}(0)y_i\Big) \\ &+ m\frac{i}{2}\int_0^t ds \int_0^t du\, y_{\mathrm{cl}}(s)K(s-u)y_{\mathrm{cl}}(u), \end{aligned} \tag{1.95}$$

where the subscript "sc" denotes semiclassical action, which in this context refers to the action along diagonal paths plus small fluctuations, evaluated in the solutions of the corresponding equations of motion. The last term of the above equation is the imaginary and temperature-dependent noise term, which acts as a Gaussian filter suppressing large deviations from the diagonal. Further, for a motion constrained to boundary conditions $y_i = y_f = 0$, meaning a motion only along the diagonal, Eq. (1.95) vanishes

$$\Phi_{\rm sc}(r_f, r_i, y_f = 0, y_i = 0) = 0. \tag{1.96}$$

The vanishing of action when evaluated along the classical path $r_c$, makes the construction of the semiclassical reduced density matrix, involving superposition (interference) of *different* classical dissipative paths solutions, a difficult task. In chapter 4, we explore a proposal to build a semiclassical approach to dissipative systems which allow in principle to observe path interference between different classical trajectories, where crucially the environment should be initiated in a *microcanonical* equilibrium state.

## 1.3. Summary

We have studied in this chapter the emergence of classicality in the closed system scenario, as an asymptotic limit for the quantum propagator, which gives rise to the classical equations of motion of the system at the level of amplitudes: as a result of the stationary condition of the action. In the same way, this asymptotic limit allows us to construct the semiclassical approximation of the density matrix, as a double sum of classical trajectories. The main contribution to this double sum comes from pairs of identical trajectories, yielding the diagonal approximation, which results in a density matrix in diagonal form (statistical mixture). On the other hand, the open system approach offers the possibility to understand the role of the environment in the emergence of this statistical mixture in the central system, through delocalization of local quantum coherence or decoherence, and the consequent emergence of classical pointer states. Further, we have shown how the classical equations of motion emerge in the Caldeira-Leggett model, in the semiclassical limit, where crucially, the stationary condition is not applied at the level of amplitudes but at the level of probabilities. This subtle difference from the closed system scenario has enormous consequences in understanding the origin of irreversibility in dissipative systems, as explored in more detail in chapter 4. The difficulty, however, to construct a semiclassical density matrix for open systems rests on, as shown in the Caldeira-Leggett model, the vanishing of the action when evaluated along the classical solutions. This makes the search for interference phenomena in dissipative open systems a problematic task. Some ideas in solving this issue will be explored in chapter 4.

# 2. Strong coupling and non-Markovian effects in the statistical notion of temperature

After introducing the basic concepts and tools of open quantum systems in the last chapter we want here to present the first of our main results, concerning the notion of temperature as an emergent quantity in strongly coupled systems. We will see how, starting from the fundamental microcanonical ensemble, temperature $T$ can be understood as a derived quantity involving two coupled systems that, in the thermodynamic limit interchange energy, and $T$ has the role of an equilibrium parameter. While this approach is presented in many textbooks and manuscripts (see for example [48]) for weakly coupled systems, the use of Saddle-Point Analysis (SPA) in this context was pioneered by Schwinger [49].

Here we generalize this idea to the case of strongly coupled quantum systems, providing a consistent generalization of temperature, and we illustrate its main features for the specific model of Quantum Brownian Motion where it leads to consistent microcanonical thermodynamics. In the coming sections we will follow closely our manuscript [24][1].

## 2.1. Introduction

In the context of statistical physics there are two ways to explain how a system $\mathcal{A}$ acquires a property associated with the thermodynamic notion of temperature [50, 51]. In the first approach, one considers the system as *weakly* coupled with a thermal bath $\mathcal{B}$ that is initially in a canonical state $\mathrm{e}^{-\beta H_{\mathcal{B}}}/Z_{\mathcal{B}}$ at temperature $T$, where $\beta = 1/KT$, $K$ is the Boltzmann constant, and $Z_{\mathcal{B}}$ is the partition function, see Fig. 2.1. If we wait long enough, $\mathcal{A}$ will equilibrate (in the sense of stationarity of macroscopic observables) and acquire itself a canonical distribution at the same temperature $T$. Here, therefore, the idea of temperature is pre-assumed from the beginning.

In the second approach, one considers instead the global system $\mathcal{A} + \mathcal{B}$ in a microcanonical distribution at total energy $E$, see Fig. (5.3). We agree with Hänggi and co-workers [48, 52, 53] that this is the conceptually foundational starting point to understand the meaning of temperature. Here $\mathcal{A}$ and $\mathcal{B}$ equilibrate due to the presence of a *weak* interaction term, and the temperature will emerge as a parameter that fixes the condition of equilibrium. *The temperature $T = T(E)$ is then a derived rather than a fundamental macroscopic property.*

[1] 

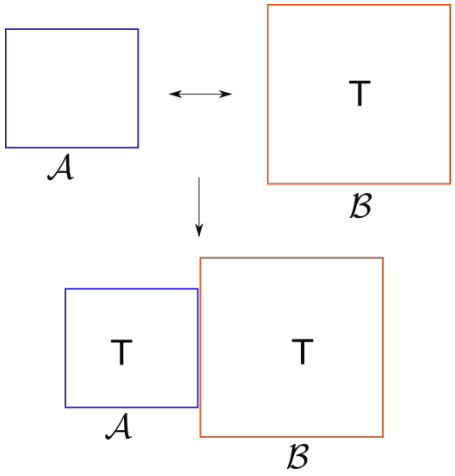


Figure 2.1: A system $\mathcal{A}$ is weakly coupled to a thermal reservoir $\mathcal{B}$ at temperature $T$. The two systems have enough time to interchange energy until an equilibrium is reached and $\mathcal{A}$ acquires a state of thermal equilibrium at the same temperature of the reservoir.


Figure 2.2: the global system $\mathcal{A}+\mathcal{B}$ is in a microcanonical equilibrium at energy $E$. The equilibrium has been reached due to the presence of a weak interaction between $\mathcal{A}$ and $\mathcal{B}$, and the temperature $T$ emerges as an equilibrium parameter.

These two approaches are equivalent in the weak-coupling regime, where the total energy $E$ is the sum of the subsystems $E_{\mathcal{A}} + E_{\mathcal{B}}$, because the interaction energy is small enough to be neglected. In this scenario the energy is an extensive quantity and the usual thermodynamic laws can be applied.

As it has been shown when going beyond the assumption of weak interactions, for strongly coupled $\mathcal{A}$ and $\mathcal{B}$, deviations from the standard thermodynamics emerge [54–57], as well as problems defining local temperature [58–61]. The equivalence between the microcanonical and the canonical approach does not hold, correlations between system and bath become important, and the system is non-extensive by nature [62–64]. In this context it is well known that when $\mathcal{A}$ is strongly coupled to a thermal bath the long time steady state of the system, contrary to the weak coupling scenario, does not take the Boltzmann form, neither in the open-quantum system approach [65–67], in the global closed thermal state scenario [68], nor in the pure state setup [69, 70].

In order to provide a consistent definition of temperature $T$ in the system-plus-bath scenario, with arbitrary coupling strength $\gamma$, we will start with a global microcanonical state at energy $E$ and generalize the Saddle-Point Analysis (SPA) of ensemble equivalence pioneered by Schwinger [49, 71].

In section 2.2 we review the relevant aspects of the emergence of temperature in the weak coupling scenario, then in section 2.3 we generalize this idea to the finite coupling case, and as an experimental relevant application, we will present the main features of this definition of temperature $T(E,\gamma)$ in the solvable case of Quantum Brownian Motion.

## 2.2. The statistical emergence of temperature from a saddle-point condition

Let us first review the weak coupling case by considering two many-body systems $\mathcal{A}$ and $\mathcal{B}$ with Hamiltonians $\hat{H}_{\mathcal{A}}$ and $\hat{H}_{\mathcal{B}}$, that in isolation have fixed energies $E_{\mathcal{A}}$, $E_{\mathcal{B}}$. When brought into *weak* thermal contact allowing them to interchange energy through a small interaction term such that $E_{\text{int}}(\gamma) \ll E_{\mathcal{A}} + E_{\mathcal{B}}$, in equilibrium the resulting global state is microcanonical

$$\hat{\rho}_{\mathcal{AB}} = \frac{\delta(E - \hat{H}_{\mathcal{AB}})}{\mathcal{G}_{\mathcal{AB}}(E)}, \tag{2.1}$$

with total energy $E = E_{\mathcal{A}}+E_{\mathcal{B}}+\mathcal{O}(\gamma)$. Here $\hat{H}_{\mathcal{AB}} = \hat{H}_{\mathcal{A}}+\hat{H}_{\mathcal{B}}+\mathcal{O}(\gamma)$ acts in $\mathcal{H}_{\mathcal{A}}\otimes\mathcal{H}_{\mathcal{B}}$ and $\mathcal{G}_{\mathcal{AB}}(E) = \text{Tr}_{\mathcal{AB}}\,\delta(E-\hat{H}_{\mathcal{AB}})$ is the microcanonical partition function. In fact, $\mathcal{G}_{\mathcal{AB}}(E)$ is the central quantity connecting statistics and thermodynamics through the Boltzmann equation

$$S(E) = K \log \mathcal{G}_{\mathcal{AB}}(E), \tag{2.2}$$

for the thermodynamic entropy $S(E)$, where $K$ is the Boltzmann constant.

It is important to note that in the microcanonical distribution the macroscopic quantity characterizing the state is the energy $E$, which is then the control parameter in this scenario. There is no a priori notion of temperature, and so we say that temperature is not a fundamental but a derived property. The emergence of temperature in this microcanonical, weak-limit scenario starts with writing the density of states, expanding the operator-valued Dirac delta function as

$$\begin{aligned} \mathcal{G}_{\mathcal{AB}}(E) &= \text{Tr}_{\mathcal{AB}}\ \delta(E - \hat{H}_{\mathcal{AB}}) \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau\, e^{iE\tau}\text{Tr}_{\mathcal{AB}}\left[e^{-i\tau\hat{H}_{\mathcal{AB}}}\right], \end{aligned} \tag{2.3}$$

where $\tau$ is an auxiliary integration variable with units of inverse energy. The operator-valued function $\delta(E-\hat{H})$ is defined as: $\delta(E-\hat{H}) = \sum_n |E_n\rangle\langle E_n|\,\delta(E-E_n)$, in the energy eigenbasis of $\hat{H}$. Defining $\text{Tr}_{\mathcal{AB}}[e^{-i\tau\hat{H}_{\mathcal{AB}}}] = Z_{\mathcal{AB}}(i\tau)$, Eq. (2.3) takes the form

$$\mathcal{G}_{\mathcal{AB}}(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau\, e^{iE\tau}e^{\log Z_{\mathcal{AB}}(i\tau)}, \tag{2.4}$$

with an associated action $\phi$

$$\begin{aligned} \phi(E,\tau) &= iE\tau + \log\, Z_{\mathcal{AB}}(i\tau) \\ &= iE\tau + \log\, Z_{\mathcal{A}}(i\tau) + \log\, Z_{\mathcal{B}}(i\tau), \end{aligned} \tag{2.5}$$

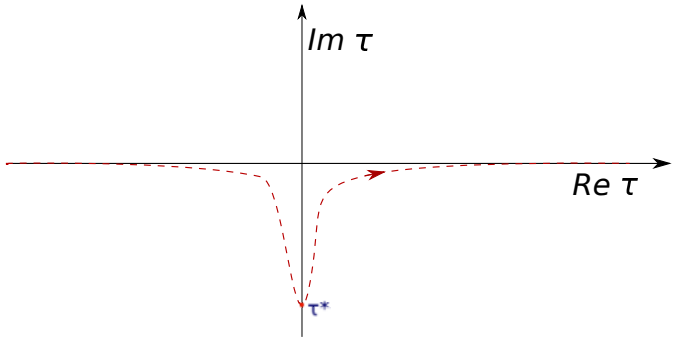


Figure 2.3: The Saddle-point condition in Eq. (2.4) admits an analytical continuation in the complex $\tau$ plane, as shown in dotted-line, and we find the saddle-point $\tau^* = -i\beta$, where we interpret $\beta$ as the inverse temperature.

where the decomposition $Z_{\mathcal{AB}} = Z_{\mathcal{A}} + Z_{\mathcal{B}}$, with $Z_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{A}}[e^{-i\tau\hat{H}_{\mathcal{A}}}]$ and $Z_{\mathcal{B}} = \mathrm{Tr}_{\mathcal{B}}[e^{-i\tau\hat{H}_{\mathcal{B}}}]$, is possible because the interaction term is small enough to be neglected. Following an idea due to Schwinger [49], for a large number of degrees of freedom $N \to \infty$, the quantities $E$ and $\log Z_{\mathcal{AB}}$ are large (allowing rapid oscillations in the exponential) and we can solve the integral in Eq. (2.4) using the Saddle-Point-Approximation (SPA). The saddle-point condition

$$\frac{d}{d\tau}\phi(E,\tau)\bigg|_{\tau=\tau^*} \stackrel{!}{=} 0 \tag{2.6}$$

admits an analytical continuation over the lower half of the complex $\tau$ plane, as shown in Fig. 2.3, where we find the sole saddle-point $\tau^* = -i\beta$, with $\beta$ satisfying

$$iE + i\frac{d}{d\beta}\log Z_{\mathcal{A}}(\beta)\bigg|_{\beta=i\tau^*} + i\frac{d}{d\beta}\log Z_{\mathcal{B}}(\beta)\bigg|_{\beta=i\tau^*} \stackrel{!}{=} 0. \tag{2.7}$$

By interpreting the real solution $\beta = 1/KT$ as the inverse temperature and $Z_i(\beta) = Z_i(i\tau^*)$ as the canonical partition function, then $\bar{E}_i = -\frac{d}{d\beta}\log Z_i(\beta)$ is the mean internal energy of each subsystem, and the relation

$$E = \bar{E}_{\mathcal{A}}(\beta = i\tau^*) + \bar{E}_{\mathcal{B}}(\beta = i\tau^*) \tag{2.8}$$

gives a condition on how the total energy is distributed between systems $\mathcal{A}$ and $\mathcal{B}$ when they are brought into contact. This microscopic analysis is thus used as the definition of both thermal equilibrium and of the inverse temperature that fixes this condition.

Before we make this microscopic construction complete and see how $\beta(E)$ can indeed be interpreted as the thermodynamic temperature, we find important to complete the analysis of [49] by discussing the regime of validity of the SPA, as well as the behavior of the error terms in the thermodynamic limit. In order to bring Eqs. (2.4,2.5) to the form required by the SPA, we consider first the situation where the total number of particles $N = N_{\mathcal{A}} + N_{\mathcal{B}}$ and energy $E$ are distributed in such a way that the ratios

$\nu_{\mathcal{A}} = N_{\mathcal{A}}/N, \nu_{\mathcal{B}} = N_{\mathcal{B}}/N, u = E/N$ converge to non-zero constants when $N \to \infty$. Within this usual definition of thermodynamic limit applied to both subsystems $\mathcal{A}, \mathcal{B}$, the ratios $\log z_{\mathcal{A}} = N_{\mathcal{A}}^{-1} \log Z_{\mathcal{A}}, \log z_{\mathcal{B}} = N_{\mathcal{B}}^{-1} \log Z_{\mathcal{B}}$ also converge to finite values, and the phase $\phi(E, \tau)$ in Eq. (2.5) takes the form

$$\phi(E, \tau) = N \left[ iu\tau + \nu_{\mathcal{A}} \log z_{\mathcal{A}}(i\tau) + \nu_{\mathcal{B}} \log z_{\mathcal{B}}(i\tau) \right]. \tag{2.9}$$

Substitution of Eq. (2.9) brings Eq. (2.4) to the form suitable for SPA, and rigorously identifies the large parameter as $N$. From the general theory we then conclude that the error in the evaluation of $\mathcal{G}_{\mathcal{AB}}(E)$ in Eq. (2.4) by means of SPA is of order $\mathcal{O}(1/\sqrt{N})$ and it remains bounded as long as $d^2\phi/d\tau^2 \neq 0$.

With these observations in mind, let us use Eqns. (2.2) and (2.4) with the solution established by Eq. (2.7) to obtain

$$\mathcal{G}_{\mathcal{AB}}(E) = \mathrm{e}^{\frac{S(E)}{K}} = \frac{\mathrm{e}^{\beta E + \log Z_{\mathcal{AB}}(\beta)}}{\sqrt{2\pi \frac{\partial^2 \log Z_{\mathcal{AB}}(\beta)}{\partial \beta^2}}} \left[ 1 + \mathcal{O}(N^{-1/2}) \right], \tag{2.10}$$

which by introducing the Helmholtz free energy $F(\beta) = -\frac{1}{\beta} \log Z_{\mathcal{AB}}(\beta)$, immediately gives the well known thermodynamic relation [71]

$$S(E)/K = \beta E - \beta F(\beta) \iff F = E - TS(E). \tag{2.11}$$

If there exist many solutions to Eq. (2.6) over the imaginary $\tau$ axes, for example: $\tau_1^* = -i\beta_1, \tau_2^* = -i\beta_2$, with $S_1(E) > S_2(E)$, we must choose the solution $\tau_1^*$ in Eq. (2.10) in accordance with the principle of maximum entropy, and neglecting exponentially small corrections $\sim \mathrm{e}^{S_2 - S_1}$.

In the approach of Schwinger, the focus of the SPA analysis was to provide a way to justify the ensemble equivalence as follows. Following a similar procedure as the one leading to Eq. (2.4), we write down the microcanonical density matrix $\hat{\rho}_{\mathcal{AB}}$ in Eq. (2.1) as

$$\hat{\rho}_{\mathcal{AB}}(E) = \frac{1}{2\pi \mathcal{G}_{\mathcal{AB}}(E)} \int_{-\infty}^{\infty} d\tau \, \mathrm{e}^{i\tau E} \mathrm{e}^{\log Z_{\mathcal{AB}}(i\tau)} \frac{\mathrm{e}^{-i\tau \hat{H}_{\mathcal{AB}}}}{Z_{\mathcal{AB}}(i\tau)}, \tag{2.12}$$

where we have multiplied and divided by $Z_{\mathcal{AB}}(i\tau)$. The microcanonical expectation value of an observable $\hat{O}$ acting on the global system can then be written in the form

$$\langle \hat{O} \rangle_E = \frac{1}{2\pi \mathcal{G}_{\mathcal{AB}}(E)} \int_{-\infty}^{\infty} d\tau \, \mathrm{e}^{i\tau E} \mathrm{e}^{\log Z_{\mathcal{AB}}(i\tau)} \langle \hat{O} \rangle_{i\tau}, \tag{2.13}$$

where we define

$$\langle \hat{O} \rangle_{i\tau} = \mathrm{Tr}_{\mathcal{AB}}[\hat{O} \mathrm{e}^{-i\tau \hat{H}_{\mathcal{AB}}} / Z_{\mathcal{AB}}(i\tau)]. \tag{2.14}$$

In the thermodynamic limit, provided $\langle \hat{O} \rangle_{i\tau}$ varies slowly with respect to $\tau$ [71], the integral in Eq. (2.13) can also be solved by SPA, resulting in $\langle \hat{O} \rangle_E \approx \langle \hat{O} \rangle_{\beta(E)}$, where $\beta(E)$ is the solution of Eq. (2.7). This is the meaning of equivalence of ensembles, according to Schwinger. Note that Eq. (2.13) is a mathematical identity which relates the expectation

value of a global observable $\hat{O}$ calculated in the microcanonical equilibrium with the quantity $\langle\hat{O}\rangle_{i\tau}$, which in the thermodynamic limit will give the canonical expectation value of the observable evaluated at the inverse temperature $\beta(E)$. This identity then does not refer to any dynamical process of equilibration in time. The topic of dynamical equilibration or relaxation goes beyond the formalism developed here.

In summary, Eq. (2.8) establishes a relation of energy equilibrium between two many-body systems. The condition of equilibrium is fixed by the inverse temperature $\beta$ coming from the SPA analysis of Eq. (2.6) in the thermodynamic limit. We establish this limit considering, for example, a many-body global system $\mathcal{A}+\mathcal{B}$ with a constant energy per particle, where the total energy scales with the number of particles $N$. In that case the thermodynamic limit $N\to\infty$ gives the relation Eq. (2.10). It is satisfactory to see how the SPA analysis formalizes the difference between the scenario of mutual equilibrium, where both subsystems are macroscopic and the temperature emerges from the distribution of the total energy as the two systems get a finite fraction, and the bath scenario where $\nu_{\mathcal{A}}=0$ in Eq. (2.9), and the temperature of the subsystem is simply inherited from the temperature of the bath. In this last scenario the function $\mathrm{e}^{\log Z_{\mathcal{A}}(i\tau)}=Z_{\mathcal{A}}(i\tau)$ is smooth and does not participate of the SPA condition.

## 2.3. Finite-coupling regime

After this revision of the key aspects of the emergence of temperature in composite weakly interacting systems, we now proceed to extend these ideas to systems with non-negligible interaction Hamiltonian $\hat{H}_{\mathrm{int}}$. The key point that allows for this generalization is that the SPA analysis that naturally leads to the concept of temperature is not restricted to $\gamma\to 0$ at all, and in fact its only requirement is consistency with the thermodynamic limit $N\to\infty$. While the global microcanonical equilibrium state in the case of finite interaction energy is

$$\hat{\rho}_{\mathcal{AB}}=\frac{\delta(E-\hat{H}_{\mathcal{A}}-\hat{H}_{\mathcal{B}}-\hat{H}_{\mathrm{int}})}{\mathcal{G}_{\mathcal{AB}}(E)}, \tag{2.15}$$

and the density of states is still given by Eq. (2.4), now $Z_{\mathcal{AB}}(i\tau)$ can not be unambiguously decomposed in general in terms of the bare Hamiltonians $\hat{H}_{\mathcal{A}}$ and $\hat{H}_{\mathcal{B}}$ [72]. However, our key observation is that as long as we can solve the integral in Eq. (2.4) by SPA, the resulting real solution for $\beta$, which now depends not only on the total energy $E$ but also on the parameters of the interaction, characterizes the condition of thermal equilibrium between $\mathcal{A}$ and $\mathcal{B}$, thus providing the statistical definition of temperature for systems with finite coupling. To support this claim we will now study the consistency and consequences of this definition in a solvable example.

As a specific microscopic model that allows for almost full analytical treatment and remains of high experimental relevance, we consider now a microcanonical modification of the widely used open-system approach to QBM as introduced in chapter. 1. Here $\mathcal{A}$ consists of a quantum harmonic oscillator linearly coupled to a bath $\mathcal{B}$ of $N$ non-

interacting harmonic oscillators. The total Hamiltonian reads

$$\begin{aligned}\hat{H}_{\mathcal{AB}} = &\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{q}^2 \\ &+ \frac{1}{2}\sum_{n=1}^{N}\left[\frac{\hat{p}_n^2}{m_n} + m_n\omega_n^2\left(\hat{q}_n - \frac{c_n}{m_n\omega_n^2}\hat{q}\right)^2\right],\end{aligned} \tag{2.16}$$

where $\hat{p}$ and $\hat{q}$ are momentum and position operators of the coupled harmonic oscillator with bare frequency $\omega_0$ and mass $m$, and $\hat{p}_n, \hat{q}_n$ the momentum and position operators of the $n$th bath oscillator with frequency $\omega_n$ and mass $m_n$ coupled with the central system through characteristic $c_n$ fixed for a given model of the bath. The bath and interactions are characterized by the bare and coupled spectral densities that distribute the frequencies $\omega_n$ like

$$I(\omega) = \pi\sum_{n=1}^{N}\delta(\omega-\omega_n) = \kappa\omega^2 e^{-\omega/\omega_D} \tag{2.17a}$$

$$J(\omega) = \pi\sum_{n=1}^{N}\frac{c_n^2}{2m\omega_n}\delta(\omega-\omega_n) = m\gamma\omega e^{-\omega/\omega_D}, \tag{2.17b}$$

with cut-off Drude frequency $\omega_D$ and so called damping parameter $\gamma$, which is a function of the parameters $c_n^2$ characterizing the system-bath coupling strength. The parameter $\kappa$ is a characteristic of the bath with units of $\omega^{-3}$ such that $\int_0^\infty d\omega I(\omega)/\pi = N$. In order to use Eq. (2.4), we construct $Z_{\mathcal{AB}}(i\tau)$ of the QBM model by analytical continuation of the Matsubara frequencies $\nu_n = \frac{2\pi n}{\hbar i\tau}$ from the known result [46], to get

$$Z_{\mathcal{AB}}(i\tau) = Z_{\mathcal{B}}(i\tau)\frac{1}{\hbar i\tau\omega_0}\prod_{n=1}^{\infty}\frac{\nu_n^2(\omega_D+\nu_n)}{(\omega_0^2+\nu_n^2)(\omega_D+\nu_n)+\nu_n\gamma\omega_D}. \tag{2.18}$$

Here the imaginary temperature partition function $Z_{\mathcal{B}}(i\tau)$ of $\mathcal{B}$, using the spectral density from Eq. (2.17a), reads

$$\log Z_{\mathcal{B}}(i\tau) = -i\tau E_0 + \frac{2\kappa\zeta(4)}{(\hbar i\tau)^3}, \tag{2.19}$$

where $E_0 = 3\kappa\hbar\omega_D^4$ is the zero point energy of the bath, and $\zeta(x)$ is the Riemann zeta function. In this way we arrive at

$$\log Z_{\mathcal{AB}}(i\tau) = \log Z_{\mathcal{B}}(i\tau) + \log\tilde{Z}(i\tau), \tag{2.20}$$

where the effective $\tilde{Z}$, related to the coupled harmonic oscillator, has an explicit form in terms of Gamma functions $\Gamma$ [46],

$$\tilde{Z}(i\tau) = \frac{\hbar i\tau\omega_0\Gamma(\hbar i\tau\lambda_1/2\pi)\Gamma(\hbar i\tau\lambda_2/2\pi)\Gamma(\hbar i\tau\lambda_3/2\pi)}{4\pi^2\Gamma(\hbar i\tau\omega_D/2\pi)}, \tag{2.21}$$

with $\lambda_1, \lambda_2$ and $\lambda_3$ being the roots of the polynomial expression in $\nu_n$ that appears in the denominator of Eq. (2.18), and carry the dependence on $\gamma, \omega_D$ and $\omega_0$.

Interestingly, as shown in [73], for systems that have an interaction that involves only relative coordinates, like in Eq. (2.16), the *classical* partition function does not depend at all on the coupling

$$\log Z^{\text{classic}}_{\mathcal{AB}}(i\tau) = \log Z^{\text{classic}}_{\mathcal{B}}(i\tau) + \log Z^{\text{classic}}_{\mathcal{A}}(i\tau),$$

and therefore the temperature $\beta$ is independent of $\gamma$, regardless how strong the interaction is. This means that for the model in Eq. (2.16) *the dependence of the temperature on the coupling strength is a purely quantum effect.*

Before going further we make an important remark. Since our model consists of a single harmonic oscillator (system $\mathcal{A}$) linearly coupled to many harmonic oscillators (system $\mathcal{B}$), we find here the situation where the SPA analysis requires $\nu_{\mathcal{A}} = 0$ as discussed in the last part of section 2.2. Since the function $\tilde{Z}$ in Eq. (2.20) encloses the effect of both the single harmonic oscillator plus interaction terms, we must subtract from Eq. (2.20) the term $\log Z_{\mathcal{A}}(i\tau)$ due to the bare central oscillator, meaning that we are considering $Z_{\mathcal{A}}(i\tau)$ smooth enough not to let it participate in the SPA analysis of Eq. (2.4).

With this in mind we now use Eqns. (2.4, 2.19, 2.20) to identify the action

$$\phi(i\tau) = i(E - E_0)\tau + \frac{2\kappa\zeta(4)}{(\hbar i\tau)^3} + \log \tilde{Z}(i\tau) - \log Z_{\mathcal{A}}(i\tau). \tag{2.22}$$

Solving the integral in Eq. (2.4) by SPA, using the saddle-point condition in Eq. (2.6), and again, looking for real solutions $\beta = i\tau^*$, we get

$$\begin{aligned} E - E_0 - \frac{6\kappa\zeta(4)}{\hbar^3}\frac{1}{\beta^4} = \frac{1}{\beta} - \frac{\hbar\omega_0}{2}\coth\Big(\frac{\beta\hbar\omega_0}{2}\Big) \\ + \frac{\hbar}{2\pi}\left\{\omega_D\psi(1+\hbar\beta\omega_D/2\pi) - \sum_{i=1}^{3}\lambda_i\psi(1+\hbar\beta\lambda_i/2\pi)\right\}, \end{aligned} \tag{2.23}$$

where we have inserted Eq. (2.21) into (2.22). Note the subtracted energy of the bare oscillator $\frac{\hbar\omega_0}{2}\coth\Big(\frac{\beta\hbar\omega_0}{2}\Big)$. Here $\psi(x) = \frac{d}{dx}\log\Gamma(x)$ denotes the Digamma function. Equation (2.23) establishes the equilibrium relation for the total energy $E$ between system $\mathcal{B}$ and the interaction energy, where the *l.h.s* is related with the energy of the bath and the *r.h.s* accounts for the energy of interaction. In the regime where $\gamma = 0$ the *r.h.s* of Eq. (2.23) is zero. In this case the derived temperature is given by the bath. This is the common scenario in the weak-coupling canonical approach, where the central system acquires a temperature given by the constant temperature of the canonical thermal bath. We will show that an interaction term that couples linearly the system with each degree of freedom of the bath gives rise to an interaction energy which affects the resulting equilibrium temperature. The divergences affecting Eq. (2.23) for $\omega_D \to \infty$, arise from the well known [74] divergences of the ground state energy of the coupled harmonic oscillator $\epsilon_0$,

$$\epsilon_0 = \frac{\hbar}{2\pi}\left[\lambda_1\log[\omega_D/\lambda_1] + \lambda_2\log[\omega_D/\lambda_2] + \lambda_3\log[\omega_D/\lambda_3]\right], \tag{2.24}$$

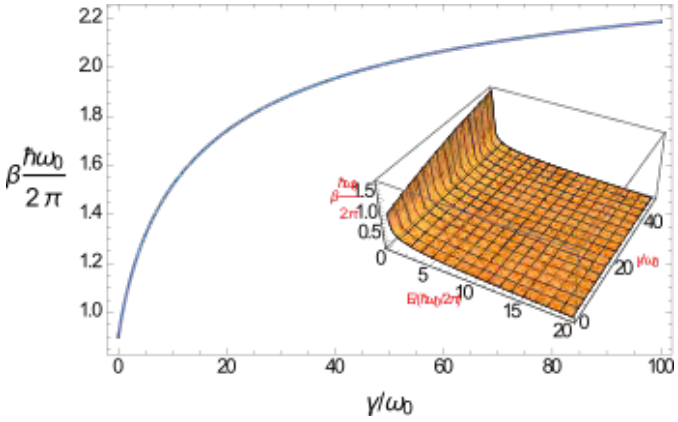


Figure 2.4: Inverse temperature $\beta(\gamma)$ for given values $\kappa\omega_0^3 = 5$, $\omega_D/\omega_0 = 10$, and $E/\left(\frac{\hbar\omega_0}{2\pi}\right) = 0.2$, showing the increase of $\beta$ with $\gamma$ near the ground state energy. Inset shows the variation of $\beta(E,\gamma)$ for a large range of energies, showing a monotonic decrease with $E$.

but are readily renormalized by redefining $\tilde{Z} \to \tilde{Z} \times e^{\beta\epsilon_0}$ to obtain a global zero ground state energy. The new relation Eq. (2.23) for renormalized energy finally reads

$$\begin{aligned} E - \frac{6\kappa\zeta(4)}{\hbar^3}\frac{1}{\beta^4} = \frac{1}{\beta} &+ \frac{\hbar}{2\pi}\left\{\omega_D\psi(1+\hbar\beta\omega_D/2\pi) - \omega_D\log\omega_D\right\} \\ &- \frac{\hbar}{2\pi}\sum_{i=1}^{3}\left(\lambda_i\psi(1+\hbar\beta\lambda_i/2\pi) - \lambda_i\log\lambda_i\right) \\ &- \frac{\hbar\omega_0}{2}\coth\left(\frac{\beta\hbar\omega_0}{2}\right) + \frac{\hbar\omega_0}{2}, \end{aligned} \tag{2.25}$$

where we have made use of the Vieta relation $\lambda_1 + \lambda_2 + \lambda_3 = \omega_D$ [46]. The solution of Eq. (2.25) for $\beta$ (fixing the energy equilibrium condition for our model) accordingly defines the inverse temperature in the finite coupling regime. This solution $\beta(E,\gamma)$, our main result, depends on the interaction $\gamma$, the total energy $E$, but also the bath parameters $\kappa$ and $\omega_D$.

Coming back to the issue of SPA vs weak coupling expansions, we stress again that in a model where the total energy $E$ scales with the number of particles $N$, in solving Eq. (2.4) by SPA we are neglecting terms of $\mathcal{O}(1/\sqrt{N})$, which is justified in the thermodynamic limit for large number of particles [71]. Still, the SPA approximation does not depend on any perturbative expansion of the interaction parameter $\gamma$ and thus our results are valid beyond the weak-coupling limit.

In Fig. 2.4 we show the numerical solution $\beta(E,\gamma)$ of Eq. (2.25) for given values of $\kappa$ and $\omega_D$ and for energy near the renormalized ground state, where quantum effects are more visible. A clear variation of the temperature as a function of $\gamma$ is observed, showing that the interaction energy has a sensible effect in the derived temperature. In the inset of Fig. 2.4 can be observed that $\beta$ is a monotonous function of the total energy $E$. From

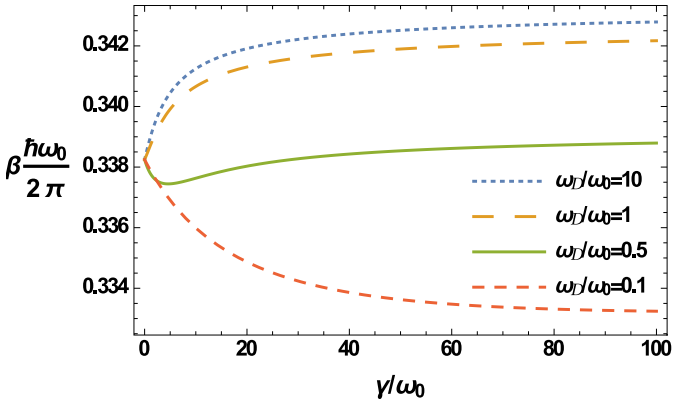


Figure 2.5: $\beta(\gamma)$ for parameters $\kappa\omega_0^3 = 5$ and $E/\left(\frac{\hbar\omega_0}{2\pi}\right) = 10$, showing the increasing of $\beta$ in the Markovian regime and its change of behavior in the non-Markovian case.

Eq. (2.25), and using the asymptotic expansion of Digamma functions, we obtain that for $\beta \to \infty$, $E \to 0$, as expected.
For large energies the change of $\beta$ with $\gamma$ is less evident, but still can be appreciated in Fig. 2.5. Remarkably in this regime the behavior of $\beta$ with $\gamma$ is strongly affected by the tunning parameter $\omega_D/\omega_0$, that also quantifies the degree of memory of the bath or non-Markovianity [75]. This surprising connection between the dependence of the temperature on the coupling and the time scale $2\pi/\omega_D$ associated to memory effects in the environment is also shown by the explicit dependence of $\beta$ on the Drude frequency in Fig. 2.6.

We can provide a physical interpretation of the peculiar dependence of $d\beta/d\gamma$ on the Drude frequency $\omega_D$ for our results in the following way. In the *Markovian regime* Fig. 2.5 suggest that the action from the bath on the central system mostly determines the energy equilibrium condition: the energy-flow follows the natural direction from bath to system to reach equilibrium. Moreover, it can be shown that the *r.h.s* of (2.25) grows with $\gamma$ in this regime. That explains the growing behavior of $\beta$ with $\gamma$ in this case. On the other hand, in the *non-Markovian regime* Fig. 2.5 suggest that is the action from the system on the bath which determines the equilibrium condition: in this case the direction of energy-flow goes from system to bath. It can be shown as well that the contribution of the *r.h.s* of (2.25) in this case follows a decreasing or increasing behavior as a function of $\gamma$, depending on the particular range of values of $\omega_D/\omega_0$ within the non-Markovian regime. This is reflected in the peculiar behavior appearing in Fig. 2.5. We want to emphasize that the results obtained here go beyond any finite-order expansion around the weak-coupling scenario. Fig. 2.7 shows the contrast between the solution for temperature obtained in the first order expansion for $\gamma$ in Eq. (2.25) and that obtained from the full expression. The characteristic saturation behavior clearly indicates the breakdown of any finite-order approximation in powers of $\gamma$.

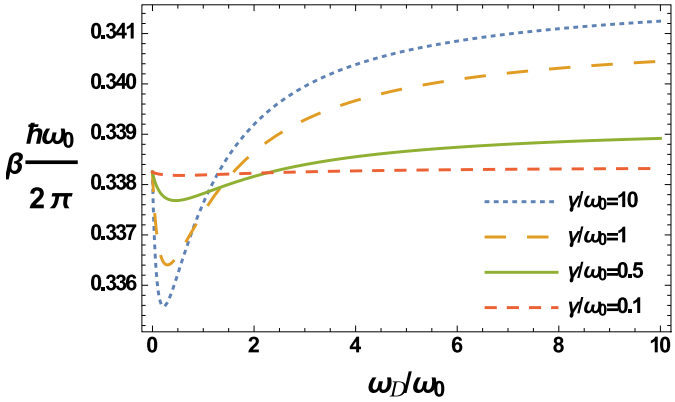


Figure 2.6: $\beta(\omega_D)$ for parameters $\kappa\omega_0^3 = 5$ and $E/\left(\frac{\hbar\omega_0}{2\pi}\right) = 10$, showing the explicit dependence of $\beta$ with the Drude frequency and its change of behavior from Markovian to non-Markovian regime.

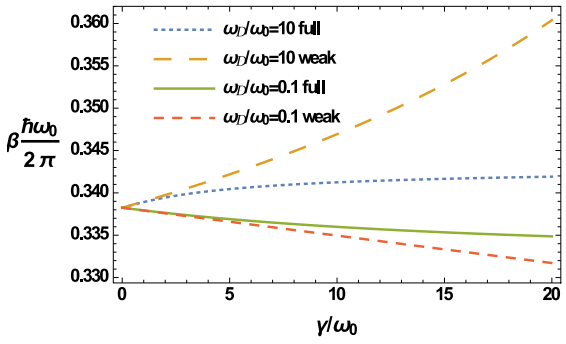


Figure 2.7: Contrast between the temperature solution at first order expansion in $\gamma$ and the full results, showing the characteristic saturation behavior of the full result in contrast with the first order perturbative expansion in $\gamma$.

## 2.4. Microcanonical thermodynamic relations and ensemble equivalence

After having obtained the inverse temperature $\beta(E,\gamma)$ as a function of the energy and the finite coupling strength, we can calculate thermodynamic potentials in the finite-coupling regime. We start with Eq. (2.10), from which the entropy of the global system in the limit $N \to \infty$ can be calculated by

$$\log Z_{\mathcal{AB}}(\beta) = S(E)/K - \beta E. \tag{2.26}$$

Recognizing that $\beta(E,\gamma)$ is a function of $E$, we get

$$\frac{1}{K}\frac{\partial S}{\partial E} = \beta + \frac{\partial \beta}{\partial E}\left(E + \frac{\partial}{\partial \beta}\log Z_{\mathcal{AB}}\right), \tag{2.27}$$

and since $\frac{\partial}{\partial \beta}\log Z_{\mathcal{AB}} = -E$, we finally obtain the thermodynamic relation

$$\frac{1}{K}\frac{\partial S}{\partial E} = \beta(E,\gamma). \tag{2.28}$$

Following Ref. [76] we may also calculate the entropy for the coupled oscillator as

$$\frac{S_{\mathcal{A}}}{K} = \log \tilde{Z}(\beta) - \beta\frac{\partial}{\partial \beta}\log \tilde{Z}(\beta), \tag{2.29}$$

where the dressed partition function $\tilde{Z}$ is taken from Eq. (2.21) and evaluated at the solution $\beta(E,\gamma)$ given by the SPA condition. The term $-\frac{\partial}{\partial \beta}\log \tilde{Z}(\beta)$ is the thermodynamic mean energy of the coupled oscillator evaluated at $\beta(E,\gamma)$. Figure 2.8 illustrates the behavior of $S_{\mathcal{A}}$ as a function of the total energy $E$ for various values of the coupling $\gamma$. As can be observed, $S_{\mathcal{A}}$ is a positive quantity that becomes zero for $E = 0$, in nice accordance with the third law of thermodynamics. The entropy is also a monotonically increasing function of $E$ and $\gamma$. This latter feature accounts for the decrease in purity of the reduced density matrix $\mathrm{Tr}_{\mathcal{B}}\ \hat{\rho}_{\mathcal{AB}}$ with increasing $\gamma$.

Finally, let us consider the finite-coupling version of the ensemble equivalence. Whenever the solution of the integral in Eq. (2.13) is justified by SPA, the saddle-point condition will give a relation between the expectation value of any smooth operator calculated in the microcanonical ensemble and the one evaluated in the canonical case, *but for a temperature given by the solution $\beta(E,\gamma)$ in the finite-coupling regime.* The same considerations also hold for the reduced density matrix describing the subsystem $\mathcal{A}$ and, in that case, the relation for the expectation value of an observable $\hat{O}_{\mathcal{A}}$ is given as

$$\langle \hat{O}_{\mathcal{A}} \rangle_E \approx \langle \hat{O}_{\mathcal{A}} \rangle_{\beta(E,\gamma)}\,, \tag{2.30}$$

providing the sought extension of the equivalence of ensembles for systems with finite-coupling, in the thermodynamic limit. Accordingly, in Fig. 2.9 we show the expectation value for the squared position operator of the coupled oscillator evaluated at the solution

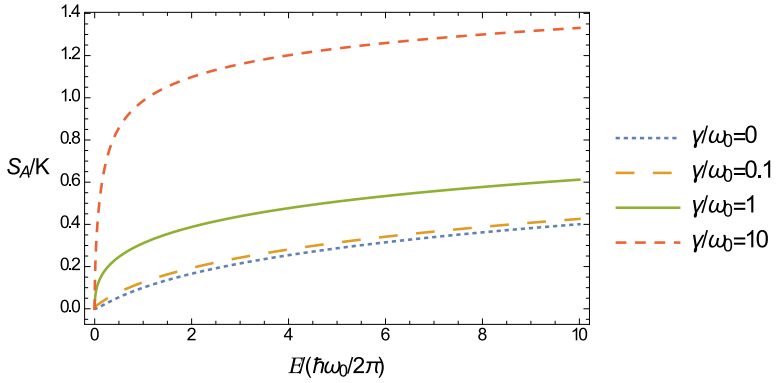


Figure 2.8: Subsystem entropy $S_{\mathcal{A}}(E,\gamma)$ for parameters $\kappa\omega_0^3 = 5$ and $\omega_D/\omega_0 = 10$. The entropy of the subsystem $\mathcal{A}$ is parametrically larger when the system-depended damping $\gamma$ is large and also increases with the energy, and becomes zero for $E = 0$, in accordance with the laws of thermodynamics.

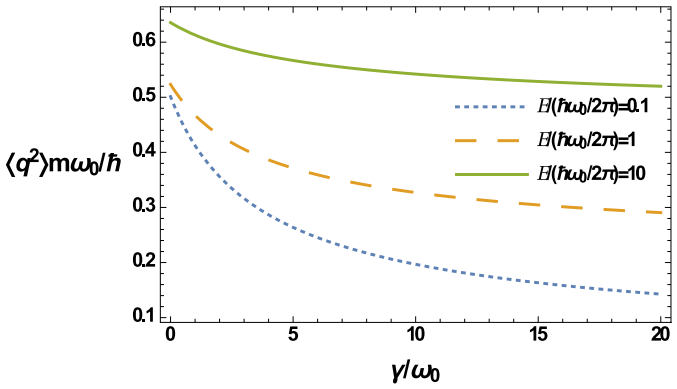


Figure 2.9: $\langle q^2\rangle(\gamma)$ for parameters $\kappa\omega_0^3 = 5$ and $\omega_D/\omega_0 = 10$. As expected the particle gets more localized with increasing $\gamma$ and its squared position expectation value increases with $E$.

$\beta(E,\gamma)$. As expected $\langle q^2 \rangle$ grows with the energy $E$ and the particle is getting more localized with the increase of the damping parameter $\gamma$, as the bath monitors the position of the central particle [77].

It is interesting to note that a similar behavior of the entropy and the expectation value of the squared position with respect to $\gamma$ in the QBM model is found in the canonical thermal bath approach [46, 76]. This is actually a non-trivial result due to the fact that our microcanonical thermodynamics is based on $\beta(E,\gamma)$, which is a SPA condition solution that involves $\gamma$. One could imagine a situation where an observable in Eq. (2.13) has a non-smooth dependence with the integration variable $\tau$, and therefore this dependence must be included in the SPA condition. In such scenario the equilibrium temperature becomes itself a function of the particular observable and our notion of ensemble equivalence must be accordingly modified.

## 2.5. Summary

In this chapter, starting from the fundamental microcanonical distribution, we have studied the emergence of temperature $T$ in the finite coupling regime of open quantum systems. Following the approach pioneered by Schwinger, resulting in $T = T(E)$ as an emergent quantity that establishes the condition of equilibrium between two weakly coupled subsystems at energy $E$, we have shown that in the finite and strong coupling regime, $T = T(E,\gamma)$ also depends on the parameter $\gamma$ that characterize the strength of the interaction. We have applied this idea to the paradigmatic Quantum Brownian Motion model and studied the main features of this notion of temperature, confirming that $T(E,\gamma)$ is a monotonically increasing function of the total energy $E$, and showing a clear variation of $T$ with $\gamma$, which is a purely quantum effect particularly visible near the ground state energy. The entropy of the coupled oscillator, which now depends on $\gamma$, is a positive quantity that starts from zero for $E = 0$ and increases monotonically with $E$ and $\gamma$. Remarkably, we found also, for large energies, an unexpected dependence on the memory properties of the bath: while $T(E,\gamma)$ decreases as a function of the interaction parameter $\gamma$ in the Markovian regime, the behavior is more complex in the non-Markovian case.

# 3. Semiclassical treatment of decoherence in chaotic systems

In this chapter we will explore the effect of decoherence in the semiclassical limit on a system with classically chaotic dynamics. As shown in chapter 1, decoherence is a purely quantum phenomenon due to the effect of *delocalization* of local quantum correlations when a system is coupled to a large environment. On the other hand, a system with classically chaotic behavior experiences universal properties that enable us to construct systematically quantum corrections to the diagonal approximation given in Eq. (1.26), and in this way, allow us to study quantum corrections on a system subject to decoherence. We will see that in order to make these corrections visible we need to let the system itself experience coherent effects by, for example, inserting the system initially inside an open cavity from which it may scape, and measuring only local observables within the cavity. We find that the competing effects of interference and decoherence lead to a universal non-monotonous form for the survival probability depending only on the universality class, coupling strength and macroscopic parameters of the cavity.

In section 3.1 we will review some important concepts and tools related with the semiclassical quantum corrections in a system with classically chaotic limit. Section 3.2 is devoted to study the interplay between coherent and decoherence effects in a chaotic system, starting with the general aspects of decoherence due to the coupling of a particle to a bath reservoir within the Caldeira-Leggett model, as already shown in chapter 1. Then we review the main features of the quantum survival probability, which involves a scenario where the particle is inside a cavity from which it may escape. At the end of the section the main technical aspects of this chapter is presented, where we develop the semiclasscial treatment of the particle inside a cavity coupled to a bath, and study the first quantum correction to the evolution of the Wigner function, in the semiclassical limit. Finally, we provide some concluding remarks in section 3.3. For the main aspects of this chapter, starting from section 3.2, we follow closely our manuscript in [25][1].

## 3.1. Classical chaos and Sieber-Richter orbit pairs

From the vast literature in chaotic systems (see for example [37, 78–80]), here we only mention some properties useful to understand the quantum correction for correlated trajectories applied in the next sections. We consider classical Hamiltonian dynamics in $d$-dimensions. That is, given a point in phase-space

$$\mathbf{x} = (\mathbf{q}, \mathbf{p})^T, \tag{3.1}$$

[1] ©[2021] American Physical Society.

with dimension $2d$, its time evolution is given by a Hamiltonian $H\big(\mathbf{x}(t),t\big)$, according to

$$\dot{\mathbf{x}}(t) = \Sigma\Big[\frac{\partial H}{\partial \mathbf{x}}\big(\mathbf{x}(t),t\big)\Big]^T, \tag{3.2}$$

with the symplectic matrix $\Sigma = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Each phase-space trajectory is uniquely determined by an initial condition $\mathbf{x}_0 = (\mathbf{q}_0, \mathbf{p}_0)^T$, such that $\mathbf{x}(t) = \mathbf{x}(t; \mathbf{q}_0, \mathbf{p}_0)$.
A main attribute of chaotic systems is its exponentially sensitive dependence on initial conditions. Let us assume two nearby initial points in phase-space $\mathbf{x}_0$ and $\mathbf{x}_0' = \mathbf{x}_0 + \delta\mathbf{x}_0$. At time $t$, under the Hamiltonian evolution, the separation between the two trajectories is given by $\delta\mathbf{x}(t) = \mathbf{x}(t) - \mathbf{x}'(t)$. In the limit of small initial separation $\delta\mathbf{x}_0$ and long times, there is at least one direction in which a chaotic system displays exponential separation of trajectories

$$\delta\mathbf{x}(t) \sim \mathrm{e}^{\lambda(\mathbf{x}_0, \delta\mathbf{x}_0)t}\delta\mathbf{x}_0, \tag{3.3}$$

where $\lambda(\mathbf{x}_0, \delta\mathbf{x}_0) > 0$ is called the Lyapunov exponent in the given direction. [2] The direction in which the separation grows exponentially is called *unstable*. For autonomous Hamiltonian systems the phase-space volume is conserved (usually constrained to a sub-manifold of phase-space with constant energy), and then for each direction with positive Lyapunov exponent $\lambda$ there is always a direction of negative grow $-\lambda$. This direction is called *stable*, while along $\lambda = 0$ is known as neutral direction. On every point along a trajectory we can then place a local coordinate system spanned by unit vectors $\hat{e}_i$ pointing along the stable, unstable and neutral directions, with $i = 1, 2, ..., 2d$, as depicted in Fig. 3.1. In particular, the stable and unstable manifolds are sub-manifolds of phase-space containing all points $\mathbf{x}$ whose trajectories starting at $\mathbf{x}_0$ converge (stable) or diverge (unstable) to each other, in the limit of long times $t \to \infty$. If it is possible to build a local coordinate with non-vanishing stable and unstable directions for almost every point in the available phase-space, the dynamics is called *hyperbolic* [81]. This property enable us to build families of correlated trajectories, which is a key ingredient in the Sieber-Richter orbit pairs construction we will discuss soon.

Likewise, a key property of chaotic systems is *ergodicity*: if given enough time, a typical trajectory will approach arbitrarily close any point in the available phase-space. Thus, in the limit of long times, a time-average of a function of the trajectory will be equal to a phase-space average of the function

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T dt\; f(\mathbf{x}(t;\mathbf{x}_0)) = \frac{1}{\Omega}\int d^{2d}x\; f(\mathbf{x}), \tag{3.4}$$

where $\Omega$ is the volume of the available phase-space of the system.

*Sieber-Richter orbit pairs.* Exponential sensitivity under small changes on initial conditions, being a hallmark of chaos which implies almost impossible long-term predictions,

[2] Throughout this chapter we will consider only systems with a uniform Lyapunov exponent $\lambda$ in the available phase-space.

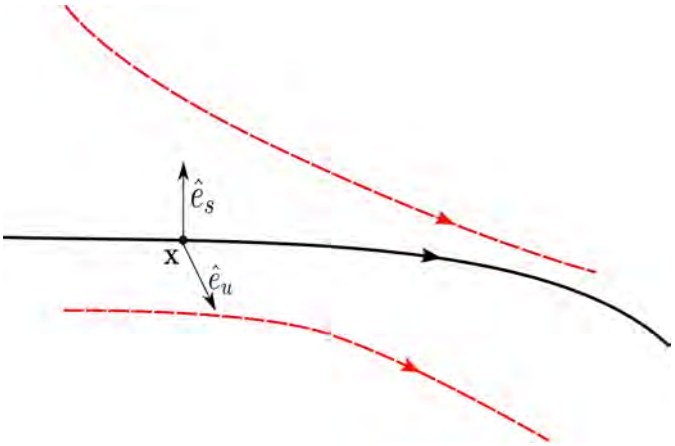


Figure 3.1: Illustration of a point $\mathbf{x}$ on a trajectory in phase-space where a local coordinate system is displayed, with stable and unstable directions. Along the unstable direction $\hat{e}_u$, nearby trajectories (dashed-lines) tend to separate apart with exponential growth, while along the stable direction $\hat{e}_s$, a nearby trajectory approaches the original one exponentially, for long times. Along the trajectory there is a neutral direction. The arrows show the direction of time.

has nevertheless a beautiful and very useful consequence: instability of trajectories depending on the initial value problem implies *exponential stability* of the *boundary value* problem [82]. This means that for a given trajectory, with specific initial and final position, but not specific momentum, a small perturbation of the endpoints will create a new trajectory which approaches exponentially close the original one during the given time span $t \gg 1/\lambda$. This stability condition requires the dynamic to be hyperbolic, and as a consequence, trajectories of a chaotic system tend to form *families* or bunches in phase-space. In each family, trajectories are hardly distinguishable if a weak-resolution or coarse-grained process is assumed, and therefore they have arbitrarily small action differences. Each family can then be in principle specified by a single trajectory, and if the trajectory happens to have *self-crossings* (in configuration-space) during its evolution, the exponential stability guarantees the existence of another trajectory within the family, which differs only by reconnections inside the self-crossing, as shown in Fig. 3.2. This key observation allowed Sieber and Richter [39, 83] to develop a theory of pairs of correlated trajectories differing inside the *encounter* region, where the self-crossing appears, yielding small action difference, which was decisive to understand universal energy spectral fluctuations [84–86], and universal features in quantum transport [87] [88].

Figure. 3.2 illustrates a typical Sieber-Richter orbit pair $(\gamma, \gamma')$ which differs in a so-called 2-encounter region. The trajectory $\gamma'$ has a small-angle self-crossing in configuration space, and its correlated partner $\gamma$ displays an *avoiding* crossing, where the two *stretches* of the trajectory remain very close to each other along the encounter. Outside the encounter (in the *links*) the pair of trajectories are exponentially close, but after leaving the encounter, one trajectory follows the time-reversed path of the other,

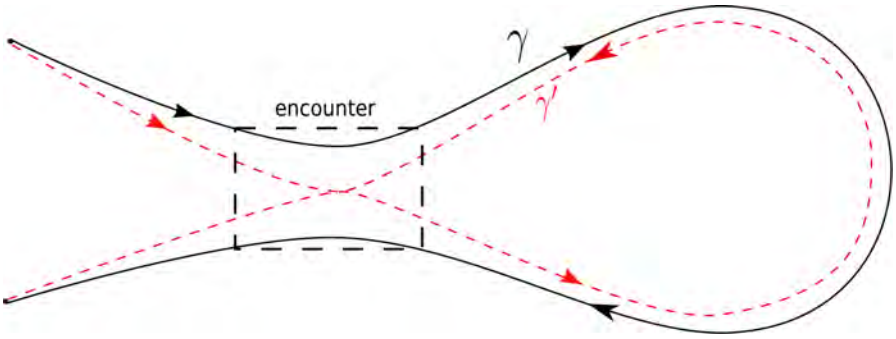


Figure 3.2: A typical Sieber-Richter pair of trajectories. The $\gamma'$ trajectory has a self-crossing in configuration space, and its partner $\gamma$ displays an avoiding crossing, where the two stretches of the trajectory remain very close, defining an encounter region. On the right, the two trajectories form a loop, one following the time-reversed path of the other. This figure is for a system with $d = 2$, and time-reversal symmetry. The picture is in configuration space and the arrows show the direction of momentum.

forming a *loop*, as shown in Fig. 3.2. The existence of this configuration of correlated trajectories for long times is due to the exponential stability of the boundary problem discussed above. This 2-encounter diagram requires the system to have time-reverse invariance. Families of trajectories with $l$ stretches forming an encounter region may exist, but in this chapter we only consider 2-encounter diagrams with a small action difference $S_\gamma - S_{\gamma'} \sim \mathcal{O}(\hbar)$, because they yield the first-order quantum correction to the diagonal approximation in Eq. (1.26) (see section 1.1.2).

### 3.1.1. Action difference and density of trajectories

To calculate the action difference of a 2-encounter diagram we place a Poincaré surface of section $\mathcal{P}$ (a plane which intersects the trajectory in phase-space transversal to the flow) at any point inside the encounter, as shown in Fig. 3.3 (for a more detailed discussion, see [78]). The trajectory $\gamma$ first reaches $\mathcal{P}$ at time $t'$ and then, after leaving the encounter, forms a loop and returns back to the encounter, reaching again $\mathcal{P}$ a second time at $t''$. Let us assume for simplicity, and according to the systems we will study in the next sections, $d = 2$, but the main idea holds also for higher dimensions. Given hyperbolicity, $\mathcal{P}$ is spanned by one stable $\hat{e}_s$ and one unstable $\hat{e}_u$ direction. Inside the encounter the two trajectories $\gamma, \gamma'$ are different form each other, but remain close. In this region we can describe one trajectory in terms of a local coordinate system localized on the other trajectory. As shown in Fig. 3.3, we select a reference point in phase-space $\mathbf{x}_\gamma$ at time $t'$ and construct a local coordinate system $(s, u)$, based on the stable and unstable local manifold, where $t_u$ is the time trajectory $\gamma'$ needs to leave the encounter (to escape the linearized regime) in the unstable direction, and in a similar way is defined $t_s$ along the stable direction. In this way the whole trajectory is divided into four parts: three links and the encounter region. Outside the encounter, in the links, $\gamma$ and $\gamma'$ are exponentially

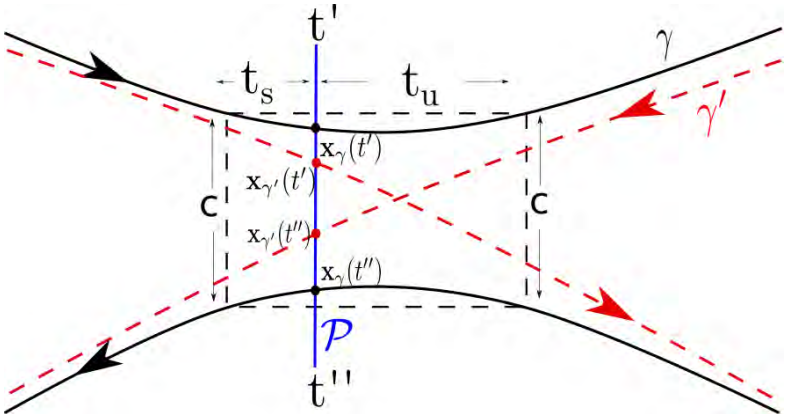


Figure 3.3: A Poincaré surface of section $\mathcal{P}$ is placed inside the encounter, and there we select a reference point in phase-space $\mathbf{x}_\gamma(t')$ of the trajectory $\gamma$, when it first reaches $\mathcal{P}$ at time $t'$. A local reference frame is constructed at this point with $(s, u)$ the local stable and unstable manifold. Using this frame, the trajectory $\gamma'$ can be described within the linerized regime inside the encounter.

close and the action difference vanishes. In the second link, there is a loop in which $\gamma$ and $\gamma'$ have switched partners, and then one trajectory follows the time-reversed path of the other. The time the first stretch needs to travel the encounter is denoted $t_{\text{enc}}$, and is given by $t_{\text{enc}} = t_u + t_s$, and the duration of the loop is called $t_{\text{loop}}$. Having fixed the point $\mathbf{x}_\gamma(t')$, the phase-space location of $\mathbf{x}_\gamma(t'')$ on the second stretch is given by

$$\mathcal{T}\mathbf{x}_\gamma(t'') - \mathbf{x}_\gamma(t') = s\hat{e}_s(\mathbf{x}_\gamma(t')) + u\hat{e}_u(\mathbf{x}_\gamma(t')), \tag{3.5}$$

where $\mathcal{T}$ is the time-reverse operator, which reverses the direction of momentum. When $\mathcal{P}$ is moved along the encounter, the components $u$ and $s$ will change according to Eq. (3.3), stretching and shrinking in the unstable and stable direction respectively. However, due to the symplectic structure of the Hamiltonian flow [78], the symplectic surface element $\Delta S$ remains constant

$$\Delta S = su. \tag{3.6}$$

Thus the exact location of the reference point inside the encounter is irrelevant. This invariant surface element determines the properties of the encounter region. We need to introduce a small constant bound $c > 0$, as shown in Fig. 3.3, which determines the maximum value of the components $s$ and $u$ before leaving the linearized regime

$$|s|,\ |u| \leq c. \tag{3.7}$$

With this considerations the duration of the encounter stretch is given by

$$t_{enc}(s,u) = t_u + t_s = \frac{1}{\lambda}\log\frac{c}{|u|} + \frac{1}{\lambda}\log\frac{c}{|s|} = \frac{1}{\lambda}\log\left(\frac{c^2}{|s||u|}\right), \tag{3.8}$$

which is then determined by the symplectic surface $\Delta S$.

In a similar way we can specify the partner orbit $\gamma'$ inside the encounter from the reference point. The first stretch of $\gamma'$ traverse now the encounter with exponentially growing separation from the first stretch of $\gamma$, and the second stretch of $\gamma'$ approaches exponentially the second stretch of $\gamma$, as can be seen in Fig. 3.3. Then in the $(u, s)$ basis we can write

$$\mathbf{x}_{\gamma'}(t') = \begin{pmatrix} u \\ 0 \end{pmatrix}, \ \mathcal{T}\mathbf{x}_{\gamma'}(t'') = \begin{pmatrix} 0 \\ s \end{pmatrix}. \tag{3.9}$$

To calculate the action difference $S_\gamma - S_{\gamma'}$ accumulated inside the encounter it is convenient to imagine each trajectory has fixed energy $E$, which is the energy of the submanifold of the available phase-space. The details of the calculation can be found in [78]. Here we only sketch the main idea.

The action evaluated along a path from an initial position $\mathbf{q}'$ to a final position $\mathbf{q}$ during a time span $t$ (see Eq. (1.8)), can be transformed into an action evaluated for paths with fixed energy $E$ between the same endpoints, according to

$$S_0(\mathbf{q}, \mathbf{q}', E) = S(\mathbf{q}, \mathbf{q}', t) + Et, \tag{3.10}$$

where to define the energy-dependent action, the time argument has to be fixed such that

$$\frac{\partial}{\partial E} S_0(\mathbf{q}, \mathbf{q}', E) = t(\mathbf{q}, \mathbf{q}', E). \tag{3.11}$$

Starting at an arbitrary point $\mathbf{q}', \mathbf{p}'$, where $\mathbf{p}' = -\frac{\partial}{\partial \mathbf{q}'} S_0$, the increment along the path is given by $dS_0(\mathbf{q}, \mathbf{q}', E) = \mathbf{p} \cdot d\mathbf{q}$. The momentum becomes a function of the position, and in this way the action along the trajectory is given by

$$S_0 = \int \mathbf{p} \cdot d\mathbf{q}. \tag{3.12}$$

Now the idea is to select two exponentially close points in configuration space $\mathbf{q}'_\gamma$ and $\mathbf{q}'_{\gamma'}$, on the left link in Fig. 3.3, and evaluate the action difference using Eq. (3.12). First we can calculate the accumulated action from a piece of trajectory ending at the Poincaré plane (see Fig. 3.3): from $\mathbf{q}'_\gamma$ to $\mathbf{q}_\gamma(t')$ and from $\mathbf{q}'_{\gamma'}$ to $\mathbf{q}_{\gamma'}(t')$. Assuming the initial points are exponentially close, the action difference reads

$$\begin{aligned} S_\gamma - S_{\gamma'} &\approx \int_{\mathbf{q}'_\gamma}^{\mathbf{q}_\gamma(t')} d\mathbf{q} \cdot \mathbf{p}(\mathbf{q}, \mathbf{q}'_\gamma) - \int_{\mathbf{q}'_\gamma}^{\mathbf{q}_{\gamma'}(t')} d\mathbf{q} \cdot \mathbf{p}(\mathbf{q}, \mathbf{q}'_\gamma) \\ &= \int_{\mathbf{q}_{\gamma'}(t')}^{\mathbf{q}_\gamma(t')} d\mathbf{q} \cdot \mathbf{p}(\mathbf{q}, \mathbf{q}'_\gamma), \end{aligned} \tag{3.13}$$

where to obtain the second line a contour integral along an arbitrary path from $\mathbf{q}_{\gamma'}(t')$ to $\mathbf{q}_\gamma(t')$ was used, due to the fact that $\mathbf{p}(\mathbf{q}, \mathbf{q}'_\gamma)$ is a unique function of $\mathbf{q}$. That path can be selected to run in $\mathcal{P}$ and, as shown in Fig. 3.4, it runs along the unstable axes. It is not difficult to show that similar calculations along the complete trajectories give a total accumulated action difference which equals the closed contour integral in $\mathcal{P}$

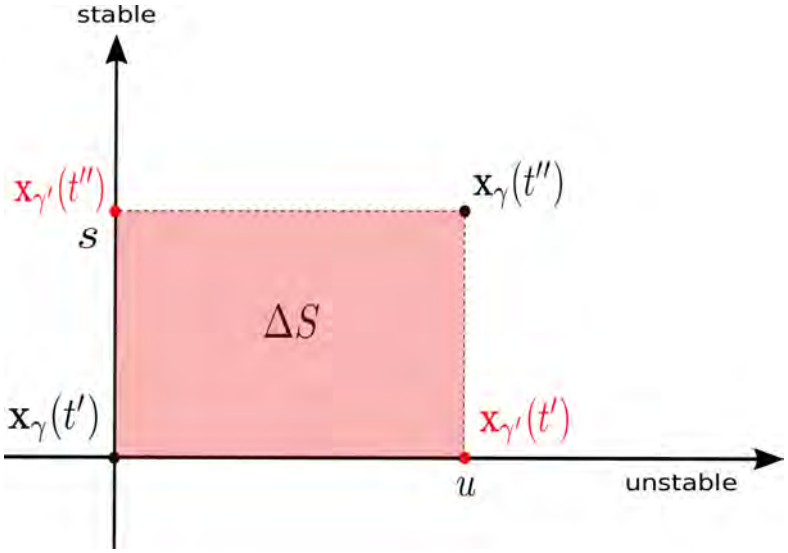


Figure 3.4: A local Poincaré plane is spanned by the stable and unstable directions. The plane is pierced by the pair of trajectories at points $\mathbf{x}_\gamma(t'), \mathbf{x}_{\gamma'}(t'), \mathbf{x}_\gamma(t'')$ and $\mathbf{x}_{\gamma'}(t'')$, forming a parallelogram whose area is the invariant symplectic surface $\Delta S = su$. This surface turns out to be the total action difference between the pair of trajectories.

$$S_\gamma - S_{\gamma'} = \oint d\mathbf{q} \cdot \mathbf{p}, \tag{3.14}$$

which is an integral around the parallelogram shown in Fig. 3.4. In this way the total action difference is then equal to the area of this parallelogram, giving finally

$$S_\gamma - S_{\gamma'} = \Delta S = su, \tag{3.15}$$

yielding the canonically invariant surface given in Eq. (3.6).

The final ingredient to characterize Sieber-Richter orbit pairs is the *density* of trajectories with a 2-encounter and action difference $\Delta S = su$. We need to calculate the expected number of close 2-encounters in a typical long trajectory. To this end, let us consider the probability that, given a trajectory which pierces a Poincaré surface in a point at some time $\tau$, then $\mathcal{P}$ contains a second piercing of the trajectory with separation $(ds, du)$, during a time interval $\tau + d\tau$, calculated from the initial piercing point. Due to ergodicity, and the fact that for a long trajectory of time $t$, the second piercing is statistically independent of the first, this probability is uniform, and is given by $dsdud\tau/\Omega(E)$, where $\Omega(E) = \int d\mathbf{Q}d\mathbf{P}\delta(E - H_{\mathcal{A}}(\mathbf{Q}, \mathbf{P}))$ is the volume of the energy shell of energy $E$. The expected number of such piercings through a given section $\mathcal{P}$ in the time interval $(\tau, \tau + d\tau)$ with components in $(s, s + ds) \times (u, u + du)$ corresponds then to the Liouville measure $1/\Omega$ [78, 89]. Finally, we need to integrate over the piercing time, and due to the fact that the exact location of $\mathcal{P}$ inside the encounter is not important, we also need to integrate over the time $t'$ of the first piercing. Thus, we weight the encounter with its

duration $t_{\rm enc}$ to avoid over-counting, and in this way we arrive at the desired density of 2-encounters for a trajectory of total duration $t$

$$\omega_t(s,u) = \frac{\int dt' \int d\tau}{t_{\rm enc}(s,u)\Omega}. \tag{3.16}$$

This finishes the characterization of 2-encounters of the Sieber-Richter orbit pairs that we will use in the coming sections.

## 3.2. Interplay between coherent and incoherent effects in chaotic systems

The phenomenon of decoherence was studied in chapter 1, where it has been related to the loss of local coherence between states of a system, due to its coupling to many degrees of freedom of an environment. Being a dynamical process, this gradual loss of coherence has been observed already in many experiments [90–93]. In this section we want to study the interplay between coherent effects in a chaotic system and decoherence due to environmental coupling.

The interplay between coherent decaying due to the opening of the system to a coherent continuum (as in scattering systems) and decoherence, (usually modeled by coupling to a large set of uncontrolled degrees of freedom) takes a further twist if one is interested in studying the regime of large systems or high quantum numbers, the so-called mesoscopic regime [94]. In this case, the microscopic description takes advantage of the universal quantum signatures of systems with chaotic classical limit that are explored by means of asymptotic analysis based on path integrals [78]. In this way, the interplay between quantum coherence, decoherence and quantum signatures of chaos is a pillar of modern physics, with broad applications, from the theory of quantum transport [95], to the precise understanding of the quantum-classical transition [7].

In previous works the universal quantum corrections to classical decay in open chaotic systems were computed [36] in the spirit of the semiclassical approach to mesoscopic transport as sketched in the last section. Our objective here is to extend these ideas in a way that addresses the key impact of decoherence. In order to account for the emergence of universal quantum signatures of classically chaotic dynamics, the proper tools are those of semiclassical analysis where quantum phenomena are described in terms of a highly non-trivial use of classical information around classical solutions. Specifically, quantum interference is explained in terms of interfering classical paths, and, as we will show here, its degrading due to decoherence is explained in terms of decoherence functionals evaluated themselves along pairs of classical solutions. A key finding of our analysis is that in the limit of weak-coupling the leading classical contribution to the decoherence processes can be shown to vanish, and therefore all its effects arise from quantum interference, fully captured by the semiclassical theory of correlated solutions to produce universal results.

To start, we first review some aspects of decoherence in the Caldeira-Leggett model and the quantum survival probability, before jumping to the full semiclassical treatment.

### 3.2.1. Decoherence in the Caldeira-Leggett model

For the sake of completeness in this chapter we briefly present the general aspects of the Caldeira-Leggett model already studied in chapter 1, but now for a system with $d = 2$ dimensions, each coupled to an environment of harmonic oscillators. We consider a system $\mathcal{A}$ in two dimensions, each dimension coupled to a $N$-particle environment of harmonic oscillators $\mathcal{E}$. The total Hamiltonian reads

$$\hat{H} = \hat{H}_{\mathcal{A}} + \hat{H}_{\mathcal{E}} + \hat{H}_{\mathcal{AE}}, \tag{3.17}$$

where

$$\hat{H}_{\mathcal{A}} = \frac{\hat{\mathbf{P}}^2}{2m} + \hat{V}(\hat{\mathbf{Q}}) \tag{3.18}$$

is the Hamiltonian of the central system such that $\mathbf{Q} = (Q_1, Q_2)$ and $\mathbf{P} = (P_1, P_2)$. Each degree of freedom is coupled to an identical environment, whose total bare Hamiltonian is $\hat{H}_{\mathcal{E}} = \hat{H}_{\mathcal{E},1} + \hat{H}_{\mathcal{E},2}$, with

$$\hat{H}_{\mathcal{E},i} = \sum_{k=1}^{N} \frac{1}{2}\Big(\hat{p}_{k,i}^2/m_k + m_k\omega_k^2\hat{q}_{k,i}^2\Big), \tag{3.19}$$

for $i = 1, 2$, and $\hat{H}_{\mathcal{AE}}$ the interaction energy between $\mathcal{A}$ and $\mathcal{E}$. We will choose an interaction which couples linearly each position operator of the central system $\hat{\mathbf{Q}}$ with the position operator of each environment mode $\hat{q}_k$, with $k = 1, ..., N$; which reads

$$\begin{aligned}\hat{H}_{\mathcal{AE}} = &-\hat{Q}_1 \otimes \sum_{k=1}^{N} g_{k,1}\hat{q}_{k,1} - \hat{Q}_2 \otimes \sum_{k=1}^{N} g_{k,2}\hat{q}_{k,2} \\ &+\hat{Q}_1^2 \sum_{k=1}^{N} \frac{g_{k,1}^2}{2m_k\omega_k^2} + \hat{Q}_2^2 \sum_{k=1}^{N} \frac{g_{k,2}^2}{2m_k\omega_k^2}.\end{aligned} \tag{3.20}$$

The last term in Eq. (3.20) compensates for the coupled-induced renormalization of the potential. While Eq. (3.20) will in general produce dissipation as well as decoherence on $\mathcal{A}$, in this chapter we will consider the regime of "pure decoherence", neglecting dissipative effects, an approximation that is fully justified due to the vast separation of time scales between these two mechanisms (see Eq. (1.70)). That is, we will be only interested in the decoherence effects that $\mathcal{E}$ produces on the central system. The whole system $\mathcal{A}+\mathcal{E}$ evolves under $\hat{H}$, with the time evolution being described by the associated propagator given by

$$K(\mathbf{Q}_f, \mathbf{q}_f, t; \mathbf{Q}_i, \mathbf{q}_i) = \langle \mathbf{Q}_f, \mathbf{q}_f | \, \mathrm{e}^{-\frac{i}{\hbar}\hat{H}t} \, | \mathbf{Q}_i, \mathbf{q}_i \rangle \,, \tag{3.21}$$

with the vector $\mathbf{q}$ defined as $\mathbf{q} = (q_{1,1}, ..., q_{N,1}, q_{1,2}, ..., q_{N,2})$. In the Feynman path integral approach the propagator has the form

$$K(\mathbf{Q}_f, \mathbf{q}_f, t; \mathbf{Q}_i, \mathbf{q}_i) = \int \mathcal{D}[\mathbf{Q}(s), \mathbf{q}(s)] \mathrm{e}^{\frac{i}{\hbar}R[\mathbf{Q},\mathbf{q}]}, \tag{3.22}$$

which is a path integral over all paths with boundary conditions $\mathbf{Q}_i = \mathbf{Q}(0), \mathbf{Q}_f = \mathbf{Q}(t)$, $\mathbf{q}_i = \mathbf{q}(0), \mathbf{q}_f = \mathbf{q}(t)$, and where $R$ is the total action $R = R_{\mathcal{A}} + R_{\mathcal{E}} + R_{\mathcal{AE}}$. A general initial state $\rho_{\mathcal{AE}}(0)$ will evolve as

$$\begin{aligned}\rho_{\mathcal{AE}}(\mathbf{Q}_f, \mathbf{Q}'_f, \mathbf{q}_f, \mathbf{q}'_f, t) = \int d\mathbf{Q}_i d\mathbf{Q}'_i d\mathbf{q}_i d\mathbf{q}'_i K(\mathbf{Q}_f, \mathbf{q}_f, t; \mathbf{Q}_i, \mathbf{q}_i) \\ \times K^*(\mathbf{Q}'_f, \mathbf{q}'_f, t; \mathbf{Q}'_i, \mathbf{q}'_i)\rho_{\mathcal{AE}}(0),\end{aligned} \tag{3.23}$$

and the reduced dynamics of the central system is obtained after tracing out the degrees of freedom of the environment, $\rho_{\mathcal{A}}(t) = \mathrm{Tr}_{\mathcal{E}}\Big[\rho_{\mathcal{AE}}(t)\Big]$. Choosing a factorized initial state $\rho_{\mathcal{AE}}(0) = \rho_{\mathcal{A}}(0) \otimes \rho_{\mathcal{E}}(0)$, the reduced density matrix gives

$$\rho_{\mathcal{A}}(\mathbf{Q}_f, \mathbf{Q}'_f, t) = \int d\mathbf{Q}_i d\mathbf{Q}'_i \rho_{\mathcal{A}}(0) \int \mathcal{D}[\mathbf{Q}(s)]\mathcal{D}[\mathbf{Q}'(s)] \mathrm{e}^{\frac{i}{\hbar}(R_{\mathcal{A}}[\mathbf{Q}] - R_{\mathcal{A}}[\mathbf{Q}'])} \mathcal{F}[\mathbf{Q}, \mathbf{Q}'], \tag{3.24}$$

where $\mathcal{F}[\mathbf{Q}, \mathbf{Q}']$ is the Feynman-Vernon influence functional given by

$$\begin{aligned}\mathcal{F}[\mathbf{Q}, \mathbf{Q}'] = \int_{(\mathbf{q}_i, \mathbf{q}'_i) \to \mathbf{q}_f} d\mathbf{q}_f d\mathbf{q}_i d\mathbf{q}'_i \rho_{\mathcal{E}}(0) \int \mathcal{D}[\mathbf{q}]\mathcal{D}[\mathbf{q}'] \\ \times \mathrm{e}^{\frac{i}{\hbar}\left(R_{\mathcal{E}}[\mathbf{q}] + R_{\mathcal{AE}}[\mathbf{Q}, \mathbf{q}] - R_{\mathcal{E}}[\mathbf{q}'] - R_{\mathcal{AE}}[\mathbf{Q}', \mathbf{q}']\right)}.\end{aligned} \tag{3.25}$$

If we assume the initial state $\hat{\rho}_{\mathcal{E}}(0) = \hat{\rho}_{\mathcal{E},1}(0) \otimes \hat{\rho}_{\mathcal{E},2}(0)$ to be a thermal state for $\mathcal{E}$ at inverse temperature $\beta = 1/\kappa_B T$,

$$\hat{\rho}_{\mathcal{E}} = \frac{\mathrm{e}^{-\beta \hat{H}_{\mathcal{E}}}}{Z_{\mathcal{E}}}, \tag{3.26}$$

with $Z_{\mathcal{E}} = Z_{\mathcal{E},1} \times Z_{\mathcal{E},2}$, the influence functional has an exact representation, and the reduced density matrix is accordingly given by

$$\rho_{\mathcal{A}}(\mathbf{Q}_f, \mathbf{Q}'_f, t) = \int d\mathbf{Q}_i d\mathbf{Q}'_i \rho_{\mathcal{A}}(0) \int \mathcal{D}[\mathbf{Q}]\mathcal{D}[\mathbf{Q}'] \mathrm{e}^{\frac{i}{\hbar}\left(R_{\mathcal{A}}[\mathbf{Q}] - R_{\mathcal{A}}[\mathbf{Q}'] - R^F[\mathbf{Q}, \mathbf{Q}']\right)} \mathrm{e}^{-R^d[\mathbf{Q}, \mathbf{Q}']/\hbar}. \tag{3.27}$$

The effective action in $R^F$ is responsible for dissipation of energy of the particle and thus for the relaxation process. Neglecting this term in our approximation we only keep the decoherence action $R^d$, which, assuming both baths have an identical spectral density, reads

$$R^d[\mathbf{Q}, \mathbf{Q}'] = \int_0^t ds \int_0^s du (\mathbf{Q}(s) - \mathbf{Q}'(s))^T \kappa(s-u)(\mathbf{Q}(u) - \mathbf{Q}'(u)), \tag{3.28}$$

which involves a mixture of off-diagonal components $\mathbf{Q} - \mathbf{Q}'$ of the density matrix along paths mediated by the bath kernel

$$\kappa(s-u) = \frac{1}{\pi} \int_0^\infty d\omega J(\omega) \coth\left(\beta\hbar\omega/2\right) \cos\omega(s-u). \tag{3.29}$$

Here the integral is over a continuum of bath-oscillators frequencies $\omega$. If we choose an Ohmic spectral density associated with the bath such that $J(\omega) = \Gamma\omega$, in the limit of high temperatures, $\beta \to 0$, by using $\coth\left(\beta\hbar\omega/2\right) \sim 2/\hbar\omega\beta$, the kernel transforms into

$$\kappa(s-u) = \frac{2\Gamma}{\hbar\beta}\delta(s-u), \tag{3.30}$$

and the decoherence term in the action takes the form

$$R^d[\mathbf{Q},\mathbf{Q}'] = \frac{2\Gamma}{\hbar\beta}\int_0^t ds|\mathbf{Q}(s)-\mathbf{Q}'(s)|^2. \tag{3.31}$$

In this way, inserting Eq. (3.31) into Eq. (3.27), we see that $R^d$ is responsible for the suppression of quantum coherence between paths $\mathbf{Q}$ and $\mathbf{Q}'$ due to the coupling of the central system to the environment of bath oscillators.

All together, in the high-temperature regime, Eq. (3.27) reads

$$\rho_{\mathcal{A}}(\mathbf{Q}_f,\mathbf{Q}'_f,t) = \int d\mathbf{Q}_i d\mathbf{Q}'_i \rho_{\mathcal{A}}(0)\int \mathcal{D}[\mathbf{Q}]\mathcal{D}[\mathbf{Q}']\mathrm{e}^{\frac{i}{\hbar}(R_{\mathcal{A}}[\mathbf{Q}]-R_{\mathcal{A}}[\mathbf{Q}'])}\mathrm{e}^{-\alpha\int_0^t ds|\mathbf{Q}(s)-\mathbf{Q}'(s)|^2}, \tag{3.32}$$

where we have defined a new coupling-strength constant $\alpha = \frac{2\Gamma}{\hbar\beta}$, subduing the whole parameter dependence of the decoherence action. To make further progress, as Eq. (3.32) represents still a formidable problem, we will assume that $\alpha$ is classically small so that the coupling with the environment does not affect the classical dynamics of the central system, only the coherence between pair of paths $\mathbf{Q},\mathbf{Q}'$. This weak-coupling regime, usually justified even for realistic models, will enable us to evaluate Eq. (3.32) semiclassically. Thus, we have a model for decoherence without dissipation process. The main assumption is that the coupling with the bath is classically small such that the central system only experiences a loss of coherence of the relative states $\mathbf{Q},\mathbf{Q}'$. This is also justified if we note that in these models the decoherence time scale is much more faster than the dissipative time scales induced by the environment [46, 96].

### 3.2.2. Particle in a chaotic cavity and quantum survival probability

In [97] the authors considered a particle moving in two dimensions, initially inside a cavity of area $A$. The cavity has a hole of size $l$ from which the particle can escape. At the purely classical level, it is known that the probability $\rho_{\mathrm{cl}}$ to find the particle inside the cavity at time $t$, the so-called survival probability, has the form [36]

$$\rho_{\mathrm{cl}} = \mathrm{e}^{-t/\tau_D}, \tag{3.33}$$

for cavities supporting classical chaotic dynamics. This result is valid for times longer than the Lyapunov time $1/\lambda$, with $\lambda$ the Lyapunov exponent (assumed uniform). Here, $1/\tau_D$ is the escape rate, given in terms of the dwell time $\tau_D = \Omega(E)/(2lp)$, where $p$ is the momentum of the particle. In [97], using semiclassical techniques, quantum corrections to the classical survival probability were studied, and a universal quantum enhancement

for underlying classical chaotic dynamics was predicted. At first-order in $\hbar$, it takes the form of a correction $\delta\rho_{\rm qm}$,

$$\delta\rho_{\rm qm} = {\rm e}^{-t/\tau_D}\frac{t^2}{2T_H\tau_D}, \tag{3.34}$$

where $T_H = \Omega/(2\pi\hbar)$ is the Heisenberg time. This quantum enhancement of the decaying classical survival probability is a *coherent* effect coming from interference between pair of trajectories. In the following, we will study the interplay between this quantum survival probability and the *decoherence* process as implied by Eq. (3.32). That is, we will consider a particle that is coupled *both* to a continuum through an opening of size $l$ of the cavity that produces coherent effects, and to an environment that suppresses such effects by decoherence.

### 3.2.3. Semiclassical treatment

As reported for the first time in [97, 98], in general coherent corrections to the classical dynamics of observables, like the survival probability, manifest themselves only when the observable itself is defined within a finite region of an otherwise unbounded system. In this spirit, the state of the particle $\mathcal{A}$ inside the cavity under the influence of $\mathcal{E}$ will evolve using Eq. (3.32), but projected onto the area of the open cavity.

We implement the semiclassical approach to Eq. (3.32) taking into account that, in our weak-coupling scenario, the classical solutions of the saddle-point analysis (SPA) in Eq. (3.32) are given by the stationary condition of the bare action $R_{\mathcal{A}}$. This leads us to consider the application of SPA at the level of the amplitudes, the so-called semiclassical approximation to the quantum mechanical propagator studied already in chapter 1 [28]. Within the semiclassical approximation, the propagator takes the form

$$K_{\rm sc}(\mathbf{Q}_f, t; \mathbf{Q}_i, 0) = \frac{1}{2\pi\hbar}\sum_{\tilde{\gamma}:\mathbf{Q}_i\to\mathbf{Q}_f} A_{\tilde{\gamma}}{\rm e}^{\frac{i}{\hbar}R^{\tilde{\gamma}}_{\mathcal{A}}}, \tag{3.35}$$

as a sum over classical paths $\tilde{\gamma}$ connecting points $\mathbf{Q}_i \to \mathbf{Q}_f$, during time $t$. The van Vleck-Gutzwiller amplitude

$$A_{\tilde{\gamma}} = \left|\det\Big(-\frac{\partial^2 R^{\tilde{\gamma}}_{\mathcal{A}}}{\partial\mathbf{Q}_f\partial\mathbf{Q}_i}\Big)\right|^{1/2}{\rm e}^{-i\pi\mu_{\tilde{\gamma}}/2}, \tag{3.36}$$

contains, besides the stability factor, the number of focal points $\mu_{\tilde{\gamma}}$ of the trajectory. Substitution of Eq. (3.35) into the general expression for evolution of the state in Eq. (3.32), gives

$$\begin{aligned}\rho^{\rm sc}_{\mathcal{A}}(\mathbf{Q}_f, \mathbf{Q}'_f, t) =& \frac{1}{(2\pi\hbar)^2}\int_A d\mathbf{Q}_i d\mathbf{Q}'_i \rho_{\mathcal{A}}(\mathbf{Q}_i, \mathbf{Q}'_i, 0)\\ &\sum_{\tilde{\gamma}:\mathbf{Q}_i\to\mathbf{Q}_f}\sum_{\tilde{\gamma}':\mathbf{Q}'_i\to\mathbf{Q}'_f} A_{\tilde{\gamma}}A^*_{\tilde{\gamma}'}{\rm e}^{\frac{i}{\hbar}(R^{\tilde{\gamma}}_{\mathcal{A}}-R^{\tilde{\gamma}'}_{\mathcal{A}})}{\rm e}^{-\alpha\int_0^t ds|\mathbf{Q}_{\tilde{\gamma}}(s)-\mathbf{Q}_{\tilde{\gamma}'}(s)|^2},\end{aligned} \tag{3.37}$$

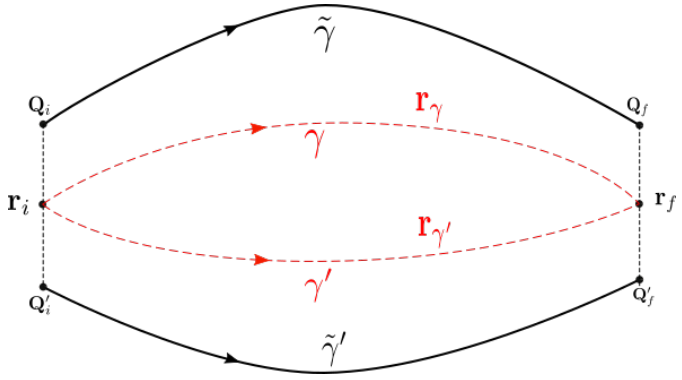


Figure 3.5: From the double sum in Eq. (3.37) we build a pair of trajectories $(\gamma, \gamma')$, with small action difference and ending points $\mathbf{r}_i = (\mathbf{Q}_i + \mathbf{Q}'_i)/2$, $\mathbf{r}_f = (\mathbf{Q}_f + \mathbf{Q}'_f)/2$. By this the paths $\mathbf{r}_\gamma(s)$ and $\mathbf{r}_{\gamma'}(s)$ are constructed, which are involved in the decoherence contribution of Eq. (3.39). The picture is in configuration space and the arrows show the direction of momentum.

thus taking the form of a double sum over classical paths. Since the semiclassical approximation in Eq. (3.37) is valid when the bare action of the central system $R_\mathcal{A}$ is much greater than $\hbar$, the sum over pairs of trajectories contains highly oscillatory terms that cancels out each other, unless the pair difference is of order $\hbar$, $R^{\tilde{\gamma}}_\mathcal{A} - R^{\tilde{\gamma}'}_\mathcal{A} \sim \mathcal{O}(\hbar)$. Following the usual semiclassical methods [10], the important contributions to the double sum come from those pairs of trajectories with small action difference. In the double sum of Eq. (3.37) we construct a pair of trajectories $(\gamma, \gamma')$ with ending points $\mathbf{r}_i = (\mathbf{Q}_i + \mathbf{Q}'_i)/2$, $\mathbf{r}_f = (\mathbf{Q}_f + \mathbf{Q}'_f)/2$, as shown in Fig. 3.5. In a final step we expand the action $R^{\tilde{\gamma}}_\mathcal{A}$ around the path $\gamma$,

$$R^{\tilde{\gamma}}_\mathcal{A}(\mathbf{Q}_i, \mathbf{Q}_f) \approx R^{\gamma}_\mathcal{A}(\mathbf{r}_i, \mathbf{r}_f) - \mathbf{P}^i_\gamma \cdot \mathbf{y}_i/2 + \mathbf{P}^f_\gamma \cdot \mathbf{y}_f/2, \tag{3.38}$$

and similarly $R^{\tilde{\gamma}'}_\mathcal{A}$ around $\gamma'$. Thus Eq. (3.37) reads now

$$\rho^{\mathrm{sc}}_\mathcal{A}(\mathbf{r}_f + \mathbf{y}_f/2, \mathbf{r}_f - \mathbf{y}_f/2, t) = \int_A d\mathbf{r}_i d\mathbf{y}_i \rho_\mathcal{A}(\mathbf{r}_i + \mathbf{y}_i/2, \mathbf{r}_i - \mathbf{y}_i/2, 0)$$
$$\frac{1}{(2\pi\hbar)^2} \sum_{\gamma:\mathbf{r}_i\to\mathbf{r}_f} \sum_{\gamma':\mathbf{r}_i\to\mathbf{r}_f} A_\gamma A^*_{\gamma'} \mathrm{e}^{\frac{i}{\hbar}(R^\gamma_\mathcal{A} - R^{\gamma'}_\mathcal{A})} \mathrm{e}^{-\frac{i}{\hbar}(\mathbf{P}^i_\gamma + \mathbf{P}^i_{\gamma'})\cdot\mathbf{y}_i/2} \mathrm{e}^{\frac{i}{\hbar}(\mathbf{P}^f_\gamma + \mathbf{P}^f_{\gamma'})\cdot\mathbf{y}_f/2} \mathrm{e}^{-\alpha\int_0^t ds |\mathbf{r}_\gamma(s) - \mathbf{r}_{\gamma'}(s)|^2}, \tag{3.39}$$

where we have used the classical identities (see also section 1.1.2) [29]

$$\begin{aligned} \frac{\partial R^\gamma_\mathcal{A}}{\partial \mathbf{r}_i} &= -\mathbf{P}^i_\gamma(\mathbf{r}_i, \mathbf{r}_f, t), \\ \frac{\partial R^\gamma_\mathcal{A}}{\partial \mathbf{r}_f} &= \mathbf{P}^f_\gamma(\mathbf{r}_i, \mathbf{r}_f, t), \end{aligned} \tag{3.40}$$

for the initial and final momentum for the path $\gamma$, and similarly for the path $\gamma'$. The

integral over $\mathbf{y}_i$ can now be performed to obtain

$$\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i,(\mathbf{P}^i_\gamma+\mathbf{P}^i_{\gamma'})/2,0\Big)=\frac{1}{(2\pi\hbar)^2}\int d\mathbf{y}_i\rho_{\mathcal{A}}(\mathbf{r}_i+\mathbf{y}_i/2,\mathbf{r}_i-\mathbf{y}_i/2,0)\mathrm{e}^{-\frac{i}{\hbar}(\mathbf{P}^i_\gamma+\mathbf{P}^i_{\gamma'})\cdot\mathbf{y}_i/2}, \tag{3.41}$$

where the initial Wigner function [99] with initial momentum $(\mathbf{P}^i_\gamma+\mathbf{P}^i_{\gamma'})/2$ appears, to arrive at the expression

$$\begin{aligned}\rho^{\mathrm{sc}}_{\mathcal{A}}(\mathbf{r}_f+\mathbf{y}_f/2,\mathbf{r}_f-\mathbf{y}_f/2,t)=\int_A d\mathbf{r}_i\sum_{\gamma:\mathbf{r}_i\to\mathbf{r}_f}\sum_{\gamma':\mathbf{r}_i\to\mathbf{r}_f}A_\gamma A^*_{\gamma'}\\ \times\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i,(\mathbf{P}^i_\gamma+\mathbf{P}^i_{\gamma'})/2,0\Big)\mathrm{e}^{\frac{i}{\hbar}(R^\gamma_{\mathcal{A}}-R^{\gamma'}_{\mathcal{A}})}\mathrm{e}^{\frac{i}{\hbar}(\mathbf{P}^f_\gamma+\mathbf{P}^f_{\gamma'})\cdot\mathbf{y}_f/2}\mathrm{e}^{-\alpha\int_0^t ds|\mathbf{r}_\gamma(s)-\mathbf{r}_{\gamma'}(s)|^2}.\end{aligned} \tag{3.42}$$

As shown in chapter 1, a fully phase-space representation is obtained after multiplying Eq. (3.42) by $\mathrm{e}^{-\frac{i}{\hbar}\mathbf{p}_f\cdot\mathbf{y}_f}$, and integrating over the variable $\mathbf{y}_f$. The left-hand side of Eq. (3.42) transforms then into the Wigner function of the central system at time $t$ and momentum $\mathbf{p}_f$, and the right-hand side gives just a delta function after the $\mathbf{y}_f$-integration.

All together, we obtain the important result for the time evolution of the Wigner function (compare to Eq. (1.26) in the closed-system scenario)

$$\begin{aligned}\mathcal{W}^{\mathrm{sc}}_{\mathcal{A}}(\mathbf{r}_f,\mathbf{p}_f,t)=\int_A d\mathbf{r}_i\sum_{\gamma:\mathbf{r}_i\to\mathbf{r}_f}\sum_{\gamma':\mathbf{r}_i\to\mathbf{r}_f}A_\gamma A^*_{\gamma'}\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i,(\mathbf{P}^i_\gamma+\mathbf{P}^i_{\gamma'})/2,0\Big)\\ \times\mathrm{e}^{\frac{i}{\hbar}(R^\gamma_{\mathcal{A}}-R^{\gamma'}_{\mathcal{A}})}\delta\Big(\mathbf{p}_f-(\mathbf{P}^f_\gamma+\mathbf{P}^f_{\gamma'})/2\Big)\,\mathrm{e}^{-\alpha\int_0^t ds|\mathbf{r}_\gamma(s)-\mathbf{r}_{\gamma'}(s)|^2},\end{aligned} \tag{3.43}$$

involving a sum over pairs of trajectories starting at point $\mathbf{r}_i$ and ending at $\mathbf{r}_f$, with the constraint in their final momentum. As mentioned before, the integration in Eq. (3.43) runs over the area $A$ of the cavity, as appropriate for the calculation of expectation values of observables of the form $\hat{O}\chi_A(\hat{q})$, where $\chi_A(q)$ is the corresponding characteristic function. In the following subsections we will assume that we have introduced a local time average in Eq. (3.43) in order to smooth out highly oscillatory terms in the double sum.

### Diagonal approximation

Eq. (3.43) represents the semiclassical approximation of the Wigner function of the central system, at time $t$, projected on a cavity of area $A$, evolved from the initial Wigner function. From the pairs of trajectories in Eq. (3.43), which have small action difference, those which are identical, $\gamma=\gamma'$, correspond to the leading-order contribution. This is the so-called diagonal approximation. In this case Eq. (3.43) reads

$$\mathcal{W}^{\mathrm{dg}}_{\mathcal{A}}(\mathbf{r}_f,\mathbf{p}_f,t)=\int_A d\mathbf{r}_i\sum_{\gamma:\mathbf{r}_i\to\mathbf{r}_f}|A_\gamma|^2\mathcal{W}_{\mathcal{A}}(\mathbf{r}_i,\mathbf{P}^i_\gamma,0)\delta(\mathbf{p}_f-\mathbf{P}^f_\gamma), \tag{3.44}$$

where naturally the decoherence contribution has disappeared since it would involve off-diagonal terms. It is important to note that, for a system constrained in a closed area,

we can use the amplitude $|A_\gamma|^2 = \det\left|\frac{\partial \mathbf{P}_\gamma^f}{\partial \mathbf{r}_i}\right|$, as a Jacobian transformation from initial position to final momentum, to get

$$\begin{aligned}\mathcal{W}_{\mathcal{A}}^{\mathrm{dg}}(\mathbf{r}_f,\mathbf{p}_f,t) &= \int d\mathbf{P}_f \delta(\mathbf{p}_f-\mathbf{P}_f)\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{P}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{P}_f,t)\Big)\\ &= \mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{p}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{p}_f,t)\Big),\end{aligned} \tag{3.45}$$

which says that the Wigner function at time $t$ is simply obtained in terms of the initial Wigner function by rigidly transporting backwards its values along the solution of the classical equations of motion $(\mathbf{r}_f,\mathbf{p}_f) = (\mathbf{r}_f(\mathbf{r}_i,\mathbf{p}_i,t),\mathbf{p}_f(\mathbf{r}_i,\mathbf{p}_i,t))$. This is Eq. (1.27), the so-called Truncated Wigner approximation [33, 100–102], expressing in the semiclassical limit the evolution of quantum mechanical states by means of classical evolution of the corresponding Wigner function. In the case of interest here, however, we project the Wigner function in a cavity and thus Eq. (3.44) gives the diagonal approximation of the projected Wigner function, which allows us to calculate local observables inside the cavity. Using the sum rule for open systems [103], and assuming a state with a well-defined mean energy $E_0$, we get

$$\begin{aligned}\mathcal{W}_{\mathcal{A}}^{\mathrm{dg}}(\mathbf{r}_f,\mathbf{p}_f,t) &= \int_A d\mathbf{P}_f \delta(\mathbf{p}_f-\mathbf{P}_f)\mathrm{e}^{-t/\tau_D}\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{P}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{P}_f,t)\Big)\\ &= \mathrm{e}^{-t/\tau_D}\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{p}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{p}_f,t)\Big),\end{aligned} \tag{3.46}$$

where $1/\tau_D$ is the classical escape rate at energy $E_0$. Equation (3.46) results in an exponential decay of the projected Wigner function inside the cavity. In particular, the probability to find the particle inside the cavity at time $t$ can be obtained as $\int_A d\mathbf{r}_f d\mathbf{p}_f \mathcal{W}_{\mathcal{A}}^{\mathrm{dg}}(\mathbf{r}_f,\mathbf{p}_f,t)$, and gives the result for the classical survival probability in [97]. While in the diagonal approximation the decohrence factor in Eq. (3.43) cancels out, the leading-order quantum correction to Eq. (3.43) for a chaotic system, the so-called loop contributions, involves pairs of correlated trajectories which are not identical all the time and thus could reveal interference effects between the involved paths. This is the topic of the next subsection.

### Loop corrections

The leading order quantum correction to the time evolution of the projected Wigner function in Eq. (3.43) comes from pairs of trajectories $\gamma,\gamma'$ which are identical to each other except in a so-called self-encounter region [39], where they remain close to each other but switch partners, as studied in section 3.1, and is shown in Fig. 4.1. In this scenario there are three diagrams whose contributions have to be added within the leading-order loop correction: when the encounter takes place at the beginning (or at the end) of the trajectory, called 1-leg-loops, and when the encounter is fully developed in the region between the endpoints of the trajectory, called 2-leg-loops. Let us sketch the calculation for the contribution of the 2-leg diagram. We place a Poincaré surface of section $\mathcal{P}$ at any point inside the encounter, as shown in Fig. 3.3. The trajectory $\gamma$

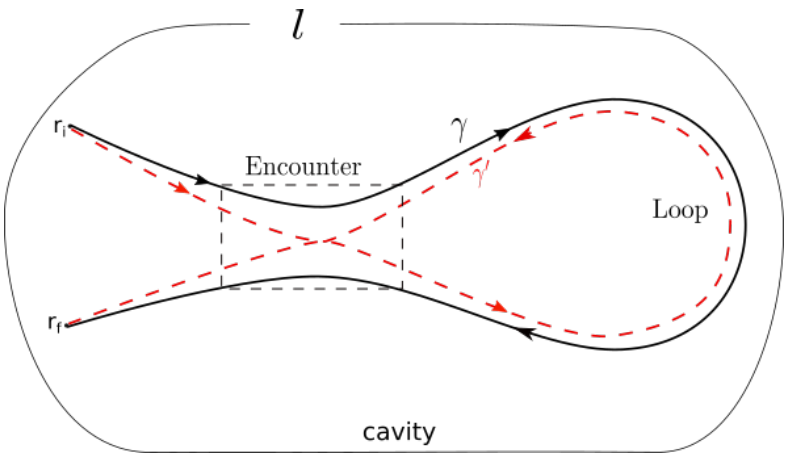


Figure 3.6: A typical pair of correlated trajectories $\gamma$, $\gamma'$ inside the cavity. The trajectories differ from each other inside the encounter region where they change partners, but remain close, and after leaving the encounter they form a loop, one trajectory following the time-reversed path of the other. The draw is in configuration space and the arrows show the direction of the momentum. This is an example of a 2-leg diagram where the encounter is fully developed between the endpoints.

first reaches $\mathcal{P}$ at time $t'$ and then, after leaving the encounter, forms a loop and returns back to the encounter, reaching again $\mathcal{P}$ a second time at $t''$. The key observation is that the decoherence term inside the loop is no longer zero. Moreover, since being $\gamma$ the time-reversed of $\gamma'$, the paths $\mathbf{r}_\gamma(s)$ and $\mathbf{r}_{\gamma'}(s)$ can be treated as uncorrelated through the loop. The important role of this type of non-diagonal suppression has been studied in the framework of closed systems by calculating its effect on the loss of purity [104].

With this division of the trajectory the decoherence term itself splits into

$$\begin{aligned}\int_0^t |\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)|^2 = &\int_0^{t'-t_s} |\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)|^2 + \int_{t'-t_s}^{t'+t_u} |\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)|^2 \\ &+ \int_{t'+t_u}^{t'+t_u+t_{\text{loop}}} |\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)|^2 + \int_{t'+t_u+t_{\text{loop}}}^{t'+2t_u+t_s+t_{\text{loop}}} |\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)|^2 \\ &+ \int_{t'+2t_u+t_s+t_{\text{loop}}}^{t} |\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)|^2,\end{aligned} \tag{3.47}$$

where the first and last integrals represent the first and third link respectively. There $\gamma$ and $\gamma'$ are exponentially close and thus the integrals vanish.

*Inside the loop.* The important contribution to decoherence comes from pairs of trajectories inside the loop. To calculate this contribution we apply ergodic arguments: due to the chaotic nature of the system we transform the time integral of the squared difference in Eq. (3.47) into a variance of position $\sigma^2$. To this end we add to the integrand the phase-space average position value $\langle \mathbf{r} \rangle_{E_\gamma}$, where $E_\gamma$ denotes the energy of the trajectory

$\gamma$, which is the same energy of $\gamma'$, and write

$$\begin{aligned}\int_{t'+t_u}^{t'+t_u+t_{\rm loop}} & d\tau|\mathbf{r}_\gamma(\tau)-\langle\mathbf{r}\rangle_{E_\gamma}+\langle\mathbf{r}\rangle_{E_\gamma}-\mathbf{r}_{\gamma'}(\tau)|^2 \\ &= \int_{t'+t_u}^{t'+t_u+t_{\rm loop}} d\tau\,\Big(|\mathbf{r}_\gamma(\tau)-\langle\mathbf{r}\rangle_{E_\gamma}|^2+|\mathbf{r}_{\gamma'}(\tau)-\langle\mathbf{r}\rangle_{E_\gamma}|^2 \\ &\quad +2(\mathbf{r}_\gamma(\tau)-\langle\mathbf{r}\rangle_{E_\gamma})^T\cdot(\mathbf{r}_{\gamma'}(\tau)-\langle\mathbf{r}\rangle_{E_\gamma})\Big) \\ &= 2t_{\rm loop}\,\langle(\mathbf{r}-\langle\mathbf{r}\rangle_{E_\gamma})^2\rangle := \,2t_{\rm loop}\sigma^2.\end{aligned} \tag{3.48}$$

To obtain the last line we use the relation

$$\frac{1}{T}\int_0^T d\tau f(\mathbf{r}_\gamma(\tau),\mathbf{p}_\gamma(\tau))=\langle f(\mathbf{r},\mathbf{p})\rangle_{E_\gamma}\,, \tag{3.49}$$

to change the time integral into phase-space average $\langle f\rangle_{E_\gamma}$, with $\langle\mathbf{r}-\langle\mathbf{r}\rangle_{E_\gamma}\rangle=0$, and the fact that $(\gamma,\gamma')$ are uncorrelated inside the loop.

*Inside the encounter.* When the pair $(\gamma,\gamma')$ traverses the encounter for the first time, that is in the time interval $[t'-t_s,t'+t_u]$, the difference $\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)$ at any time $\tau$ within the interval, calculated from the reference point $\mathbf{x}_\gamma$, is given in the linearized regime by

$$\mathbf{r}_\gamma(\tau)-\mathbf{r}_{\gamma'}(\tau)=-u\mathrm{e}^{\lambda(\tau-t')}\tilde{e}_u(\mathbf{x}_\gamma(\tau)), \tag{3.50}$$

where $u$ ($s$) is the coordinate in the unstable (stable) manifold, and $\tilde{e}_u(\mathbf{x}_\gamma(\tau))$ is a local unit vector pointing in the unstable direction at time $\tau$. With this considerations the decoherence term inside the encounter during the first time interval can be evaluated to give

$$\int_{t'-t_s}^{t'+t_u} d\tau|\mathbf{r}_\gamma(s)-\mathbf{r}_{\gamma'}(\tau)|^2=u^2\int_{t'-t_s}^{t'+t_u}d\tau\,\mathrm{e}^{2\lambda(\tau-t')}|\tilde{e}_u(\mathbf{x}_\gamma(\tau))|^2, \tag{3.51}$$

where, in the semiclassical limit the precise time-dependence of $\tilde{e}_u(\mathbf{x}_\gamma(\tau))$ is effectively averaged over the phase space in order to take it out of the time integral as a constant $\eta$, whose exact value will not play any role in the final result. In this way the last equation gives

$$\int_{t'-t_s}^{t'+t_u} d\tau|\mathbf{r}_\gamma(s)-\mathbf{r}_{\gamma'}(\tau)|^2=\eta\frac{c^2}{2\lambda}\Big(1-\Big(\frac{su}{c^2}\Big)^2\Big), \tag{3.52}$$

where the factor $c$ is a classical scale constant characterizing the linearized regime. When a similar calculation is carried out for the second time interval inside the encounter, we obtain finally the total contribution of the decoherence term

$$\int_0^t d\tau|\mathbf{r}_\gamma(s)-\mathbf{r}_{\gamma'}(\tau)|^2=\eta\frac{c^2}{\lambda}\Big(1-\Big(\frac{su}{c^2}\Big)^2\Big)+2t_{\rm loop}\sigma^2. \tag{3.53}$$

On the other hand, the action difference is taken from Eq. (3.15), as $R_{\mathcal{A}}^{\gamma}-R_{\mathcal{A}}^{\gamma'}=su$, and the density of trajectories from Eq. (3.16). Finally, we perform the sum over $\gamma$ by

taking $|A_\gamma|^2$ in Eq. (3.43) as a Jacobian transformation, using the sum rule as in the diagonal approximation in Eq. (3.46).

Further, as shown in [97], due to the encounter time a trajectory needs in order to close itself forming a self-crossing, we take into account that the quantum survival probability is augmented by the factor $\mathrm{e}^{t_{\mathrm{enc}}/\tau_D}$, and using Eq. (3.53), the first quantum correction to Eq. (3.43) is finally given by

$$\begin{aligned}\mathcal{W}_{\mathcal{A}}^{\mathrm{loop}}(\mathbf{r}_f,\mathbf{p}_f,t)_{2-\mathrm{legs}} =&\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{p}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{p}_f,t)\Big)\\ &\int_{-c^2}^{c^2} dsdu \int_{t_s}^{t-2t_u-t_s} dt' \int_0^{t-t'-2t_u-t_s} dt_{\mathrm{loop}}\\ &\times \frac{\mathrm{e}^{-(t-t_{\mathrm{enc}}(s,u))}}{\Omega t_{\mathrm{enc}}(s,u)}\mathrm{e}^{-\alpha\eta\frac{c^2}{\lambda}(1-(\frac{su}{c^2})^2)}\mathrm{e}^{-\alpha 2t_{\mathrm{loop}}\sigma^2},\end{aligned} \tag{3.54}$$

where the limits of the integration reflect the fact that we need a minimum time $t_u + t_s$ to form an encounter region (the variables $(s, u)$ can not grow beyond the limit $c$), and the encounter time reads $t_{\mathrm{enc}} = \lambda^{-1}\log\big(c^2/|su|\big)$. An integral similar to Eq. (3.54) is obtained for the contribution of the 1-leg diagrams, but the time intervals for $t'$ and $t_{\mathrm{loop}}$ have to be adjusted to account for the fact that encounters at the beginning or at the end of the trajectory do not have time to fully develop. We evaluate the integral in (3.54), and the one coming from 1-leg diagrams, in the semiclassical regime where $\lambda\tau_D$, $c^2/\hbar \to \infty$, while $\alpha/\lambda \to 0$, to get

$$\begin{aligned}\mathcal{W}_{\mathcal{A}}^{\mathrm{loop}}(\mathbf{r}_f,\mathbf{p}_f,t) =&\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{p}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{p}_f,t)\Big)\\ &\times\left[\frac{\tau_d^2}{T_H\tau_D}\mathrm{e}^{-t/\tau_D}\Big(\mathrm{e}^{-t/\tau_d}-1\Big)+\frac{\tau_d}{T_H\tau_D}t\,\mathrm{e}^{-t/\tau_D}\right],\end{aligned} \tag{3.55}$$

where we introduced the *decoherence time*,

$$\tau_d = (2\alpha\sigma^2)^{-1}, \tag{3.56}$$

with the variance $\sigma^2$ giving an estimate of the average separation in position of two correlated trajectories. Equation (3.55) is our main result. As shown in Fig. 3.7, it gives an analytical result for the interplay between the quantum enhancement due to coherent interference effects from correlated trajectories inside the encounter region [97], illustrated in red (dashed) line, and on the other hand, the diminishing of the quantum survival probability, compared with the vanishing-coupling result. This diminishing is due to decoherence effects depending on the temperature and the coupling strength, coming from uncorrelated trajectories inside the loop, which give rise to the term $\mathrm{e}^{-2\alpha\sigma^2 t}$.

In the short-time regime, obtained by expanding $\mathrm{e}^{-t/\tau_d}$ for small $t/\tau_d$, Eq. (3.55) reads

$$\begin{aligned}\mathcal{W}_{\mathcal{A}}^{\mathrm{loop}}(\mathbf{r}_f,\mathbf{p}_f,t) =&\mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{p}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{p}_f,t\Big)\\ &\times\mathrm{e}^{-t/\tau_D}\left[\frac{t^2}{2T_H\tau_D}-\frac{t^3}{6T_H\tau_D\tau_d}+\mathcal{O}(t^4/(\tau_d^2T_H\tau_D))\right],\end{aligned} \tag{3.57}$$

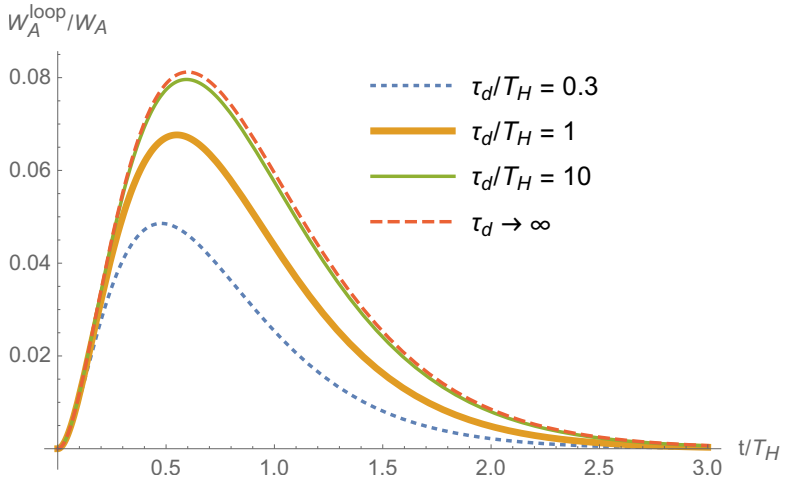


Figure 3.7: Plot of the first quantum correction $\mathcal{W}_{\mathcal{A}}^{\text{loop}}/\mathcal{W}_{\mathcal{A}}$ to the survival probability, as a function of the ratio $t/T_H$, for a dwell time $\tau_D/T_H = 0.3$, and different decoherence characteristic time $\tau_d/T_H$. The graphic shows a diminishing of the first quantum correction to the survival probability, compared to the vanishing-coupling result, due to the coupling of the system to the environment. The red (dashed) line, $\tau_d \to \infty$, represents the correction for vanishing coupling.

and we identify in the quadratic time-dependence the well-known result for the first quantum correction to the survival probability found in [97], (see Eq. (3.34)). It is important to observe that when we close the cavity, $\tau_D \to \infty$, the loop contribution $\mathcal{W}_{\mathcal{A}}^{\text{loop}}(\mathbf{r}_f, \mathbf{p}_f, t)$ in Eq. (3.55) vanishes. So in the closed-cavity scenario, and when the system is only coupled to a bath which produces decoherence in position, all quantum loop corrections cancel out in the semiclassical limit. This cancellation of quantum loop corrections for a closed system with classically chaotic dynamics points to an extremely robust character of the diagonal approximation (and of the Truncated Wigner method), and can be understood as a generalization of the very nontrivial loop cancellation order by order in $\hbar$ shown in [98] for the integrated probability, where it simply accounts for unitarity of quantum evolution. The fact that loop corrections to the more fundamental (non-integrated) Wigner function, as we obtained, manifest only when the system is open is indeed a fascinating observation for which a clear physical mechanism is still not at hand.

*Ehrenfest-time effects.* As a final stage we calculate explicitly the dependence of our result on the Ehrenfest-time, defined as the time scale above which quantum interference becomes important in chaotic systems. Following [97] we distinguish between the Ehrenfest time of the closed system, $t_E^c = \lambda^{-1} \log(\mathcal{L}/\lambda_B)$, and the open Ehrenfest time, $t_E^o = \lambda^{-1} \log\left(l^2/\mathcal{L}\lambda_B\right)$, where $\lambda_B$ is the de Broglie wavelength, and $\mathcal{L}$ is the size of the system. This choice implies $c^2 = l^2\hbar/\mathcal{L}\lambda_B$ [36]. As shown in [105], for a cavity with opening size $l$, we require the encounter stretches to escape the encounter when their separation is of the order $l$, in order for them to leave the encounter in an uncorrelated

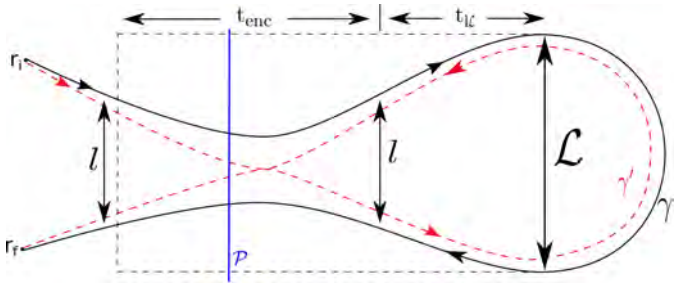


Figure 3.8: In the case of non-vanishing Ehrenfest time, when the stretches escape the encounter they need to be separated a distance of the order of the cavity opening size $l$ in order for them to leave the encounter region in a uncorrelated manner. And to form a loop the stretches have to be separated a distance of the order of the size of the cavity $\mathcal{L}$.

manner. Moreover, as shown in Fig. 3.8, on the right-hand side of the encounter the stretches should be separated a distance of the order of the size of he cavity $\mathcal{L}$, in order to close themselves forming a loop. This imposes a minimum time of the loop, which is $2t_{l\mathcal{L}}$, where $t_{l\mathcal{L}} = \lambda^{-1}\log(\mathcal{L}/l)$. Indeed, with this considerations it is clear that the variance in position should be of the order of the size of the cavity, giving $\tau_d = (2\alpha\mathcal{L}^2)^{-1}$. With these restrictions, and redefining appropriately the time limits, we solve the integrals in Eq. (3.54), introducing a step function $\theta(t-2(t_{enc}+t_{l\mathcal{L}}))$, establishing a minimal time of the trajectory. By doing similar calculation for the 1-leg diagrams, we finally obtain

$$\begin{aligned}\mathcal{W}_{\mathcal{A}}^{\text{loop}}(\mathbf{r}_f,\mathbf{p}_f,t) =& \mathcal{W}_{\mathcal{A}}\Big(\mathbf{r}_i(\mathbf{r}_f,\mathbf{p}_f,t),\mathbf{p}_i(\mathbf{r}_f,\mathbf{p}_f,t)\Big)\\ &\times\left[\frac{\tau_d^2}{T_H\tau_D}\mathrm{e}^{-(t-t_E^o)/\tau_D}\left(\mathrm{e}^{-(t-2t_E^o)/\tau_d}-\mathrm{e}^{-2t_{l\mathcal{L}}/\tau_d}\right)\right.\\ &\left.+\frac{(t-2t_E^e)\tau_d}{T_H\tau_D}\mathrm{e}^{-(t-t_E^o)/\tau_D}\mathrm{e}^{-2t_{l\mathcal{L}}/\tau_d}\right]\theta(t-2t_E^e),\end{aligned} \tag{3.58}$$

with $2t_E^e = t_E^o + t_E^c$. This completes the full semiclassical analysis. Notice that in the limit $\tau_d \to \infty$, and using $t_{l\mathcal{L}} = t_E^e - t_E^o$, Eq. (3.58) becomes the Ehrenfest-time-dependent result obtained in [97].

## 3.3. Summary

In this chapter, we provide a complete picture of the effect of decoherence on the coherent quantum corrections to classical population decay in chaotic cavities. It begins with the construction of the semiclassical Wigner representation of a chaotic particle weakly coupled to an environment within the Caldeira-Legget model. This representation (Eq. (3.43)) consists of a double sum of classical trajectories, and we show that it is the difference between these pairs of trajectories that generates an exponential decay

in the Wigner function, due to positional decoherence. Coherent effects due to path interference are made explicit when projecting this Wigner function in an open cavity, appropriate to calculate local observables inside it. We find the first-order quantum correction due to path interference to the time evolution, which leads to a universal non-monotonous form depending on the properties of the cavity and the bath-coupling parameters. In particular, the interplay between a coherent enhancement of the survival probability, coming from correlated trajectories inside an encounter region, and on the other hand, the decoherence effect coming from uncorrelated trajectories inside a loop produces a diminishing of the quantum survival probability compared to the scenario of vanishing-coupling. Our analysis is completed by calculating the explicit dependence of this first-order quantum correction on the Ehrenfest-time.

# 4. Semiclassical analysis of an open Bose-Hubbard model

In this chapter we will study a two-site Bose-Hubbard model coupled to an environment. We investigate the dissipation process of the system and, by considering an environment in an initial microcanonical state, we propose an approach which may allow for the first time the observation of interference effects of dissipative classical trajectories. In section 4.1 we calculate the propagation amplitude of the model, and investigate in detail the relation between the boundary conditions inherent to the quantum amplitude and the time-reversal invariance of the associated equations of motion. A subject where the literature is contradictory. Section 4.2 is devoted to the study of the reduced density matrix of the system and its associated semiclassical analysis. Finally, in section 4.3 we use the approach from chapter 2 and consider the environment initially in a micorcanonical state, which in principle, may allow to observe interference effects in open systems.

The two-site Bose-Hubbard (dimer) model has been used as an important model to understand tunneling phenomena [106], whose simplicity makes is useful for analytical treatment. Moreover, the general study of many-body systems coupled to an environment have many important applications, for example in entanglement engineering and quantum information processing [107–113], to mention only few. We consider is a composite system $\mathcal{AE}$ with Hamiltonian of the form

$$\hat{H} = \hat{H}_{\mathcal{A}} + \hat{H}_{\mathcal{E}} + \hat{H}_{\mathcal{AE}}, \tag{4.1}$$

where the environment $\mathcal{E}$ consists of $\mathcal{N}$ harmonic oscillators, each with natural frequency $\omega_k$, linearly coupled to the central system $\mathcal{A}$, being the latter a two-site Bose-Hubbard (BH) model, such that

$$\hat{H}_{\mathcal{A}} = -h(\hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1) + \frac{g}{2}\sum_{j=1}^{2} \hat{N}_j(\hat{N}_j - 1), \tag{4.2}$$

where $h$ is the hopping strength, $g$ the on-site interaction energy, and the particle-number operator for each site $\hat{N}_j = \hat{b}_j^\dagger \hat{b}_j$, is given in terms of the creation and annihilation operators $\hat{b}_j^\dagger$ and $\hat{b}_j$, respectively. The environment and interaction Hamiltonian have the form

$$\hat{H}_{\mathcal{E}} + \hat{H}_{\mathcal{AE}} = \sum_{k=1}^{\mathcal{N}} \Big( \omega_k \hat{\psi}_k^\dagger(s)\hat{\psi}_k(s) + \gamma_k \hat{N}_1(s)\big(\hat{\psi}_k^\dagger(s) + \hat{\psi}_k(s)\big) + \frac{\gamma_k^2}{\omega_k}\hat{N}_1^2 \Big) \equiv \hat{H}_L. \tag{4.3}$$

Here $\gamma_k$ is the strength coupling, and $\hat{\psi}_k = \frac{1}{\sqrt{2}}\big(\hat{q}_k + i\hat{p}_k\big)$, in terms of the conjugate quadrature operators $(\hat{q}_k, \hat{p}_k)$ for each mode in $\mathcal{E}$. The system is then coupled to the environment on one site through the operator $\hat{N}_1$, and since $\hat{N} = \hat{N}_1 + \hat{N}_2$ commutes with $\hat{H}$, the total number of particles $N$ is a conserved quantity. The last term in the second equality of Eq. (4.3) corresponds to a counter-term necessary to remove a renormalization of the potential due to the coupling, as shown in chapter 1.

## 4.1. Amplitude: boundary conditions, and time-reversal invariance

The quantum amplitude propagator $K$ can be written as a Feynman path integral in the form

$$\begin{aligned} K(r_f, \mathbf{q}_f, t; r_i, \mathbf{q}_i, 0) = \int \mathcal{D}[r(s), \theta(s)]\mathcal{D}[\mathbf{q}(s), \mathbf{p}(s)] \\ \exp i\left( \int_0^t ds\ (\dot{r}(s)\theta(s) - H_{\mathcal{A}}(r,\theta)) + \int_0^t ds\ (\mathbf{p}(s)\cdot\dot{\mathbf{q}}(s) - H_L(\mathbf{p},\mathbf{q},r))\right), \end{aligned} \tag{4.4}$$

ordering terms apart, with boundaries $r(t) = r_f, r(0) = r_i$, $\mathbf{q}(t) = \mathbf{q}_f$, and $\mathbf{q}(0) = \mathbf{q}_i$. We have defined the vector $\mathbf{q} = (q_1, ..., q_{\mathcal{N}})$, in a similar form the vector $\mathbf{p}$, and introduced the canonical variables $(N_j, \theta_j)$ of the system $\mathcal{A}$, through $b_j = \sqrt{N_j}\mathrm{e}^{i\theta_j}$. With this, the variables $r = N_1 - N_2$ and $\theta = (\theta_1 - \theta_2)/2$ have been introduced. The use of these variables in the Feynman propagator has some subtleties [114], which are of no importance when we take later the semiclassical limit. We also set $\hbar = 1$ since, as shown below, the semiclassical limit will depend only on the total number of particles $N$ within $\mathcal{A}$. The dot in Eq. (4.4) denotes derivative with respect to time. The bare Hamiltonian for $\mathcal{A}$ in Eq. (4.4) reads

$$H_{\mathcal{A}}(r,\theta) = -h\sqrt{N^2 - r^2}\cos 2\theta + \frac{g}{2}\left(\frac{1}{2}(N^2 + r^2) - N\right). \tag{4.5}$$

Being Eq. (4.4) quadratic in $\mathbf{q}$ and $\mathbf{p}$, the latter variables can be integrated exactly, yielding

$$\begin{aligned} K(r_f, \mathbf{q}_f, t; r_i, \mathbf{q}_i, 0) = \prod_{k=1}^{\mathcal{N}} \frac{1}{\sqrt{2\pi\hbar\sin\omega_k t}} \int \mathcal{D}[r(s), \theta(s)] \\ \exp i\left(\mathcal{R}[\mathbf{q}_f, \mathbf{q}_i, r] + \int_0^t ds\ (\dot{r}(s)\theta(s) - H_{\mathcal{A}}(r,\theta))\right), \end{aligned} \tag{4.6}$$

where the effective action $\mathcal{R}$ reads

$$\begin{aligned} \mathcal{R} = \sum_{k=1}^{\mathcal{N}} \left( \frac{1}{\sin\omega_k t}\left(\frac{1}{2}(q_{f,k}^2 + q_{k,i}^2)\cos\omega_k t - q_{f,k}q_{i,k} - \sqrt{2}q_{f,k}\gamma_k a_k[r]\right.\right. \\ \left.\left. -\sqrt{2}q_{i,k}\gamma_k b_k[r] - \gamma_k^2 c_k[r]\right) + \gamma_k^2 d_k[r] - \gamma_k^2 e_k[r]\right). \end{aligned} \tag{4.7}$$

In the last equation we have introduced the functionals

$$\begin{aligned} a_k[r] &= \int_0^t ds\ N_1(r(s)) \sin\omega_k s,\ b_k[r] = \int_0^t ds\ N_1(r(s)) \sin\omega_k(t-s) \\ c_k[r] &= \int_0^t ds \int_0^t du\ N_1(r(s)) N_1(r(u)) \sin(\omega_k s) \sin\omega_k(t-u) \\ d_k[r] &= \int_0^t ds \int_0^s du\ N_1(r(s)) N_1(r(u)) \sin\omega_k(s-u) \\ e_k[r] &= \int_0^t ds\ \frac{N_1(r(s))^2}{\omega_k}, \end{aligned} \tag{4.8}$$

using the relation $N_1(r) = (r+N)/2$.
It is surprising that at this point some confusion has existed by trying to identify the non-local in time functionals above with dissipative contributions of the corresponding classical equations of motion for $\mathcal{A}$ [115, 116]. Nevertheless, out of an amplitude, with its corresponding boundary conditions, it is not possible to derive a dissipative equation of motion, which necessarily implies the break of time-reversal symmetry. Explicitly, the classical ($c$) equations of motion for $\mathcal{A}$, obtained by the stationary condition of the effective action $\mathcal{R}$, is given by

$$\begin{aligned} \frac{\delta\mathcal{R}[r]}{\delta r(s)}\Big|_{r_c} &= \frac{1}{2}\sum_{k=1}^{\mathcal{N}} \Bigg( -\sqrt{2}\gamma_k q_{f,k} \frac{\sin\omega_k s}{\sin\omega_k t} - \sqrt{2}\gamma_k q_{i,k} \frac{\sin\omega_k(t-s)}{\sin\omega_k t} \\ -2\gamma_k^2 \frac{\sin\omega_k s}{\sin\omega_k t} \int_0^t du\ r_c(u) \sin\omega_k(t-u) &- 2\frac{\gamma_k^2}{\omega_k} r_c(s) - 2\gamma_k^2 \int_0^s du\ r_c(u) \sin\omega_k(u-s) \Bigg), \end{aligned} \tag{4.9}$$

which is actually a time-reverse invariant equation. That is, $\tilde{r}_c(s) \equiv r_c(t-s)$ also obeys Eq. (4.9). Note that Eq. (4.9) contains a *non-causal* term: the equation of motion at time $s$, accordingly, contains information about the trajectory at later times $u > s$. This non-causal contribution is often removed by appealing to "physical reasons" not entirely clear (for example by eliminating from the equations of motion the advanced Green function) [117]. It is worth mentioning that even if we propagate an initial state of $\mathcal{E}$, for example a coherent state, $\sim \int dq_{k,i} \mathrm{e}^{i\mathcal{R}} \mathrm{e}^{-q_{k,i}^2/2}$, the resulting contribution to the equations of motion is time-reverse invariant as well. This general property has its root in the connection of the *boundary value problem* implicit in the construction of the amplitude Eq. (4.6), and the time-reversal invariance of the associated equations of motion [118]. The stationary condition of the action from the propagator involves the finding of those paths with *fixed* boundary points. On the contrary, a dissipative equation of motion needs to break the time-reversal invariance, which is a property compatible with *initial conditions*. In [118] the author proposes a formalism which consists of doubling the degrees of freedom of the system, to introduce a new trajectory evolving "backwards" in time, whose job is to break the time-reversal symmetry of the resulting effective action at level of the amplitudes.
However, as noticed already long time ago [119], it is interesting that the breaking

of time-symmetry happens precisely at the level of *probabilities*, due to the interaction between the system and the environment. This breaking of time-symmetry characterizes a *physical process involving forward and backward paths*, as it will be seen below. Let us see how this process works by constructing the propagating function associated with the density matrix, which involves the product of two propagators $KK^*$, in the spirit of the path integral approach to the Caldeira-Leggett model.

## 4.2. Density matrix and dissipative equations of motion

The density matrix at time $t$, evolved from an initial state, for the joint system $\mathcal{AE}$, is given by

$$\begin{aligned}\rho_{\mathcal{AE}}(r_f, r'_f, \mathbf{q}_f, \mathbf{q'}_f, t) = \int dr_i dr'_i d\mathbf{q}_i d\mathbf{q'}_i K(r_f, \mathbf{q}_f, t; r_i, \mathbf{q}_i) \\ \times K^*(r'_f, \mathbf{q'}_f, t; r'_i, \mathbf{q'}_i)\rho_{\mathcal{AE}}(r_i, r'_i, \mathbf{q}_i, \mathbf{q'}_i),\end{aligned} \tag{4.10}$$

which comprises forward ($K$) and backward ($K^*$) paths. The physical meaning of an environment $\mathcal{E}$ is connected to the fact that *for all practical purposes* an observer does not have complete knowledge about all the degrees of freedom within $\mathcal{E}$. This is reflected in the usual choice of the initial state of the environment as one of *statistical nature*. Moreover, due to the impossibility to access all the environmental degrees of freedom at any time within the evolution, the process of *tracing out* the environment is carried out. This *lack of knowledge* about the details of the environment is crucial to understand the effective emergence of irreversibility, as shown below, and is actually also related to the quantum-to-classical transition problem, as studied in section 1.2.1.

With this in mind, we trace out the degrees of freedom of $\mathcal{E}$ in Eq. (4.10) to obtain the reduced density matrix for $\mathcal{A}$, $\hat{\rho}_{\mathcal{A}}(t) = \mathrm{Tr}_{\mathcal{E}}\ \hat{\rho}_{\mathcal{AE}}(t)$. Using relative $\mathbf{x} = \mathbf{q} - \mathbf{q}'$, and center of mass coordinates $\mathbf{r} = (\mathbf{q} + \mathbf{q}')/2$, and assuming, as usual, a factorized initial state, such that $\hat{\rho}_{\mathcal{AE}}(0) = \hat{\rho}_{\mathcal{A}}(0) \otimes \hat{\rho}_{\mathcal{E}}(0)$, we obtain

$$\begin{aligned}\rho_{\mathcal{A}}(r_f, r'_f, t) = \int dr_i dr'_i d\mathbf{z} d\mathbf{z}^* W_0(\mathbf{z}, \mathbf{z}^*)\rho_{\mathcal{A}}(r_i, r'_i) \\ \times \int \mathcal{D}[r, r', \theta, \theta'] \mathrm{e}^{i(S_{\mathcal{A}}[r,\theta] - S_{\mathcal{A}}[r',\theta'])} \mathrm{e}^{i\tilde{\mathcal{R}}[r,r',\mathbf{z},\mathbf{z}^*]}.\end{aligned} \tag{4.11}$$

Here we have introduced the Wigner function of the environment $W_0(\mathbf{z}, \mathbf{z}^*)$, with position $\mathbf{r}_i$ and momentum $\mathbf{p}_i$, through $\mathbf{z} = \mathbf{r}_i + i\mathbf{p}_i$. The bare action of the system $\mathcal{A}$ can be read from Eq. (4.6) as $S_{\mathcal{A}} = \int_0^t ds\ (\dot{r}(s)\theta(s) - H_{\mathcal{A}}(r, \theta))$, and the new effective action involves

forward and backward paths in the form

$$\begin{aligned}\tilde{\mathcal{R}} = \sum_{k=1}^{\mathcal{N}} \Bigg( & -\frac{\gamma_k}{2\sqrt{2}} \int_0^t ds \, \big(r(s) - r'(s)\big)\big(z_k \mathrm{e}^{-i\omega_k s} + z_k^* \mathrm{e}^{i\omega_k s}\big) \\ & + \frac{\gamma_k^2}{4} \int_0^t ds \int_0^s du \, \Big(r(s)r'(u) - r(u)r'(s) + r(s)r(u) \\ & - r'(s)r'(u) + 2N\big(r(s) - r'(s)\big)\Big) \sin\omega_k(s-u) \\ & - \frac{\gamma_k^2}{2\omega_k} \int_0^t ds \, \Big(r(s) - r'(s)\Big)\Big(\frac{r(s) + r'(s)}{2} + N\Big)\Bigg).\end{aligned} \tag{4.12}$$

Finally, we change coordinates to $y = r - r'$ and $R = (r + r')/2$, in order to obtain

$$\begin{aligned}\tilde{\mathcal{R}} = \sum_{k=1}^{\mathcal{N}} \Bigg( & -\frac{\gamma_k}{2\sqrt{2}} \int_0^t ds \, y(s)(z_k \mathrm{e}^{-i\omega_k s} + z_k^* \mathrm{e}^{i\omega_k s}) \\ & - \frac{\gamma_k^2}{2\omega_k} \int_0^t ds \int_0^s du \, y(s)\dot{R}(u) \cos\omega_k(s-u) \\ & - \frac{\gamma_k^2}{2\omega_k} \int_0^t ds \, y(s)\big(N + R(0)\big) \cos\omega_k s \Bigg),\end{aligned} \tag{4.13}$$

where an integration by parts has been used. The double integral in Eq. (4.13) gives a contribution to the equations of motion of the diagonal coordinate $R$, which reads

$$\frac{\delta}{\delta y(s)} \int_0^t ds \int_0^s du \, y(s)\dot{R}(u) \cos\omega_k(s-u) = \int_0^s du \, \dot{R}_c(u) \cos\omega_k(s-u), \tag{4.14}$$

yielding a causal, history-dependent term, associated to dissipation of energy (compare to Eq. (4.9)). Thus, the trace operation involving the final states of the uncontrollable environment transforms the original boundary problem, with its associated time invariance, into a problem compatible with initial conditions, breaking the time invariance. It is important to note that this result is independent of the initial state of the environment. Moreover, the partial-trace operation may be understood as a *coarse-grained* quantum channel [120], which corresponds to a lack of information about the composite system, reducing the total degrees of freedom, and in this context, yielding an effective irreversible dynamics (dissipation), for large $\mathcal{N}$. In appendix A we show that an equation of motion with broken time-reversal symmetry is indeed a consequence of the properties and symmetries of the Feynman-Vernon influence functional, regardless of any details of the subsystems.

Due to the total particle number conservation, we can take the semiclassical limit in Eq. (4.11), for large $N$ in the central BH system [121]. Let us forget for a moment about the first line in the effective action Eq. (4.13), which depends on the initial environmental

state. With all this, from Eq. (4.11) we read the total action

$$\begin{aligned}\Phi \equiv & S_{\mathcal{A}} - S'_{\mathcal{A}} + \tilde{\mathcal{R}} = (\theta_R y)\big|_0^t - \int_0^t ds\Big(y(s)\dot{\theta}_R(s) - \dot{R}(s)\theta_y(s)\Big) \\ & - \int_0^t ds\Big(H_{\mathcal{A}}(R+y/2,\theta_R+\theta_y/2) - H_{\mathcal{A}}(R-y/2,\theta_R-\theta_y/2)\Big) \\ & - \frac{1}{2}\int_0^t ds(R(0)+N)y(s)\gamma(s) - \frac{1}{2}\int_0^t ds\int_0^s du\; y(s)\dot{R}(u)\gamma(s-u),\end{aligned} \tag{4.15}$$

where the conjugate variable to $y$ is defined, $\theta_y = \theta - \theta'$, and similarly the conjugate to $R$, as $\theta_R = (\theta+\theta')/2$. We also have introduced the damping function

$$\gamma(s) = \int_0^\infty d\omega \frac{J(\omega)}{\pi\omega}\cos\omega s, \tag{4.16}$$

in terms of the *spectral density* of the environment $J(\omega) = \pi\sum_{k=1}^{\mathcal{N}}\gamma_k^2\delta(\omega-\omega_k)$. The first step to obtain the semiclassical approximation to Eq. (4.11) consists in expanding the action Eq. (4.15) around the diagonal $R(s)$, considering *small variations* in $(y(s),\theta_y(s))$. That means, we want to investigate the evolution of the system around the diagonal. Doing so, from the expansion

$$\begin{aligned}& H_{\mathcal{A}}(R+y/2,\theta_R+\theta_y/2) - H_{\mathcal{A}}(R-y/2,\theta_R-\theta_y/2) \\ & \quad = \frac{\partial H_{\mathcal{A}}(R,\theta_R)}{\partial R}y + \frac{\partial H_{\mathcal{A}}(R,\theta_R)}{\partial\theta_R}\theta_y + \mathcal{O}(y^3,\theta_y^3),\end{aligned} \tag{4.17}$$

we neglect higher than second-order terms, and as a further step we re-scale the diagonal and relative coordinates with the total number of particles, according to $R \to NR$, $y \to Ny$. The re-scaled variables belong to the interval of values $-1 \le R \le 1$, and $-2 \le y \le 2$. Crucially, as discussed in [121] for the closed HB model, when acting on a Fock-state of $N$ particles the creation and annihilation operator involved in the dimmer each gain a prefactor of the order $\mathcal{O}(\sqrt{N})$. Thus, by increasing the number of particles terms like $\hat{b}^\dagger\hat{b}$ in Eq. (4.2) scale as $N$, while the interaction term proportional to $g$ ($\hat{N}^2$) scales as $N^2$. In this case, in the limit $N\to\infty$ the interaction terms governs the system dynamics, yielding either a Mott insulating or a clustering state. To avoid this scenario we demand the on-site interaction strength $g$ scales as $1/N$. Similarly, in order to obtain an action which scales as $N$, we also need to impose the requirement that the damping parameter $\gamma(s)$ scales as $1/N$. With all these considerations, we arrive at the "quasi-classical (qc)" action

$$\begin{aligned}\Phi = & N(\theta_R y)\big|_0^t + N\int_0^t ds\;\theta_y(s)\Big(\dot{R}(s) - \frac{\partial H_{\mathcal{A}}(R,\theta_R)}{\partial\theta_R}\Big) \\ & - N\int_0^t ds\;y(s)\Bigg(\dot{\theta}_R(s) + \frac{\partial H_{\mathcal{A}}(R,\theta_R)}{\partial R} + \frac{1}{2}(R(0)+1)\gamma(s) \\ & + \frac{1}{2}\int_0^s du\;\dot{R}(u)\gamma(s-u)\Bigg) \to \frac{1}{\hbar_e}\Phi_{qc},\end{aligned} \tag{4.18}$$

from which we identify $1/N \equiv \hbar_e$ as an *effective Planck constant* that controls the semiclassical limit, $N \to \infty$. Observe that Eq. (4.18) does not include yet the first term in Eq. (4.13). The usual procedure, as studied also in section 1.2.2, consists in choosing a canonical initial state for $\mathcal{E}$ at given inverse temperature $\beta$, such that its Wigner function reads

$$W_0(\mathbf{z}, \mathbf{z}^*) = \prod_{k=1}^{\mathcal{N}} \frac{1}{\pi} \tanh\Big(\frac{\beta\omega_k}{2}\Big) \mathrm{e}^{-\tanh\left(\frac{\beta\omega_k}{2}\right)|z_k|^2}. \tag{4.19}$$

Inserting Eqns. (4.19,4.18) into Eq. (4.11), and integrating the variables $\mathbf{z}$, we obtain

$$\begin{aligned}\rho^{qc}_{\mathcal{A}}(R_f, y_f, t) = \int dR_i dy_i\ \rho_{\mathcal{A}}(R_i, y_i) \int \mathcal{D}[R, \theta_R]\mathcal{D}[y, \theta_y] \\ \times \mathrm{e}^{\frac{i}{\hbar_e}\Phi_{qc}[R,\theta_R,y,\theta_y]} \mathrm{e}^{-\frac{1}{\hbar_e}\mathcal{R}_d[y]},\end{aligned} \tag{4.20}$$

where the *decoherence* action $\mathcal{R}_d$, quadratic in $y$, is given by

$$\mathcal{R}_d = \int_0^t ds \int_0^s du\ y(s)y(u)\mathcal{K}(s-u), \tag{4.21}$$

with the temperature-dependent kernel

$$\mathcal{K}(s) = \int_0^\infty d\omega\ \frac{J(\omega)}{\pi} \coth\left(\frac{\beta\omega}{2}\right) \cos\omega s. \tag{4.22}$$

As can be seen from Eq. (4.20), this action is responsible for the extinction of the relative coordinates (coherences), acting as a Gaussian filter (noise) that prevents excursions far away from the diagonal. In this scenario, we showed in chapter 1 that it is possible to integrate out the "noise" paths $(y, \theta_y)$ in Eq. (4.20), thus obtaining a generalized Lagnevin equation for the classical diagonal motion, which consists of the dissipative part plus a fluctuating force determined by the noise. We may integrate the paths $\theta_y$ in Eq. (4.20), yielding a delta functional (up to a normalization constant)

$$\begin{aligned}\rho^{qc}_{\mathcal{A}}(R_f, y_f, t) = \int dR_i dy_i\ \rho_{\mathcal{A}}(R_i, y_i) \int \mathcal{D}[R, \theta_R]\mathcal{D}[y] \\ \times\ \delta\Big(\dot{R}(s) - \frac{\partial H_{\mathcal{A}}(R, \theta_R)}{\partial \theta_R}\Big) \mathrm{e}^{\frac{i}{\hbar_e}\Phi_{qc}[R,\theta_R,y,]} \mathrm{e}^{-\frac{1}{\hbar_e}\mathcal{R}_d[y]},\end{aligned} \tag{4.23}$$

which imposes a restriction on the paths $R(s), \theta_R(s)$. Taking into account this delta functional, and varying the action with respect to the relative coordinate $y$, yield the equations of motion

$$\begin{aligned}&\dot{\theta}_R(s) + \frac{\partial H_{\mathcal{A}}(R, \theta_R)}{\partial R} + \frac{1}{2}(R(0)+1)\gamma(s) + \frac{1}{2}\int_0^s du\ \dot{R}(u)\gamma(s-u) = i\int_0^t du\ y(u)\mathcal{K}(s-u), \\ &\dot{R}(s) - \frac{\partial H_{\mathcal{A}}(R, \theta_R)}{\partial \theta_R} = 0.\end{aligned} \tag{4.24}$$

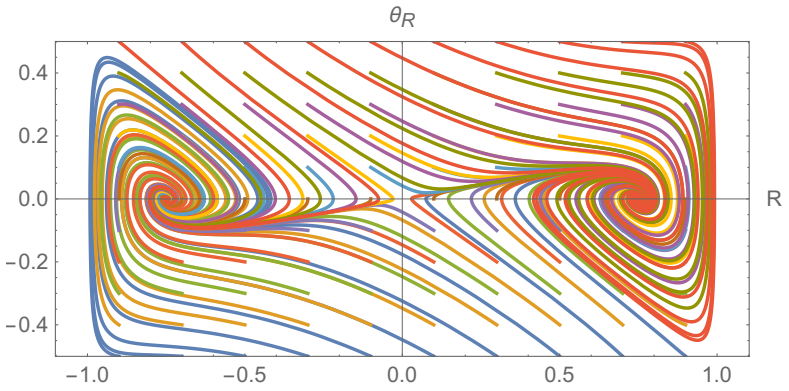


Figure 4.1: Phase-space portrait of the classical evolution from Eq. (4.24), for an Ohmic spectral density, with damping $\gamma = 0.5$, and system parameter $g/h = -3$. In this regime there are two attractors, where, depending on initial conditions, a trajectory will end up for long times, in virtue of the dissipation process.

Notice that these are equations compatible with *initial data*. The first is a complex equation, but in cases where we are interested only in the classical (diagonal) evolution, setting $y = 0$, gives a history-dependent dissipative term, as discussed already in Eq. (4.14). This term is responsible for the relaxation process of the system. The stationary points are given by $(R = 0, \theta_R = \pi n/2)$, and $(R = \pm\sqrt{\alpha^2 - 4}/\alpha, \theta_R = \pi n/2)$, with $n = 0, \pm 1, ...$, and the system interaction parameter $\alpha = g/h$. Figure. 4.1 shows the phase-space portrait for the diagonal motion in Eq. (4.24), for an Ohmic spectral density in the continuum of environmental modes, $J(\omega) = 2\gamma\omega$, and for the choice of parameters $\alpha = -3$, $\gamma = 1/2$. Depending on the initial condition, a trajectory will end up in one of the two attractors shown in the figure, determined by the stationary points. We emphasize that the superscript $(qc)$ in Eq. (4.20) refers to the approximation which led to the action $\Phi_{qc}$. Finally, evaluating Eq. (4.23) along the classical diagonal paths, Eq. (4.24), or setting $y(s) = 0$, the action vanishes. The vanishing of the action evaluated along the classical solutions for $R$ makes the search for interference effects in dissipative systems a difficult task.

## 4.3. System coupled to a microcanonical environment

In chapter 2 we have investigated how, if starting from the fundamental microcanoncial distribution, a generalized concept of temperature can be derived for strongly coupled systems. This rises the question about which new features could emerge if a system is coupled to an environment initially in a microcanonical state. In the previous sections we learned that the dissipation process of the system $\mathcal{A}$ is independent of the initial state of $\mathcal{AE}$. This process depends only on the interaction Hamiltonian, which defines the dynamical observable *monitored* by the environment. On the other hand, the decoherence or noise action in Eq. (4.21), depends strongly on the initial state, and in particular,

propagating a canonical thermal state produces a pure temperature-dependent decoherence contribution. However, as shown below, setting the initial state microcanonical transforms the kernel in Eq. (4.21) into a complex quantity, allowing the possibility to observe interference effects. Thus, let us start considering at $t = 0$, $\hat{\rho}^0_{\mathcal{E}}(E)$ a microcanonical state at a given energy $E$,

$$\hat{\rho}^0_{\mathcal{E}}(E) = \frac{\delta(E - \hat{H}_{\mathcal{E}})}{\mathcal{G}_{\mathcal{E}}(E)}, \tag{4.25}$$

with the density of states $\mathcal{G}_{\mathcal{E}}(E) = \mathrm{Tr}_{\mathcal{E}}\, \delta(E - \hat{H}_{\mathcal{E}})$. Following similar steps as in chapter 2, the microcanonical state can be obtained through an inverse Laplace transform of Eq. (4.19) for complex values $\beta = i\tau$, such that the Wigner function of $\hat{\rho}^0_{\mathcal{E}}(E)$ reads (see Eq. (2.12))

$$W_0(\mathbf{z}, \mathbf{z}^*, E) = \frac{1}{2\pi \mathcal{G}_{\mathcal{E}}(E)} \int_{-\infty}^{\infty} d\tau\, \mathrm{e}^{i\tau E} \mathrm{e}^{\log Z_{\mathcal{E}}(i\tau)} W_0(\mathbf{z}, \mathbf{z}^*, i\tau), \tag{4.26}$$

where $W_0(\mathbf{z}, \mathbf{z}^*, i\tau)$ represents Eq. (4.19) evaluated at $\beta = i\tau$, and $Z_{\mathcal{E}}(i\tau) = \mathrm{Tr}_{\mathcal{E}}[e^{-i\tau \hat{H}_{\mathcal{E}}}]$. We now insert Eqns. (4.26,4.18) into Eq. (4.11), taking into account the first term in Eq. (4.13). Further, integrating the variables $(\mathbf{z}, \mathbf{z}^*)$, and the $(\theta_R, \theta_y)$ variables, we obtain, up to a Jacobian, the important result

$$\begin{aligned} \rho^{qc}_{\mathcal{A}}(R_f, y_f, t) = \frac{1}{2\pi \mathcal{G}_{\mathcal{E}}(E)} \int_{-\infty}^{\infty} d\tau\, \mathrm{e}^{i\tau E} \mathrm{e}^{\log Z_{\mathcal{E}}(i\tau)} \\ \times \sqrt{2\pi\hbar_e} \int dR_i dy_i\, \rho_{\mathcal{A}}(R_i, y_i) \int \mathcal{D}[R]\mathcal{D}[y] \times \delta\Big(\dot{R}(s) - \frac{\partial H_{\mathcal{A}}(R, \theta_R)}{\partial \theta_R}\Big) \mathrm{e}^{\frac{i}{\hbar_e}\Sigma[R,y]}. \end{aligned} \tag{4.27}$$

Here the action reads

$$\begin{aligned} \Sigma = (\theta_R[R]y)\big|_0^t - \int_0^t ds\, y(s) \Bigg( \dot{\theta}_R\big(R(s), \dot{R}(s)\big) + \frac{\partial H_{\mathcal{A}}}{\partial R} + \frac{1}{2}(R(0) + 1)\gamma(s) \\ + \frac{1}{2} \int_0^s du\, \dot{R}(u)\gamma(s-u) + \frac{1}{2} \int_0^t du\, y(u) \mathcal{K}_\tau(s-u) \Bigg), \end{aligned} \tag{4.28}$$

where now $\theta_R[R(s), \dot{R}(s)]$ is a functional of each trajectory $R(s)$, imposed by the delta in Eq. (4.27). The $\tau$-dependent kernel is given by

$$\mathcal{K}_\tau(s) = \int_0^\infty d\omega\, \frac{J(\omega)}{\pi} \cot\left(\frac{\tau\omega}{2}\right) \cos \omega s. \tag{4.29}$$

An explicit evaluation of the $\omega$ integral in Eq. (4.29) for complex values of $\tau$ is given in appendix B. On the other hand, the resulting path integrals in Eq. (4.27) involve diagonal trajectories $R$, and *small* relative trajectories $y$, with $R(0) = R_i,\ R(t) = R_f$ and $y(0) = y_i,\ y(t) = y_f$. Similarly to Eq. (4.24), taking into account the delta functional,

variations of Eq. (4.28) with respect $y$ yield

$$\begin{aligned}\dot{\theta}_R(s) + \frac{\partial H_{\mathcal{A}}}{\partial R} + \frac{1}{2}(R(0)+1)\gamma(s) + \frac{1}{2}\int_0^s du\ \dot{R}(u)\gamma(s-u) = -\int_0^t du\ y(u)\mathcal{K}_\tau(s-u),\\ \dot{R}(s) - \frac{\partial H_{\mathcal{A}}(R,\theta_R)}{\partial \theta_R} = 0.\end{aligned} \tag{4.30}$$

While variation of the action with respect to $R$ gives

$$\begin{aligned}\ddot{y}(s)\frac{\partial \theta_R}{\partial \dot{R}} + \dot{y}(s)\Big(\frac{d}{ds}\frac{\partial \theta_R}{\partial \dot{R}} - \frac{\partial \theta_R}{\partial R}\Big) + y(s)\frac{\partial^2 H_{\mathcal{A}}}{\partial R^2}\\ + \frac{1}{2}y_f\gamma(t-s) - \frac{1}{2}\int_s^t du\ \dot{y}(u)\gamma(s-u) = 0.\end{aligned} \tag{4.31}$$

Observe that Eq. (4.31) corresponds to a dissipative equation for $y$, but for the time-reversed evolution, and being a second-order linear differential equation, has a unique solution given the boundary conditions. In particular, for $y_i = y_f = 0$, $y$ vanishes. Thus, for every classical trajectory $R_\alpha$ there exists an associated solution $y[R_\alpha]$ with the given boundary conditions, satisfying the system of Eqns. (4.30,4.31). Notice that the path $y$ only appears on the right-hand-side in the first Eq. (4.30). Thus, a further simplification consists in solving Eq. (4.30) for $R$, neglecting the right-hand-side, obtaining in this way dissipative real classical paths $R_\alpha$, fulfilling the boundary conditions. Then, inserting $R_\alpha$ into Eq. (4.31) yields classical real paths $y[R_\alpha]$, carrying information about the dissipative solutions $R_\alpha$.
With all these considerations, finally, for a large number of particles, $\hbar_e \to 0$, we solve Eq. (4.27) by SPA and obtain the semiclassical ($sc$) result

$$\begin{aligned}\rho^{sc}_{\mathcal{A}}(R_f, y_f, t) =& \frac{1}{2\pi \mathcal{G}_{\mathcal{E}}(E)}\int_{-\infty}^{\infty} d\tau\ \mathrm{e}^{i\tau E}\mathrm{e}^{\log Z_{\mathcal{E}}(i\tau)}\\ &\times \sqrt{2\pi\hbar_e}\int dR_i dy_i\ \rho_{\mathcal{A}}(R_i, y_i) \sum_{\alpha:\ R_i, y_i \to R_f, y_f} A_\alpha \mathrm{e}^{\frac{i}{\hbar_e}\Sigma_\alpha}.\end{aligned} \tag{4.32}$$

The action evaluated along the classical paths reads

$$\Sigma_\alpha = (\theta_R[R_\alpha]y[R_\alpha])\big|_0^t + \frac{1}{2}\int_0^t ds \int_0^t du\ y[R_\alpha(s)]\mathcal{K}_\tau(s-u)y[R_\alpha(u)], \tag{4.33}$$

and $A_\alpha$ denotes the fluctuations of $R$ and $y$ along their classical solutions. Formally,

$$A_\alpha = \int \mathcal{D}[\delta R]\mathcal{D}[\delta y]\ \mathrm{e}^{\frac{i}{2\hbar_e}\delta^2\Sigma[R_\alpha, \delta R, y_\alpha, \delta y]}. \tag{4.34}$$

A complete calculation and analysis of $A_\alpha$ is work in progress.
In summary, allowing the relative paths to be small but different from zero, they *carry information about each diagonal path*, and thus, Eq. (4.32) reveals in principle *interference* between different dissipative trajectories $R_\alpha$. One should remember, however, that

we still need to solve the $\tau$-integral in Eq. (4.32). We may solve this integral, as shown in chapter 2, by SPA in the thermodynamic limit, for a large number of particles in $\mathcal{E}$, using a contour on the lower-half of the complex $\tau$-plane. This contour is required to guarantee the analyticity of $\mathrm{e}^{\log Z_{\mathcal{E}}(i\tau)} = \mathrm{Tr}\,\mathrm{e}^{-i\tau\hat{H}_{\mathcal{E}}}$ [49], and the saddle-point on the imaginary $\tau$-axis was identified in chapter 2 as the emergent temperature. If the saddle-point has only a pure imaginary value, then Eq. (4.33) yields a decaying contribution (decoherence) in Eq. (4.32). It is interesting, however, to investigate in this context the role of complex saddle-points, since they produce an oscillatory (interference) contribution in Eq. (4.33). Actually, the oscillatory part in the trace of the propagator plays an important role in spectral statistics [28, 84, 122], and even though in the thermodynamic limit these oscillatory contributions may be hard to visualize, in the present context they deserve more attention. Particularly, for strongly coupled systems, we have seen in chapter 2 that the non-vanishing interaction energy leads to a coupling-dependent notion of temperature. There the eventual appearance of complex saddle-points was not of interest, because we were only interested in real temperatures. However, in the current scenario this possibility may play an important role. For instance, initializing the global $\mathcal{AE}$ system in a microcanonical state, like that in Eq. (2.15), would yield a term $\mathrm{e}^{\log Z_{\mathcal{AE}}(i\tau)}$ which now takes into account the interaction between the subsystems. Accordingly, solving by SPA the $\tau$ integral in Eq. (4.32) would give as a result an equation of the form in Eq. (2.22), which may have complex saddle-points. This initial state, however, produces in the reduced density matrix of the system an extra path integral over complex paths [47], which admittedly, in general could be prohibitive difficult to solve. Future work will investigate this possibility more extensively.

## 4.4. Summary

We have studied the path integral approach of a two-site Bose-Hubbard model, with one of its sites coupled to an environment. The dissipation process in the semiclassical limit has been analyzed in great detail, where it was shown how considering the final states of the uncontrollable environment as unknown (trace operation), is the clue to understanding the dynamical emergence of irreversibility in dissipative processes, much in the same way that ignoring the environmental degrees of freedom is the clue to understanding the emergence of classical robust states, as shown in chapter 1. Further, using the ideas developed in chapter 2, we have considered the effect of an environment initially in a microcanonical, instead of the usual canonical state, and shown in this scenario the possibility to observe interference between different dissipative classical trajectories, in the semiclassical limit of a large number of particles within the central system, a phenomenon that is notoriously hard to produce. We hope these results may open a new direction in the study of open quantum systems with microcanonical environments.

# 5. Semiclassical analysis of work statistics

The interplay between quantum phenomena and classical thermodynamics is an important area in the study of work and energy exchange on small quantum systems [123–127]. The semiclassical methods studied so far in this thesis are quite suitable to handle these problems, in virtue of the possibility to use classical information in order to see interference effects. In this chapter we propose a semiclassical approach to quantum work distribution, which allows in principle to study quantum interference phenomena. This is a work still in progress and we hope the results obtained here may help to push forward studies into this fascinating direction. Sections 5.1 and 5.2 are intended to review main concepts related with work distribution, including classical and quantum fluctuation relations. This will settle the ground for section 5.3, where a path integral formalism for work is investigated, suitable for semiclassical analysis. Finally, in the last sections we develop, using the van Vleck-Gutzwiller formalism, a semiclassical approach to the characteristic function of work, for closed and open systems, and study the quantum-classical correspondence. The chapter closes with some concluding remarks and discussions of open problems faced in this approach.

## 5.1. Classical relations

We consider in this chapter the response of a classical and quantum system, due to the action of an external classical force. This process can be characterized by the change of energy contained in the system, we consider therefore non-autonomous systems. That is, we deal here with a classical system with a Hamiltonian of the form

$$H(\mathbf{x}, \lambda_t) = H_0(\mathbf{x}) - \lambda_t \, Q(\mathbf{x}), \tag{5.1}$$

with $\mathbf{x} = (\mathbf{q}, \mathbf{p})$, and a given time-dependent *force protocol* $\lambda_t$, acting on the system during the time interval $[0, \tau]$. The time evolution of the system is given by Hamilton's equations of motion Eq. (3.2). To each initial point in phase-space $\mathbf{x}_0$ we assign accordingly a point $\mathbf{x}_t$ at $t \in [0, \tau]$, specified by the value of the force protocol, organized in their order of appearance within the time span

$$\mathbf{x}_t = \varphi_{t,0}[\mathbf{x}_0, \lambda]. \tag{5.2}$$

The flow $\varphi$ is then a function of the initial condition $\mathbf{x}_0$ and a *functional* of the force protocol $\lambda$. We assume $H_0$ to be time-reversal invariant, and that $Q(\mathbf{x})$ has a defined parity, namely $\varepsilon_Q = \pm 1$.
It is important now to introduce the principle of *microreversibility*, obeyed by non-autonomous systems, such that the flow under the backward protocol $\tilde{\lambda}_t = \lambda_{\tau - t}$, is

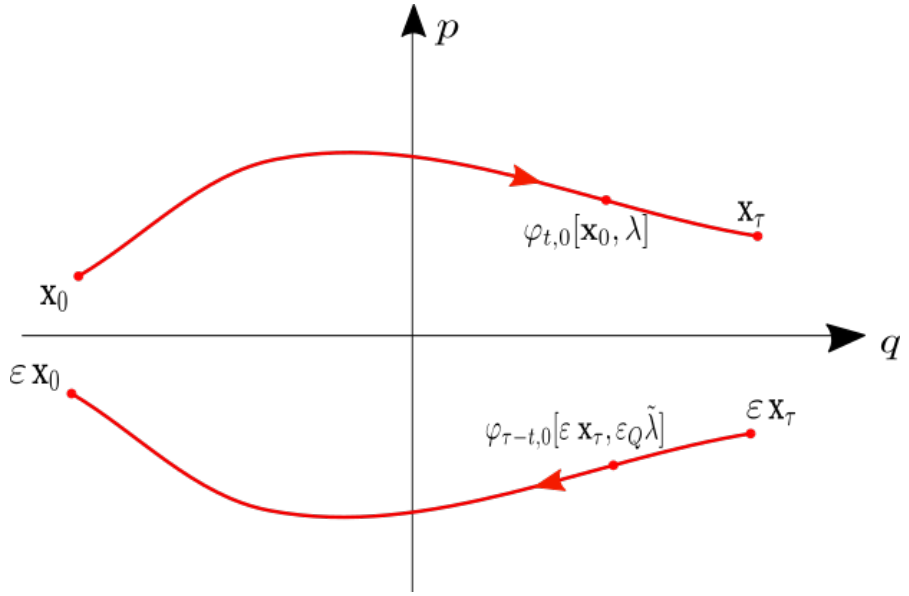


Figure 5.1: Diagram of the microreversibility principle showing the relation between a point at time $t$, evolved from $t = 0$, with the Hamiltonian flow in the forward force protocol, $\varphi_{t,0}[\mathbf{x}_0, \lambda]$, and the point evolved with the reversed protocol, from $t = \tau$, $\varphi_{\tau-t,0}[\varepsilon\ \mathbf{x}_\tau, \varepsilon_Q\tilde{\lambda}]$. The arrows on the trajectories show the direction of time.

related to the flow under the forward protocol $\lambda_t$, like

$$\varphi_{t,0}[\mathbf{x}_0, \lambda] = \varepsilon\ \varphi_{\tau-t,0}[\varepsilon\ \mathbf{x}_\tau, \varepsilon_Q\tilde{\lambda}]. \tag{5.3}$$

Above $\varepsilon\ \mathbf{x} = \varepsilon\ (\mathbf{q}, \mathbf{p}) = (\mathbf{q}, -\mathbf{p})$ is the time-reversal operation, as illustrated in Fig. 5.1. This principle establishes the possibility to reverse the evolution of a process even for non-autonomous dynamics, by reversing the force protocol. Let us consider a phase-space function $B(\mathbf{x})$, such that $B(\varepsilon\mathbf{x}) = \varepsilon_B B(\mathbf{x})$, with $\varepsilon_B = \pm 1$. Its temporal evolution is given by

$$B_t = B(\varphi_{t,0}[\mathbf{x}_0, \lambda]). \tag{5.4}$$

Now, if we choose different initial conditions $\mathbf{x}_0$, then different trajectories $B_t$ are realized. For example, assume at $t = 0$ the system is prepared in a Gibbs equilibrium state, such that the initial conditions are sampled from the distribution

$$\rho_0(\mathbf{x}_0) = \frac{\mathrm{e}^{-\beta H_0(\mathbf{x}_0)}}{Z_0}, \tag{5.5}$$

with the partition function $Z_0 = \int d\mathbf{x}_0\ \mathrm{e}^{-\beta H_0(\mathbf{x}_0)}$, and inverse temperature $\beta$. In this way, the trajectory $B_t$ becomes a *random quantity.*

Let us introduce

$$W_0[\mathbf{x}_0, \lambda] = \int_0^\tau dt\ \lambda_t \dot{Q}_t, \tag{5.6}$$

known as *exclusive work*, which is a function of $\mathbf{x}_0$, through $Q_t = Q(\varphi_{t,0}[\mathbf{x}_0, \lambda])$, and a functional of the force protocol $\lambda$. The dot represents derivation with respect to time. Using Eq. (5.1) we see that the total derivative with respect to time of the full Hamiltonian is given by $\frac{dH}{dt} = -\dot{\lambda}_t Q(\mathbf{x})$. Thus we obtain

$$\frac{d}{dt}H_0(\mathbf{x}_t) = \frac{d}{dt}\big(H + \lambda_t Q\big) = \lambda_t \dot{Q}(\mathbf{x}_t). \tag{5.7}$$

And in this way Eq. (5.6) becomes

$$W_0[\mathbf{x}_0, \lambda] = \int_0^\tau dt\ \lambda_t \dot{Q}_t = H_0(\mathbf{x}_\tau[\mathbf{x}_0, \lambda]) - H_0(\mathbf{x}_0), \tag{5.8}$$

namely, the difference of the energy associated to the bare Hamiltonian $H_0$, refereed accordingly, as its internal energy. The forces affect the system's energy by moving the system from one region of phase-space to another region, but the forces itself do not appear in the definition of the system's energy.

An alternative approach consists in considering the full Hamiltonian as the energy of the system. Then the energy landscape changes with time as we manipulate the forces $\lambda_t$. In this case it is appropriate to define the *inclusive work* $W$, by

$$\begin{aligned} W[\mathbf{x}_0, \lambda] = &- \int_0^\tau dt\ \dot{\lambda}_t Q(\mathbf{x}_t) = \int d\lambda_t \frac{\partial H}{\partial \lambda_t} \\ &= H(\mathbf{x}_\tau, \lambda_\tau) - H(\mathbf{x}_0, \lambda_0). \end{aligned} \tag{5.9}$$

Now, let us assume an ensemble of Hamiltonian trajectories $\mathbf{x}_t$. This ensemble evolves in phase-space, with a density given by [128]

$$f(\mathbf{x}, t) = \langle \delta(\mathbf{x} - \mathbf{x}_t) \rangle\,, \tag{5.10}$$

where the angular bracket denotes the ensemble average. The density $f$ obeys the Louville equation

$$\frac{\partial f}{\partial t} = \big\{H, f\big\}, \tag{5.11}$$

with the Poisson brackets $\big\{A, B\big\} = \partial A/\partial \mathbf{q} \cdot \partial B/\partial \mathbf{p} - \partial A/\partial \mathbf{p} \cdot \partial B/\partial \mathbf{q}$. In general, Eq. (5.11) does not have a simple solution, for example, if the dynamics is chaotic. We can calculate the work in Eq. (5.6) for each trajectory $\mathbf{x}_t$ in the ensemble, ending at a given time $t$. Since $\dot{Q}_t = \big\{Q_t, H\big\}$, we obtain

$$\begin{aligned} W_0(t) = \int_0^t du\ \lambda_u \big\{Q_u, H\big\} &= \int_0^t du\ \big\{\lambda_u Q_u, H_0 - \lambda_u Q_u\big\} \\ &= \int_0^t du\ \big\{\lambda_u Q_u, H_0\big\}. \end{aligned} \tag{5.12}$$

On the other hand, let us consider the following *weighted* phase-space density

$$g_0(\mathbf{x}, t) = \langle \delta(\mathbf{x} - \mathbf{x}_t) \mathrm{e}^{-\beta W_0(t)} \rangle\,. \tag{5.13}$$

From which we obtain

$$\frac{\partial g_0}{\partial t} = \big\{H, g_0\big\} - \beta g_0 \big\{\lambda_t Q_t, H_0\big\}. \tag{5.14}$$

If we start from an ensemble initially prepared in an *equilibrium* state $\rho^{eq}$, and since $W_0(0) = 0$, then

$$g_0(\mathbf{x}, 0) = f(\mathbf{x}, 0) = \rho^{eq}(\mathbf{x}, \lambda_0), \tag{5.15}$$

and thus the solution to Eq. (5.14) is *stationary*

$$g_0(\mathbf{x}, t) = \frac{\mathrm{e}^{-\beta H_0(\mathbf{x})}}{Z(\lambda_0)} = \rho^{eq}(\mathbf{x}, \lambda_0), \tag{5.16}$$

with $Z(\lambda_t) = \int d\mathbf{x}\, \mathrm{e}^{-\beta H(\mathbf{x},\lambda_t)}$. This means that even if $f(\mathbf{x}, t)$ is a complicated function of time, like in chaotic dynamics, the weighted density $g_0(\mathbf{x}, t)$ is stationary, if we start from an equilibrium distribution. A similar expression can be derived for the inclusive work, by setting

$$W(t) = -\int_0^t du\ \dot{\lambda}_u Q_u, \tag{5.17}$$

and defining the weighted density

$$g(\mathbf{x}, t) = \left\langle \delta(\mathbf{x} - \mathbf{x}_t) \mathrm{e}^{-\beta W(t)} \right\rangle. \tag{5.18}$$

And for an equilibrium initial state $g(\mathbf{x}, 0) = f(\mathbf{x}, 0) = \rho^{eq}(\mathbf{x}, \lambda_0)$, one obtains [128]

$$g(\mathbf{x}, t) = \frac{1}{Z(\lambda_0)} \mathrm{e}^{-\beta H(\mathbf{x},\lambda_t)} = \frac{Z(\lambda_t)}{Z(\lambda_0)} \rho^{eq}(\mathbf{x}, \lambda_t), \tag{5.19}$$

which is not constant, but proportional to the equilibrium distribution corresponding to the value of $\lambda$ at time $t$. In summary we have then

$$\begin{aligned} \left\langle \delta(\mathbf{x} - \mathbf{x}_t) \mathrm{e}^{-\beta W_0(t)} \right\rangle &= \rho^{eq}(\mathbf{x}, \lambda_0) \\ \left\langle \delta(\mathbf{x} - \mathbf{x}_t) \mathrm{e}^{-\beta W(t)} \right\rangle &= \frac{Z(\lambda_t)}{Z(\lambda_0)} \rho^{eq}(\mathbf{x}, \lambda_t). \end{aligned} \tag{5.20}$$

Finally, evaluating Eq. (5.20) at $t = \tau$, and integrating over the phase-space we obtain

$$\begin{aligned} \left\langle \mathrm{e}^{-\beta W_0} \right\rangle &= 1 \\ \left\langle \mathrm{e}^{-\beta W} \right\rangle &= \frac{Z(\lambda_\tau)}{Z(\lambda_0)} = \mathrm{e}^{-\beta \Delta F}, \end{aligned} \tag{5.21}$$

where the free energy $F$ has been introduced. These relations, first obtained in [129], are known as the Jarzynski equalities, or non-equilibrium work theorems.

Before going further, let us study another approach which actually uses the microreversibility principle to derive the above relations. Coming back to the phase-space function $B_t$ in Eq. (5.4), we want to calculate the quantity

$$\begin{aligned} \left\langle \exp\left[\int_0^\tau ds\ u_s B_s\right] \mathrm{e}^{-\beta W_0} \right\rangle = \int d\mathbf{x}_0\ \frac{\mathrm{e}^{-\beta(H_0(\mathbf{x}_0)+W_0)}}{Z_0} \\ \times \exp\left[\int_0^\tau ds\ u_s B(\varphi_{\mathbf{s},\mathbf{0}}[\mathbf{x_0}, \lambda])\right], \end{aligned} \tag{5.22}$$

where we have introduced a test function $u_s$. It is worth noting that the last expression is a functional of the force protocol $\lambda$. Making the change of variables $\mathbf{x}_0 \to \mathbf{z}_\tau$, with unity Jacobian due to the fact that time evolution is a canonical transformation, using the work definition in Eq. (5.8), denoting $\rho_0(\mathbf{x}_0) = \frac{\mathrm{e}^{-\beta(H_0(\mathbf{x}_t)+W_0)}}{Z_0}$, and using Eq. (5.3), the last equation reads

$$\begin{aligned} &\int d\mathbf{x}_\tau \; \rho_0(\mathbf{x}_\tau) \exp\left[\int_0^\tau ds \; u_s B(\varepsilon\varphi_{\tau-\mathbf{s},\mathbf{0}}[\varepsilon\mathbf{x}_\tau, \varepsilon_{\mathbf{Q}}\tilde{\lambda}])\right] \\ &= \int d\mathbf{x'}_\tau \; \rho_0(\mathbf{x'}_\tau) \exp\left[\int_0^\tau ds \; u_{\tau-s}\varepsilon_B B(\varphi_{\mathbf{s},\mathbf{0}}[\mathbf{x'}_\tau, \varepsilon_{\mathbf{Q}}\tilde{\lambda}])\right]. \end{aligned} \tag{5.23}$$

In order to obtain the second line we use $\mathbf{x}_\tau \to \mathbf{x'}_\tau = \varepsilon\mathbf{x}_\tau$, and also $s \to \tau - s$. Finally, since $H_0$ is time-reversal invariant, then $\rho_0(\mathbf{x}) = \rho_0(\varepsilon\mathbf{x})$, and defining the time-reversed test function $\tilde{u}_t = u_{\tau-t}$, from Eqns. (5.22,5.23), we get

$$\left\langle \mathrm{e}^{\left[\int_0^\tau ds \; u_s B_s\right]} \mathrm{e}^{-\beta W_0} \right\rangle_\lambda = \left\langle \mathrm{e}^{\int_0^\tau ds \; \tilde{u}_s \varepsilon_B B_s} \right\rangle_{\varepsilon_Q\tilde{\lambda}}, \tag{5.24}$$

where now we have made explicit that the left-hand-side is governed by the time evolution of the full Hamiltonian in the presence of the forward protocol $\lambda$, and the right-hand-side is determined by the dynamics for the time-reversed protocol $\varepsilon_Q\tilde{\lambda}$. Setting $u = 0$ in Eq. (5.24), we obtain the first equation in Eq. (5.21), namely

$$\langle \mathrm{e}^{-\beta W_0} \rangle_\lambda = 1. \tag{5.25}$$

This equation establishes that the work $W_0$ done on any system, whose initial state is thermal, at inverse temperature $\beta^{-1}$, has an exponential expectation value independent of any details of the system. Actually, since $\mathrm{e}^{-\beta W_0}$ is a convex function [123], it follows that

$$\langle W_0 \rangle_\lambda \geq 0, \tag{5.26}$$

which says that, on average, a Hamiltonian system may only absorb energy, when it is perturbed out of equilibrium by an external force. This is a manifestation of the second law of thermodynamics.

Let us further define the *work probability density function* $P_0$ (PDF) as

$$P_0[W_0, \lambda] = \int d\mathbf{x}_0 \; \rho_0(\mathbf{x}_0)\delta(W_0 - H_0(\mathbf{x}_\tau) + H_0(\mathbf{x}_0)). \tag{5.27}$$

Notice that the only random quantity appearing in Eq. (5.27) is $\mathbf{x}_0$ (sampled from the initial equilibrium distribution), and the functional dependence with $\lambda$ comes from the term $\mathbf{x}_\tau = \varphi_{\tau,0}[\mathbf{x}_0, \lambda]$. By similar arguments that gave rise to Eq. (5.24), using the microreversibility principle Eq. (5.3), one can show [123]

$$\frac{P_0[W_0, \lambda]}{P_0[-W_0, \varepsilon_Q\tilde{\lambda}]} = \mathrm{e}^{\beta W_0}, \tag{5.28}$$

which is called the Bochkov-Kuzovlev work fluctuation relation [128], and says that the probability that work $W_0 > 0$ is injected into the system is larger, by a factor $\mathrm{e}^{\beta W_0}$, than the probability that the same work is being absorbed under the reversed protocol. Another manifestation of the second law of thermodynamics.

Analogously, using the inclusive work Eq. (5.9), the following relation can be obtained

$$\left\langle \mathrm{e}^{\left[\int_0^\tau ds\ u_s B_s\right]} \mathrm{e}^{-\beta W} \right\rangle_\lambda = \frac{Z(\lambda_\tau)}{Z(\lambda_0)} \left\langle \mathrm{e}^{\int_0^\tau ds\ \tilde{u}_s \varepsilon_B B_s} \right\rangle_{\varepsilon_Q \tilde{\lambda}}, \tag{5.29}$$

with the reference equilibrium state on the right-hand-side of the last equation given by $\rho^\beta(\mathbf{x}, \tilde{\lambda}_0) = \rho^\beta(\mathbf{x}, \lambda_\tau)$, where $\rho^\beta(\mathbf{x}, \lambda_t) = \mathrm{e}^{-\beta H(\mathbf{x}, \lambda_t)}/Z(\lambda_t)$. And again, setting $u = 0$, the second equation in Eq. (5.21) can be derived. In the case of inclusive work, the PDF is given by

$$P[W, \lambda] = \int d\mathbf{x}_0\ \rho_0(\mathbf{x}_0, \lambda_0) \delta(W - H(\mathbf{x}_\tau, \lambda_\tau) + H(\mathbf{x}_0, \lambda_0)). \tag{5.30}$$

And for later purposes we define the *characteristic function of work*, as the Fourier transform of $P[W, \lambda]$

$$\begin{aligned} G[u, \lambda] &= \int dW \mathrm{e}^{iuW} P[W, \lambda] \\ &= \int d\mathbf{x}_0\ \mathrm{e}^{iu(H(\mathbf{x}_\tau, \lambda_\tau) - H(\mathbf{x}_0, \lambda_0))} \mathrm{e}^{-\beta H(\mathbf{x}_0, \lambda_0)} / Z(\lambda_0) \\ &= \int d\mathbf{x}_0\ \exp\left[ iu \int_0^\tau ds\ \dot{\lambda}_s \frac{\partial H(\mathbf{x}_s, \lambda_s)}{\partial \lambda_s} \right] \frac{\mathrm{e}^{-\beta H(\mathbf{x}_0, \lambda_0)}}{Z(\lambda_0)}. \end{aligned} \tag{5.31}$$

Finally, similar to Eq. (5.28), for the inclusive work the fluctuation relation reads [130]

$$\frac{P[W, \lambda]}{P[-W, \varepsilon_Q \tilde{\lambda}]} = \mathrm{e}^{\beta(W - \Delta F)}. \tag{5.32}$$

It is important to note that the non-equilibrium work theorem Eq. (5.21), as well as the fluctuation relations in Eqns. (5.28,5.32), *were obtained using only the mircoreversibility principle and the initial equilibrium state.* Similar relations are also found in the quantum case.

## 5.2. Quantum relations

Work is a process, which means that it is actually not a state of the system (its differential is not exact). In the quantum theory this implies that work can not be represented by a Hermitian operator, whose eigenvalues can be determined in a single projective measurement [131]. That is why a definition of quantum work suitable to describe a process is necessary. One common definition is the so-called *two-point measurement* definition of quantum work $w$ [131]. In the quantum scenario we deal with a system with Hamiltonian operator

$$\hat{H}(\lambda_t) = \hat{H}_0 - \lambda_t \hat{Q}. \tag{5.33}$$

Now the equilibrium state is the density matrix

$$\hat{\rho}(\lambda_t) = \mathrm{e}^{-\beta\hat{H}(\lambda_t)}/Z(\lambda_t), \tag{5.34}$$

with the partition function $Z(\lambda_t) = \mathrm{Tr}\ \mathrm{e}^{-\beta\hat{H}(\lambda_t)}$. The states are evolved according to the unitary time evolution operator $\hat{U}$, obeying the Schrödinger equation

$$i\hbar\partial_t\hat{U}_{t,0}[\lambda] = \hat{H}(\lambda_t)\hat{U}_{t,0}[\lambda], \tag{5.35}$$

with $\hat{U}_{0,0} = \hat{1}$. If at time $t = 0$ the eigenvalue $E_n^{\lambda_0}$ of $\hat{H}(\lambda_0)$, and later at $t = \tau$ the eigenvalue $E_m^{\lambda_\tau}$ of $\hat{H}(\lambda_\tau)$, are obtained, the measured *inclusive* work is defined as

$$w_{m,n} = E_m^{\lambda_\tau} - E_n^{\lambda_0}. \tag{5.36}$$

It is important to note that this definition of quantum work has an intrinsic statistical nature, due to the quantum measurement process. And accordingly, this definition can not take into account quantum interference effects in the energy basis, which are destroyed by the measurement process. The quantum work fluctuation relations also make use of the microreversibility in quantum mechanics, which takes the form [123,132]

$$\hat{U}_{t,\tau}[\lambda] = \hat{T}^\dagger\hat{U}_{\tau-t,0}[\tilde{\lambda}]\hat{T}, \tag{5.37}$$

where $\hat{T}$ is the time-reversal operator, whose action on a given state $\psi$ is $\hat{T}\psi = \psi^*$, if $\psi$ is in coordinate representation, in the absence of spin degrees of freedom. Using the group property of the time evolution operator, $\hat{U}_{t,\tau}[\lambda] = \hat{U}_{t,0}[\lambda]\hat{U}_{\tau,0}[\lambda]$, and since by definition $\hat{U}_{0,\tau}[\lambda] = \hat{U}_{\tau,0}^{-1}[\lambda]$, we can write Eq. (5.37) as

$$\hat{U}_{t,0}[\lambda]\hat{U}_{0,\tau}[\lambda] = \hat{T}^\dagger\hat{U}_{\tau-t,0}[\tilde{\lambda}]\hat{T}. \tag{5.38}$$

From which we can write, using an initial state $|i\rangle$, the following expression

$$\hat{U}_{t,0}[\lambda]\,|i\rangle = \hat{T}^\dagger\hat{U}_{\tau-t,0}[\tilde{\lambda}]\hat{T}\hat{U}_{\tau,0}[\lambda]\,|i\rangle\,. \tag{5.39}$$

Finally, denoting the evolved state at time $t$ as $|\psi_t\rangle = \hat{U}_{t,0}[\lambda]\,|i\rangle$, and the final ($t = \tau$) state as $|f\rangle = \hat{U}_{\tau,0}[\lambda]\,|i\rangle$, we arrive at the relation

$$\hat{T}\,|\psi_t\rangle = \hat{U}_{\tau-t,0}[\tilde{\lambda}]\hat{T}\,|f\rangle\,, \tag{5.40}$$

which expresses the time-reversed evolution due to the backward force protocol $\tilde{\lambda}$, in analogy with the classical case. An illustration of this is shown in Fig. 5.2. Let us suppose the system is initially prepared in the canonical state

$$\hat{\rho}(\lambda_0) = \mathrm{e}^{-\beta\hat{H}(\lambda_0)}/Z(\lambda_0). \tag{5.41}$$

At any time $t$ we can calculate the instantaneous energy eigenstates of the system as

$$\hat{H}(\lambda_t)\,|\psi_{n,\gamma}^{\lambda_t}\rangle = E_{n,\gamma}^{\lambda_t}\,|\psi_{n,\gamma}^{\lambda_t}\rangle\,, \tag{5.42}$$

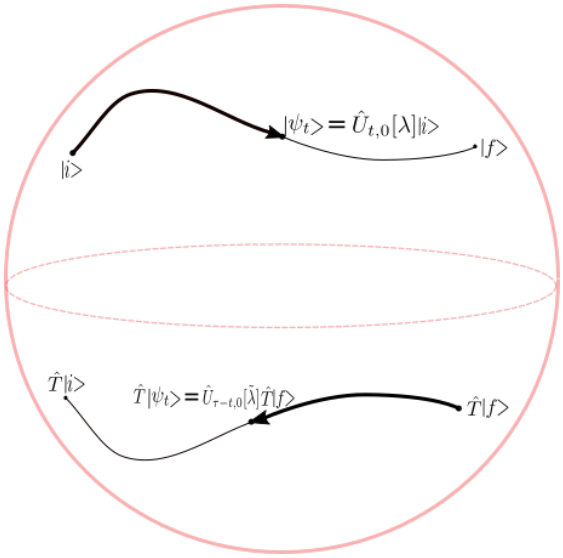


Figure 5.2: Microreversibility principle in quantum mechanics showing a quantum state, in the hypersphere with unity radius in the Hilbert space of the system, evolved by the unitary operator $\hat{U}_{t,0}[\lambda]$, according to the forward protocol, and the time-reversed state, which evolves by $\hat{U}_{\tau-t,0}[\tilde{\lambda}]$ according to the reversed protocol.

where $n$ denotes the quantum-number indexing the energy eigenstates, and $\gamma$ denotes all further quantum numbers necessary to specify an energy eigenstate. With this we can calculate the quantum work distribution as follows. At $t = 0$ the first measurement of the Hamiltonian $\hat{H}(\lambda_0)$ is performed, yielding an outcome $E_n^{\lambda_0}$, with probability [1]

$$p_n^0 = g_n \mathrm{e}^{-\beta E_n^{\lambda_0}} / Z(\lambda_0), \tag{5.43}$$

with $g_n$ representing the degeneracy of the $n$-level energy state. After the measurement the system is found to be in the state

$$\hat{\rho}_n = \frac{\hat{\Pi}_n^{\lambda_0} \hat{\rho}(\lambda_0) \hat{\Pi}_n^{\lambda_0}}{p_n^0}, \tag{5.44}$$

with the projection operator given by

$$\hat{\Pi}_n^{\lambda_0} = \sum_{\gamma} |\psi_{n,\gamma}^{\lambda_0}\rangle \langle \psi_{n,\gamma}^{\lambda_0}| . \tag{5.45}$$

At any time $t$ after the first measurement the state of the system will be determined by the unitary time evolution

$$\hat{\rho}_n(t) = \hat{U}_{t,0}[\lambda] \hat{\rho}_n \hat{U}_{t,0}^{\dagger}[\lambda]. \tag{5.46}$$

[1] Let the system be in a state $\hat{\rho}$, $\{|n\rangle\}$ be a basis, and $\hat{\Pi}_n = |n\rangle\langle n|$ the projector operator. Then if we make a (Von-Neumann) measurement in the basis, after the measurement the system will be in one of the eigenstates, say $|m\rangle$, with probability $p_m = \langle m|\hat{\rho}|m\rangle = \mathrm{Tr}[|m\rangle\langle m|\hat{\rho}]$. The final state will read $\hat{\rho}_m = |m\rangle\langle m| = \frac{\hat{\Pi}_m \hat{\rho} \hat{\Pi}_m}{\mathrm{Tr}[\hat{\Pi}_m \hat{\rho} \hat{\Pi}_m]}$. Notice that this is a non-linear operation on the state $\hat{\rho}$ [16].

Finally, at time $\tau$ a second energy measurement (of $\hat{H}(\lambda_\tau)$) is performed, which gives $E_m^{\lambda_\tau}$ with probability

$$p_{m|n}[\lambda] = \mathrm{Tr}\Big[\hat{\Pi}_m^{\lambda_\tau}\hat{\rho}_n(\tau)\Big]. \tag{5.47}$$

Then, the *probability density function* to observe the work $w$ is given by

$$P[w,\lambda] = \sum_{m,n}\delta\big(w-(E_m^{\lambda_\tau}-E_n^{\lambda_0})\big)p_{m|n}[\lambda]p_n^0. \tag{5.48}$$

One can compare this equation with Eq. (5.30) in the classical case. It is useful to define the *characteristic function of work* as

$$G[u,\lambda] = \int dw\ \mathrm{e}^{iuw}P[w,\lambda]. \tag{5.49}$$

It has been shown in [133] that Eq. (5.49) can be written as a two-point quantum correlation function, given by

$$\begin{aligned} G[u,\lambda] =& \Big\langle \mathrm{e}^{iu\hat{H}^H(\lambda_\tau)}\mathrm{e}^{-iu\hat{H}(\lambda_0)}\Big\rangle \\ =& \mathrm{Tr}\Big[\mathrm{e}^{iu\hat{H}^H(\lambda_\tau)}\mathrm{e}^{-iu\hat{H}(\lambda_0)}\mathrm{e}^{-\beta\hat{H}(\lambda_0)}\Big]/Z(\lambda_0), \end{aligned} \tag{5.50}$$

where we use the Heisenberg picture representation

$$\hat{H}^H(\lambda_\tau) = \hat{U}_{\tau,0}^\dagger[\lambda]\hat{H}(\lambda_\tau)\hat{U}_{\tau,0}[\lambda]. \tag{5.51}$$

As a further step we can write

$$\mathrm{e}^{iu\hat{H}^H(\lambda_\tau)}\mathrm{e}^{-iu\hat{H}(\lambda_0)} = \hat{\mathcal{T}}e^{iu(\hat{H}^H(\lambda_\tau)-\hat{H}(\lambda_0))}, \tag{5.52}$$

by using the time-ordered operator $\hat{\mathcal{T}}$. And in this way Eq. (5.50) can be written as

$$\begin{aligned} G[u,\lambda] =& \mathrm{Tr}\Big[\hat{\mathcal{T}}e^{iu(\hat{H}^H(\lambda_\tau)-\hat{H}(\lambda_0))}\mathrm{e}^{-\beta\hat{H}(\lambda_0)}\Big]/Z(\lambda_0) \\ =& \mathrm{Tr}\Big[\hat{\mathcal{T}}\exp\Big(iu\int_0^\tau dt\dot{\lambda}_t\frac{\partial\hat{H}^H(\lambda_t)}{\partial\lambda_t}\Big)\mathrm{e}^{-\beta\hat{H}(\lambda_0)}\Big]/Z(\lambda_0), \end{aligned} \tag{5.53}$$

which gives an equation analogous to Eq. (5.31). Using Eq. (5.51), equation (5.53) can be written as

$$Z(\lambda_0)G[u,\lambda] = \mathrm{Tr}\Big[\hat{U}_{\tau,0}^\dagger[\lambda]\mathrm{e}^{iu\hat{H}(\lambda_\tau)}\hat{U}_{\tau,0}[\lambda]\mathrm{e}^{-iu\hat{H}(\lambda_0)}\mathrm{e}^{-\beta\hat{H}(\lambda_0)}\Big]. \tag{5.54}$$

On the other hand, the mircorreversibility principle in Eq. (5.37), for $t=0$ assumes the form

$$\hat{U}_{0,\tau}[\lambda] = \hat{U}_{\tau,0}^\dagger[\lambda] = \hat{T}^\dagger\hat{U}_{\tau,0}[\tilde{\lambda}]\hat{T}, \tag{5.55}$$

and with this we obtain

$$\begin{aligned} Z(\lambda_0)G[u,\lambda] =& \mathrm{Tr}\Big[\hat{T}^\dagger \hat{U}_{\tau,0}[\tilde{\lambda}]\hat{T}\mathrm{e}^{iu\hat{H}(\lambda_\tau)}\hat{T}^\dagger \hat{U}^\dagger_{\tau,0}[\tilde{\lambda}]\hat{T}\mathrm{e}^{-iu\hat{H}(\lambda_0)}\mathrm{e}^{-\beta\hat{H}(\lambda_0)}\hat{T}^\dagger\hat{T}\Big] \\ =& \mathrm{Tr}\Big[\hat{T}^\dagger \hat{U}_{\tau,0}[\tilde{\lambda}]\mathrm{e}^{-iu^*\hat{H}(\lambda_\tau)}\hat{U}^\dagger_{\tau,0}[\tilde{\lambda}]\mathrm{e}^{iu^*\hat{H}(\lambda_0)}\mathrm{e}^{-\beta\hat{H}(\lambda_0)}\hat{T}\Big] \\ =& \mathrm{Tr}\Big[\mathrm{e}^{-\beta\hat{H}(\lambda_0)}\mathrm{e}^{-iu\hat{H}(\lambda_0)}\hat{U}_{\tau,0}[\tilde{\lambda}]\mathrm{e}^{iu\hat{H}(\lambda_\tau)}\hat{U}^\dagger_{\tau,0}[\tilde{\lambda}]\Big], \end{aligned} \tag{5.56}$$

where due to the antilinearity of $\hat{T}$, the identity $\mathrm{Tr}\ \hat{T}^\dagger A\hat{T} = \mathrm{Tr}A^\dagger$ was used. As a last step, by employing the cycle property of the trace, we arrive at the important result

$$\begin{aligned} Z(\lambda_0)G[u,\lambda] =& \mathrm{Tr}\Big[\hat{U}^\dagger_{\tau,0}[\tilde{\lambda}]\mathrm{e}^{i(-u+i\beta)\hat{H}(\lambda_0)}\hat{U}_{\tau,0}[\tilde{\lambda}]\mathrm{e}^{-i(-u+i\beta)\hat{H}(\lambda_\tau)}\mathrm{e}^{-\beta\hat{H}(\lambda_\tau)}\Big] \\ =& Z(\lambda_\tau)G[-u+i\beta,\tilde{\lambda}]. \end{aligned} \tag{5.57}$$

The fluctuation relation comes by applying the inverse Fourier transform to the last expression, and then we get

$$\frac{P[w,\lambda]}{P[-w,\tilde{\lambda}]} = \mathrm{e}^{\beta(w-\Delta F)}, \tag{5.58}$$

with the free energy given by $F(\lambda_t) = -\beta^{-1}\log Z(\lambda_t)$. Equation (5.58) is the quantum analogous of the classical fluctuation relation Eq. (5.32), and is called the quantum fluctuation theorem [133]. This relation was obtained, as in the classical case, using the microreversibility principle and the initial state of statistical nature. Finally, integrating Eq. (5.58) with respect to $w$ yields

$$\langle \mathrm{e}^{-\beta w}\rangle_\lambda = \mathrm{e}^{-\beta\Delta F}, \tag{5.59}$$

which is the quantum Jarzynski equality, analogous to Eq. (5.21).
Two important remarks are at place. First, instead of a canonical initial state, one can use an initial microcanonical state at energy $E$

$$\hat{\rho}_0(E) = \frac{\delta\big(E-\hat{H}(\lambda_0)\big)}{\mathcal{G}(E,\lambda_0)}, \tag{5.60}$$

with the density of states $\mathcal{G}(E,\lambda_0) = \mathrm{Tr}\ \delta\big(E-\hat{H}(\lambda_0)\big)$. In this scenario the derived *microcanonical fluctuation relations* read [134]

$$\frac{P[E,w,\lambda]}{P[E+w,-w,\tilde{\lambda}]} = \mathrm{e}^{\big(S(E+w,\lambda_\tau)-S(E,\lambda_0)\big)/K_B}, \tag{5.61}$$

where $S(E,\lambda_t) = K_B\log\mathcal{G}(E,\lambda_t)$ is the Boltzmann thermodynamic equilibrium entropy, and the probability density of work is given by

$$P[E,w,\lambda] = \frac{1}{\mathcal{G}(E,\lambda_0)}\ \mathrm{Tr}\ \delta\big(\hat{H}^H(\lambda_\tau)-E-w\big)\delta\big(\hat{H}^H(\lambda_0)-E\big). \tag{5.62}$$

And second, the *exclusive* version of quantum work can be also defined as [135]

$$w_0^{m,n} = e_m - e_n, \tag{5.63}$$

with $e_k$ being the eigenvalues of $\hat{H}_0$. In the next section we will present a treatment of quantum work based on the path integral formalism, which in principle could allow the possibility to observe interference effects. And we will also show our approach to build the semiclassical characteristic function of work based on the path integral construction.

## 5.3. Path integral and quantum work

In [136] the authors present a novel approach to study quantum work based on Feynman path integral. In this subsection we will summarize the construction following [136] and at the end we present our approach in order to build a semiclassical characteristic function of work.
Under consideration is a quantum system whose Hamiltonian, similar to Eq. (5.33), reads

$$\hat{H}(\lambda_t) = \frac{\hat{\mathbf{p}}^2}{2m} + \hat{V}(\lambda_t, \hat{\mathbf{x}}), \tag{5.64}$$

which describes a particle with $d$ degrees of freedom, momentum operator $\hat{\mathbf{p}}$, position operator $\hat{\mathbf{x}}$, and mass $m$, under the influence of the external force protocol $\lambda_t$, which drives the system out of equilibrium. As before, the force protocol will act during the time span $[0, \tau]$. The starting point is the characteristic function of work, given by Eq. (5.54), which, using the cyclic property of the trace, can be written as

$$G[u, \lambda] = \mathrm{Tr}\Big[\hat{U}_{\tau,0} \mathrm{e}^{-iu\hat{H}(\lambda_0)} \hat{\rho}(\lambda_0) \hat{U}^{\dagger}_{\tau,0} \mathrm{e}^{iu\hat{H}(\lambda_\tau)}\Big], \tag{5.65}$$

where for simplicity of notation we now drop the explicit functional dependence on $\lambda$, and $\hat{\rho}(\lambda_0)$ is the initial equilibrium state Eq. (5.41). The path integral expression of Eq. (5.65) can be obtained by noticing first that, due to the definition of path integrals, the following relations hold

$$\begin{aligned} \langle \mathbf{x}_f | \, \hat{U}_{\tau,0} \mathrm{e}^{-iu\hat{H}(\lambda_0)} \, | \mathbf{x}_i \rangle &= \int \mathcal{D}[\mathbf{x}] \mathrm{e}^{\frac{i}{\hbar} S_1^u[\mathbf{x}]}, \\ \langle \mathbf{y}_i | \, \hat{U}^{\dagger}_{\tau,0} \mathrm{e}^{iu\hat{H}(\lambda_\tau)} \, | \mathbf{y}_f \rangle &= \int \mathcal{D}[\mathbf{y}] \mathrm{e}^{-\frac{i}{\hbar} S_2^u[\mathbf{y}]}, \end{aligned} \tag{5.66}$$

comprising paths from $\mathbf{x}(0) = \mathbf{x}_i,\ \mathbf{y}(0) = \mathbf{y}_i$ to $\mathbf{x}(\tau) = \mathbf{x}_f,\ \mathbf{y}(\tau) = \mathbf{y}_f$, and the actions given by

$$\begin{aligned} S_1^u[\mathbf{x}] &= \int_0^{\hbar u} dt\ \mathcal{L}[\lambda_0, \mathbf{x}(t)] + \int_{\hbar u}^{\tau + \hbar u} dt\ \mathcal{L}[\lambda_{t-\hbar u}, \mathbf{x}(t)], \\ S_2^u[\mathbf{y}] &= \int_0^{\tau} dt\ \mathcal{L}[\lambda_t, \mathbf{y}(t)] + \int_{\tau}^{\tau + \hbar u} dt\ \mathcal{L}[\lambda_\tau, \mathbf{y}(t)]. \end{aligned} \tag{5.67}$$

The Lagrangian of the system reads

$$\mathcal{L}[\lambda_s, \mathbf{x}(s)] = \frac{m}{2} \dot{\mathbf{x}}^2(s) - V[\lambda_s, \mathbf{x}(s)]. \tag{5.68}$$

Thus, using Eq. (5.66) we obtain from Eq. (5.65) the path integral form of the characteristic function of work as

$$G[u,\lambda] = \int d\mathbf{x}_i d\mathbf{y}_i d\mathbf{x}_f d\mathbf{y}_f \delta(\mathbf{x}_f - \mathbf{y}_f) \int \mathcal{D}[\mathbf{x}]\mathcal{D}[\mathbf{y}] \times \mathrm{e}^{\frac{i}{\hbar}\left(S_1^u[\mathbf{x}] - S_2^u[\mathbf{y}]\right)} \rho(\mathbf{x}_i, \mathbf{y}_i), \tag{5.69}$$

where $\rho(\mathbf{x}_i, \mathbf{y}_i) = \langle \mathbf{x}_i | \, \hat{\rho}(\lambda_0) \, | \mathbf{y}_i \rangle$. Finally, using the identity [136]

$$S_1^u[\mathbf{x}] = S_2^u[\mathbf{x}] + \hbar u W_u[\mathbf{x}], \tag{5.70}$$

with the *quantum work functional* defined as

$$W_u[\mathbf{x}] = \int_0^\tau dt \, \frac{1}{\hbar u} \int_0^{\hbar u} ds \, \dot{\lambda}_t \frac{\partial V[\lambda_t, \mathbf{x}(t+s)]}{\partial \lambda_t}, \tag{5.71}$$

we arrive at the path integral expression for the characteristic function of work

$$G[u,\lambda] = \int d\mathbf{x}_i d\mathbf{y}_i d\mathbf{x}_f d\mathbf{y}_f \delta(\mathbf{x}_f - \mathbf{y}_f) \int \mathcal{D}[\mathbf{x}]\mathcal{D}[\mathbf{y}] \times \mathrm{e}^{\frac{i}{\hbar}\left(S_2^u[\mathbf{x}] - S_2^u[\mathbf{y}]\right)} \rho(\mathbf{x}_i, \mathbf{y}_i) \mathrm{e}^{iuW_u[\mathbf{x}]}. \tag{5.72}$$

Notice that Eq. (5.72) involves the work functional $W_u$ along the forward path $\mathbf{x}$. This result can be compared with Eq. (5.53). The advantage of Eq. (5.72) is due to the fact that it explicitly expresses the quantum work along individual paths, and in principle could help us to deepen our understanding of quantum work in the semiclassical limit, as shown below.

## 5.4. Semiclassical analysis of the characteristic function of work

In this section we will use Eq. (5.72) in order to construct a semiclassical expression based on the van Vleck-Gutzwiller propagator. We will see how the classical limit of work distribution emerges from the diagonal approximation. The first step consists in expanding the action difference and the work functional in Eq. (5.72) in terms of $\hbar$ as follows. From Eq. (5.67) we obtain

$$S_2^u[\mathbf{x}] - S_2^u[\mathbf{y}] = S[\mathbf{x}] - S[\mathbf{y}] + \hbar u \frac{1}{2} m\Big(\dot{\mathbf{x}}^2(\tau) - \dot{\mathbf{y}}^2(\tau)\Big) + \mathcal{O}((\hbar u)^2), \tag{5.73}$$

where we have used the fact that $\mathbf{x}(\tau) = \mathbf{y}(\tau)$, and $S[\mathbf{x}] = \int_0^\tau dt \, \mathcal{L}[\mathbf{x}(t), \dot{\mathbf{x}}(t), t]$. On the other hand, from Eq. (5.71) we have

$$W_u[\mathbf{x}] = \int_0^\tau dt \, \frac{1}{\hbar u} \left( \hbar u \dot{\lambda}_t \frac{\partial V[\lambda_t, \mathbf{x}(t)]}{\partial \lambda_t} + \frac{(\hbar u)^2}{2} \dot{\lambda}_t \dot{\mathbf{x}}(t) \cdot \frac{\partial^2 V[\lambda_t, \mathbf{x}(t)]}{\partial \lambda_t \partial \mathbf{x}(t)} + \mathcal{O}(\hbar^3) \right). \tag{5.74}$$

In order to obtain the semiclassical approximation of Eq. (5.72) we keep the first two terms in Eq. (5.73), and the first term in Eq. (5.74). We also consider accordingly $W_u[\mathbf{x}]$

smooth compared with $S[\mathbf{x}]/\hbar$, arriving at the *semiclassical characteristic function of work*

$$G^{sc}[u,\lambda] = \int d\mathbf{x}_i d\mathbf{y}_i d\mathbf{x}_f\ \rho(\mathbf{x}_i,\mathbf{y}_i)\frac{1}{(2\pi\hbar)^d}\sum_{\tilde{\gamma}:\,\mathbf{x}_i\to\mathbf{x}_f}\sum_{\tilde{\gamma}':\,\mathbf{y}_i\to\mathbf{x}_f} A_{\tilde{\gamma}}A^*_{\tilde{\gamma}'} \\ \times\, \mathrm{e}^{\frac{i}{\hbar}(S_{\tilde{\gamma}}-S_{\tilde{\gamma}'})}\mathrm{e}^{ium\left(\dot{\mathbf{x}}^2_{\tilde{\gamma}}(\tau)-\dot{\mathbf{y}}^2_{\tilde{\gamma}'}(\tau)\right)/2}\mathrm{e}^{iu\int_0^\tau dt\ \dot{\lambda}_t\frac{\partial V[\lambda_t,\mathbf{x}_{\tilde{\gamma}}(t)]}{\partial\lambda_t}}. \tag{5.75}$$

In the last expression, $\tilde{\gamma}$ and $\tilde{\gamma}'$ are classical trajectories with $\mathbf{x}_{\tilde{\gamma}}(0)=\mathbf{x}_i$, $\mathbf{y}_{\tilde{\gamma}'}(0)=\mathbf{y}_i$, $\mathbf{x}_{\tilde{\gamma}'}(\tau)=\mathbf{y}_{\tilde{\gamma}'}(\tau)=\mathbf{x}_f$, solutions of the classical equations of motion, which come from the stationary condition of the action $S_{\tilde{\gamma}}$ and $S_{\tilde{\gamma}'}$, respectively. The stability matrix $A_{\tilde{\gamma}}$ contains already the Maslov indices, and the work functional is evaluated along the forward classical path $\mathbf{x}_{\tilde{\gamma}}$. As a further step, following chapter 1, we look for pairs of trajectories $\gamma,\gamma'$ with small action difference $S_\gamma - S_{\gamma'} \sim \mathcal{O}(\hbar)$, because they survive the rapidly oscillatory contribution of the action difference in Eq. (5.75), as shown in Fig. 1.2. Introducing center of mass $\mathbf{r}=(\mathbf{x}+\mathbf{y})/2$ and relative coordinates $\xi=\mathbf{x}-\mathbf{y}$, and after expanding the action $S_{\tilde{\gamma}}$ around $\gamma$, and similarly $S_{\tilde{\gamma}'}$ around $\gamma'$ (see Eq. (1.22)), we obtain

$$G^{sc}[u,\lambda] = \int d\mathbf{r}_i d\mathbf{r}_f \sum_{\gamma:\,\mathbf{r}_i\to\mathbf{r}_f}\sum_{\gamma':\,\mathbf{r}_i\to\mathbf{r}_f} A_\gamma A^*_{\gamma'}\ \mathcal{W}_0\big(\mathbf{r}_i,(\mathbf{p}_i^\gamma+\mathbf{p}_i^{\gamma'})/2\big) \\ \times\, \mathrm{e}^{\frac{i}{\hbar}(S_\gamma-S_{\gamma'})}\mathrm{e}^{ium\dot{\mathbf{r}}(\tau)\dot{\xi}(\tau)}\mathrm{e}^{iu\int_0^\tau dt\ \dot{\lambda}_t\frac{\partial V[\lambda_t,\mathbf{r}_\gamma(t)]}{\partial\lambda_t}}, \tag{5.76}$$

where as usual, $\mathcal{W}_0\big(\mathbf{r}_i,(\mathbf{p}_i^\gamma+\mathbf{p}_i^{\gamma'})/2\big)$ denotes the initial Wigner function, with $\mathbf{p}_i^\gamma$ and $\mathbf{p}_i^{\gamma'}$ the initial momentum of the trajectory $\gamma$ and $\gamma'$, respectively. Above it is understood $\dot{\mathbf{r}}(\tau)=\big(\dot{\mathbf{r}}_\gamma(\tau)+\dot{\mathbf{r}}_{\gamma'}(\tau)\big)/2$, and $\dot{\xi}(\tau)=\dot{\mathbf{r}}_\gamma(\tau)-\dot{\mathbf{r}}_{\gamma'}(\tau)$.

### Quantum-classical correspondence

From Eq. (5.76) the *diagonal approximation*, $\gamma=\gamma'$, yields the classical characteristic function of work as (see Eq. (1.27))

$$G^{dg}[u,\lambda] = \int d\mathbf{r}_i d\mathbf{p}_i \mathcal{W}_0\big(\mathbf{r}_i,\mathbf{p}_i\big)\mathrm{e}^{iu\int_0^\tau dt\ \dot{\lambda}_t\frac{\partial V[\lambda_t,\mathbf{r}(t)]}{\partial\lambda_t}}, \tag{5.77}$$

which coincides with the classical result, Eq. (5.31), taking into account that in the semiclassical limit the Wigner function converges to the classical phase-space distribution. It is worth mentioning that, without obtaining our result Eq. (5.76), the quantum-classical correspondence Eq. (5.77) was also derived from Eq. (5.72) in [136]. On the other hand, in [137,138] the quantum-classical correspondence was studied by exploiting the analogy between Eq. (5.65) and the fidelity amplitude, in the so-called dephasing representation [139], which, however, does not take into account explicitly pairs of trajectories, as it is the case in our formula Eq. (5.76). At this point it is instructive to rewrite the classical functional of work, noticing that the integrand equals the total time-derivative of the Hamiltonian

$$\int_0^\tau dt\ \dot{\lambda}_t\frac{\partial V[\lambda_t,\mathbf{r}(t)]}{\partial\lambda_t} = \int_0^\tau dt\ \frac{dH}{dt} = H(\lambda_\tau,\varphi_{\tau,0}[\mathbf{z}_0,\lambda]) - H(\lambda_0,\mathbf{z}_0), \tag{5.78}$$

with $\mathbf{z} = (\mathbf{r}, \mathbf{p})$, and the Hamiltonian flow $\varphi$ given accordingly by Eq. (5.2). With this result, Eq. (5.76) can be written as

$$\begin{aligned} G^{sc}[u,\lambda] = \int d\mathbf{r}_i d\mathbf{r}_f \sum_{\gamma:\, \mathbf{r}_i \to \mathbf{r}_f} \sum_{\gamma':\, \mathbf{r}_i \to \mathbf{r}_f} A_\gamma A^*_{\gamma'}\, \mathcal{W}_0\big(\mathbf{r}_i, (\mathbf{p}_i^\gamma + \mathbf{p}_i^{\gamma'})/2\big) \\ \times \mathrm{e}^{\frac{i}{\hbar}(S_\gamma - S_{\gamma'})} \mathrm{e}^{ium\dot{\mathbf{r}}(\tau)\dot{\xi}(\tau)} \mathrm{e}^{iu\left(H(\lambda_\tau, \varphi^\gamma_{\tau,0}[\mathbf{z}_0^\gamma, \lambda]) - H(\lambda_0, \mathbf{z}_0^\gamma)\right)}, \end{aligned} \tag{5.79}$$

where we have made explicit the dependence of the energy difference with the forward path $\gamma$. It is clear then that Eq. (5.79) involves an average of the energy difference between the initial and final time of the protocol followed by all classical trajectories $\gamma$, weighted by the action difference of all possible pairs of "close" classical trajectories $(\gamma, \gamma')$. From Eq. (5.79) the diagonal approximation becomes

$$\begin{aligned} G^{dg}[u,\lambda] &= \int d\mathbf{r}_i d\mathbf{p}_i \mathcal{W}_0\big(\mathbf{r}_i, \mathbf{p}_i\big) \mathrm{e}^{iu\left(H(\lambda_\tau, \varphi_{\tau,0}[\mathbf{z}_0, \lambda]) - H(\lambda_0, \mathbf{z}_0)\right)} \\ &= \Big\langle \mathrm{e}^{iu\left(E(\lambda_\tau, \mathbf{z}_\tau) - E(\lambda_0, \mathbf{z}_0)\right)} \Big\rangle_{\mathbf{r}_i, \mathbf{p}_i}, \end{aligned} \tag{5.80}$$

written as a phase-space average over initial conditions $\mathbf{z}_0 = (\mathbf{r}_0, \mathbf{p}_0)$. Notice that the energy difference depends on the chosen force protocol and the initial point $\mathbf{z}_0$, which accordingly determines the final point $\mathbf{z}_\tau = \varphi_{\tau,0}[\mathbf{z}_0, \lambda]$.

So far we have studied a non-autonomous system subject to an external force, but otherwise isolated. One interesting possibility is to extend our semiclassical analysis to a system which, besides the driving external force, is coupled to an environment. This is the topic of the next section.

## 5.5. Path integral quantum work of a system coupled to an environment

Following [136] we consider a one-dimensional system $\mathcal{A}$ with Hamiltonian Eq. (5.64), coupled to an environment $\mathcal{E}$ of harmonic oscillators, using the Caldeira-Leggett model studied in chapter 1. The global Hamiltonian reads then

$$\hat{H}(\lambda_t) = \hat{H}_{\mathcal{A}}(\lambda_t) + \hat{H}_{\mathcal{E}} + \hat{H}_{\mathcal{A}\mathcal{E}}, \tag{5.81}$$

where the central system Hamiltonian reads

$$\hat{H}_{\mathcal{A}}(\lambda_t) = \frac{\hat{p}^2}{2m} + \hat{V}(\lambda_t, \hat{x}), \tag{5.82}$$

the environment Hamiltonian is a collection of $N$ harmonic oscillators

$$\hat{H}_{\mathcal{E}} = \sum_{k=1}^{N} \frac{1}{2}\Big(\hat{p}_k^2/m_k + m_k\omega_k^2 \hat{q}_k^2\Big), \tag{5.83}$$

with $\hat{p}_k$, $\hat{q}_k$ momentum and position operator of each harmonic oscillator with natural frequency $\omega_k$ and mass $m_k$. The interaction Hamiltonian is given by

$$\hat{H}_{\mathcal{AE}} = -\hat{x} \otimes \sum_{k=1}^{N} g_k \hat{q}_k + \hat{x}^2 \sum_{k=1}^{N} \frac{g_k^2}{2m_k\omega_k^2}, \tag{5.84}$$

which comprises a coupling between the position operator of the system $\mathcal{A}$ with each position of the environment, with strength $g_k$. The only time-dependence in Eq. (5.81) is given by the force protocol acting on the central system $\mathcal{A}$. Thus, *the work done on the open system $\mathcal{A}$ coincides with the work done on the total system $\mathcal{AE}$*. Then, analogously to Eq. (5.36), we can write the quantum work as

$$w_{m,n} = E_m^{\lambda_\tau} - E_n^{\lambda_0}, \tag{5.85}$$

with $E_l^{\lambda_t}$ the instantaneous energy eigenvalue of $\hat{H}(\lambda_t)$. We measure then the total energy at the beginning and at the end of the force protocol process. This definition is independent of the coupling strength between $\mathcal{A}$ and $\mathcal{E}$. In the strong-coupling regime, however, the interaction energy becomes important, and the usual identification of heat as the environment energy change is no longer possible. How to define heat in this scenario is an open issue [123], which nevertheless, does not affect the work statistics discussed in this section. Using Eq. (5.65) we can write

$$G[u,\lambda] = \mathrm{Tr}_{\mathcal{AE}}\Big[\hat{U}_{\mathcal{AE}}(\tau,0)\mathrm{e}^{-iu\hat{H}(\lambda_0)}\hat{\rho}_{\mathcal{AE}}(\lambda_0)\hat{U}^{\dagger}_{\mathcal{AE}}(\tau,0)\mathrm{e}^{iu\hat{H}(\lambda_\tau)}\Big], \tag{5.86}$$

with the system initialized in the state

$$\hat{\rho}_{\mathcal{AE}}(\lambda_0) = \hat{\rho}_{\mathcal{A}}(\lambda_0) \otimes \mathrm{e}^{-\beta\hat{H}_{\mathcal{E}}}/Z_{\mathcal{E}}, \tag{5.87}$$

where the initial state of the environment is a canonical state at inverse temperature $\beta$. As shown in section 5.2, the initial state of the central system should be an equilibrium state in order to the fluctuation relations to become valid. However, we leave here $\hat{\rho}_{\mathcal{A}}(\lambda_0)$ undetermined, mainly because it will not change the semiclassical analysis below. We trace out the environmental degrees of freedom in Eq. (5.86), using the result Eq. (1.64), namely

$$\begin{aligned}\langle x_f|\,\hat{\rho}_{\mathcal{A}}(\tau)\,|x'_f\rangle = &\int dx_i dx'_i\;\rho_{\mathcal{A}}(x_i,x'_i)\\ &\times\int_{x_i\to x_f}\mathcal{D}x\int_{x'_i\to x'_f}\mathcal{D}x'\;\mathrm{e}^{i\left(S_{\mathcal{A}}[x]-S_{\mathcal{A}}[x']-S^F[x,x']\right)/\hbar}\;\mathrm{e}^{-S^{\mathcal{N}}[x,x']/\hbar},\end{aligned} \tag{5.88}$$

in terms of the reduced density matrix $\hat{\rho}_{\mathcal{A}}(t) = \mathrm{Tr}_{\mathcal{E}}\left[\hat{\rho}_{\mathcal{AE}}(t)\right]$. The bare action reads $S_{\mathcal{A}} = \int_0^\tau dt\;\mathcal{L}_{\mathcal{A}}(x(t),\dot{x}(t),t)$. The noise (decoherence) $S^{\mathcal{N}}$, and friction action $S^F$, are given accordingly by Eqns. (1.65,1.66). Performing similar calculations as those which led to Eq. (5.72), we obtain

$$\begin{aligned}G[u,\lambda] = &\int dx_i dx'_i dx_f dx'_f \delta(x_f - x'_f)\rho(x_i,x'_i)\\ &\times\int\mathcal{D}[x]\mathcal{D}[x']\mathrm{e}^{\frac{i}{\hbar}\left(S_2^u[x]-S_2^u[x']-S_F^u[x,x']\right)}\mathrm{e}^{-\frac{1}{\hbar}S^u_{\mathcal{N}}[x,x']}\mathrm{e}^{iuW_u[x]}.\end{aligned} \tag{5.89}$$

In the last equation $S_2^u$ can be read from Eq. (5.67), in terms of the bare Lagrangian $\mathcal{L}_\mathcal{A}$, the work functional is the same as Eq. (5.71), and the $u$-dependent noise and friction actions read

$$\begin{aligned} S^u_\mathcal{N}[x,x'] =& \int_0^{\tau+\hbar u} dt \int_0^t ds\ \big(x(t)-x'(t)\big)K(t-s)\big(x(s)-x'(s)\big), \\ S^u_F[x,x'] =& m\int_0^{\tau+\hbar u} dt \int_0^t ds\ \big(x(t)-x'(t)\big)\gamma(t-s)\Big(\frac{\dot x(s)+\dot x'(s)}{2}\Big) \\ &+ m\frac{x(s)+x'(s)}{2}\int_0^{\tau+\hbar u} ds\ \gamma(s)\big(x(s)-x'(s)\big), \end{aligned} \tag{5.90}$$

with the environment auto-correlation function $K(s)$ and damping kernel $\gamma(s)$ given by Eq. (1.67). Equation (5.89) is the path integral characteristic function of work of an open system $\mathcal{A}$ coupled to an environment. We proceed to derive a semiclassical approximation to this equation.

### Semiclassical analysis

Similar to Eq. (5.73), we expand $S_2^u[x]-S_2^u[x']$ in terms of $\hbar$, and changing to center of mass $r=\frac{x+x'}{2}$ and relative coordinates $y=x-x'$, we additionally perform an expansion around $r$, assuming $y$ to be small, in the same spirit as in section 1.2.3 (see Eqns. (1.71,1.72))

$$\begin{aligned} S_2^u[x]-S_2^u[x'] =& -m\dot r_i y_i - \int_0^\tau ds\ y(s)\bigg(\frac{d}{ds}\frac{\partial}{\partial\dot r}\mathcal{L}_\mathcal{A}(r,\dot r)-\frac{\partial}{\partial r}\mathcal{L}_\mathcal{A}(r,\dot r)\bigg) \\ &+\hbar u m\dot r_f\dot y_f + \mathcal{O}(y^3,\dot y^3)+\mathcal{O}((\hbar u)^2), \end{aligned} \tag{5.91}$$

where we have used the fact that $y(\tau)=y_f=0$. Similarly, expanding Eq. (5.90) in $\hbar$ we obtain

$$\begin{aligned} S^u_\mathcal{N}[y] =& \int_0^\tau dt\int_0^t ds\ y(t)K(t-s)y(s)+\mathcal{O}((\hbar u)^2), \\ S^u_F[r,y] =& m\int_0^\tau dt\int_0^t ds\ y(t)\gamma(t-s)\dot r(s) + mr_i\int_0^\tau ds\ \gamma(s)y(s)+\mathcal{O}((\hbar u)^2). \end{aligned} \tag{5.92}$$

Finally, the work functional becomes

$$W_u[r,y]=\int_0^\tau dt\ \dot\lambda_t\bigg(\frac{\partial V[\lambda_t,r(t)]}{\partial\lambda_t}+\frac{y(t)}{2}\frac{\partial^2V[\lambda_t,r(t)]}{\partial\lambda_t\partial r}+\mathcal{O}(y^2)\bigg)+\mathcal{O}(\hbar u). \tag{5.93}$$

Keeping the lowest order terms in Eqns. (5.91,5.92,5.93), and inserting them in Eq. (5.89) yields

$$\begin{aligned} G[u,\lambda] =& \int dr_i dy_i dr_f\ \rho(r_i+y_i/2,r_i-y_i/2)\int_{y_i\to0}\mathcal{D}y \\ &\int_{r_i\to r_f}\mathcal{D}r\ \mathrm{e}^{\frac{i}{\hbar}\left(-m\dot r_i y_i-\int_0^\tau ds\ y(s)\left(\frac{d}{ds}\frac{\partial}{\partial\dot r}\mathcal{L}_\mathcal{A}(r,\dot r)-\frac{\partial}{\partial r}\mathcal{L}_\mathcal{A}(r,\dot r)\right)+\hbar u m\dot r_f\dot y_f-S_F[r,y]\right)} \\ &\times\mathrm{e}^{-\frac{1}{\hbar}S^\mathcal{N}[y]}\mathrm{e}^{iu\int_0^\tau dt\ \dot\lambda_t\left(\frac{\partial V[\lambda_t,r(t)]}{\partial\lambda_t}+\frac{y(t)}{2}\frac{\partial^2V[\lambda_t,r(t)]}{\partial\lambda_t\partial r}\right)}, \end{aligned} \tag{5.94}$$

where the noise action is given by

$$S_{\mathcal{N}}[y] = \frac{1}{2}\int_0^\tau dt \int_0^\tau ds\; y(t)K(t-s)y(s), \tag{5.95}$$

and the friction action by

$$S_F[r,y] = m\int_0^\tau dt \int_0^t ds\; y(t)\gamma(t-s)\dot{r}(s) + mr_i\int_0^\tau ds\;\gamma(s)y(s). \tag{5.96}$$

As before, we consider the functional work in Eq. (5.94) as smooth compared to the rapid oscillations of the other terms.
At this point we propose two approaches in order to derive a semiclassical expression from Eq. (5.94).
The first approach consists in considering the dynamical evolution along the center of mass $r(s)$, and treating accordingly the small coordinates $y(s)$ as fluctuating paths coupled to noise. This will give the diagonal (classical) evolution of the characteristic function of work. For this purpose, we apply a Hubbard-Stratonovich transformation to Eq. (5.94), introducing an auxiliary noise path $\eta$, reading (normalization constant apart)

$$\mathrm{e}^{-\frac{1}{2\hbar}\int_0^\tau dt\int_0^\tau ds\; y(t)K(t-s)y(s)} = \int \mathcal{D}\eta\; \mathrm{e}^{\frac{i}{\hbar}\int_0^\tau dt\;\eta(t)y(t)}\mathrm{e}^{-\frac{1}{2\hbar}\int_0^\tau dt\int_0^\tau ds\;\eta(t)K^{-1}(t-s)\eta(s)}, \tag{5.97}$$

where $K^{-1}$ is the functional inverse of $K(s)$. In this way, inserting Eq. (5.97) into Eq. (5.94), we obtain

$$\begin{aligned} G[u,\lambda] = \int dr_f dr_i \int \mathcal{D}\eta\mathcal{D}y\mathcal{D}r\; \mathcal{W}(r_i,p_i)\mathrm{e}^{-\frac{1}{2\hbar}\int_0^\tau dt\int_0^\tau ds\;\eta(t)K^{-1}(t-s)\eta(s)} \\ \times \exp\frac{i}{\hbar}\Bigg[-\int_0^\tau ds\; y(s)\Bigg(m\ddot{r}(t) + V'(\lambda_t,r(t)) + m\int_0^t ds\;\gamma(t-s)\dot{r}(s) \\ + mr_i\gamma(s) - \frac{\hbar u}{2}\dot{\lambda}_t\frac{\partial^2 V[\lambda_t,r(t)]}{\partial\lambda_t\partial r} - \eta(t)\Bigg)\Bigg]\mathrm{e}^{iu\int_0^\tau dt\;\dot{\lambda}_t\left(\frac{\partial V[\lambda_t,r(t)]}{\partial\lambda_t}\right)}. \end{aligned} \tag{5.98}$$

Above we have employed the bare Lagrangian $\mathcal{L}_{\mathcal{A}} = \frac{1}{2}m\dot{r}^2 - V(\lambda_t,r)$, and introduced the initial Wigner function $\mathcal{W}(r_i,p_i)$, with momentum $p_i = m\dot{r}_i$. Being the exponent in Eq. (5.98) linear in $y$, we may integrate the relative paths, yielding a $\delta$-functional, which accordingly imposes a restriction over the $r$-paths, giving rise to the classical equation of motion for $r$. Thus, we arrive at classical the limit (c)

$$\begin{aligned} G^c[u,\lambda] = \int dr_f dr_i \int \mathcal{D}\eta\; \mathrm{e}^{-\frac{1}{2\hbar}\int_0^\tau dt\int_0^\tau ds\;\eta(t)K^{-1}(t-s)\eta(s)}\int \mathcal{D}r \\ \times \delta\Big(m\ddot{r}(t) + V'(\lambda_t,r(t)) + m\int_0^t ds\;\gamma(t-s)\dot{r}(s) + mr_i\gamma(s) - \eta(t)\Big)\mathrm{e}^{iuW_c[r]}, \end{aligned} \tag{5.99}$$

where the equation inside the delta functional, namely

$$m\ddot{r}(t) + V'(\lambda_t, r(t)) + m\int_0^t ds\ \gamma(t-s)\dot{r}(s) + mr_i\gamma(s) = \eta(t), \tag{5.100}$$

is the Langevin equation, describing a particle dissipating energy with a memory-dependent kernel, and a fluctuating noise force $\eta$, as discussed in detail in section 1.2.3. In Eq. (5.99) the classical work functional

$$W_c[r] = \int_0^\tau dt\ \dot{\lambda}_t\left(\frac{\partial V[\lambda_t, r(t)]}{\partial \lambda_t}\right), \tag{5.101}$$

evaluated along each trajectory $r$, solution of the equation of motion in Eq. (5.100) with boundary conditions $r(0) = r_i$, $r(\tau) = r_f$. Above we have dropped the contribution $\frac{\hbar u}{2}\dot{\lambda}_t\frac{\partial^2 V[\lambda_t, r(t)]}{\partial\lambda_t \partial r}$, which we consider negligibly small. As we know from chapter 1, the equation of motion inside the delta functional represents a classical evolution involving a history-dependent dissipative contribution. Notice that $\dot{\lambda}_t\frac{\partial V[\lambda_t, r_\gamma(t)]}{\partial\lambda_t}$ in general can not be written as a change of energy of the open system $\mathcal{A}$. Instead Eq. (5.101) can be read as the total supply power due to the force protocol, on a system which at the same time is dissipating energy in virtue of its coupling to an environment. The result Eq. (5.99) has the form of an average of the classical functional of work over all classical paths. The same limit was obtained in [136], and shows the quantum-classical correspondence for the open system scenario.

There exist a possibility to arrive at a semiclassical expression from Eq. (5.94), as a particular application of our results from chapter 4. There, initializing the environment in a microcanonical, instead of the usual canonical state, allows us to capture, in principle, interference effects coming from relative non-vanishing paths $y_c(s)$, carrying information about the dissipative trajectories $r_c(s)$. Using Eq. (4.26) for the initial state of the environment, with $\beta = i\alpha$, and accordingly the result Eq. (4.32), the semiclassical characteristic function of work for a system coupled to a *microcanonical* environment at energy $E$ reads

$$\begin{aligned} G^{sc}[u,\lambda] =& \frac{1}{2\pi\mathcal{G}_{\mathcal{E}}(E)}\int_{-\infty}^{\infty} d\alpha\, \mathrm{e}^{i\alpha E}\mathrm{e}^{\log Z_{\mathcal{E}}(i\alpha)}\int dr_f dr_i \\ & \sum_{\gamma: r_i, y_i \to r_f, 0} \mathcal{W}(r_i, p_i^\gamma) A_\gamma \mathrm{e}^{\frac{i}{\hbar}\left(-\int_0^\tau dt\int_0^t ds\ y[r_\gamma(t)]K_\alpha(t-s)y[r_\gamma(s)]\right)} \\ & \times \mathrm{e}^{iu\left(m\dot{r}_f\dot{y}_f + \int_0^\tau dt\ \dot{\lambda}_t\left(\frac{\partial V[\lambda_t, r_\gamma(t)]}{\partial\lambda_t} + \frac{y[r_\gamma(t)]}{2}\frac{\partial^2 V[\lambda_t, r_\gamma(t)]}{\partial\lambda_t\partial r}\right)\right)}, \end{aligned} \tag{5.102}$$

where $r_\gamma$ are the classical trajectories, solutions of the equations of motion, obtained after variation of the highly oscillatory action in Eq. (5.98). The equations of motion read

$$\begin{aligned} & m\ddot{r}_c(s) + V'(\lambda_s, r_c(s)) + m\int_0^s du\ \gamma(s-u)\dot{r}_c(u) + mr_i\gamma(s) = -\int_0^\tau du\ y(u)K_\alpha(s-u), \\ & m\ddot{y}_c(s) + y_c(s)V''(\lambda_s, r(s)) - m\int_s^\tau du\ \gamma(u-s)\dot{y}_c(u) = 0, \end{aligned} \tag{5.103}$$

fulfilling $r(0) = r_i$, $r(\tau) = r_f$. Here $y[r_\gamma]$ is the unique solution for $y$ of Eq. (5.103), for each $r_\gamma$, with boundary conditions $y(0) = y_i$, $y(\tau) = 0$. Above, $\mathcal{G}_\mathcal{E}(E)$ refers to the density of states of the environment, $A_\gamma$ contains the fluctuations of the paths $r$ and $y$ around their classical solutions, and the $\alpha$-dependent kernel $K_\alpha$ can be read from Eq. (4.29). Equation (5.102) comprises interference between different classical trajectories, with the evolution not only along the diagonal, but also along small relative paths $y$. Notice that the same procedure developed in this section can be applied to a many-body central system $\mathcal{A}$, like the Bose-Hubbard model studied in chapter 4, where the semiclassical limit is understood as the thermodynamic limit of large number of particles in $\mathcal{A}$. This opens the possibility to investigate the work statistics on a many-body system coupled to an environment.

## 5.6. Summary

In this chapter, we have developed a semiclassical approach to the characteristic function of work for a quantum system subject to an external force. For an isolated non-autonomous system, this has the form of a double sum over pairs of classical trajectories Eq. (5.76), solutions of the system Hamilton's equation of motion. The double sum can in principle reveal coherent effects between pairs of correlated trajectories. In this case, however, the difficulty resides in the fact that the system energy is not a conserved quantity, and then the methods used in chapter 3 are no longer directly applicable. How to find in this scenario, systematic pairs of correlated trajectories, that survive after an average or smoothing process has taken place, is an open issue. The quantum-classical correspondence can be derived from Eq. (5.76) applying the diagonal approximation, which yields to Eq. (5.80). Further, we have extended the semiclassical analysis to the case where the system, besides acting on by an external force, is coupled to an environment. In this case, as already investigated in chapters 1 and 4, the derivation of a semiclassical expression is more involved. The quantum-classical correspondence, Eq. (5.99), comprises an evolution of the open system along the center of mass. This equation involves an average of the classical work-functional over classical trajectories, which are solutions of the equation of motion producing dissipation of energy, in virtue of the environmental coupling, besides supply power, due to the external force. A key contribution of our work is the result in Eq. (5.102), obtained by using the proposal from chapter 4, where the environment is initialized in a microcanonical distribution at a given energy. This allows the semiclassical analysis involving non-vanishing relative coordinate trajectories, which carry information about the center of mass classical evolution. In the open system scenario, we additionally face the problem of how to calculate, in a systematic way, interference effects between trajectories that are dissipating energy to the environment. In many situations an open system can have different stationary points towards it will approach for long times, depending on the initial conditions and parameters of the system. Thus, the possibility to see interference processes between trajectories approaching different stationary points is exciting and deserves more analysis. Finally, the formalism developed here can be applied to situations where $\mathcal{A}$ is a

many-body system, and even to scenarios like thermal quantum machines, where the search for quantum effects is an ever-growing area.

# Summary and outlook

In this final part of the thesis, we summarize our main results and give some perspectives concerning possible directions toward future research. A detailed summary is given at the end of each chapter.
The main objective of the thesis was the study of open quantum systems, which we understand here as systems coupled with large environments, in the semiclassical limit of large actions/or a large number of particles within the system. When calculating the semiclassical propagator, one main difference compared with the closed-system scenario is that the classical equations of motion, obtained by the stationary condition of the associated action, must be derived at the level of probabilities, not at the level of amplitudes. One may observe, for instance, that Eq. (1.25) represents the semiclassical density matrix of the closed-system, where each of the two propagators has been calculated in the semiclassical limit (van Vleck-Gutzwiller), obtaining an equation of motion involving only one propagator (amplitude). On the contrary, finding of the equations of motion in an open system involves the stationary condition of an effective action (see Eq. (1.76)), with a structure comprising correlated "forward" and "backward" paths (two propagators). Thus, only at the level of probabilities the classical equation of motion emerges in the open system approach, giving rise to the Langevin equation for the Caldeira-Leggett model, as shown in Eq. (1.93). This interplay between forward and backward paths yields precisely an effective action with a real part giving rise to dissipation of energy in the equations of motion, and an imaginary contribution (which makes the usual semiclassical analysis problematic, if one has to deal with complex paths), producing decoherence in the basis of the interaction Hamiltonian. When evaluating along the quasi classical diagonal coordinate, the semiclassical action vanishes. This property of open system contributes to making the standard semiclassical approach (that in this scenario means looking for superposition of different dissipative classical trajectories) a challenging task.

In chapter 2 we have seen that if a composite system is described by the fundamental microcanonical equilibrium state at some energy $E$, using an approach pioneered by Schwinger by making use of SPA techniques, one may explain the familiar notion of temperature $T(E)$ as a derived property, which establishes the condition of equilibrium between the subsystems. For weakly coupled systems this approach shows the well-known equivalence of the canonical and microcanonical ensemble in the thermodynamic limit. We have extended these ideas to the case where the interaction energy between the subsystems is not negligible. In this case, of course, the energy of the composite system is no longer an extensive quantity. Still, one can define a temperature of equilibrium that depends on the interaction parameter. We have applied this idea to the paradigmatic Quantum Brownian Motion model and studied the main features of this notion of tem-

perature, confirming that it is a monotonically increasing function of the total energy $E$, and showing a clear variation of $T$ with the interaction parameter, being this feature a purely quantum effect particularly visible near the ground state energy. Further, a generalized version of ensemble equivalence has been derived, and interestingly, we show that our notion of temperature fulfills consistent microcanonical thermodynamics.
It would be interesting to extend these ideas to the case where the subsystems are allowed to interchange particles. In that case, similar ideas yield an analytical continuation of the Grand Canonical partition function, analogous to Eq. (2.4), allowing fluctuations of energy and the number of particles. Then, SPA can be employed, resulting in a coupling-dependent temperature and a chemical potential, establishing the condition of particle equilibrium. There exist, of course, the challenge to apply the formalism to a specific model beyond QBM, but the main ideas in principle can be extended according to these lines.

In chapter 3 we have made use of the semiclassical methods for action correlations in classically chaotic systems to investigate how decoherence, arising from the system coupled to an environment, affects coherence effects, coming from quantum population decay in a chaotic cavity. The key point is interference between pairs of correlated classical trajectories, which in a chaotic system display a universal signature involving encounter regions and loops. Coherent enhancement of the survival probability comes from correlated trajectories inside an encounter, and on the other hand, the decoherence effect arises from uncorrelated trajectories inside a loop. This interplay produces a diminishing in the first-order quantum correction to the classical survival probability, as compared to the scenario of vanishing-coupling (see Eq. (3.55) and Fig 3.7).
One interesting extension would be to investigate quantum corrections in the semiclassical limit when the environment has memory effects. In this non-markovian regime, obtaining the effect of decoherence inside a loop is more involved, and it is not clear that universal results could be reached in this scenario. As a final remark, we should observe that the employ of Sieber-Richter orbit pairs was possible in this case because the only effect of the environment on the system was decoherence, leaving accordingly the classical dynamics (the bare action) intact.

Chapter 4 deals with a Bose-Hubbard system describing a Josephson junction subject to dissipation and decoherence in virtue of environmental coupling. We studied in detail the time-reversal symmetry character of the equations of motion associated with action amplitudes. The quantum amplitude propagator involves boundary conditions on the paths associated with its path integral representation, thus yielding equations of motion, by the stationary action principle, with time-reversal symmetry, essential to describe conservative systems. An open system, however, requires the action of two propagators in order to obtain its classical equation of motion. Crucially, it is the uncontrollable character of the environment, with its related trace procedure, that gives rise to dissipative, and consequently time-reversal-broken equations of motion for the system. Thus, irreversibility may be understood as an emergent property of open systems subject to huge and, for all practical purposes, uncontrollable environments.

Further, using the ideas developed in chapter 2, we have considered the effect of an environment initially in a microcanonical, instead of the usual canonical state, and shown in this scenario the possibility to observe interference between different dissipative classical trajectories, in the semiclassical limit of a large number of particles within the central system, a phenomenon that is notoriously hard to produce. We hope these results may open a new direction in the study of open quantum systems with microcanonical environments. The explicit calculation of the fluctuations in Eq. (4.34) and the analysis of the conditions under which we may obtain complex saddle-points solution for $\tau$ in Eq. (4.32) are work in progress.

Finally, chapter 5 was devoted to the study of non-autonomous systems. Namely, a quantum system subject to an external force producing work. Specifically, the path integral expression of the characteristic function of quantum work was analyzed in the semiclassical limit, based on the two-point-measurement definition of quantum work. For an isolated non-autonomous system this has the form of a double sum over pairs of classical trajectories (see Eq. (5.76)), solutions of the system Hamilton's equation of motion. The double sum can in principle reveal coherent effects between pairs of correlated trajectories. In this case, however, the difficulty resides in the fact that the system's energy is not a conserved quantity, and then the methods used in chapter 3 are no directly applicable. One interesting possibility to explore is the study of a force protocol with periodic time function, and to investigate with the help of Floquet theory under which conditions Sieber-Richter orbit pairs may apply.
We also have extended the semiclassical analysis to the case of an open system and showed the quantum-classical correspondence, involving the classical work-functional over classical trajectories, which are solutions of the equation of motion producing dissipation of energy, in virtue of the environmental coupling, besides supply power, due to the external force. And as a final step, by applying the results from chapter 4 we obtained Eq. (5.102), where the environment is initialized in a microcanonical distribution at a given energy. This allows the semiclassical analysis involving non-vanishing relative coordinate trajectories, carrying information about the center of mass evolution. In the open system scenario, we additionally face the problem of how to calculate, in a systematic way, interference effects between trajectories that are dissipating energy to the environment. In many situations an open system can have different stationary points towards it will approach for long times, depending on the initial conditions and parameters of the system. Thus, the possibility to see interference processes between trajectories approaching different stationary points is exciting, and deserves more analysis.

# A. Equations of motion based on the influence functional symmetries

In this appendix we follow [43,119] in order to show the emergence of classical equations of motion with broken time-reversal symmetry, in virtue of properties and symmetries of the Feynman-Vernon influence functional, independent of any details of the systems. As usual, let us consider a system $\mathcal{A}$ coupled to an environment $\mathcal{E}$. If we do not care, or do not have control over the final states of the environment, after tracing out its degrees of freedom we obtain the reduced density matrix for $\mathcal{A}$. We will focus on the transition probability that the central system found at time $s = 0$ in position $Q(0) = Q_i$, may be found at later time $s = t$ in position $Q(t) = Q_f$. This process is described by the reduced density matrix, reading

$$\rho_{\mathcal{A}}(Q_f, Q_f; t) = \int dQ_i \; \rho_{\mathcal{A}}(Q_i, Q_i; 0) \int \mathcal{D}Q\mathcal{D}Q' \; \mathrm{e}^{\frac{i}{\hbar}(S[Q]-S[Q'])}\mathcal{F}[Q, Q'], \tag{A.1}$$

comprising paths from $Q(0) = Q'(0) = Q_i$ to $Q(t) = Q'(t) = Q_f$. The action $S[Q]$ is the bare action of the central system, and $\mathcal{F}[Q, Q]$ is the Feynman-Vernon influence functional [43], describing the effects on $\mathcal{A}$ due to the environment. Any $\mathcal{F}[Q, Q']$ can always be written as

$$\mathcal{F}[Q, Q'] = \mathrm{e}^{\Pi[Q,Q']}\mathrm{e}^{i\Sigma[Q,Q']}, \tag{A.2}$$

with $\Pi$ and $\Sigma$ real functionals. Moreover, $\mathcal{F}$ has the symmetry property

$$\mathcal{F}[Q, Q] = 1, \tag{A.3}$$

for those paths fulfilling the above boundary conditions. This implies

$$\Pi[Q, Q] = \Sigma[Q, Q] = 0. \tag{A.4}$$

A further symmetry of the influence functional reads $\mathcal{F}[Q, Q'] = \mathcal{F}^*[Q', Q]$, which accordingly implies

$$\begin{aligned} \Pi[Q, Q'] =& \Pi[Q', Q], \\ \Sigma[Q, Q'] =& -\Sigma[Q', Q]. \end{aligned} \tag{A.5}$$

To obtain the classical equations of motion we need to calculate the first variations of the actions $\Pi$ and $\Sigma$ with respect to the paths $Q, Q'$. Using center of mass $r = (Q + Q')/2$ and relative $y = Q - Q'$ coordinates, we observe that due to the symmetry in Eq. (A.5) $\Pi$ is an even functional of $y$, at least quadratic, such that

$$\Pi[r + y/2, r - y/2] = \Pi[r - y/2, r + y/2]. \tag{A.6}$$

Moreover, the symmetry in Eq. (A.4) implies $\Pi[r, r] = 0$, and in this way, an expansion of $\Pi[r + y/2, r - y/2]$ around $r$ shows that *the first variations of* $\Pi$ *along the diagonal vanishes*. Thus, for paths such that $Q = Q'$, the equation of motion, obtained by variation of the total action in Eq. (A.1), reads

$$\delta S[Q] + \int_0^t ds\ \Sigma_Q[Q, Q; s]\delta Q(s)ds = 0, \tag{A.7}$$

where $\Sigma_Q$ denotes variation with respect to the path $Q$. Finally, writing the bare action as $S[Q] = \int_0^t ds\ \mathcal{L}(Q, \dot{Q}, s)$, the equation of motion becomes

$$\frac{d}{ds}\frac{\partial \mathcal{L}}{\partial \dot{Q}} - \frac{\partial \mathcal{L}}{\partial Q} + \Sigma_Q[Q, Q; s] = 0. \tag{A.8}$$

As a final step, we should prove that the functional $\Sigma_Q$ depends only on the past history, to show that the equation of motion has indeed broken the time-reversal symmetry. Let us expand $\Sigma[Q + \delta Q, Q]$ around $(Q, Q)$, to write

$$\Sigma[Q + \delta Q, Q] = \int_0^t ds\ \Sigma_Q[Q, Q]\delta Q(s). \tag{A.9}$$

Choosing the variations such that $\delta Q(u) = 0$, for $u \geq s$, and $\delta Q(u)$ otherwise arbitrary, we obtain

$$\Sigma[Q + \delta Q, Q] = \int_0^s du\ \Sigma_Q[Q, Q; u]\delta Q(u). \tag{A.10}$$

Now, in virtue of the symmetry Eq. (A.3), if $Q = Q'$ at times $u \geq s$, then $\mathcal{F}[Q, Q']$ does not depend on the properties of $Q(u)$ in this time interval [43]. Thus, due to the chosen variations $\delta Q$, the above statement applies also to both sides of Eq. (A.10), and then we see that $\Sigma_Q$ does not depend on any property of $Q(u)$ for $u > s$. This shows that the functional $\Sigma_Q$ can be considered as a generalized induced force, producing dissipation [119].

# B. Environment autocorrelation function for complex arguments

In this appendix we give sense to the expression involving the environment autocorrelation function in Eq. (4.29), namely

$$\mathcal{K}_\tau(s) = \int_0^\infty d\omega \; \frac{J(\omega)}{\pi} \cot\left(\frac{\tau\omega}{2}\right) \cos\omega s, \tag{B.1}$$

for complex values of $\tau$. This integral diverges for the simple Ohmic spectral density. Thus, we should consider the case of an spectral density with a Drude cut-off frequency $\omega_D$, such that

$$J(\omega) = \gamma\omega \frac{\omega_D^2}{\omega^2 + \omega_D^2}, \tag{B.2}$$

which acts as a filter for frequencies greater than the cut-off $\omega_D$. Then, we aim to solve the integral

$$\mathcal{K}_\tau(s) = \frac{\gamma\omega_D^2}{2\pi} \int_{-\infty}^\infty d\omega \; \frac{\omega}{\omega^2 + \omega_D^2} \cot\left(\frac{\tau\omega}{2}\right) \cos\omega s, \tag{B.3}$$

using a contour in the complex $\omega$-plane. Above we have extended the integral limit using the fact that the integrand is an even function of $\omega$. First, we identify the poles of the first part of the integrand, by writing

$$\frac{\omega}{\omega^2 + \omega_D^2} = \frac{\omega}{(\omega - i\omega_D)(\omega + i\omega_D)} \equiv g(\omega). \tag{B.4}$$

While for a value $\tau = \tau_1 - i\beta$, with $\tau, \beta$ real, and $\beta > 0$, we obtain

$$cot\Big(\frac{\tau\omega}{2}\Big) = i\frac{(1 + \mathrm{e}^{-i\tau_1\omega}\mathrm{e}^{-\beta\omega})}{(1 - \mathrm{e}^{-i\tau_1\omega}\mathrm{e}^{-\beta\omega})}, \tag{B.5}$$

whose poles are given at

$$\omega_n = \tau_1\nu_n + i\beta\nu_n. \tag{B.6}$$

In terms of the Matsubara frequencies $\nu_n = \frac{2\pi n}{|\tau|^2}$, with $n = 0, \pm1, ....$ The location of the poles are shown in Fig B.1. Accordingly we write Eq. (B.3) as

$$\mathcal{K}_\tau(s) = \frac{\gamma\omega_D^2}{2\pi}\frac{i}{2} \int_{-\infty}^\infty d\omega \; g(\omega) \frac{1 + \mathrm{e}^{-\omega(\beta + i\tau_1)}}{1 - \mathrm{e}^{-\omega(\beta + i\tau_1)}} \Big(\mathrm{e}^{i\omega|s|} + \mathrm{e}^{-i\omega|s|}\Big). \tag{B.7}$$

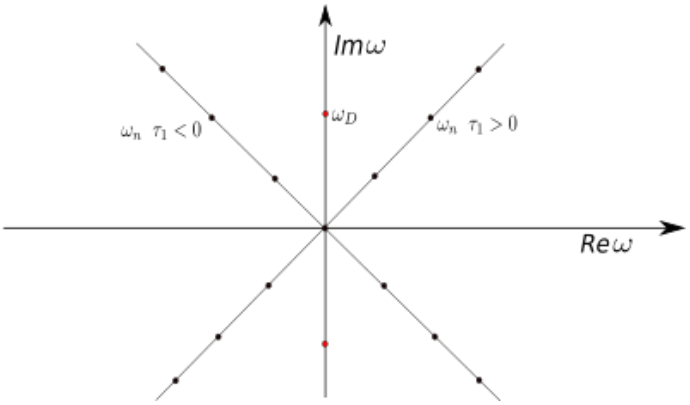


Figure B.1: The black dots show the poles $\omega_n$ of the factor in Eq. (B.5), while red dots represent the poles of the function $g(\omega)$ in Eq. (B.4). The two lines in the complex plane depend accordingly on the sign of $\tau_1$.

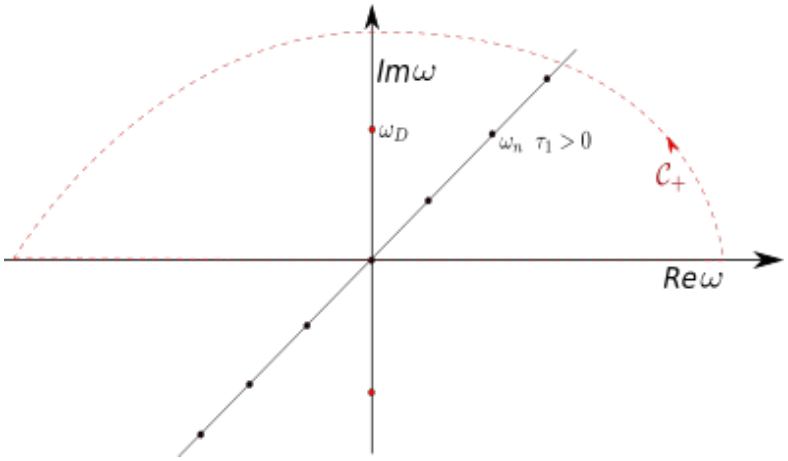


Figure B.2: The contour $\mathcal{C}_+$ used to solve the integral in Eq. (B.8) in the upper-half of the plane, which employing the residue theorem yields the result shown in the equation. A similar contour, but on the lower-half of the plane, is used to solve the integral in Eq. (B.9).

Thus, if $\tau_1 > 0$, we choose the contours shown in Fig B.2. On the upper-half contour $\mathcal{C}_+$, using $z = \mathrm{Re}\,\omega + i\,\mathrm{Im}\,\omega$, and employing the residue theorem, we obtain

$$\begin{aligned}\frac{\gamma\omega_D^2}{2\pi}\frac{i}{2}\oint_{\mathcal{C}_+} dz\; g(z)\frac{1+\mathrm{e}^{-z(\beta+i\tau_1)}}{1-\mathrm{e}^{-z(\beta+i\tau_1)}}\mathrm{e}^{iz|s|} =& \frac{\gamma\omega_D^2}{2\pi}\frac{i}{2}\Bigg[2\pi i\frac{2}{\beta+i\tau_1}\sum_{n=1}^{\infty} g(\omega_n)\mathrm{e}^{i\omega_n|s|} \\ &+ 2\pi i\frac{1+\mathrm{e}^{-i\omega_D(\beta+i\tau_1)}}{1-\mathrm{e}^{-i\omega_D(\beta+i\tau_1)}}\frac{\mathrm{e}^{-\omega_D|s|}}{2}\Bigg].\end{aligned} \tag{B.8}$$

Above we have used the fact that $g(\omega_n = 0) = 0$. In a similar way, on the lower-half contour $\mathcal{C}_-$ the calculation yields

$$\begin{aligned}\frac{\gamma\omega_D^2}{2\pi}\frac{i}{2}\oint_{\mathcal{C}_-} dz\; g(z)\frac{1+\mathrm{e}^{-z(\beta+i\tau_1)}}{1-\mathrm{e}^{-z(\beta+i\tau_1)}}\mathrm{e}^{-iz|s|} =& -\frac{\gamma\omega_D^2}{2\pi}\frac{i}{2}\Bigg[2\pi i\frac{2}{\beta+i\tau_1}\sum_{n=-1}^{-\infty} g(\omega_n)\mathrm{e}^{-i\omega_n|s|} \\ &+ 2\pi i\frac{1+\mathrm{e}^{i\omega_D(\beta+i\tau_1)}}{1-\mathrm{e}^{i\omega_D(\beta+i\tau_1)}}\frac{\mathrm{e}^{-\omega_D|s|}}{2}\Bigg],\end{aligned} \tag{B.9}$$

where the clock-wise direction on the contour has been taken into account. Finally, summing up both results, and after some algebra, we obtain

$$\mathcal{K}_\tau(s) = \frac{\gamma\omega_D^2}{2\pi}\frac{i}{2}\left[2\pi i\frac{4}{\beta+i\tau_1}\sum_{n=1}^{\infty}\frac{\omega_n}{\omega_n^2+\omega_D^2}\mathrm{e}^{i\omega_n|s|} + 2\pi\mathrm{e}^{-\omega_D|s|}\cot\left(\frac{\omega_D}{2}(\beta+i\tau_1)\right)\right], \tag{B.10}$$

which comprises an infinite sum over Matsubara frequencies, involving the complex $\tau$, and a decaying function of the cut-off $\omega_D$. On the other hand, if $\tau_1 < 0$, the same arguments apply, but the contours are exchanged, giving rise to the same final result.

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Dissipation of energy and the loss of quantum coherence are the main hallmarks of open quantum systems, which refers to a system coupled to many degrees of freedom of an uncontrollable environment. Due to this coupling, the system gradually loses its quantum properties and behaves more “classical”.

On the other hand, in the regime of large quantum numbers, semiclassical theory helps to understand quantum systems using information about their classical limit, allowing to observe interference effects between classical trajectories.

This thesis aims is to use the semiclassical approach to study open quantum systems. In this work, a novel notion of temperature for strongly coupled systems is developed. as well as a semiclassical treatment of decoherence in classically chaotic systems. Further, a new approach to catch interference between dissipative classical trajectories is studied, which opens the possibility to observe path interference in quantum thermodynamics.

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