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# Quantizing Lévy Flights

## Extending the Caldeira-Leggett model for velocity-dependent coupling forces in dissipative systems

*Since its very beginning, quantum mechanics has been developed to deal with systems on the atomic or sub-atomic scale. For many decades, there has been no reason to think about its application to macroscopic systems. Actually, macroscopic objects have even been used to show how bizarre quantum effects would appear if quantum mechanics were applied beyond its original realm. [...] due to recent advances in the design of systems on the meso- and nanoscopic scales, as well as in cryogenic techniques, this situation has changed drastically.*

—Amir Ordaçgi Caldeira [11, p. 1]


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## Abstract

Brownian motion is the random-walk behavior exhibited by a particle when subjected to a bath composed of smaller particles that constantly undergo collisions with the Brownian particle. Its trajectory is described by the Langevin equation, which has several technical problems for constructing a quantum version of the model. Most notably, there is a velocity dependence in the equation of motion, which makes direct canonical quantization problematic; energy is not conserved due to diffusion. To solve this problem, Anthony James Leggett and Amir Ordaçgi Caldeira, modeled the bath as a collection of harmonic oscillators, which allowed them to close the system, derive the Langevin equation in the appropriate (classical) limit for the ohmic regime, and investigate quantum aspects of Brownian motion.

Building on this Caldeira-Leggett model, this research suggests to change the interaction between the Brownian particle and the bath to depend on the velocity of the particle in a general way. We derive a generalized velocity-dependent Langevin equation with memory effects and multiplicative noise. First, when we reduce to a coupling linear in velocity the memory disappears and we find a Langevin-type equation that resembles the equation for the self-interaction of an electron with its own radiation field, i.e. the Abraham-Lorentz equation, in the superohmic regime. Second, when we make the approximation that the second derivative of the coupling is negligible, a particular non-polynomial coupling reproduces a force term that gives rise to Lévy flights as encountered in ultracold-atoms experiments, e.g. *Sisyphus* laser cooling.

We also use the path-integral quantization method to construct a quantum version for our generalized velocity-dependent Caldeira-Leggett model. After tracing out the bath, it turns out to be possible to find an effective action without a special choice for the form of the coupling; hence, it remains completely general. Reducing to the linear-velocity case, we obtain an effective action that can be interpreted as a bath-induced resistance to a change in velocity of the Brownian system—on top of classical inertia terms. For the effective action corresponding with the Lévy flight model, further numerical research is desirable.

Last, we will also discuss future possibilities of engineering environments in such a way that they are friendly to coherence, which has many applications—for example, suppressing decoherence for quantum computers.

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# 1 Introduction

## 1.1 Quantizing dissipative systems: the problem and the solution(s)

The story of this thesis is a story of dissipation. Dissipative systems are 'open', in the sense that they are in contact with a surrounding environment which it is constantly interacting with. Of course, this is always the case for a realistic system, since a perfect vacuum will never be achieved; albeit for technologically imperfect vacuum pumps, cosmic microwave photons, or, at the very least, spontaneously appearing particle-antiparticle pairs. But these interactions are usually so small that they are inconsequential; after all, it is the great merit of science to theoretically isolate certain parts of the world and give an explanatory theory for such a subsystem on itself. It is quite a different thing, though, when the mathematical model itself is not 'closed'. This happens when one gives a phenomenological description of the observations, while the assumption cannot be made that the part which is left out of the description is negligible.

The paradigmatic example of an open system is Brownian motion: the random-walk behavior of a colloid particle suspended in some medium such as water—as depicted at the left of Figure 1. The equation that describes the motion of such a 'Brownian particle' is the Langevin equation, written down by Paul Langevin in 1906. This is a phenomenological model: although the water plays a crucial role in the dynamics of the system, as water molecules bombard the Brownian particle from all directions and at all times, the motion of the water molecules themselves is not described.

It has historically proven difficult to successfully construct quantum-mechanical versions of open systems. The reason for this is twofold. First, since the system is continuously exchanging energy with its environment, energy is not conserved. Therefore, a Hamiltonian or Lagrangian description with the Langevin equation as its corresponding dynamics, will have an explicit time-dependence. Second, the dynamics of an open system is practically irreversible, because the environmental degrees of freedom are usually too many to keep track of. Hence, familiar schemes of quantization, canonical or via the path integral, are not straightforwardly in accord with the uncertainty principle.

Multiple solutions have been proposed to solve this problem. In the seventies, some proposed to adjust the Schrödinger equation to incorporate dissipative effects, most prominently by Kostin [40] and Nelson [63]. It was proposed by Dekker to modify the canonical quantization method to include complex variables. Another promising method is to use the Lindblad formalism, which is a master equation that preserves the trace and positivity of the density matrix and reproduces the Schrödinger equation under certain conditions. These are all demanding paths by themselves; we will consider a fourth route.

As early as 1959, Magalinskii suggested the elegant solution of including the environment itself into the description such that one ends up with a closed system [51]. He suggested to describe the bath as an infinite set of harmonic oscillators. In 1963, Feyn-

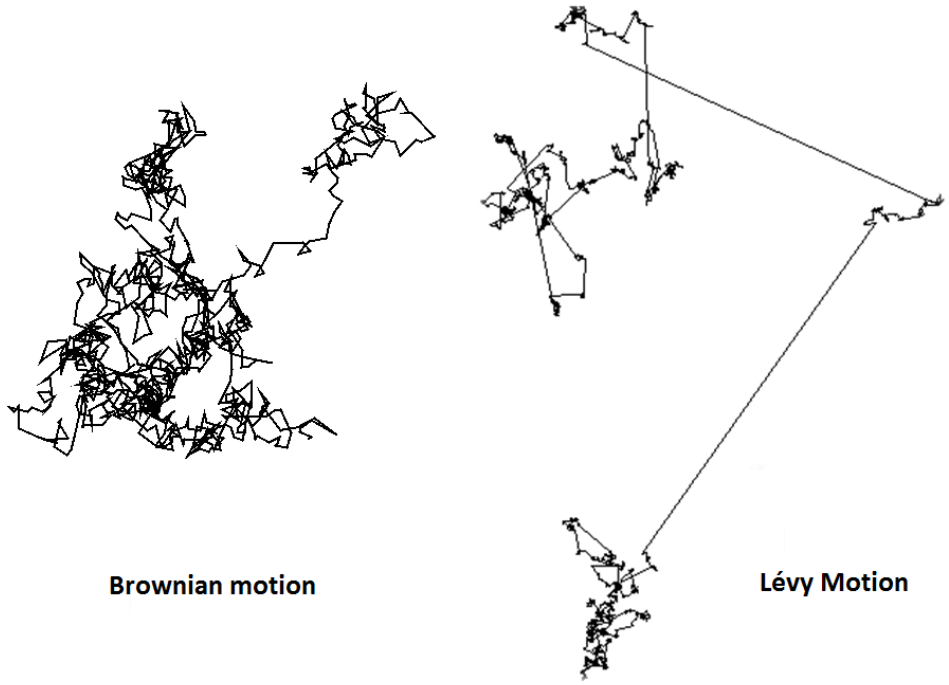


Figure 1: Left: The random-walk behavior of a Brownian particle. Right: Lévy motion; the system performs a random walk most of the time, which is sometimes interrupted by a long Lévy flight. Picture extracted from http://www.crm.umontreal.ca/~physmath/images/gallery.dir/.

man and Vernon developed a way to quantize such a system using the path-integral method [19]. Today, this model is often referred to as Caldeira-Leggett model, due to Caldeira and Leggett's proof that this model is also applicable to situations where the dissipation is very strong, which had a large impact on the theory quantum tunneling and the study of macroscopic quantum phenomena [8] [9]. In addition, at the quantum level, not only energy leaks into the environment, the coherence of quantum states also dissipates—a phenomenon known as decoherence, which the model also treats well. In short, the Caldeira-Leggett model is a successful description of quantum Brownian motion in a closed formalism.

Many simple physical systems adhere to the random-walk behavior of Brownian motion. Nevertheless, more complex motions are also found in nature. We will focus on Lévy motion, which performs the random walk for most of the time, but which has occasionally large 'jumps', which are the so-called 'Lévy flights'—as depicted at the right of Figure 1. Lévy distributions are the generalization of the Gaussian distribution in the sum of large numbers of independent variables in cases where the variances of the variables diverge. This result is known as the generalized central limit theorem. Lévy distributions are characterized by power-law tails and divergent moments. Hence, in contrast to the Gaussian-distributed momentum of Brownian motion, the Lévy dis-

tribution has a much wider support, a property called having 'heavy tails'. This, then, corresponds to a much larger probability for making long jumps. Lévy statistics occurs, for example, on the stock market [55], the migration patterns of the albatross [79], or in hopping processes in polymer physics [66].

Another area where Lévy flights occur is in laser cooling experiments. Laser cooling of atoms provides an ideal case study for the application of Lévy statistics in a privileged situation, where statistical models can be derived from first principles. In an experiment by Sagi, in 2012, anomalous spatial diffusion was directly studied by imaging the expansion of neutral $^{87}Rb$ atoms in a one-dimensional optical lattice. The atomic distributions at different times was given by a Lévy distribution [69].

In a theoretical work of Marksteiner, Ellinger, and Zoller, it is shown that Lévy flights should occur in Sisyphus laser cooling [56]. This cooling technique aims to cool an atom cloud down by pointing laser lights at it from all directions. Although the thermal fluctuations of individual atoms within the cloud are very small, sometimes a Lévy flight occurs as a result of the spontaneous emission of a photon by an excited atom [52]; the recoil that results from the emission corresponds, then, to the Lévy flight.

## 1.2 This Thesis: a velocity-dependent Caldeira-Leggett model

This thesis aims to modify the Caldeira-Leggett model in such a way that it will incorporate Lévy behavior. The goal is to find a closed Lagrangian description of Lévy motion, which would then allow for direct quantization—either canonically or via the path integral. In other words, we are searching for a closed quantum theory of Lévy systems.

The original Caldeira-Leggett Lagrangian couples the coordinate of the Brownian particle linearly to the particle of the bath. The strategy we will follow is to modify this coupling to one that depends on the velocity of the Brownian particle in a very general way, while still being coupled to the bath coordinates. With such a closed description in hand, we will quantize the system using path-integral quantization.

It turns out that in certain limiting cases, and for a specific non-polynomial choice for the form of the velocity coupling, such a strategy allows one to reproduce the force term from Marksteiner, Ellinger and Zoller's research that gives rise to Lévy flights in Sisyphus cooling. In the low-velocity limit, this result reduces to a linear-velocity coupling. For this linear-velocity case, we find, for cubically superohmic baths, an equation that has the same form as the equation of motion of an self-interacting electron in a cavity, i.e. the Abraham-Lorentz equation. We find this, without assuming an electron model or other fundamental physics. We also construct an effective action corresponding to the modified Caldeira-Leggett Lagrangian. That is, we integrate out the bath coordinates, leaving us only with an effective dynamics for the Brownian system. It turns out, that such an effective action can be found without considering specific cases for the velocity coupling, and is, therefore, completely general.

Summarizing, one can distinguish three main results in this thesis. First, the reproduction of Lévy flights in ultracold-atom experiments. Second, the derivation of an

equation similar to the Abraham-Lorentz equation, for linear-velocity coupling and a superohmic bath. Third, a quantum-mechanical effective action for completely general coupling forces.

## 1.3 Outline of the Thesis

This thesis contains four main chapters; respectively, they deal with setting up the framework for open systems, closing the system via the Caldeira-Leggett approach, modifying the Caldeira-Leggett model to general velocity-dependent coupling, and quantizing this modified model.

Specifically, in Chapter 2 we will discuss four subjects. First, we will discuss the theory of Brownian motion as it was developed by Einstein, Langevin and others. Second, we will discuss the phenomenon of decoherence from a very general perspective. Third, we will derive some results from linear-response theory that will be needed for the Caldeira-Leggett model. And last, we will discuss the occurrence of Lévy flights in Sisyphus cooling. In Chapter 3, we thoroughly discuss the Caldeira-Leggett model and the derivation of the Langevin equation from it. In Chapter 4, we apply the same methods as in Chapter 3 to the modified Caldeira-Leggett Lagrangian, resulting in a modified Langevin equation with multiplicative noise and memory effects. In Section 4.2, we discuss a general polynomial approach, the linear-velocity case, and the coupling that gives rise to Lévy flights. In the final chapter, Chapter 5, we derive the path-integral formalism and discuss the Feynman-Vernon functional integral approach. Furthermore, we derive the quantization of the free particle and the forced harmonic oscillator, and we derive the effective action for the modified Caldeira-Leggett model.

**A few remarks about notations:**

- Throughout the thesis, we will deal with coupling constants denoted by $C_k$, $C'_k$, $\bar{C}_k$ and $\tilde{C}_k$. In principle, these distinction are unimportant in the context of a single section. However, taking the thesis as a whole, the distinction refers to coordinate-coordinate coupling, general-coordinate coupling, linear-velocity coupling and general-velocity coupling, respectively.
- In other cases, 'primes' will indicate partial derivatives with repects to the argument of the function. Hence, $F'[\dot{Q}]$ is shothand for $\partial F[\dot{Q}]/\partial\dot{Q}$.
- I will stick to 'Mermin's imperative', i.e. giving every equation a number, such that it can always be referenced [58].

# 2 Open Dissipative Systems

> "[T]he human mind is built to identify for each event a definite cause and can therefore have a hard time accepting the influence of unrelated or random factors."
>
> —Leonard Mlodinow [59, p. xi]

## 2.1 The Theory of Brownian Motion

### 2.1.1 Einstein's approach: the Diffusion equation

Brownian motion is the behavior of a system undergoing random fluctuations, of which the paradigmatic example is a particle suspended in a liquid bath. The first scholar to notice this effect, was the Dutch plant physiologist Jan Ingenhousz in 1785, who observed the irregular movement of coal dust particles on the surface of an alcohol suspension under a microscope [34]. Almost half a century later, in 1828, the botanist Robert Brown observed a very similar effect when observing particles of the pollen of plants in water; see Figure 2 for a sketch of the observation. In the heydays of vitalism, this irregular movement was originally ascribed a biological origin, caused by 'swimming' living creatures in the fluid. Through further experiments, Brown established this was a highly problematic explanation of what he saw:

> "I was led next to inquire whether this property continued after the death of the plant [...], the particles [...] were found in motion equally evident with that observed in the living plant; specimens of several plants, some of which had been dried and preserved in an herbarium for upwards of twenty years, and others not less than a century, still exhibited the molecules or smaller spherical particles in considerable numbers, and in evident motion [...]."[7, p. 469]

Although the 1860s and '70s saw the rise of the kinetic theory of molecules developed most prominently by Boltzmann, Gibbs and Maxwell, controversy about the ontological status of molecules reigned. During his *annus mirabilis* 1905, Einstein hypothesized, using the kinetic theory, that the physical origin of the by-then called Brownian particles lay in their continuous interaction with other particles, too small to be seen through the microscope [16]; see Figure 3.

For Einstein, the framework was mainly based on *diffusion*: the flow of particles, e.g. as a result of a density gradient from a high density area to a low density area, which he described using Fick's law [24]. In modern notation, Fick's first law states that the net particle flux $J(x)$ through a barrier of length $L$ is proportional to the density gradient due to the difference in particle pressure on either side of that area,

$$J(x) \equiv \frac{d\mathcal{N}(x,t)}{dt} = -D\frac{d\mathcal{N}(x,t)}{dx}, \tag{2.1}$$

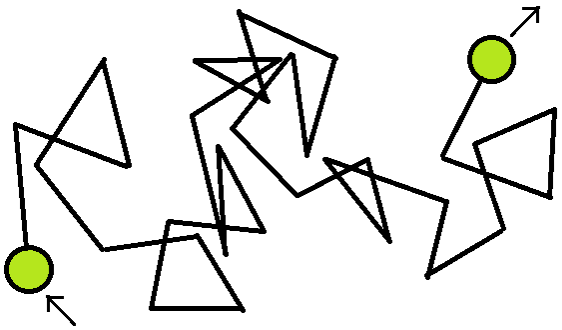

Figure 2: A sketch of what Robert Brown must have seen under his microscope: the jiggling around of a Brownian particle from the initial position to the final position. This movement has become known as the 'Random walk'.

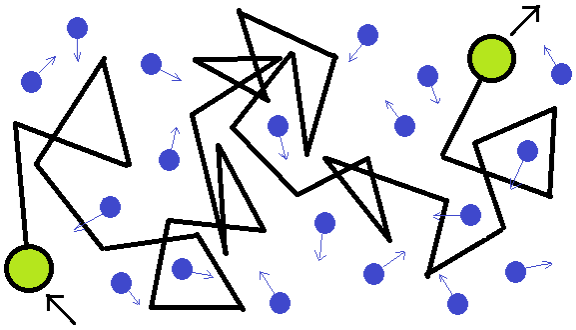

Figure 3: Einstein's theoretical explanation of Brownian motion: the Brownian particle is repeatedly bombarded by smaller particles, unseen through the microscope. These smaller particles are described by the kinetic theory of Maxwell, Boltzmann, and Gibbs, serving (historically) as strong empirical indication of the merit of the kinetic theory of gases.

where $\mathcal{N}(x,t) = n(x,t)/L$ is the number of particles $n(x,t)$ per area and $D$ is called the diffusion constant; see also Figure 4. The minus sign is conventional, due the choice of the positive $x$-direction (being to the right in the Figure).

Starting with the particle density $\mathcal{N}(x,t)$ at some point in time, we want to predict the rate of change of this density in terms of the density gradient. Assuming locality and conservation of the total number of particles leads to the continuity equation: some particles will enter a certain area (due to the density gradient) and some will leave it, such that their rate of change is [71, pp. 5–6]

$$\frac{d\mathcal{N}(x,t)}{dt} = -\frac{dJ(x)}{dx}. \tag{2.2}$$

Combined with Eq. (2.1) we arrive at the diffusion equation,[1]

$$\frac{d\mathcal{N}(x,t)}{dt} = D\frac{d^2\mathcal{N}(x,t)}{dx^2}. \tag{2.4}$$

Now, taking an initial state for the density of $N$ particles, $\rho(x_1,...,x_M;t=0) = \delta(x)$, [75, p. 201], where all particle starts out in the origin, the solution of the diffusion equation (2.4)–as can easily be checked–is the Maxwell-Boltzmann distribution

$$\mathcal{N}(x,t) = \frac{N}{\sqrt{4\pi Dt}}\exp\left[-\frac{x^2}{4Dt}\right], \tag{2.5}$$

which describes the spreading of the particle density function, i.e. diffusion, as it becomes de-localized as time goes on.

We can reformulate the above approach in terms of a 'random-walk' that the Brownian particle performs, as Figure 2 shows. Every step in time $\Delta t$, the Brownian particle makes jumps in a *random* direction with arbitrary distance $\Delta x$. Using Eq. (2.4)–which can now interpreted as a probability density–one can calculate the expectation values of the mean distance traveled, and the mean-square displacement of the Brownian particle. On average, the distance traveled by one ($N = 1$) particle (or 'first moment')

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} dx\ x\ \mathcal{N}(x,t) = \frac{1}{\sqrt{4\pi Dt}}\int_{-\infty}^{\infty} dx\ x\ \exp\left[-\frac{x^2}{4Dt}\right] = 0 \tag{2.6}$$

vanishes, due to the odd integrand—as it should for random step-direction. The mean

[1] This is easily generalized to three dimensions, relying on the fundamental assumption of statistical physics that a particle is equally likely to move in any direction, i.e. isotropy, such that

$$\frac{d\mathcal{N}(\vec{x},t)}{dt} = \tilde{D}\vec{\nabla}^2\mathcal{N}(\vec{x},t), \tag{2.3}$$

for $\tilde{D} = D/3$. This is also known as Fick's second law.

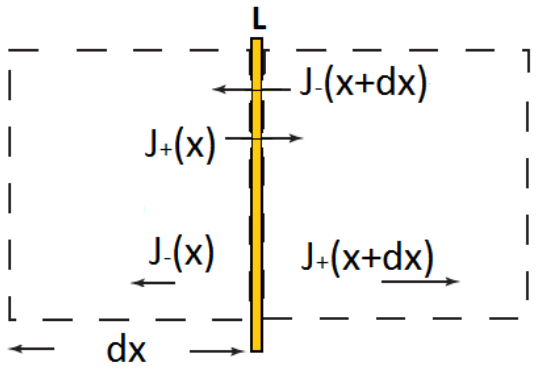


Figure 4: Fick's law. The particle flux $J(x)$ is the number of particles per unit time passing through the area A (in yellow). The subscript '+' indicates particles traveling to the right, '−' indicates particles traveling to the left. The rate of diffusion is given by the diffusion constant $D$.

squared displacement (or 'second moment') is

$$\langle x^2(t)\rangle = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} dx\ x^2\ \exp\left[-\frac{x^2}{4Dt}\right] = 2Dt, \tag{2.7}$$

where we performed the Gaussian integral. For one step $\Delta x$, the diffusion coefficient is then given by

$$D = \frac{\langle(\Delta x)^2\rangle}{2\Delta t}, \tag{2.8}$$

which is Einstein's relation. Through the relation (2.8), Einstein's theory provided a theoretical expression for the diffusion coefficient in terms of the size of the atoms (assuming spherical atoms) [16, p. 17]. Since the diffusion coefficient can be experimentally measured, Jean Perrin found a way to measure Avogrado's number [64]. Intuitively, to find this number one needs to measure the value of a *macroscopic quantity* (of a pure material) and the value of this quantity for a *single* particle. Perrin measured the charge of a mole of electrons and divided it by the charge on a single electron (using Millikan's well-known result [54]), obtaining a value of Avogadro's number of the number of particles per mole.[2]

The diffusion equation (2.4) is an example of the Fokker-Planck equation in the

[2]Contrary to popular belief, Amadeo Avogadro did not estimate or publish on what is now known as 'Avogadro's number' (the number of particles of an ideal gas in a given volume). In the early nineteenth century, Avogadro posed the hypothesis that equal volumes of different gases (at the same temperature and pressure) contain the same number of particles. It was Josef Loschmidt, *using the kinetic theory of gases*, in 1865, who first gave an estimate of the number of particles in a cubic centimeter of a gas: he estimated the Loschmidt constant at $2.6867773 \times 10^{25} m^{-3}$ [50]. Jean Perrin, in his 1908 measurement of this number, coined the term 'Avogadro's constant'.

case of Brownian particles in a fluid. The Fokker-Planck equation is a master equation, which, in general, describes the evolution of a probability function $P(x,t)$, and reads [75, p. 193–196]

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}A(x)P + \frac{1}{2}\frac{\partial^2}{\partial x^2}B(x)P, \tag{2.9}$$

for real differentiable functions $A(x)$ and $B(x) > 0$. For Brownian motion, the probability interpretation comes in by interpreting Eq. (2.4) as an *average* particle flow in the diffusion equation—after all, in practice we are wholly ignorant of the precise microstate of the system and, therefore, retort to the ensemble approach. In this context, the first term on the right-hand side of Eq. (5.1.1) is called the 'drift term' and the second term is called the 'fluctuation term'. In the words of Einstein, "[w]e can look upon the dynamic equilibrium condition considered here as a superposition of two processes proceeding in opposite directions."[16, p. 10]. In equilibrium, hence, when the left-hand side vanishes, these forces should cancel each other out. These two processes are the influence of a fluctuation force on the one hand, and a process of diffusion on the other. This is an example of the *fluctuation-dissipation theorem*, which we will derive more generally in the next two sections.

### 2.1.2 Langevin's approach: velocity-dependent force balance

In 1906, Paul Langevin provided a mathematical framework for Einstein's theory of Brownian motion, using a stochastic differential equation for the motion of the Brownian particle, subject to a friction force and a fluctuation force [44]. Starting from Newton's second law for a system of mass $M$ and position vector $\vec{x}(t)$, he wrote

$$M\frac{d\vec{v}}{dt} = \vec{F}_{\text{friction}} + \vec{f}(t) \quad \text{and} \quad \vec{v} = \frac{d\vec{x}}{dt}, \tag{2.10}$$

First, there is a friction force (or "viscous drag"), representing the friction that the Brownian particle will experience and which will be responsible for dissipation; this force is proportional to the velocity of the particle and its mass, where the proportionality constant is the friction coefficient $\eta$, hence

$$\vec{F}_{\text{friction}} = -\eta\vec{v}. \tag{2.11}$$

The second force should represent the influence of the bath on the Brownian particle. According to Langevin, this force is "rapidly and unpredictably varying" [44]. We will call it the *fluctuation force* $f(t)$, since it will give rise to bath-driven fluctuations. It is then natural to make the step to modeling this force in a *stochastically*—The function $f(t)$ itself is now taken from an *ensemble* of functions each endowed with a certain probability weight. Although, in reality, $f(t)$ is uniquely defined and deterministic, it is unattainable regarding the large number of degrees of freedom of the bath. This step from a unique deterministic force towards an stochastic one is not always apparent in the literature, due to a loose use of the word 'random' [77, cf.]. The task that arises,

then, is determining the distribution of this ensemble.

In principle, the system would also feel external forces, such as gravity. For generality, then, we include an external force $\vec{F}_{\text{ext}} = -\vec{\nabla}V(x)$, for $V(x)$ the external potential. The Langevin equation reads

$$M\frac{d\vec{v}}{dt} + \vec{\nabla}V(x) + \eta\vec{v} = \vec{f}(t). \tag{2.12}$$

This is a stochastic differential equation: it can only be solved if we specify a probability distribution for the different functions $f(t)$. Without this specification, the Langevin equation is meaningless; hence, we will speak here of the Langevin equations (plural), to indicate that only the form of Eq. (2.12) is not the end of the story.

First, since the collisions between the Brownian particle and the bath constituents are supposed to be random both in direction and in strength, the fluctuation force should vanish on average,[3]

$$\langle f_i(t)\rangle = 0, \tag{2.15}$$

where the index $i \in \{x, y, z\}$ indicates the direction. Second, one must specify the duration of one collision, say $|t - t'|$, between the particles meeting each other at time $t$ and leaving each other at time $t'$. As long as the relevant times are larger than the collision time, one can conveniently use the delta distribution. Effectively, one assumes that all collisions are–for all practical purposes–instantaneous and uncorrelated to each other. Hence, we postulate the two-point correlation function

$$\langle f_i(t)f_j(t')\rangle = \alpha\delta_{ij}\delta(t - t'), \tag{2.16}$$

for the Kronecker delta $\delta_{ij}$, Dirac's delta distribution $\delta(t - t')$ and $\alpha$ a constant, which will be determined later. The delta-peaked two-point correlation function of Eq. (2.16) is usually referred to as 'white noise'. This assumption, called the *relaxation-time approximation*, breaks down at timescales where the microscopics of single collisions kicks in, i.e. $t < \tau$, for the so-called relaxation time $\tau$ the average time between two collisions.[4]

[3]Technically, the ensemble average is taken the initial values with respect to the unperturbed canonical classical equilibrium state

$$\langle ...\rangle = \int_{\text{phase space}} d\alpha^{(0)} \;\; \rho \times (...), \tag{2.13}$$

for the usual probability density of a classical statistical ensemble,

$$\rho = Z^{-1}\exp\left[-\frac{H}{k_B T}\right], \tag{2.14}$$

for partition function $Z$, Hamiltonian $H$, and $d\alpha^{(0)}$ a volume element of the phase space of initial conditions. The integral ranges over all possible values.

[4]Often one encounters another requirement, namely that the mass of the Brownian particle must be sufficiently high with respect to the other particles of the bath, i.e. $M \gg m$. However, this is not

For more realistic modeling, Eq. (2.16) should be sharply peaked, but with finite width equal to the duration of a single collision. This is the so-called Itô-Stratonovich dilemma . The function $f_i$ in Eq. (2.16) is singular, while–in reality–it should be a proper stochastic function (the Stratonovich approach). Hence, the trade-off is pragmatic: the delta distribution (the Itô approach) is easier to handle, but physically not well defined. In the words of Nico van Kampen, "[...] whenever the delta function stands for a sharp, but not infinitely sharp peak the Stratonovich interpretation is appropriate. The Itô interpretation cannot even be formulated unless $\tau$ is strictly zero" [75, Chapter IX-5, p. 232] There will be two places in which this approximation will play a role, though. Firstly, it will be consistent with the demand of taking the frequency cut-off $\Omega$ to infinity when treating the Caldeira-Leggett model. Secondly, when absorbing a 'spurious drift' term into the ensemble average in Eq. (3.41). We will discuss this then.

In other concerns, this nuance can be overlooked by keeping in mind that we can safely work within the relaxation-time approximation, $\tau$ very small, i.e. as long as other timescales a much larger than this single collision time, the delta distribution can be taken for convenience. In other words, after each collision the bath has the time to recover to equilibrium faster than the Brownian particle can. Therefore, such a system is called 'memory-less'.[5]

Let us simplify to zero external field $V(x) = 0$ and motion in one dimension.[6] For an initial condition for the velocity of the Brownian particle, say $v(0) = v_0$, the Langevin equation (2.12) can be solved explicitly. We multiply both sides of the equation by an integrating factor $\exp \eta t/M$, and obtain

$$\frac{d}{dt}\left(ve^{\frac{\eta}{M}t}\right) = \frac{1}{M}f(t)e^{\frac{\eta}{M}t}. \tag{2.17}$$

By integrating over time, we obtain

$$v(t) = v_0 e^{-\frac{\eta}{M}t} + \frac{1}{M}\int_0^t dt' f(t')e^{-\frac{\eta}{M}(t-t')}. \tag{2.18}$$

Taking the ensemble average, and utilizing Eq. (2.15), we find

$$\langle v(t)\rangle = v_0 e^{-\frac{\eta}{M}t}, \tag{2.19}$$

a strict theoretical requirement, since one can use the parameter $M$ and work in different high- or low-mass regimes later. Experimentally, though, to be visible as a Brownian particle in a bath (such as Brown's pollen in water) the mass is usually much higher—if this were not the case, the particle would be indistinguishable from bath constituents.

[5]The requirement of having 'no memory' often coincides with the *Markov property* that the probability of a future state does not depend on the current state. Nevertheless, this is not always the case, and is conceptually very different; see (again) Bacciagaluppi's [1] and the accurate remarks in Van Kampen's seven-paged [76].

[6]The results are trivially extended to three dimensions.

since the integrating factor is uncorrelated with the force. Hence, as time progresses, it is likely to find the particle slowing down.

Now, taking the square of of Eq. (2.18), we can calculate the correlation

$$\begin{aligned}\left\langle v^2(t)\right\rangle &= v_0^2 e^{-2\frac{\eta}{M}t} + \frac{e^{-2\frac{\eta}{M}t}}{M^2}\int_0^t dt' \int_0^t dt'' \left\langle f(t')f(t'')\right\rangle e^{\frac{\eta}{M}(t'+t'')} \\ &= v_0^2 e^{-2\frac{\eta}{M}t} + \frac{\alpha}{M^2} e^{-2\frac{\eta}{M}t}\int_0^t dt' e^{2\frac{\eta}{M}t'} \\ &= v_0^2 e^{-2\frac{\eta}{M}t} + \frac{\alpha}{2M\eta}(1 - e^{-2\frac{\eta}{M}t}),\end{aligned} \tag{2.20}$$

where we have used Eq. (2.16) in the second line. The cross term vanishes gain by ising Eq. (2.15).

Now, we can relate the friction force coefficient $\eta$ to the fluctuation coefficient $\alpha$ by employing our knowledge about the root-mean-square velocity of any classical system, since it must satisfy the equipartition theorem. Every degree of freedom that is quadratic in the Hamiltonian, will contribute a factor $1/2\, k_B T$ to the internal energy, for Boltzmann's constant $k_B$ and absolute temperature $T$.

$$\left\langle v^2\right\rangle = \frac{k_B T}{M} \tag{2.21}$$

Thus, after the system has equilibrated for $t \to \infty$, we can equate the right-hand sides of Eqs. (2.20) and (2.21), and find

$$\alpha = 2\eta k_B T. \tag{2.22}$$

This is the simplest form of the fluctuation-dissipation relation. That such a relation can be obtained by the initial information about the equilibrium system, through the equipartition theorem, is why the Langevin equations are so successful in making predictions: it enables for a precise macroscopic description between the fluctuation term that causes random collisions with the Brownian particle and the friction term which tries to damp these collisions down exponentially. In equilibrium, these opposing forces, as Einstein described in the quote above, balance each other out. The white noise requirement of Eq. (2.16) now reads

$$\left\langle f_i(t) f_j(t')\right\rangle = 2\eta k_B T \delta_{ij}\delta(t - t'), \tag{2.23}$$

Now that we have seen the framework of the classical system, we will briefly discuss an example for quantum mechanics. Benguria and Kac [5] discussed generalizing the

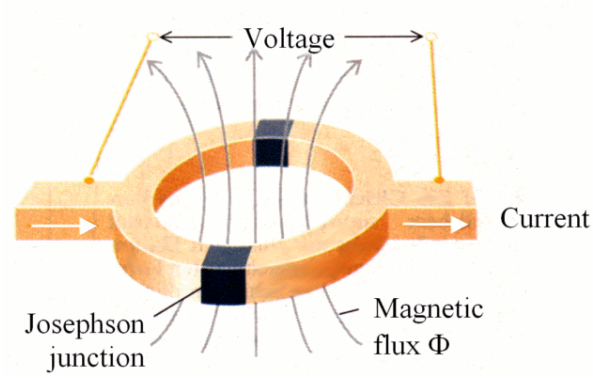


Figure 5: Sketch of an experimental set-up of a Josephson Junction apparatus. A circular current creates an magnetic ring in which individual flux quanta can be confined. Then, for the right settings, these can escape one by one though the Josephson Junction (in black). The dissipation of the flux quanta $\phi$ is described by Eq. (2.25).

fluctuation force to a quantum force, while maintaining Eq. (2.12). In one dimension, this reads

$$\langle f^q(t) f^q(t') \rangle = \frac{\eta}{2\pi} \int_0^\Omega d\omega \exp[-i\omega(t-t')] \hbar\omega \coth\left[\frac{\hbar\omega}{2k_B T}\right], \tag{2.24}$$

below a certain cut-off frequency $\Omega$. This is called *coloured noise*. Intuitvely, the correlation functions change due to Heisenberg's principle: $\langle \hat{x}\hat{p} \rangle = 1/2\imath\hbar$, see [41, Chapter 8] for full derivations of quantum noises. The cut-off corresponds to the reciprocal of the relaxation timescale $\tau$, and therefore only works for long-time behaviour of the system. For high temperatures $k_B T \gg \hbar\omega$ and the cut-off $\Omega \to \infty$, this coincides with the classical case of Eq. 2.23, while for low temperatures quantum modeling becomes possible. This approach has been used by Koch, Van Harlingen and Clarke to investigate Josephson junctions [39].

One of the most remarkable lessons of physics is that often the use of an identical mathematical description is applicable to widely differing physical systems. The Langevin equation is one such mathematical description; developed to treat Brownian motion, it can also be applied to the dynamics of the order parameter in a second-order phase transition [32], and works well for describing the noise of individual magnetic flux quanta $\phi$ in a non-linear capacitor circuit (an in-parallel-connected $RLC$-circuit with resistance $R$, capacitor $C$ and non-linear part $L$) [11]. The coordinate of the flux quanta of the last example obey

$$C\ddot{\phi} + \frac{RC}{L}\dot{\phi} + \frac{1}{L}\phi = I(t); \quad \langle I(t) \rangle = 0; \quad \langle I(t) I(t') \rangle = \frac{2RCk_B T}{L}\delta(t-t'), \tag{2.25}$$

where $I(t)$ is a fluctuation current. This model has had great success in the description of superconducting quantum interference devices (SQUIDs) and their application to

quantum computing. As this is a macroscopic system (it is an electrical circuit), a quantum version of this system will be very interesting, because it will describe quantum dissipation (i.e. decoherence) for macroscopic degrees of freedom. Hence, quantum effects are visible at the macroscopic level (as they are in SQUIDs).

## 2.2 Decoherence for general composite systems

We have seen in Chapter 2 that in open system energy can leak into the environment (dissipation). For quantum systems, an additional quantity can 'leak', namely coherence. This is due to the entanglement of the quantum system with the constituents of the bath surrounding it. These constituents, in turn, 'carry away' the coherence, which effectively brings about a dynamical localization of the system, see Figure 6; this phenomenon is called *decoherence*. For environments which behave 'ohmically', i.e. where diffusion behaves as in the case of Brownian motion, decoherence arises for fairly general interaction Hamiltonians (written as interaction between particles' relative position, which they always are). For non-ohmic baths, where diffusion is 'anomalous', one would intuitively assume that coherence effects will be heavily affected, but this is not yet fully understood—we will come back to this throughout the thesis.

In the next chapters, we will explore the Caldeira-Leggett Lagrangian, and, in Chapter 5, we will use path-integral quantization with the final goal of tracing out the environmental degrees of freedom and investigating decoherence properties. For this reason, we will discuss the phenomenon of decoherence in a general setting, and in the operator formalism. This will be necessary to understand the concept of integrating out the environmental degrees of freedom in the path-integral formalism. Also it will help understand how general decoherence is.

Let us start with a very general superposition of a quantum state $|\Psi\rangle = \sum_i c_i |\psi\rangle$, relative to some orthonormal basis set $\{|\psi\rangle\}$ and coefficients $c_i$. This will be our system of interest, which we intend to measure. Say we perform a measurement using (interact with) a measurement device $\mathcal{M}$ with eigenstates $\{|m_i\rangle\}$ such that this apparatus will become entangled with the system (subscript 0 will indicate the initial state). Hence,

$$|\Psi'\rangle = \sum_i c_i |\psi_i\rangle |m_0\rangle \xrightarrow{H_1} \sum_i c_i |\psi_i\rangle |m_i\rangle , \tag{2.26}$$

which is governed by a (general) interaction Hamiltonian $H_1$ (surely, such a Hamiltonian must exist for the apparatus to qualify as a measurement device).[7]

[7] The *measurement problem of quantum mechanics* revolves around making empirical sense of Eq. (2.26), since the right-hand side again describes a superposition, while we do not observe such (possiby macroscopic) superpositions in everyday life; hence we are faced with an explanatory gap. It will not help, for eample, to measure this superposition with another measurement device $\mathcal{M}_2$, because the superposition is contagious: $\sum_i c_i |\psi_i\rangle |m_{1,0}\rangle |m_{2,0}\rangle \xrightarrow{H_1} \sum_i c_i |\psi_i\rangle |m_{1,i}\rangle |m_{2,0}\rangle \xrightarrow{H_2} \sum_i c_i |\psi_i\rangle |m_{1,i}\rangle |m_{2,i}\rangle$, *ad infinitum*. It is this problem, and the empirical indication that quantum theory can be used to

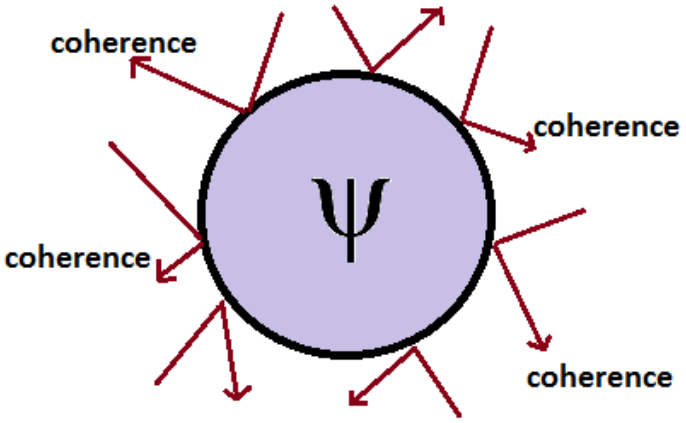


Figure 6: Decoherence, the environmental states (red arrows) continuously bombard (interact with) the quantum-mechanical system of interest $\Psi$ (the blue 'ball'), carrying away the coherence of the system, which in turn loses its off-diagonal terms in the density matrix. For ohmic environments, this turns out to happen for very general interaction Hamiltonians (written as interaction between particles' relative position, which they always are). For non-ohmic baths, this is not yet fully understood.

A system like this can, in practice, never really be closed—neutrino's, the cosmic microwave background, or imperfect vacua, will always interfere; the only closed system is the entire universe. So, we can choose to take into account all of the environment $\mathcal{E}$, with corresponding eigenstates $\{|\epsilon_i\rangle\}$, in a Hilbert space $\mathcal{H}_{tot} = \mathcal{H}_\Psi \otimes \mathcal{H}_\mathcal{M} \otimes \mathcal{H}_\mathcal{E}$. The complete state will then evolve as

$$|\Phi\rangle = \sum_i c_i |\psi_i\rangle |m_0\rangle |\epsilon_0\rangle \xrightarrow{H_1} \sum_i c_i |\psi_i\rangle |m_i\rangle |\epsilon_0\rangle \xrightarrow{H_2} \sum_i c_i |\psi_i\rangle |m_i\rangle |\epsilon_i\rangle . \tag{2.27}$$

Even when its influence of the environment is too large to be safely ignored, these $\{|\epsilon_i\rangle\}$ are hard to control in an experimental set-up, since we are dealing with an large ensemble. In this case it is helpful to switch to the density operator formalism, since it can combine classical statistical ensembles and superpositions.[8] For the state $|\Phi\rangle$ the total density operator is

$$\hat{\rho}_{\Psi\mathcal{M}\mathcal{E}} = \sum_{j,k} c_j c_k^\dagger |\psi_j\rangle |m_j\rangle |\epsilon_j\rangle \langle\psi_k| \langle m_k| \langle\epsilon_k| . \tag{2.28}$$

describe macroscopic entities such as SQUIDS, that led Amir Caldeira to write his book on dissipation for macroscopic quantum systems [11, p. 2] and led Anthony Leggett to ask the scientific community to create larger and larger macroscopic superpositions to test the limits of the theory [46].

[8]The density operator of a system of quantum states $|\psi_i\rangle$ is defined as $\hat{\rho} = \sum_i w_i |\psi_i\rangle \langle\psi_i|$, with weights $w_i$. These weights are the classical probabilities of the ensemble to be in a certain state (they are *not* quantum amplitude coefficients). See also Ref. [6, pp. 104-135].

besides being uncontrollable, the environment is most often also uninteresting; after all, we are interested in the system we are measuring. Thus, the strategy is to use the reduced density matrix of the system by tracing out the environmental degrees of freedom $\{|\epsilon\rangle\}$,[9]

$$\hat{\rho}_{\Psi\mathcal{M}} = Tr_{\mathcal{H}_\mathcal{E}}\{\hat{\rho}_{\Psi\mathcal{M}\mathcal{E}}\} = \sum_{j,k} c_j c_k^\dagger \left|\psi_j\right\rangle \left|m_j\right\rangle \left\langle\psi_k\right| \left\langle m_k\right| \left\langle\epsilon_j|\epsilon_k\right\rangle . \tag{2.29}$$

We can use this density operator to calculate the expectation value of some observable $\hat{O}$,[10]

$$\langle O\rangle := Tr\{\hat{\rho}_{\Psi\mathcal{M}\mathcal{E}}\hat{O}\} = Tr_{\mathcal{H}_\mathcal{E}}\hat{\rho}_{\Psi\mathcal{M}}\hat{O}_{\Psi\mathcal{M}}. \tag{2.30}$$

The crucial assumption is the orthogonality of environmental states, which must depend on the Hamiltonian of these states. However, usually one appeals to the high dimensionality of $\mathcal{H}_\mathcal{E}$ compared to $\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{M}$. There is a very large amount of air molecules, CMB photons, etc.. Many specific models, with corresponding Hamiltonians, have been worked out and they all show that these states are orthogonal or become so on times smaller than thermalization times, which are summed up in [37, pp. 64–68]. Thus, we can set

$$\langle\epsilon_i|\epsilon_j\rangle \approx \delta_{ij}. \tag{2.31}$$

This now leads to the disappearance of interference terms (the cross terms) in the superposition of the reduced system,

$$\hat{\rho}_{\mathcal{S}\mathcal{A}} = Tr_{\mathcal{H}_\mathcal{E}}[\hat{\rho_{\mathcal{S}\mathcal{A}\mathcal{E}}}] = \sum_j |c_j|^2 \Big( \left|\psi_j\right\rangle \left\langle\psi_j\right| \otimes \left|a_j\right\rangle \left\langle a_j\right| \Big). \tag{2.32}$$

This diagonalization of the density operator signals loss of coherence of the combined 'system plus apparatus', as phase relations dissipate into the environment due to the entanglement with the system. Even if the interaction between the system and the environment is very weak, there will still be a significant effect due to the large number of particles entangling to the system.[11]

[9] Assuming $M = M_{\Psi\mathcal{M}} \otimes \mathbf{1}_\mathcal{E}$, i.e. the apparatus does (effectively) not interact with the environment—as a proper measurement device should.

[10] This density operator expectation value is mathematically equivalent with the state operator expectation, since

$$\begin{aligned}\langle A\rangle &:= \sum_i w_i \langle\psi|A|\psi\rangle = \sum_i w_i \sum_{j,k} \langle\psi|\nu_j\rangle \langle\nu_j|A|\mu_k\rangle \langle\mu_k|\psi\rangle \\ &= \sum_{j,k} \langle\mu_k| \sum_i w_i \left|\psi\right\rangle \left\langle\psi\right| \left|\nu_j\right\rangle \langle\nu_j|A|\mu_k\rangle = \sum_{j,k} \langle\mu_k|\,\hat{\rho}\,|\nu_j\rangle \langle\nu_j|A|\mu_k\rangle = Tr\{\hat{\rho}A\},\end{aligned}$$

where in the second step we have inserted two auxiliary identities.

[11] Without this result, the idea that superpositions can be confined to the microscopic realm could have been maintained—for example by assuming a Heisenberg cut. We now realize that also macroscopic systems can, if we take macroscopic systems as agglomerates of quantum systems, fall prey to

## 2.3 Linear Response Theory and Dissipation

For future reference, we derive some important results from linear-response theory. In particular, two things will be imporant. First, the so-called Kubo formula quantifies the response of a two-point correlation function to a perturbation. Second, this will give us a spectral representation of the dynamic susceptibility of a system as it reacts to an external change, e.g. in the case of placing a Brownian particle into a bath, which will do in Chapter 3.

In linear response theory, the goal is to understand how correlation functions, such as Eq. (2.23), change when we apply a fluctuation force $f(t)$ on the system. In general, this is a very difficult task, but we can make the simplifying assumption that the response to the disturbances of the bath degrees of freedom $q_i(t)$ are *linear* in the perturbing force or forces. Hence, let us write

$$\delta q(t) = \int_0^t dt' \chi(t-t') f(t'), \tag{2.33}$$

where $\delta q(t)$ is the reaction to $f(t)$; and $\chi(t-t')$ is called the 'response function', which we have assumed to be time-translation invariant. Now, we take the Fourier transformation[12] of both sides of Eq. (2.33),

$$\begin{aligned}\int \frac{d\omega}{2\pi} \delta q(\omega) e^{-i\omega t} &= \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \chi(\omega') f(\omega) \int dt' e^{-i(\omega-\omega')t'} e^{-i\omega t} \\ &= \int \frac{d\omega}{2\pi} \int \frac{d\omega}{2\pi} \chi(\omega') f(\omega) 2\pi\delta(\omega-\omega') e^{-i\omega t} = \int \frac{d\omega}{2\pi} \chi(\omega) f(\omega) e^{-i\omega t}. \end{aligned} \tag{2.35}$$

Therefore, we see that the response and the source *decouple* in frequency space [49],

$$\delta q(\omega) = \chi(\omega) f(\omega) \tag{2.36}$$

Thus, the response is local in frequency: a perturbation at a specific frequency will

the indefiniteness of quantum mechanics [2]. Furthermore, even if the system $\Psi$ is initially in a pure state, its reduced dynamics (that is, after the environment is integrated out) will be in a mixed state. Only the combined system of $\Psi$ and the environment behaves as a pure state, satisfying ordinary Schrödinger dynamics.

[12] Our conventions for the Fourier transformation of a function of time $h(t)$ and a function of frequency $f(\omega)$ are as follows,

$$h(\omega) = \int_{-\infty}^{\infty} dt\ h(t) e^{i\omega t} \ \text{ and } \ h(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} h(\omega) e^{-i\omega t}, \tag{2.34}$$

where the difference between the functions $h(t)$ and $h(\omega)$ is solely indicated by their argument (although, in general, they are different).

respond with that exact same frequency. Responses at other frequencies lie beyond the linear-response approximation.

Splitting the response function into its real and imaginary parts, $\chi(\omega) = \mathrm{Re}[\chi(\omega)] + i\mathrm{Im}[\chi(\omega)]$, and writing the imaginary part as [80, p. 6]

$$\mathrm{Im}[\chi(\omega)] = \frac{1}{2i}\left(\chi(\omega) - \chi^*(\omega)\right) = \frac{1}{2i}\int_{-\infty}^{\infty} dt e^{i\omega t}\left(\chi(t) - \chi(-t)\right), \tag{2.37}$$

where the '*' denotes the complex conjugate and where we implicitly took the Fourier transform in for the last equality. We wrote it in this way to show that this part is not invariant under time-reversal. Hence, the imaginary part of the response function breaks follows an arrow of time. We will take the presence of such a term as evidence for an irreversible process, i.e. *dissipation*. In the quantum case, for entangled composite systems, the imaginary part of the response function will also include the information about *coherence*—as we will discuss in Section 2.2.

The susceptibility $\chi$ of a system is defined as the zero-frequency limit of the response function,

$$\chi = \lim_{\omega \to 0} \chi(\omega) \tag{2.38}$$

as can easily be seen from Eq. (2.33). The often-used magnetic susceptibility is defined in this way: the response of the magnetization of the groundstate Ising model to turning on an external field, or $\chi_{\mathrm{mag}} = \frac{\partial M}{\partial B}|_{\omega=0}$. In Chapter 3, we will use the spectral density $J(\omega)$, which is the susceptibility of a bath consisting of harmonic oscillators, responding to a Brownian particle being place in it. In that case, the coordinates $q_i$ of the bath respond to the perturbation of the coordinate $Q$ of the Brownian particle

$$J(\omega) = \left.\frac{\partial q}{\partial Q}\right|_{\omega=0}. \tag{2.39}$$

This can be extended to include the response at *all* frequencies, not just the ground state. For this, one use the Kramers-Kronig relations, resulting in

$$\chi(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Im}\{\chi(\omega')\}}{\omega' - \omega - i\epsilon} \tag{2.40}$$

a clear, but rather involved, derivation of this is given in [71, p. 82-85].

In order to derive the Kubo formula [42], we choose to set up linear-response theory in in a quantum-mechanical framework,[13] Eq. (2.33) can be written as the change in the

[13] All the results will reduce to the classical ones in the classical regime [71, p. 79], hence it is more

expectation value of a Hermitian operator $\hat{\mathcal{O}}$ and sources of disturbance $\phi_i(t)$, in the Heisenberg picture, is

$$\delta \left\langle \hat{\mathcal{O}}(t) \right\rangle = \int_0^t dt' \chi(t-t')\phi(t'). \tag{2.41}$$

We add a source Hamiltonian,

$$\mathcal{H}_s(t) = \phi(t)\hat{\mathcal{O}}(t), \tag{2.42}$$

which is assumed to be a small disturbance. In the interaction picture, the source Hamiltonian evolves the state as

$$|\Psi(t)\rangle_I = U(t,t_0)\,|\Psi(t_0\rangle_I\,, \tag{2.43}$$

for the evolution operator

$$U(t,t_0) = \mathcal{T}\exp\left(-i\int_{t_0}^t \mathcal{H}_s(t')dt'\right), \tag{2.44}$$

where $\mathcal{T}$ is the time-ordering operator. The density matrix of the system then evolves as $\rho(t) = U(t)\rho_0 U^{-1}(t)$, for a density matrix far in the past $t_0 \to -\infty$.

Now, taking the Hermitean operator $\mathcal{O}(t)$ with the source (2.42) turned on, we can calculate the change in the expectation value of this operator,

$$\langle \mathcal{O}(t)\rangle\,|_s = \mathrm{Tr}\rho(t)\mathcal{O}(t)\mathrm{Tr}\rho_0(t)U^{-1}(t)\mathcal{O}(t)U(t). \tag{2.45}$$

Up to linear order, this can be approximated by

$$\begin{aligned}\langle \mathcal{O}(t)\rangle\,|_s &= \mathrm{Tr}\rho(t)\left[\mathcal{O}(t) + i\int_{-\infty}^t dt'\,[\mathcal{H}_s(t'),\mathcal{O}]\right] \\ &= \langle \mathcal{O}(t)\rangle\,|_{s=0} + i\int_{-\infty}^t dt'\,\langle[\mathcal{H}_s(t'),\mathcal{O}]\rangle\,.\end{aligned} \tag{2.46}$$

The second term is the linear response $\delta\langle\mathcal{O}(t)\rangle$. Using the expression for the source, Eq. (2.42), one can write it as

$$\delta\langle\mathcal{O}(t)\rangle = i\int_{-\infty}^t dt'\,\langle[\mathcal{O}(t'),\mathcal{O}(t)]\rangle\,\phi(t') = i\int_{-\infty}^{\infty} dt'\Theta(t-t')\,\langle[\mathcal{O}(t'),\mathcal{O}(t)]\rangle\,\phi(t'), \tag{2.47}$$

general to work in this quantum-mechanical set-up.

with the Heaviside step-function $\Theta(t-t')$. From Eq. (2.47), we can read of the general Kubo formula if we compare this to Eq. (2.41):

$$\chi_{ij}(t-t') = -i\Theta(t-t')\left\langle\left[\hat{\mathcal{O}}_i, \hat{\mathcal{O}}_j\right]\right\rangle, \tag{2.48}$$

where we have generalized to multiple possible sources instead of one, labeled $i$ and $j$. This is a central relation in linear-response theory. We will consider it only for spectral representation.

Now consider a canonical ensemble of quantum systems in thermal equilibrium, such that we can write the expectation value in the Kubo formula (2.48) as

$$\chi_{ij}(t-t') = -i\mathrm{Tr}\left[\exp\left(-\beta\mathcal{H}\right)\Theta(t-t')\left[\hat{\mathcal{O}}_i, \hat{\mathcal{O}}_j\right]\right], \tag{2.49}$$

where $H$ is the Hamiltonian of the system. We take the Fourier transform of the response function (assuming it is invariant under time translations) we obtain[71, p. 94]

$$\chi_{ij}(\omega) = -i\int_0^\infty dt\exp(i\omega t)\mathrm{Tr}\left\{\exp\left(-\beta\rho\right)\left[\hat{\mathcal{O}}_i(t), \hat{\mathcal{O}}_j(0)\right]\right\}. \tag{2.50}$$

In the Heisenberg picture we have

$$\mathcal{O}(t) = U^{-1}(t)\mathcal{O}(0)U(t) \tag{2.51}$$

for the unitary evolution operator $U = \exp(-iHt)$. With Eq. (2.51), the definition of the commutator, and, through the completeness relation, we rewrite the response function as

$$\begin{aligned}\chi(\omega) = -i\int_0^\infty dt\exp(i\omega t)\sum_{mn}\exp\left(-\beta E_m\right)\{&\left\langle m\right|\hat{\mathcal{O}}\left|n\right\rangle\left\langle n\right|\hat{\mathcal{O}}\left|m\right\rangle\exp\left(i(E_m-E_n)\right.\\ &\left.-\left\langle m\right|\hat{\mathcal{O}}\left|n\right\rangle\left\langle n\right|\hat{\mathcal{O}}\left|m\right\rangle\exp\left[-i(E_m-E_n)\right]\right\}.\end{aligned} \tag{2.52}$$

Since the time integral will contain poles on the positive time axis, we include a small imaginary frequency $\epsilon$, to ensure analytic continuation[49]

$$\chi(\omega+i\epsilon) = \sum_{mn}\exp\left(-\beta E_m\right)\left[\frac{\left\langle m\right|\hat{\mathcal{O}}\left|n\right\rangle\left\langle n\right|\hat{\mathcal{O}}\left|m\right\rangle}{\omega+E_m-E_n+i\epsilon} - \frac{\left\langle m\right|\hat{\mathcal{O}}\left|n\right\rangle\left\langle n\right|\hat{\mathcal{O}}\left|m\right\rangle}{\omega-E_m+E_n+i\epsilon}\right] \tag{2.53}$$

which we can rewrite by renaming the dummy indices $n$ and $m$ for the second term

only:

$$\chi(\omega + i\epsilon) = \sum_{mn} \frac{\langle m|\,\hat{\mathcal{O}}\,|n\rangle\,\langle n|\,\hat{\mathcal{O}}\,|m\rangle}{\omega + E_m - E_n + i\epsilon}\left[\exp\left(-\beta E_m\right) - \exp\left(-\beta E_n\right)\right]. \tag{2.54}$$

When we take the limit $\epsilon \to 0$ the imaginary part remains in the form of delta functions; hence, there will remain a dissipative part of the response function, since energy is lost through it [26, for example].

$$\mathrm{Im}[\chi(\omega)] \propto \sum_{mn} \frac{\epsilon}{(\omega + E_m - E_n)^2 + \epsilon^2} \approx \sum_{mn} \delta(\omega - E_n + E_m). \tag{2.55}$$

Hence, although one might have expected this part to vanish, it leaves delta-contributions. This is a result that we will also use in Section 3.2.3.

## 2.4 The Lévy distribution and Sisyphus cooling

In 1937, the French mathematician Paul Lévy tried to find solutions to the question [48]

> When does the probability $P_N(x)$ for the sum of $N$ steps $x = x_1 + x_2 + ... + x_N$ have the same distribution $p(x)$ (up to a normalization) for the individual steps.

This is basically a question of 'when does the whole look like its parts', and hence closely related to the theory of fractals and emergent behavior. One obvious answer to the question is the Gaussian probability distribution

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{1}{2\sigma^2}x^2\right], \tag{2.56}$$

for $\sigma$ the standard deviation, since the sum of $N$ Gaussian distributions is again a Gaussian. But, Lévy found that there are additional solutions. These are called Lévy distributions, which–in Fourier space–have the following form

$$p_N(k) = \exp(-Na|k|^\beta). \tag{2.57}$$

For $\beta = 2$ and $a = \sigma^2/2$ we have Gaussian distribution. We calculate its form in $x$-space with an inverse Fourier transform, which should return a Gaussian distribution,

$$\begin{aligned} p_N(x) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \exp(\frac{-N\sigma^2}{2}|k|^2 + ikx) \\ &= \frac{1}{\sqrt{2\pi N\sigma^2}} \exp(-\frac{x^2}{2N\sigma^2}), \end{aligned} \tag{2.58}$$

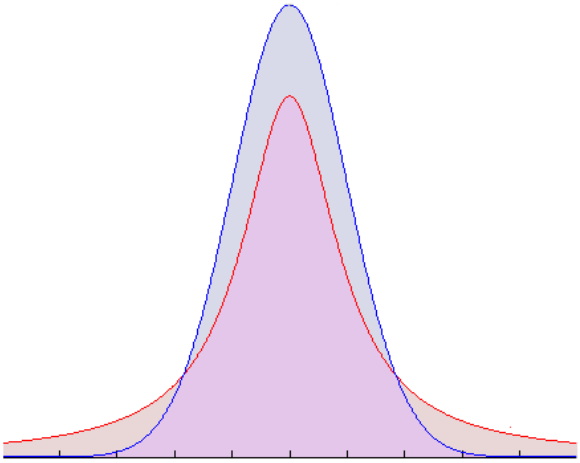

Figure 7: In blue, the Gaussian distribution. In red, the Lévy distribution. Because the support of the Lévy distribution is decaying at a much lower rate than that of the Gaussian curve, a property called 'heavy tails', the probability for a step deviating much from the mean is much higher. Such a highly-deviating step, then, corresponds to a Lévy flight.

as anticipated. This results in the random-walk behavior characteristic of Brownian motion.

For $\beta = a = 1$, however, we have the Cauchy-Lorentz or Lévy distribution, which, transformed back to $x$-space reads

$$\begin{aligned} p_N(x) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \exp(-N|k| + ikx) \\ &= \frac{1}{2\pi}\int_{-\infty}^{0} dk \exp(Nk + ikx) + \frac{1}{2\pi}\int_{0}^{\infty} dk \exp(-Nk + ikx) \\ &= \frac{1}{2\pi}\left(\frac{1}{N+ix} - \frac{1}{-N+ix}\right) = \frac{1}{\pi N}\frac{1}{1+(x/N)^2} = \frac{1}{N}p_1(x/N). \end{aligned} \tag{2.59}$$

See Figure 7 for a plot of this distribution.

Thus, we conclude that Lévy distributions are the generalization of the Gaussian distribution in the sum of large numbers of independent variables in cases where the variances of the variables diverge, which is known as the generalized central limit theorem. In contrast to the Gaussian-distributed momentum of Brownian motion, the Lévy distribution has a much wider support, a property called having 'heavy tails'. This, then, corresponds to a much larger probability for making long jumps [38].

In this thesis, we will confine ourselves to a physical intuition of the occurrence of

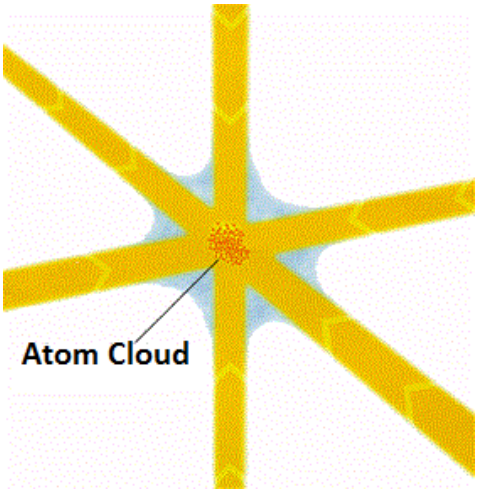


Figure 8: Laser cooling. An atom cloud is trapped by laser beams from all directions. Individual atoms inside the cloud still perform Brownian motion, as a result of thermal fluctuations. In addition, spontaneous emission of photons by excited atoms causes recoil effects that result in a fluctuation much larger than the a step of Brownian walk, i.e. the Lévy flight. Picture extracted from https://www.revolvy.com/topic/Optical%20molasses&uid=1575.

Lévy flights in the specific context of laser cooling experiments. We will discuss the technique of Sisyphus[14] laser cooling (sometimes called polarization gradient cooling), which is a type of laser cooling which allows atoms to reach temperatures below the Doppler cooling limit [52]. This is a dissipative optical lattice, where an atom cloud is subjected to laser beams from every direction. Hence, the atoms cool down, since it is energetically more favorable to move along with the gradient—see Figure 8.

At the microscopic level the atom-light interaction can be described exactly using a standard approach of quantum optics [3]. For a low intensity of the laser and in the semi-classical limit, the master equation for the density operator of the atoms can be transformed into a Fokker-Planck-type equation for a distribution function $W(x;p;t)$, as encountered in statistical physics, which can be interpreted as an atomic quasi-probability density with respect to the position $x$ and the momentum $p$ of the atom. For very fast atoms, a spatial averaging over the lattice period is allowed. The atomic momentum distribution $W(p;t)$ satisfies

$$\frac{\partial W(p,t)}{\partial t} = -\frac{\partial}{\partial p}[K(p)W(p,t)] + \frac{\partial}{\partial p}\left[D(p)\frac{\partial W(p,t)}{\partial p}\right], \tag{2.60}$$

where $K(p)$ and $D(p)$ are momentum-dependent drift and diffusion coefficients that can be expressed in terms of the microscopic parameters of the problem.

[14]Named after Sisyphus, the king of Korinthe, who cheated death and was punished by Zeus to push a boulder up a mountain for all eternity.

These laser-cooling techniques can, theoretically, be quantitatively understood in terms of non-ergodic random processes dominated by a few rare events, such as the recoil after spontaneous emission. Lévy statistics is now recognized as the best tool for studying many anomalous diffusion problems where standard statistics fail. In the context of the Lévy flights in Sisyphus cooling, Marksteiner, Ellinger, and Zoller have [56]

$$K(p) = \frac{p}{1 + p^2/p_c^2}. \tag{2.61}$$

This is the force we shall reproduce in Chapter 4.

## 2.5 Conclusion

In this chapter we discussed the fundamental basis for this thesis. This consisted of four parts. First, in Section 2.1, we looked at the theory of Brownian motion from the point of view of Einstein's diffusion and from the force balance developed by Langevin. By taking an stochastic function $f(t)$ to represent the bath, one can circumvent the epistemological problem that one cannot obtain all the microscopic information of the bath constituents in realistic situations. This fluctuation force is postulated to vanish on average. In the relaxation time approximation, i.e. when all important timescales are larger than the collision time $\tau$, we can safely assume that the two-point correlation function of the fluctuation force is proportional to the delta-distribution of Eq. (2.23), which makes the calculations easier and avoids the Itô-Stratonovich dilemma. This is a simple example of a fluctuation-dissipation relation, which we will see more often in the following two chapters.

The second important subject we have investigated is that of decoherence, which we treated in Section 2.2. Whereas in classical systems energy for subsystems is not conserved due to its leakage to the environment, for quantum systems also coherence can leak. When the environment consists of a very large number of degrees of freedom, coherence of a subsystem can be carried away by it on timescales much larger than thermal equilibration. This happens for quite general Hamiltonians, as long as interaction depend on the relative position of particles, i.e. if the potential can be written as $V(|x - x'|)$, the off-diagonal terms of the density matrix obtain a quickly-decaying exponential, which signals the damping of interference terms.

The third section 2.3, derived some important results for the response function of a system responding to a perturbation. It must be kept in mind that the response is assumed to be small, i.e. perturbations at specific frequencies will–to good approximation–only give rise to responses at that same frequency. In particular, we will use two expressions for the response function in the context of the bath susceptibility in Chapter 3, namely the Kubo formula Eq. (2.48), and the spectral representation of it in Eq. (2.40).

Last, we discussed the occurrence of Lévy flights in ultracold-atoms experiments. In particular, we have seen that these Lévy flights occur in Sisyphus laser cooling. The atoms in the cooling atom cloud perform small thermal fluctuations, i.e. the Brownian

random walk of Section 2.1. In addition to these fluctuations, there are large flights corresponding to the recoil of an atom undergoing spontaneous photon emission. The corresponding force that models this behavior, is given by Eq. (2.61); in Section 4.2.3 we will reproduce this force term.

All these for points share a common characteristic: they are open systems dealing with external influences. As we will see in the next chapter, there are problems with finding a quantum model from the mathematical framework for open systems we have developed so far. To solve these problems, we will close the system by also giving an explicit description of the constituents of the bath: the Caldeira-Leggett model.

# 3 The Caldeira-Leggett model

> "We will choose a *minimal model* which, under certain conditions, reproduces Brownian motion in the classical regime. Thus, the justification for the choice of the model will be provided *a posteriori*. However, it is worth mentioning that the employment of detailed microscopic models for some environments may show different quantum mechanical behavior, which turns out [to] be very important in some cases."
>
> —Amir Ordaçgi Caldeira [11, p. 104]

## 3.1 Limitations to the open system approach

We have seen that the theory of Brownian motion revolves around the fluctuation-dissipation relation, where the existence of an imaginary part of the response function gives rise to a dissipative part in the two-point correlation function of the fluctuation force. While it is clear that the bath plays a central role in the dynamics of the Brownian particle, its constituents do not occur explicitly in the open system models. For our purposes there are two main shortcomings of the treatment of open systems in the Einstein or Langevin set-up of the previous chapter:[15]

1. This framework for Brownian motion makes it hard to find a theory of *quantum* Brownian motion via conventional quantization techniques. The reason is that either the Lagrangian (for path-integral quantization) or the Hamiltonian (for canonical quantization) will have an explicit time-dependence in order to reproduce the velocity-dependent friction term of the Langevin equation. Hence, energy is not conserved and, although the non-conservation of energy is natural for open systems, this makes direct quantization impossible.

2. This framework is a phenomenological one, i.e. the diffusion constant $D$ or the viscosity $\eta$ can only be determined experimentally for different materials that the environment can consist of. This is to be expected, since a microscopic description of the environment was absent in the first place. In principle, it is desirable to have a theory where the origin of the viscosity of a particular medium can be explained theoretically.

These two shortcomings arise from a fundamental shortcoming of the description of Brownian motion in Section 2.1: there is no action principle that allows for the deriva-

[15] In addition to this there is also the problem of time-reversibility: due to the friction term in the Langevin equations, which is proportional to velocity, the dynamics is irreversible, even though the fundamental laws governing the particle, such as Schrödinger's or Newton's equations, are time-reversible. Hence, there is a permanent loss of information along the evolution of the system. This is a direct consequence of the the ensemble approach to the bath constituents, as is customary in statistical physics. However, we will not focus on the reversibility issue here. For a clear explanation, see Van Kampen's [76]; for a rigorous discussion of probability and time-reversibilty, see Bacciagaluppi's [1].

tion of the phenomenological Langevin equation solely in terms of the Brownian particle. Thus, we will have to address the elephant in the room: we need a microscopic description of the bath.

We can model the behavior of the environment and assume a specific interaction between the constituents of the bath and the system itself. As depicted schematically in Figure 9, we will make a conceptual cut between the system of interest and the environment.[16] The cut between system and environment is made between a particular set of degrees of freedom $\{Q_i\}$ of which we wish to obtain the dynamics and a set of (usually many more) degrees of freedom $\{q_i\}$ which we are usually ignorant of or wholly uninterested in. The strategy, then, is to describe the dynamics of the entire physical set-up (system of interest plus the environment) and integrate out the environment at a later time, leaving us only with what we wish to describe: the effective dynamics of the system of interest. The environment itself is *a priori* assumed to be in equilibrium with respect to a heat bath through the usual procedure of the taking canonical ensemble.[17]

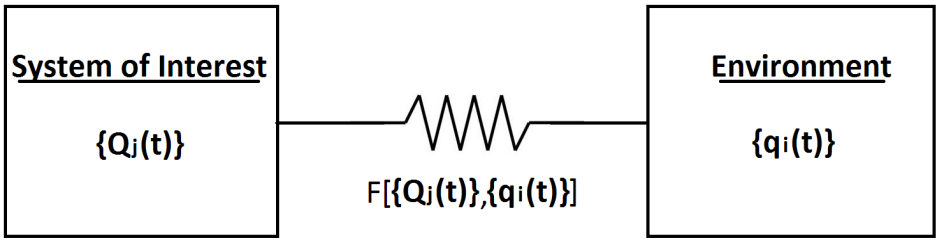


Figure 9: The Feynman-Vernon method is to explicitly make a cut between degrees of freedom in which we are interested, called the 'system', and those in which we are not, called the 'environment'. The strategy, then, is to specify a particular system-environment interaction, calculate the full dynamics of the system and environment combined, and to integrate out the environmental degrees of freedom at a later stage of the calculation.

If one follows this strategy by specifying a *Lagrangian* for the composite model, one needs to specify how the system and the environment interact (the interaction is called '$F$' in the picture). In the late 1950s, both Magalinskii [51] and Senitsky [70] envisioned the bath as a collection of harmonic oscillators, weakly coupled to the system. This strategy of 'closing' the system by describing the bath itself as a collection of harmonic oscillators has become known as the Feynman-Vernon method, who, in 1963, formulated

[16] Pay particular attention to the general formulation: from here on we will frequently call the Brownian particle 'the system of interest' or simply the 'system', since it does not have to be a particle. For example, the system of interest can be a particular species of particles, a quantum wavefunction (as we will see later on), etc.. Also, although we will use the words 'bath' and 'environment' interchangeably, 'environment' is more general, as it can be used to reference to a liquid (e.g. in the case of pollen particles in water), the air in a laboratory, or even internal degrees of freedom in a molecule.

[17] If this was not the case, the system and bath would by themselves form a completely integrable set of equations of motion.

the quantum version of the theory [19]. It was subsequently worked out by Ford, Kac, Mazur [25] and Ullersma [73] and culminated in the work of Caldeira and Leggett, who developed the approach into a full theory for quantum dissipation for harmonic systems [9], and used it for a succesful description of quantum tunneling [8]. After discussing this Caldeira-Leggett model in full detail in the current chapter, we will expand on this by including a coupling to velocity. This task will be taken up in Chapter 4 and its quantum version will be treated in Chapter 5.

## 3.2 Bilinear Coordinate-Coordinate coupling

### 3.2.1 The Caldeira-Leggett Lagrangian

The gap between phenomenological modeling and precise microscopic formulation is bridged by the Caldeira-Leggett model. It describes both the system and the bath, and their interaction by one Lagrangian, while the physical origin of this interaction is kept unspecified for generality. The bath is modeled as a collection of harmonic oscillators, linearly coupled to the system of interest. Caldeira called this a *minimal model*, since every perturbation of the bath can be approximated by a harmonic potential. Hence, the validity of this model is restricted to weak perturbations of the bath.[18] Note that this does not imply that the induced dissipation is necessarily weak; the large number of environmental degrees of freedom quarantees that we can describe strongly dissipative systems. The Lagrangian is as follows,

$$\mathcal{L} = \mathcal{L}_S + \mathcal{L}_B + \mathcal{L}_I + \mathcal{L}_{C.T.}, \tag{3.1}$$

where the abbreviations stand for 'system', 'bath', 'interaction' and 'counterterm', respectively.

For simplicity, we let the system be described by one generalized coordinate $Q$. The Lagrangian, in one dimension, of a particle of mass $M$, subject to an external potential $V(Q)$, reads

$$\mathcal{L}_S = \frac{1}{2}M\dot{Q}^2 - V(Q). \tag{3.2}$$

The bath is modeled as a collection of $N$ harmonic oscillators, labeled by an index $k$, with masses $m_k$, coordinates $q_k(t)$, and at natural frequencies $\omega_k$,

$$\mathcal{L}_B = \frac{1}{2}\sum_{k=1}^{N} m_k\dot{q}_k^2 - \frac{1}{2}\sum_{k=1}^{N} m_k\omega_k^2 q_k^2. \tag{3.3}$$

In principle, the number $N$ of harmonic oscillators[19] is very large, such that we can

[18] We will consider an extension of the coupling, towards more general perturbations, in Section 3.3.

[19] When we turn to the quantum theory, the harmonic oscillators are automatically identified as bosonic particles, but fermionic baths can also be modeled in this way, albeit it through the intermediate process of bosonization, as explained in Hedegård and Caldeira's [31].

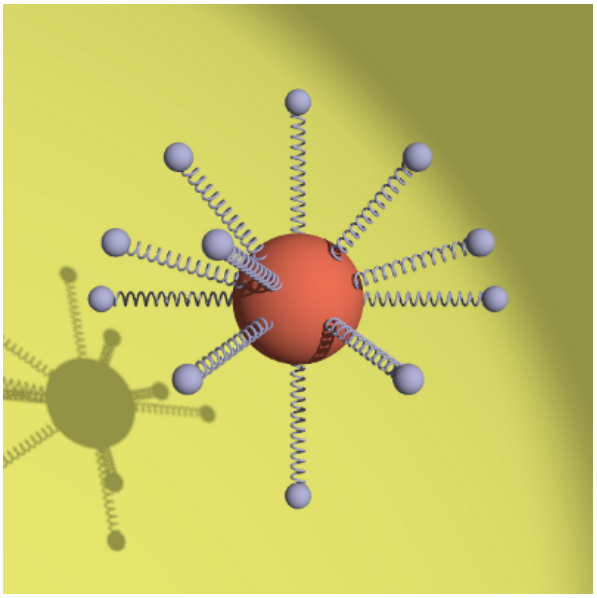

Figure 10: The harmonic coupling of the system to the bath; the bath constituents (the small grey particles) are coupled to the system (in red) by a springlike interaction. Figure extracted from Ref. [35].

safely work within the thermodynamic limit, i.e. we can let $N \to \infty$ at the end of the calculation.

The interaction is of the coordinate-coordinate type, which means the system coordinate $Q$ is linearly coupled to each oscillator coordinate $q_k$, as if attached to a spring (cf. Figure 10), with 'spring constants' $C_k$,[20]

$$\mathcal{L}_I = Q \sum_{k=1}^{N} C_k q_k. \tag{3.4}$$

This interaction is the simplest one to write down (remember we are building a minimal model), but it turns out to be quite general, see Ref. [8, Appendix C]. In principle, the $C_k$ should be seen as negative constants, since springs tend to *restore* extensions We also include a counterterm,

$$\mathcal{L}_{C.T.} = -\frac{1}{2} Q^2 \sum_{k=1}^{N} \frac{C_k^2}{m_k \omega_k^2}. \tag{3.5}$$

[20] Also, there are examples of Caldeira-Leggett Lagrangians in terms of fundamental constants, such as charge, mass and the speed of light in the case of electrons interacting with electromagnetic fields [4], as we will see in Section 4.1. However, although this is a promising realization of the Caldeira-Leggett model, this is seldom necessary. Often, the information about coupling constant $C_k$ is given by the sspectral density, as explained in Section 3.2.3.

This counterterm depends on the parameters of the environment, but not on its dynamical variables. The justification for this term is that if it were absent, the minimum of the (bare) potential $V(Q)$ of the system would shift to $q_k = C_k Q/m_k\omega_k^2$ for a given $Q$, as can easily be seen by minimizing the action with respect to the bath coordinates,

$$\frac{\partial \mathcal{L}}{\partial q_i} = -m_i\omega_i^2 q_i + C_i Q \stackrel{!}{=} 0, \tag{3.6}$$

such that

$$q_i = \frac{C_i}{m_i\omega_i^2} Q. \tag{3.7}$$

Then, we see the renormalization of the potential in

$$\frac{\partial \mathcal{L}}{\partial Q} = -\frac{\partial V}{\partial Q} + \sum_{k=1}^{N} C_k q_k + Q\sum_{k=1}^{N} \frac{C_k^2}{m_k\omega_k^2} = -\frac{\partial V}{\partial Q}, \tag{3.8}$$

using Eq. (3.7). Thus, the renormalization term ensures that the minimum remains centered about the *bare* potential $V(Q)$.

In practice, however, one does not need to worry much about the counterterm, since in most cases it is impossible to observe the bare potential $V(Q)$. If one prefers an approach without the counterterm, one can construct an equivalent Lagrangian by removing the counterterm via a simple canonical transformation and replace the interaction term by a coordinate-velocity coupling

$$\tilde{\mathcal{L}}_I = Q\sum_{k=1}^{N} \tilde{C}_k \dot{q}_k; \tag{3.9}$$

see Appendix A for this procedure. The inclusion of the counterterm is, however, necessary for certain systems, but this depends on the physical model; for a discussion on various models and the role of the counterterm, see again Ref. [8, Appendix C].

Now that we have discussed the individual components of the Lagrangian, we combine them together and write the *Caldeira-Leggett Lagrangian*:

$$\mathcal{L} = \underbrace{\frac{1}{2}M\dot{Q}^2 - V(Q)}_{\text{System}} + \underbrace{\frac{1}{2}\sum_{k=1}^{N} m_k(\dot{q}_k^2 - \omega_k^2 q_k^2)}_{\text{Bath}} + \underbrace{Q\sum_{k=1}^{N} C_k q_k}_{\text{System/Bath-INT.}} - \underbrace{\frac{1}{2}Q^2\sum_{k=1}^{N}\frac{C_k^2}{m_k\omega_k^2}}_{\text{Counterterm}}. \tag{3.10}$$

The justification of the Lagrangian (3.10) will have to be *a posteriori*, by showing that the equation of motion for the system reproduces the Langevin equations (2.12), (2.15), (2.23), after the bath coordinates are eliminated.

### 3.2.2 Dynamics

The Euler-Lagrange equations for the system and the bath, obtained from Eq. (3.10), respectively, are

$$M\ddot{Q} = -\frac{\partial V(Q)}{\partial Q} + \sum_k C_k q_k - Q\sum_k \frac{C_k^2}{m_k\omega_k^2}, \tag{3.11}$$

$$m_i\ddot{q}_i = C_i Q - m_i\omega_i^2 q_i, \tag{3.12}$$

where we have suppressed the limits of the sums for brevity. It is useful to solve this set of coupled differential equations with a Laplace transformation (see Appendix B).[21] Hence, we separately transform both sides of Eq. (3.12); for the left-hand side,

$$\begin{aligned}\mathfrak{L}\{m_i\ddot{q}_i\} &= m_i\tilde{\ddot{q}}_i,\\ &= m_i[l\tilde{\dot{q}}_i - \dot{q}_i(0)],\\ &= m_i[l^2\tilde{q}_i - lq_i(0) - \dot{q}_i(0)],\end{aligned}$$

as well as the right-hand side,

$$\mathfrak{L}\{C_iQ - m_i\omega_i^2 q_i\} = C_i\tilde{Q}(l) - m_i\omega_i^2\tilde{q}_i(l).$$

for the initial conditions $q(0)$ and $\dot{q}_i(0)$.

Solving for the transformed coordinates of the harmonic oscillators gives

$$\tilde{q}_i(l) = \frac{1}{l^2+\omega_i^2}\Big[\frac{C_i}{m_i}\tilde{Q}(l) + lq_i(0) + \dot{q}_i(0)\Big]. \tag{3.13}$$

In the second and third term, we can recognize known Laplace transformations, namely $\mathfrak{L}\{\cos(at)\} = l/(a^2+l^2)$ and $\mathfrak{L}\{\sin(at)\} = a/(a^2+l^2)$.[22] This, together with the inverse transformation of the first term (using the Bromwich inverting integral (B.5)) allows us to write

$$q_i(t) = \mathfrak{L}^{-1}\{\tilde{q}_i(l)\} = \frac{1}{2\pi i}\lim_{T\to\infty}\int_{\delta+iT}^{\delta-iT} dl\Big[\frac{C_i}{m_i}\frac{\tilde{Q}(l)}{l^2+\omega_i^2}e^{lt}\Big] + f_i^{(0)}(t), \tag{3.14}$$

for a small parameter $\delta$. This is the trajectory for a harmonic oscillator of the bath,

[21] We will use two possible notations for the Laplace transformation of a function $f(t)$; either $\tilde{f}(l)$, where the tilde denotes a function in Laplace space, or $\mathfrak{L}\{f(t)\}(l)$, when we need to be more specific. Both notations are used interchangeably for pragmatic reasons.

[22] This can be easily shown with the definition of the Laplace transformation Eq. (B.1) and partial integration. Note that in the derivation of the sine, we use the linearity property: $\mathfrak{L}\{a^{-1}\sin(at)\} = a^{-1}\mathfrak{L}\{\sin(at)\} = 1/(a^2+l^2)$.

and where we have defined the fluctuation force per bath particle,

$$f_k^{(0)}(t) := q_k^{(0)} \cos(\omega_k t) + \frac{\dot{q}_k^{(0)}}{\omega_k} \sin(\omega_k t). \tag{3.15}$$

We also define the (bath-driven) fluctuation force as the sum over all the individual forces of the bath particles weighted by the coupling constants $C_i$,

$$f^{(0)}(t) := \sum_k C_k f_k^{(0)} = \sum_k C_k \left( q_k^{(0)} \cos(\omega_k t) + \frac{\dot{q}_k^{(0)}}{\omega_k} \sin(\omega_k t) \right). \tag{3.16}$$

Before focusing on evaluating the integral, we will first plug Eq. (3.14) into the equation of motion for the system (3.11),

$$M\ddot{Q} + V'(Q) + \sum_k \left\{ \frac{1}{2\pi i} \lim_{T\to\infty} \int_{\delta+iT}^{\delta-iT} dl \left[ -\frac{C_k^2}{m_k} \frac{\tilde{Q}(l)}{l^2+\omega_k^2} e^{lt} \right] + \frac{C_k^2}{m_k \omega_k^2} Q(t) \right\} = f^{(0)}(t), \tag{3.17}$$

where we have abbreviated $\partial V(Q)/\partial Q = V'(Q)$. We can simplify this by recognizing that $(\omega_i^2 + l^2)^{-1} = \omega_i^{-2}[1 - l^2/(l^2+\omega_i^2)]$, leading to

$$M\ddot{Q} + V'(Q) + \sum_k \left\{ \frac{1}{2\pi i} \lim_{T\to\infty} \int_{\delta+iT}^{\delta-iT} dl \left[ -\frac{C_k^2}{m_k \omega_k^2} \left( \tilde{Q}(l) - \frac{l^2 \tilde{Q}(l)}{l^2+\omega_k^2} \right) e^{lt} \right] + \frac{C_k^2}{m_k \omega_k^2} Q(t) \right\} = f^{(0)}(t). \tag{3.18}$$

By observing that the first term within brackets is transformed back to the original $Q(t)$, we can show the utility of the counterterm,

$$M\ddot{Q} + V'(Q) + \sum_k \left\{ \cancel{-\frac{C_k^2}{m_k \omega_k^2} Q(t)} + \frac{C_k^2}{m_k \omega_k^2} \frac{1}{2\pi i} \lim_{T\to\infty} \int_{\delta+iT}^{\delta-iT} dl \frac{l^2 \tilde{Q}(l)}{l^2+\omega_k^2} e^{lt} + \cancel{\frac{C_k^2}{m_k \omega_k^2} Q(t)} \right\} = f^{(0)}(t). \tag{3.19}$$

This leaves us with only one term to transform back, which we have suggestively called the 'friction term',

$$M\ddot{Q} + V'(Q) + \underbrace{\sum_k \frac{C_k^2}{m_k \omega_k^2} \frac{1}{2\pi i} \lim_{T\to\infty} \int_{\delta+iT}^{\delta-iT} dl \frac{l^2 \tilde{Q}(l)}{l^2+\omega_k^2} e^{lt}}_{\text{Friction Term}} = f^{(0)}(t). \tag{3.20}$$

Focusing on the friction term, we can rewrite it as a total derivative with respect to

time:

$$\sum_k \frac{C_k^2}{m_k\omega_k^2}\frac{d}{dt}\left\{\frac{1}{2\pi i}\lim_{T\to\infty}\int_{\delta+iT}^{\delta-iT} dl\frac{l\tilde{Q}(l)}{l^2+\omega_k^2}e^{lt}\right\}. \tag{3.21}$$

Next, we rewrite this Bromwich integral back in terms of the inverse Laplace transformation

$$\frac{d}{dt}\sum_k \frac{C_k^2}{m_k\omega_k^2}\mathfrak{L}^{-1}\left\{\left(\frac{l}{l^2+\omega_k^2}\right)\left(\tilde{Q}(l)\right)\right\}(t) \tag{3.22}$$

and use the convolution theorem (Eq. (B.8)) to write it as

$$\begin{aligned}
=&\frac{d}{dt}\sum_k \frac{C_k^2}{m_k\omega_k^2}\mathfrak{L}^{-1}\left\{\mathfrak{L}\{\cos(\omega_k t)\}(l)\star\mathfrak{L}\{Q(t)\}(l)\right\}(t)\\
=&\frac{d}{dt}\left\{\sum_k \frac{C_k^2}{m_k\omega_k^2}\int_0^t dt'\cos\left[\omega_k(t-t')\right]Q(t')\right\}
\end{aligned} \tag{3.23}$$

where we used the definition of convolution in the last line.

The auxiliary variable $l$ has now been transformed away from every term, which means that we have successfully performed the Laplace transformations. What remains is to evaluate the sum over oscillators $k$ and the integral over auxiliary time $t'$. We will start by transforming the sum over oscillators into an integral over frequencies, for which we need the *spectral density*.

### 3.2.3 The Spectral Density

To successfully replace $\sum_k \to \int d\omega$, one needs to specify a continuous frequency density distribution, instead of the discrete oscillator distribution. This is called the 'spectral density' $J(\omega)$, which should arise from the additional information specified by the microscopics of the bath constituents,

$$J(\omega) = \frac{\pi}{2}\sum_k \frac{C_k^2}{m_k\omega_k}\delta(\omega-\omega_k), \tag{3.24}$$

where the factor $\pi/2$ is put in for later convenience. This form follows from the Kubo formula (2.48) of linear response theory, as explained in Section 2.3, with the result given by Eq. (2.55). It models the linear response of the bath coordinates $q_i$ to a perturbation. From the Kubo formula, one can recognize it as the Fourier transformation of the retarded dynamical susceptibility of the bath oscillators,

$$J(\omega) = \text{Im}\ \mathcal{F}\left\{\Theta(t-t')\left\langle\left[\sum_k^N C_k q_k(t), \sum_k^N C_{k'}q_{k'}(t')\right]\right\rangle\right\}, \tag{3.25}$$

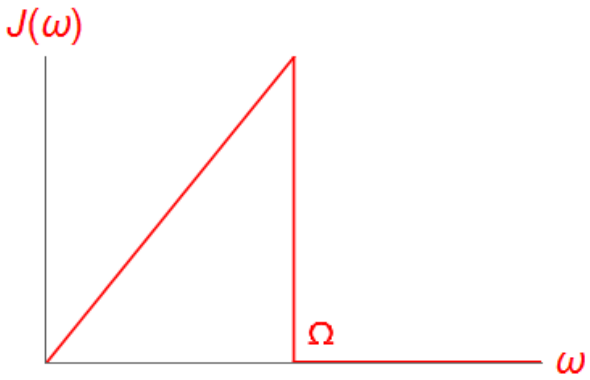


Figure 11: The ohmic spectral density function. It behaves linearly below a certain cut-off $\Omega$ and vanishes above. It is interpreted as the response at each frequency of the bath modes due to an external stimulus.

which is found by following the steps Eqs. (2.49)–(2.55), where $\langle ... \rangle$ is taken over the equilibrium state of non-interacting oscillators and–if we wish to work in the classical limit–the commutator should be replaced by the Poisson bracket. Hence, $J(\omega)$ is to be interpreted as the response to an external stimulus of the equilibrated bath–like placing a pollen particle into it–and limiting oneself to the absorbation at the lowest frequency. Hence, the expectation value in Eq. (3.25) is taken with respect to the ground state of the system, i.e. the so-called thermodynamic sum rule (cf. Eq. (2.40)).

The form of the spectral density in Eq. (3.24) allows us to convert discrete sums over oscillators into continuous integrals over frequency,

$$\sum_k \frac{C_k^2}{m_k \omega_k^2} \cos[\omega_k (t - t')] = \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega} \cos[\omega (t - t')]. \tag{3.26}$$

We now assume a specific form of the spectral density, which falls apart into three classes, which have been called the ohmic, subohmic, and superohmic cases by Leggett *et al*, which are linear, sublinear or higher polynomials in frequency, respectively [45]. Also, the spectral density vanishes for $\omega > \Omega$, i.e. a certain high-frequency cut-off $\Omega$, which fixes the timescale of the problem and is therefore inversely proportional to the relaxation time $\tau^{-1}$. Hence, we write

$$J(\omega) = \eta \omega^s \qquad \begin{cases} \text{subohmic}, & \text{if } s < 1 \\ \text{ohmic}, & \text{if } s = 1 \\ \text{superohmic}, & \text{if } s > 1 \end{cases} \tag{3.27}$$

where $\eta$ is a proportionality constant, which plays a phenomenological role here. This phenomenological input is in order to reproduce the (phenomenological) Langevin equation of the open system approach.

In most cases, the bath behaves ohmically to good approximation, but for some baths higher orders will come in to play.[23] In reality, almost no process is ever completely described by normal diffusion, but systematic errors and lack of statistics almost always obscure the small deviations. Indeed, most of the systems investigated experimentally are ohmic. However, often normal diffusion is assumed by experimentalists for the interpretation of experimental data, while deviations can be blamed on statistical errors. On the flip-side of that coin, often the opposite occurs: experimentalists obtaining an anomalous fit due to systematic errors in the experiment or the data analysis, while the underlying physics is a perfectly ordinary diffusion process with a fashionable anomalous diffusion theory of choice.[24]

Therefore, the discussion on anomalous diffusion is an important one, but might need rephrasing. We should look at at systems where the assumptions of normal diffusion are invalid *a priori*, such as in subrecoil cooling or Sisyphus cooled atoms, which we have been discussed in Section 2.4. Other examples are various, e.g. in the stock market, or dissipation of systems close to a critical point (although here experimental errors can also be very large, obscuring anomalous behavior).

Returning to the the theoretical level of this thesis, though, it is important to realize that even theoretically there are few examples of manisfestly non-ohmic baths. A prominent example, however, is the superohmic $J(\omega) \propto \omega^3$ for an electron interacting with its own radiation field, as calculated by Barone and Caldeira, where the equation of motion is the Abraham-Lorentz equation [4]. We will discuss this more thoroughly in Section 4.2.2.

### 3.2.4 Classical initial conditions: retrieving the Langevin equations

We have denoted the right-hand side of Eq. (3.19) by $f^{(0)}$. This is suggestive, since we want to show it is the fluctuation force of the Langevin equation. To show this, we must make assumptions about the initial positions and velocities of the bath particles, since these values appear in Eq. (3.16).

A reasonable choice is to assume thermodynamical equilibrium of the unperturbed bath. Then we can use the equipartition theorem in the classical limit,[25] which states that every quadratic oscillator degree of freedom will contribute $1/2k_BT$ to the total

[23] In the background of this thesis, there is always the motivation to investigate the effect of non-ohmic baths on phenomena as decoherence, and we will indicate possibilities for this in the Outlook. Peter Hänggi has several studies where he shows that coherence might be more easily preserved at high temperatures when we use subohmic chaotic baths [30]. This could play a crucial role in the search for preserving coherence in quantum computers. Moreover, this baths might be *engineered* to have the correct properties.

[24] The basis for this claim lies in a private conversation with Prof. dr. Allard Mosk, leader of the nanoLINX research group at Utrecht University.

[25] Equipartition fails in quantum mechanics, since some degrees of freedom can be hidden from view ('freeze out') due to the discreteness of energy levels. In the quantum case, we will have to use the Bose-Einstein distribution to correctly describe equilibrium. This will lead to a quantum Langevin equation, as can also be seen in Eq. (2.24).

energy; where $T$ is the temperature of the bath. For the initial conditions in the classical limit, then,[26]

$$\langle q_i(0)\rangle = \langle \dot{q}_i(0)\rangle = 0 = \langle q_i(0)\dot{q}_j(0)\rangle \tag{3.28}$$

$$\frac{1}{2}m_i \langle \dot{q}_i(0)\dot{q}_j(0)\rangle = \frac{1}{2}k_B T\delta_{ij} \tag{3.29}$$

$$\frac{1}{2}m_i\omega_i^2 \langle q_i(0)q_j(0)\rangle = \frac{1}{2}k_B T\delta_{ij}, \tag{3.30}$$

where the averages are taken over the initial values with respect to the classical equilibrium density matrix of the unperturbed bath ($B$)

$$\rho_B^{(0)} = Z_B^{-1}\exp\left[-\frac{\beta}{2}\sum_k m_k\dot{q}_k^{(0)\,2} + m_k\omega_k^2 q_k^{(0)\,2}\right], \tag{3.31}$$

which is Eq. (2.13), for our specific Lagrangian (3.10).

We now have all the ingredients to derive the Langevin equation that describes classical Brownian Motion. On average, the fluctuation force should vanish, see Eq. (2.13). Using the initial conditions (3.28), we see that it indeed vanishes:

$$\left\langle f^{(0)}(t)\right\rangle = \sum_k C_k\left(\langle q_k(0)\rangle\cos(\omega_k t) + \langle\dot{q}_k(0)\rangle\frac{\sin(\omega_k t)}{\omega_k}\right) = 0, \tag{3.32}$$

We should also calculate the two-point force correlation function in order to satisfy Eq. (2.23),

$$\begin{aligned}
&\left\langle f^{(0)}(t)f^{(0)}(t')\right\rangle = \\
&\sum_{kk'}C_kC_{k'}\left\langle\left(q_k(0)\cos(\omega_k t) + \frac{\dot{q}_k(0)}{\omega_k}\sin(\omega_k t)\right)\left(q_{k'}(0)\cos(\omega_{k'}t') + \frac{\dot{q}_{k'}(0)}{\omega_{k'}}\sin(\omega_{k'}t')\right)\right\rangle \\
&\quad = \sum_{kk'}C_kC_{k'}\langle q_k(0)q_{k'}(0)\rangle\cos(\omega_k t)\cos(\omega_{k'}t') + \sum_{kk'}C_kC_{k'}\frac{\langle\dot{q}_k(0)\dot{q}_{k'}(0)\rangle}{\omega_k\omega_{k'}}\sin(\omega_k t)\sin(\omega_{k'}t') \\
&\qquad + \sum_{kk'}C_kC_{k'}\frac{\cancelto{0}{\langle q_k(0)\dot{q}_{k'}(0)\rangle}}{\omega_k}\cos(\omega_k t)\sin(\omega_{k'}t') + \sum_{kk'}C_kC_{k'}\frac{\cancelto{0}{\langle\dot{q}_k(0)q_{k'}(0)\rangle}}{\omega_{k'}}\sin(\omega_k t)\cos(\omega_{k'}t').
\end{aligned} \tag{3.33}$$

[26] Remember that we work in one dimension.

Using the initial conditions of Eqs. (3.29) and (3.30),

$$\begin{aligned}\left\langle f^{(0)}(t)f^{(0)}(t')\right\rangle &= k_BT\sum_k \frac{C_k^2}{m_k\omega_k^2}\left[\cos(\omega_k t)\cos(\omega_k t') + \sin(\omega_k t)\sin(\omega_k t')\right] \\ &= k_BT\sum_k \frac{C_k^2}{m_k\omega_k^2}\cos[\omega_k(t-t')] \\ &= 2k_BT\int_0^\infty d\frac{\omega}{\pi}\frac{J(\omega)}{\omega}\cos[\omega(t-t')], \end{aligned} \tag{3.34}$$

where in the penultimate line we used the sum rule and we used the definition of the spectral density Eq. (3.26) in the last.

If we choose the spectral density to be ohmic, i.e. when $s = 1$ in Eq. (3.27), and if we stay away from the very short timescale regime such that we can safely let $\Omega \to \infty$ (by which we intend to say that $\Omega \ll \eta$) and work in the relaxation time approximation, we find

$$\left\langle f^{(0)}(t)f^{(0)}(t')\right\rangle = 2k_BT\eta\int_0^\Omega \frac{d\omega}{\pi}\cos\left[\omega(t-t')\right] = 2k_BT\eta\int_0^\infty \frac{d\omega}{\pi}\cos\left[\omega(t-t')\right]. \tag{3.35}$$

Using the fact that the cosine is an even function, we can extend the boundaries of the integral to the negative axis. Also, we can freely add a sine, since it is an odd function. We obtain

$$\left\langle f^{(0)}(t)f^{(0)}(t')\right\rangle = k_BT\eta\int_{-\infty}^\infty \frac{d\omega}{\pi}\left\{\cos\left[\omega(t-t')\right] + i\sin\left[\omega(t-t')\right]\right\} = k_BT\eta\int_{-\infty}^\infty \frac{d\omega}{\pi}\exp\left[i\omega(t-t')\right], \tag{3.36}$$

using Euler's relation. Now, we use the definition of the Dirac-delta distribution and find

$$\left\langle f^{(0)}(t)f^{(0)}(t')\right\rangle = k_BT\eta\int_{-\infty}^\infty \frac{d\omega}{\pi}\exp\left[i\omega(t-t')\right] = 2k_BT\eta\delta(t-t'), \tag{3.37}$$

which coincides with the white noise characteristic (2.23) of the Langevin equations.

We can also derive the final form of the friction term in Eq. (3.23) and use the

spectral density Eq. (3.26) to write

$$\frac{d}{dt}\sum_k \frac{C_k^2}{m_k\omega_k^2}\int_0^t dt' \cos\left[\omega_k(t-t')\right] Q(t') = 2\frac{d}{dt}\int_0^t dt' \int_0^\infty \frac{d\omega}{\pi}\,\frac{J(\omega)}{\omega}\cos\left[\omega(t-t')\right] Q(t'), \tag{3.38}$$

which simplifies, by assuming ohmic spectral density and performing the same integral as before, to

$$2\eta\frac{d}{dt}\int_0^t dt'\delta(t-t')Q(t') = \eta\dot{Q}(t) + 2\eta\delta(t)Q(0), \tag{3.39}$$

where the last term is a spurious 'drift' term. Physically, it is important, for it will result in the correct conditions for equilibrium for Stratonovich noise—as explained in Section 2.1.2. The spurious term shows up because we have assumed Itô noise (2.23), while in reality the two-point correlation function is supposed to be of finite width equal to the collision between the system of interest and a bath constituent. Mathematically, however, this spurious term can be absorbed in the fluctuation force if we redefine the fluctuation force as[27]

$$\bar{f}^{(0)}(t) = \sum_k^N C_k\left\{\left[q_k(0) - \frac{C_k}{m_k\omega_k^2}Q(0)\right]\cos(\omega_k t) + \frac{\dot{q}(0)_k}{\omega_k}\sin(\omega_k t)\right\}, \tag{3.40}$$

and if we take the ensemble average (2.13) with respect it to the bath *and* the coupling, instead of the bath only (see Peter Hänggi's [29] for the full calculation of the Gaussian integrals)

$$\left\langle \bar{f}^{(0)}(t)\right\rangle_{B+I} = \frac{\mathrm{Tr}_B\left[\bar{f}^{(0)}(t)\exp\left(-\beta(\mathcal{H}_B+\mathcal{H}_I)\right)\right]}{\mathrm{Tr}_B\left[\exp\left(-\beta(\mathcal{H}_B+\mathcal{H}_I)\right)\right]} \tag{3.41}$$

such that it will not change the white noise obtained in Eq. (3.37).

Finally, we can return to Eq. (3.20) and plug in the friction term (3.39) (with the spurious term absorbed in the fluctuation force). We find

$$M\ddot{Q} + V'(Q) + \eta\dot{Q} = \bar{f}^{(0)}(t). \tag{3.42}$$

All's well that ends well: this is the Langevin equation of a classical Brownian particle in an open system. Nevertheless, it is obtained from a closed composite model of the system *and* the environment and evaluating out the environment, which is the *a posteriori* justification we were looking for.

[27] The interpretation is that we have assumed that the equilibrium of the bath is re-centered to coincide with the origin of the system coordinate $Q(0)$.

## 3.3 General-coordinate coupling to the bath

Suppose we wish to expand upon the coordinate-coordinate coupling of the previous discussion and consider a coupling to the bath that is *general* in form and depends on the coordinate of the system $Q$ only. In addition we have assumed the interaction to be *separable*, i.e. the coupling constant will not be influenced by the system coordinate $Q$, i.e. a completely general $F_k[Q]$ will be assumed to simplify to $C'_k F[Q]$. This is a constraint that enforces strictly linear dissipation, which is the case for state-independent dissipation [80, p. 20]. Then, we write the Lagrangian

$$\mathcal{L} = \frac{1}{2}M\dot{Q}^2 - V(Q) + \frac{1}{2}\sum_{k=1}^{N} m_k(\dot{q}_k^2 - \omega_k^2 q_k^2) + \underbrace{F[Q]\sum_{k=1}^{N} C'_k q_k}_{\text{General System/Bath-INT.}} \underbrace{- \frac{1}{2}F[Q]^2 \sum_{k=1}^{N} \frac{C'^2_k}{m_k\omega_k^2}}_{\text{Counterterm}}. \tag{3.43}$$

The coupling constants $C'_k$ will, in general, be different from the 'spring constants' $C_k$ of the Caldeira-Leggett model; their dimension will depend on the particular realization of $F[Q]$. We have also adjusted the counterterm accordingly, to renormalize the interaction-induced effects to the bare potential [80] in a way similar to that of Eq. (3.8):

$$V_{eff}(Q) = V(Q) + \sum_{k=1}^{N} \frac{C'^2_k}{2m_k\omega_k^2} F[Q]^2. \tag{3.44}$$

We will see that this new coupling will change the Langevin equation considerably, and will lead us to a generalized Langevin equation with 'multiplicative noise', while staying true to the Fluctuation-Dissipation theorem, as we will show in Section 3.4.

The equation of motion for the system is

$$M\ddot{Q} + V'[Q] = F'[Q]\sum_k C'_k q_k - F[Q]F'[Q]\sum_k \frac{C'^2_k}{m_k\omega_k^2} \tag{3.45}$$

where $F'[Q] = \partial F[Q]/\partial Q$, and we have again suppressed the limits of the sum for brevity. The last term is entirely due to the counterterm.

The equation of motion for the harmonic oscillators of the bath is

$$m_i\ddot{q}_i + m_i\omega_i^2 q_i = C'_i F[Q], \tag{3.46}$$

which is the differential equation of a driven harmonic oscillator for a general fluctuation force. The solution can be found a standard way by Green's functional method, although we present an equivalent, but also more tedious, calculation in Appendix C,

because we think it is more insightful. The result is, Eq. (C.26),

$$q_i(t) = f_i^{(0)}(t) + \frac{C_i'}{m_i\omega_i}\int_0^t dt' \sin\left[\omega_i(t-t')F[Q(t')]\right], \tag{3.47}$$

with $f_i^{(0)}(t)$ is the harmonic force per particle defined in Eq. (3.15).

Now, we can eliminate the bath coordinates by plugging in the solution $q_i$ into the system equation of motion (3.45). We obtain

$$\begin{aligned} M\ddot{Q}(t) + V'[Q] - F'[Q(t)]\int_0^t dt' \sum_k \frac{C_k'^2}{m_k\omega_k}\sin[\omega_k(t-t')]F[Q(t')] \\ = F'[Q(t)]f^{(0)}(t) - F[Q]F'[Q]\sum_k \frac{C_k'^2}{m_k\omega_k^2}, \end{aligned} \tag{3.48}$$

for $f^{(0)}(t)$ the harmonic force defined in Eq. (3.16). We now perform a partial integration on the third term, such that we can recognize a term proportional to the velocity, which can then be identified as the friction term

$$\begin{aligned} M\ddot{Q}(t) + V'[Q] + \underbrace{F'[Q(t)]\int_0^t dt' \sum_k \frac{C_k'^2}{m_k\omega_k^2}\cos[\omega_k(t-t')]F'[Q(t')]\dot{Q}(t')}_{\text{Friction term}} \\ = \underbrace{-F'[Q(t)]F[Q(0)]\sum_k \frac{C_k'^2}{m_k\omega_k^2}\cos(\omega_k t)}_{\text{spurious initial term}} + \Xi^{(0)}(Q(t);t), \end{aligned} \tag{3.49}$$

for the anharmonic fluctuation force

$$\Xi^{(0)}(Q(t);t) = F'[Q(t)]f^{(0)}(t). \tag{3.50}$$

In Eq. (3.49) the counterterm was canceled to the $t' = t$-boundary term from the partial integration, and we have moved the other boundary term (the 'spurious' term, corresponding to $t' = 0$) of the partial integration to the right-hand side of the equation. Completely analogous to the procedure in Eq. (3.39)–(3.41), this spurious term can be included in the fluctuation force if we redefine it as

$$\bar{\Xi}^{(0)}(Q(t);t) = F'[Q(t)]\sum_k^N C_k'\left\{\left[q_k(0) - \frac{C_k'}{m_k\omega_k^2}F[Q(0)]\right]\cos(\omega_k t) + \frac{\dot{q}_k}{\omega_k}\sin(\omega_k t)\right\}, \tag{3.51}$$

and take the ensemble average with respect to the bath *and* the coupling, exactly as in Eqs. (3.41).

The generalized Langevin equation, then, becomes,

$$M\ddot{Q}(t) + V'[Q] + F'[Q(t)] \int_0^t dt' \sum_k \frac{C_k'^2}{m_k\omega_k^2} \cos[\omega_k(t-t')]F'[Q(t')]\dot{Q}(t') = \bar{\Xi}^{(0)}(Q(t);t), \tag{3.52}$$

We can proceed by using the spectral density through Eq. (3.26) to eliminate the sum over oscillators, which turns the generalized Langevin equation into

$$M\ddot{Q}(t) + V'[Q] + 2F'[Q(t)] \int_0^t dt' \int_0^\infty \frac{d\omega}{\pi} \frac{J(\omega)}{\omega} \cos\left[\omega(t-t')\right] F'[Q(t')]\dot{Q}(t') = \bar{\Xi}^{(0)}(Q(t);t), \tag{3.53}$$

In the case of ohmic dissipation and large cut-off $\Omega \to \infty$, this reduces to

$$M\ddot{Q}(t) + V'[Q] + \eta F'[Q(t)]^2\dot{Q}(t') = \bar{\Xi}^{(0)}(Q(t);t). \tag{3.54}$$

Note that 'ohmic' dissipation is interpreted as a spectral density

$$J'(\omega) = \frac{\pi}{2} \sum_k \frac{C_k'^2}{m_k\omega_k} \delta(\omega - \omega_k), \tag{3.55}$$

which only coincides with the spectral density of the previous section if we choose $F[Q] = Q$ such that $C_k' = C_k$. In general, the word 'ohmic', then, only refers to the linearity of the bath *in terms of the coupling constants*. For different coupling constants, two 'ohmic' baths will not have equal properties.
The fluctuation force $\bar{\Xi}^{(0)}(Q(t);t)$ does not lead to white noise, because, apart from the harmonically oscillating $f^{(0)}(t)$, it has an amplitude $F'[Q]$, which creates inhomogeneities. This is called *multiplicative noise*, with its characteristic correlation function

$$\left\langle \Xi^{(0)}(Q(t);t)\Xi^{(0)}(Q(t');t') \right\rangle = F'[Q(t)]F'[Q(t')] \left\langle f^{(0)}(t)f^{(0)}(t') \right\rangle = 2\eta k_B T F'[Q(t)]^2 \delta(t-t'), \tag{3.56}$$

which shows why this noise is called 'multiplicative'. The $F[Q(t)]$ can be kept outside of the ensemble average, since it does not depend on the initial values of the bath coordinates (and the trace in Eq. (3.41) is over the initial bath coordinates alone).

This multiplicative noise can physically be understood by, for example, interpreting the $F'[Q]$ as a temperature gradient. In the absence of such a temperature gradient, the noise does not depend on the position of the Brownian particle. After adding the temperature gradient, the particle will be more aggressively influenced at positions with a higher temperature than at positions with a lower temperature.

## 3.4 Fluctuation-Dissipation relation for Langevin models

In this section we intend to show that the fluctuation-dissipation relation holds in the two specific cases above, namely those of coordinate-coordinate coupling and general-coordinate coupling. In these two cases, it will take the form of a relation between the fluctuation force correlation and the memory-kernel in the friction term. The memory-kernel $\gamma(t-t')$ is the integrand of the friction term (the term proportional to velocity) in the generalized Langevin equation

$$M\ddot{Q} + V'(Q) + M\int_{-\infty}^{t} dt'\Theta(t-t')\gamma(t-t')\dot{Q}(t') = \Gamma(t), \tag{3.57}$$

for $\Gamma$ a general fluctuation force and where the Heaviside step-function $\Theta(t-t')$ has been put in to ensure causality. It is called the memory kernel, since if the integral over $t'$ can not be performed before solving the differential equation, the solution at time $t$ will depend on all the earlier times $t'$. This is what one usually calls a system with 'memory'. For predictive power, it is desirable that a system does not have memory, since information about a past state is often practically beyond reach. If a conditional probability distribution of future states of a system -conditional on past and present states, that is- does not depend on the sequence of events that preceded, it is said to have the Markov property. Thus, the behavior of the system in the future depends solely on the present state, independent of its history. In our context, the Markov property is lost when the results depend on the earlier times $t'$.[28]

The fluctuation-dissipation relation from the above Langevin equation is

$$\langle\Gamma(t)\Gamma(t')\rangle = 2\eta M k_B T\gamma(t-t'). \tag{3.58}$$

In the case of coordinate-coordinate coupling, we have already implicitly derived the fluctuation-dissipation theorem in Section 3.2.4. For ohmic dissipation, we saw that the memory-kernel was simply the delta distribution of white noise. Hence,

$$\left\langle \bar{f}^{(0)}(t)\bar{f}^{(0)}(t')\right\rangle = k_B T\delta(t-t'), \tag{3.59}$$

which is the simplest example of the fluctuation-dissipation theorem. Note that, since the integral over the delta distribution is easily performed, the solution to the Langevin equation does not depend on $t'$ and is, therefore, memory free.

If we do not assume a specific spectral density for the bath, we find the relation between the friction term and the fluctuation force correlation in the following way. Observe the right-hand side Eq. (3.38), perform the derivative with respect to time and do a partial integration. Two $Q(t)$-terms cancel, while–as we saw in Eq. (3.51)–the $Q(0)$-term can be absorbed into the fluctuation force (without changing the correlation

[28] This is strictly not true, cf footnote 5.

function), and the remaining friction term is

$$2\int_0^\infty \frac{d\omega}{\pi}\int_0^t dt' \frac{J(\omega)}{\omega}\cos\left[\omega(t-t')\right]\dot{Q}(t'). \tag{3.60}$$

Hence the memory-kernel takes the form

$$\gamma(t-t') = \frac{1}{M}\Theta(t-t')\frac{2}{\pi}\int_0^\infty d\omega \frac{J(\omega)}{\omega}\cos\left[\omega(t-t')\right]. \tag{3.61}$$

Comparing with the last line in Eq. (3.34), we observe the fluctuation-dissipation relation is obeyed

$$\left\langle f^{(0)}(t)f^{(0)}(t')\right\rangle = 2k_BT\int_0^\infty \frac{d\omega}{\pi}\frac{J(\omega)}{\omega}\cos\left[\omega(t-t')\right] = Mk_BT\gamma(t-t'). \tag{3.62}$$

Let us now turn to the generalized Langevin equation (3.53) that we found for the general coupling with $F[Q]$, and observe that the memory-kernel in the friction term (the one proportional to velocity) in Eq. (3.53), is

$$\gamma(t-t') = 2F'[Q(t)]F'[Q(t')]\int_0^\infty \frac{d\omega}{\pi}\frac{J(\omega)}{\omega}\cos\left[\omega(t-t')\right]. \tag{3.63}$$

Turning our attention to the correlation function for multiplicative noise (3.56), and using Eq. (3.62), we see that the fluctuation-dissipation theorem is again satisfied:

$$\langle\Xi(Q(t),t)\Xi(Q(t'),t')\rangle = 2F'[Q(t)]F'[Q(t')]\int_0^\infty \frac{d\omega}{\pi}\frac{J(\omega)}{\omega}\cos\left[\omega(t-t')\right] = Mk_BT\gamma(t-t'). \tag{3.64}$$

## 3.5 Conclusion

In conclusion, we have seen that by solving the coupled equations of motion, obtained from the Caldeira-Leggett model Eq. (3.10), and by eliminating the bath coordinates, we reproduce the form of the Langevin equation in the classical limit. We also proved its internal consistency by showing that it satisfies the fluctuation-dissipation theorem for all choices of the spectral density $J(\omega)$ (as long as the frequency integral does not diverge). To obtain a system without memory, one will find delta-peaked 'white' noise for ohmic spectral density $J(\omega) \propto \omega$. Hence, this justifies the choice of the Caldeira-Leggett Lagrangian and proves that we have successfully closed the dissipative system.

We have also seen that from the dynamics of a general coupling, as defined in Eq. (3.43), the result is a general Langevin equation Eq. (3.53). This similarly satisfies the fluctuation-dissipation theorem, but for the multiplicative noise of Eq. (3.56), modeling spatial inhomogeneity (such as a temperature gradient) of the Brownian system.

As a last remark: With the justification of finding the Langevin equations in the classical limit through the Caldeira-Leggett Lagrangian (3.10), we know it is a physically plausible model. One can then use path-integral quantization to find the quantum dynamics of this model, integrate out the bath, and obtain an effective non-local action, as is done in [9]. However, we will not pursue this quantization at this stage of the thesis, since it will involve much of the same derivation as we will do in Chapter 5. There, we will quantize the model for an entirely general coupling between system and environment. Then, we can retrieve the effective action for the case of coordinate-coordinate coupling, as we have seen above. For future reference, we state the result now. For imaginary time $t \to i\hbar\beta$ it reads

$$S_{eff}[\bar{Q}(\tau)] = \int_0^{\hbar\beta} d\tau \left\{ \frac{1}{2} M \dot{\bar{Q}}^2 + V(\bar{Q}) \right\} + \frac{\eta}{4\pi} \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \frac{\left[\bar{Q}(\tau) - \bar{Q}(\sigma)\right]^2}{|\tau - \sigma|^2}, \tag{3.65}$$

where the last term is called the *Caldeira-Leggett term*. This term describes a purely non-local interaction as a result of the bath medium. Its interpretation is that of friction: it is energetically more favorable for the particle to remain at the same position, since the closer they are together at successive times, the smaller the contribution of the Caldeira-Leggett effective potential is.

The next step we intend to take is to generalize the model even further, namely to general-velocity coupling.

# 4 Extending the classical model

> "[...] My view of the matter, for what its worth, is that there is no such thing as a logical method of having new ideas, or a logical reconstruction of this process."
>
> —Karl Popper [65, p. 30]

## 4.1 General velocity-coupling to the bath

In this chapter, we will generalize the Caldeira-Leggett model from a coordinate-coordinate couplinf to a coupling thta is a general function of the velocity of the Brownian particle, coupled to the coordinates of the bath oscillators. The original motivation to choose such a velocity-dependent coupling was to reproduce the force $p/(1+p^2)$ in the approach to Lévy motion in Sisyphus cooling of Marksteiner, Ellinger and Zoller [56]—as explained in Section 2.4. Realizing that the general-coordinate coupling would not give us the desired result, we chose to proceed with a completely general coupling to velocity. It turns out that such an approach is possible to reproduce the desired force in terms of velocity by choosing a specific coupling that will give us the intended result; and, hence, construct a closed effective model exhibiting Lévy behavior.

In Section 4.2.2, we will also reduce to the case where the coupling to the velocity of the Brownian particle is linear. In the superohmic case (specifically $J(\omega) \propto \omega^3$), we find an equation of motion that is remarkably similar to the Abraham-Lorentz equation, which describes a self-interacting electron.

For now, we will derive the dynamics for a general velocity coupling much in the same way as we have derived the equations of motion for the Caldeira-Leggett model in Chapter 3. The result will again be an adjusted Langevin equation, but with additional terms, which have to be treated with some care.

Thus, we leave the coordinate-coordinate coupling of the Caldeira-Leggett model behind and replace it with a general-velocity coupling $F[\dot{Q}]$ of the velocity of the Brownian particle to each of the coordinates of the bath, again assuming a separable interaction $F_i[\dot{Q}] = \tilde{C}_i F[\dot{Q}]$; note that, dimensionally, the coupling constants $\tilde{C}_i$ are not interpreted as spring constants, but have a dimension depending on the particular realization of $F[\dot{Q}]$. As before, we modify the counterterm accordingly. However, this term will obtain a different physical interpretation. For linear-velocity coupling, for example, it will renormalize the mass in the kinetic term of the system—as we will see later in the calculation. *Ceteris paribus*, we write the Lagrangian

$$\mathcal{L} = \frac{1}{2}M\dot{Q}^2 - V(Q) + \frac{1}{2}\sum_{k=1}^{N} m_k(\dot{q}_k^2 - \omega_k^2 q_k^2) + \underbrace{F[\dot{Q}]\sum_{k=1}^{N}\tilde{C}_k q_k}_{\text{General velocity interaction.}} \underbrace{-\sum_{k=1}^{N}\frac{\tilde{C}_k^2}{2m_k\omega_k^2}F^2[\dot{Q}]}_{\text{Counterterm.}}. \tag{4.1}$$

Compared to the Caldeira-Leggett model of the last chapter, the equations of motion change considerably. This is for two reasons. First, due to the time derivative in the system equation an extra term generated by the chain-rule gives rise to a $\dot{q}_i$ term, such that we must plug in the solution to the equation of motion of the bath twice. Second, the velocity coupling and the counterterm add to the kinetic part of the dynamics (i.e. the time derivative in the Euler-Lagrange equations), which, again due to the chain rule, generate additional terms. The system equation of motion reads[29]

$$M\ddot{Q} + V'(Q) + F''[\dot{Q}]\ddot{Q}\sum_k \tilde{C}_k q_k + F'[\dot{Q}]\sum_k \tilde{C}_k \dot{q}_k = \sum_k \frac{\tilde{C}_k^2}{m_k\omega_k^2}\left[F'[\dot{Q}]^2 + F[\dot{Q}]F''[\dot{Q}]\right]\ddot{Q}, \tag{4.3}$$

where the right-hand side is entirely due to the counterterm.

The bath equation of motion is again a driven harmonic oscillator equation,

$$m_i\ddot{q}_i + m_i\omega_i^2 q_i = \tilde{C}_i F(\dot{Q}), \tag{4.4}$$

with the same solution as before (Appendix C), which is

$$q_i(t) = f_i^{(0)}(t) + \frac{\tilde{C}_i}{m_i\omega_i}\int_0^t dt' \sin[\omega_i(t-t')]F[\dot{Q}(t')], \tag{4.5}$$

and its time-derivative

$$\dot{q}_i(t) = \frac{df_i^{(0)}(t)}{dt} + \frac{\tilde{C}_i}{m_i}\int_0^t dt' \cos[\omega_i(t-t')]F[\dot{Q}(t')], \tag{4.6}$$

where the differential boundary term vanishes and the fluctuation force is defined in Eqs. (3.15) and (3.16).

Let us now plug Eqs. (4.5) and (4.6) into the system equation (4.3), such that we obtain a differential equation analogous to the generalized Langevin equation. Carefully

[29] As is well known, coupling a system to velocity generates additional terms to the generalized momentum, such that it differs from the physical momentum. The generalized momentum is

$$P = \frac{\partial L}{\partial \dot{Q}} = M\dot{Q} + \sum_k \tilde{C}_k q_k F'[\dot{Q}] - \sum_k \frac{\tilde{C}_k^2}{m_k\omega_k^2}F[\dot{Q}]F'[\dot{Q}], \tag{4.2}$$

while $p_i = m_i\dot{q}_i$ still holds. Interestingly, this complication stands in the way of constructing a single-valued Hamiltonian from the Legendre transformation of the Lagrangian (4.1). For couplings $F[\dot{Q}] = \dot{Q}^n$, for $n = 1$ and $n =$ even, the momentum is still invertible. For each $n$ that gives an invertible function, there is a minimal-coupling problem to be solved—as in the Hamiltonian treatment of electrodynamics. Nevertheless, for $n =$ odd there is an ill-defined Hamiltonian. We will come back to this in the Outlook.

keeping track of all the terms, we obtain

$$M\ddot{Q}+V'[Q] + F''[\dot{Q}(t)]\ddot{Q}(t)\int_0^t dt' \sum_k \frac{\tilde{C}_k^2}{m_k\omega_k}\sin\left[\omega_k(t-t')\right]F[\dot{Q}(t')]$$
$$+ F'[\dot{Q}(t)]\int_0^t dt' \sum_k \frac{\tilde{C}_k^2}{m_k}\cos\left[\omega_k(t-t')\right]F[\dot{Q}(t')]$$
$$= -\xi^{(0)}(\dot{Q}(t);t)\ddot{Q}(t) - \zeta^{(0)}(\dot{Q}(t);t) + \sum_k \frac{\tilde{C}_k^2}{m_k\omega_k^2}\left[F'[\dot{Q}(t)]^2 + F[\dot{Q}]F''[\dot{Q}(t)]\right]\ddot{Q}(t), \tag{4.7}$$

for the velocity-dependent, amplitude-driven, fluctuation forces,

$$\xi^{(0)}(\dot{Q}(t);t) = F''[\dot{Q}(t)]f^{(0)}(t), \tag{4.8}$$

and

$$\zeta^{(0)}(\dot{Q}(t);t) = F'[\dot{Q}]\frac{df^{(0)}(t)}{dt}. \tag{4.9}$$

Let us now integrate by parts the third[30] term on the left-hand side of Eq. (4.7), which then becomes

$$-F''[\dot{Q}(t)]\ddot{Q}(t)\int_0^t dt' \sum_k \frac{\tilde{C}_k^2}{m_k\omega_k^2}\cos\left[\omega_k(t-t')\right]F'[\dot{Q}(t')]\ddot{Q}(t')$$
$$+\sum_k \frac{\tilde{C}_k^2}{m_k\omega_k^2}F''[\dot{Q}(t)]\ddot{Q}(t)F[\dot{Q}(t)] - \sum_k \frac{\tilde{C}_k^2}{m_k\omega_k^2}F''[\dot{Q}(t)]\ddot{Q}(t)F[\dot{Q}(0)]\cos(\omega_k t) \tag{4.11}$$

Note that in the first term three minus signs play a role: one from partial integration itself, one from the integration of the sine, and one from the sign of $t'$ within the sine. Now, the first boundary term will cancel to one of the counterterms (the last term on the right-hand side of Eq. (4.7)). The other boundary term depends on the initial value $\dot{Q}(0)$; this term plays the role of the spurious term that we have encountered twice in

[30] Curiously, at this stage in the calculation it seems to make more sense to actually integrate by parts the fourth term instead of the third in Eq. (4.7), because this would match the power of the parameter $\omega_k$ in both terms and allow us to add them together. However, this will lead us to a memory-kernel in terms of a sine-function

$$\bar{\gamma}(t-t') = \sum_k \frac{\tilde{C}_k^2}{m_k\omega_k}\sin\left[\omega_k(t-t')\right], \tag{4.10}$$

which we cannot integrate easily using the spectral density. Even for ohmic baths, this term would either diverge or be inconsistent with the relaxation-time approximation (physical results will depend on the cut-off in an unnatural way).

Chapter 3. This time, analogous to Eqs. (3.40) and (3.51) it can be incorporated into $\xi^{(0)}(Q(t);t)$ in the following way

$$\bar{\xi}^{(0)}(Q(t);t) = F''[\dot{Q}] \sum_k \tilde{C}_k \left\{ \left[ q_k(0) + \frac{\tilde{C}_k}{m_k \omega_k} F[\dot{Q}(0)] \right] \cos(\omega_k t) + \frac{\dot{q}_k}{\omega_k} \sin(\omega_k t) \right\}, \tag{4.12}$$

and taking the ensemble average with respect to the bath *and* interaction Hamiltonian, as in Eq. (3.41). This will cause no problems for suitable initial conditions chosen in this way.

Hence, we can rewrite the adjusted Langevin equation as

$$\begin{aligned} M\ddot{Q} + V'[Q] - F''[\dot{Q}(t)]\ddot{Q}(t) &\int_0^t dt' \sum_k \frac{\tilde{C}_k^2}{m_k \omega_k^2} \cos\left[\omega_k (t-t')\right] F'[\dot{Q}(t')]\ddot{Q}(t') \\ &+ F'[\dot{Q}(t)] \int_0^t dt' \sum_k \frac{\tilde{C}_k^2}{m_k} \cos\left[\omega_k (t-t')\right] F[\dot{Q}(t')] \\ &= -\bar{\xi}^{(0)}(\dot{Q}(t);t)\ddot{Q}(t) - \zeta^{(0)}(\dot{Q}(t);t) + \sum_k \frac{\tilde{C}_k^2}{m_k \omega_k^2} F'[\dot{Q}(t)]^2 \ddot{Q}(t). \end{aligned} \tag{4.13}$$

We will now use the spectral density of Eq. (3.26). However, this will be with $\tilde{C}_k$ instead of $C_k$, which is physically a different situation. We will discuss this difference later in the calculation. We will denote the difference in the spectral density in terms of the new coupling $\tilde{J}(\omega)$.

We can now write our first general result as

$$\begin{aligned} M\ddot{Q} + V'[Q] - 2F''[\dot{Q}(t)]\ddot{Q}(t) &\int_0^t dt' \int_0^\infty \frac{d\omega}{\pi} \frac{\tilde{J}(\omega)}{\omega} \cos\left[\omega (t-t')\right] F'[\dot{Q}(t')]\ddot{Q}(t') \\ &+ 2F'[\dot{Q}(t)] \int_0^t dt' \int_0^\infty \frac{d\omega}{\pi} \omega \tilde{J}(\omega) \cos\left[\omega (t-t')\right] F[\dot{Q}(t')] \\ &= -\bar{\xi}^{(0)}(\dot{Q}(t);t)\ddot{Q}(t) - \zeta^{(0)}(\dot{Q}(t);t) + 2\int_0^\infty \frac{d\omega}{\pi} \frac{\tilde{J}(\omega)}{\omega} F'[\dot{Q}(t)]^2 \ddot{Q}(t). \end{aligned} \tag{4.14}$$

This is as far as one can go without either specifying a specific coupling or a specific spectral density. For general coupling, it is clear that this generalized Langevin equation will definitely depend on the memory of the system. This is not problematic at all, since many interesting systems, particularly the non-linear dynamics of chaotic systems, have this feature. Also, it is often possible that, even though a system has memory, it still has some memoryless subsystems [60, p. 3], [74, good overview for circuits]. Nevertheless,

the methods involved to solve such systems, often numeric, fall beyond the scope of this research. Therefore, we will attempt to simplify Eq. (4.14) for specific cases, making necessary approximations to obtain analytical results.[31]

## 4.2 Specific choices for the velocity coupling

### 4.2.1 A polynomial coupling

In order to remain as general as we can, let us look at a coupling to a specific power $r$ of the coupling

$$\tilde{C}_k^{(r)} F[\dot{Q}] = \tilde{C}_k^{(r)} \dot{Q}^r, \tag{4.15}$$

In principle, if we want to interpret the $\tilde{C}_k$'s as spring constants, we should rescale the coupling with an inverse frequency $\omega_k$ for every time-derivative that acts on $Q$. This is important dimensionally, since every inverse time unit from a time-derivative is now canceled to an inverse frequency unit. It also makes sense physically, since the frequency of the bath oscillators defines the physical characteristic timescale of the model. Nevertheless, we will work with the $\tilde{C}_k$ (which cannot be interpreted as a spring constant) until this dimensionality issue becomes important. Following the discussion around Eq. (3.55), this will become important when we compare the spectral density of the new model $\tilde{J}(\omega)$ with the original $J(\omega)$—this is consistent with the definition of the spectral density,

$$\tilde{J}(\omega) = \frac{\pi}{2} \sum_k \frac{\tilde{C}_k^{(r)\,2}}{m_k \omega_k} \delta(\omega - \omega_k), \tag{4.16}$$

and hence one only needs to specify the relation between $C_k$ and $\tilde{C}_k$ when dealing with a specific coupling.

With the assumption (4.15), the generalized Langevin equation (4.14) becomes

$$\begin{aligned} M\ddot{Q} + V'[Q] - 2r^2(r-1)\dot{Q}^{r-2}(t)\ddot{Q}(t) \int_0^t dt' \int_0^\infty \frac{d\omega}{\pi} \frac{\tilde{J}(\omega)}{\omega} \cos\left[\omega(t-t')\right] \dot{Q}^{r-1}(t')\ddot{Q}(t') \\ + 2r\dot{Q}^{r-1}(t) \int_0^t dt' \int_0^\infty \frac{d\omega}{\pi} \tilde{J}(\omega)\omega \cos\left[\omega(t-t')\right] \dot{Q}^r(t') \\ = -r(r-1)\dot{Q}^{r-2}\bar{f}^{(0)}(t)\ddot{Q}(t) - r\dot{Q}^r \dot{f}^{(0)}(t) + 2\int_0^\infty \frac{d\omega}{\pi} \frac{\tilde{J}(\omega)}{\omega} \dot{Q}^{2r-2}(t)\ddot{Q}(t). \end{aligned} \tag{4.17}$$

[31] We will come back to the importance of modeling non-linear behavior in the Outlook.

For ohmic baths, $\tilde{J}(\omega) = \lambda\omega$, this reduces to

$$M\ddot{Q}+V'[Q] - 2\lambda r^2(r-1)\dot{Q}^{2r-3}(t)\ddot{Q}^2(t) - 2\lambda r\dot{Q}^{r-1}(t)\int_0^t dt' \int_0^\Omega \frac{d\omega}{\pi}\omega^2\cos\left[\omega(t-t')\right]\dot{Q}^r(t')$$
$$= -r(r-1)\dot{Q}^{r-2}\bar{f}^{(0)}(t)\ddot{Q}(t) - r\dot{Q}^r\dot{f}^{(0)}(t) + \frac{2\lambda\Omega}{\pi}\dot{Q}^{2r-2}(t)\ddot{Q}(t). \tag{4.18}$$

where we have used $\lambda$ for the proportionality constant of the spectral density such that it will not be confused with the viscosity $\eta$ for ohmic baths in terms of coupling constants $C_k$. One can now perform two partial integrations in $t'$, in order to evaluate the frequency integral,

$$M\ddot{Q}+V'[Q] - 2\lambda r^2(r-1)\dot{Q}^{2r-3}(t)\ddot{Q}^2(t) + 2\lambda r^2(r-1)\dot{Q}^{2r-3}(t)$$
$$+ \frac{2\lambda\Omega r^2}{\pi}\dot{Q}^{2r-2} + \frac{2\lambda r^2}{\pi}\dot{Q}^{r-1}\int_0^\Omega d\omega\cos(\omega t)\dot{Q}^{r-1}(0) - \frac{2\lambda r}{\pi}\dot{Q}^{r-1}\int_0^\Omega d\omega\sin(\omega t)\dot{Q}^r(0)$$
$$= -r(r-1)\dot{Q}^{r-2}\bar{f}^{(0)}(t)\ddot{Q}(t) - r\dot{Q}^r\dot{f}^{(0)}(t) + \frac{2\lambda\Omega}{\pi}\dot{Q}^{2r-2}(t)\ddot{Q}(t). \tag{4.19}$$

It will depend on the physical circumstances if the cut-off dependent terms are large or small, since although $\Omega$ is very large, $\lambda$ can often be related to the relaxation time, which is very small. We will discuss an example of this in the next section.

### 4.2.2 Linear-velocity coupling for a superohmic bath: Abraham-Lorentz

In the section we will discuss the generalized Langevin equation for a system of linear-velocity coupling.

$$\tilde{C}_k^{(1)}F[\dot{Q}] = \bar{C}_k\dot{Q}, \tag{4.20}$$

where we use a 'bar' to distinguish between the general-velocity case (where we had a 'tilde') and the linear-velocity case we will use now.

If we would not have included a counterterm in this model, we could easily reproduce the original Caldeira-Leggett model. In principle, in the action for the Lagrangian (4.1) and for a coupling linear in velocity (4.20), one could transfer the time-derivative in the interaction term from the particle coordinate $Q$ to the bath coordinates $q_k$, such that the action reads (again, ignoring the counterterm)

$$S = \int_0^t ds\left\{\mathcal{L}_S + \mathcal{L}_B + Q(s)\sum_{k=1}^N \bar{C}_k\dot{q}_k(s)\right\}. \tag{4.21}$$

Then, we could follow the procedure in Appendix A. There, we show the equivalence between the Lagrangian in the original Caldeira-Leggett model (3.10), which includes a counterterm proportinal to $Q^2$, and that of the above model (4.1) without that

counterterm. Hence,the original Caldeira-Leggett model is identical to Eq. (4.21) for $\bar{C}_k = C_k/\omega_k$. In our model, though, we do include a counterterm proportional to $F[\dot{Q}]^2$, which will alter the results, but will be consist with the quantum-mechanical result of Chapter 5.

For the coupling (4.20), the generalized Langevin equation (4.14) simplifies considerably, since the first derivatives of the coupling become unity, whereas the second derivatives vanish. The result is

$$M\ddot{Q}(t) + V'[Q] + 2\int_0^t dt' \int_0^\infty \frac{d\omega}{\pi}\omega \bar{J}(\omega)\cos\left[\omega(t-t')\right]\dot{Q}(t') = -\zeta^{(0)}(t) + 2\int_0^\infty \frac{d\omega}{\pi}\frac{\bar{J}(\omega)}{\omega}\ddot{Q}(t), \tag{4.22}$$

for the force

$$\zeta^{(0)} = \frac{d}{dt}\sum_k \bar{C}_k \left( q_k^{(0)}\cos(\omega_k t) + \frac{\dot{q}_k^{(0)}}{\omega_k}\sin\omega_k t \right). \tag{4.23}$$

To show that $-\zeta^{(0)}(t)$ is really a fluctuation force, one needs to calculate the average of the fluctuation force and its two-point correlation function. Using the initial conditions for classical equilibrium of the bath Eqs. (3.28)—(3.30), the average vanishes, since

$$\langle -\zeta^{(0)}(t)\rangle = -\frac{d}{dt}\sum_k \bar{C}_k \left[ \cancelto{0}{\left\langle q_k^{(0)}\right\rangle}\cos(\omega_k t) + \cancelto{0}{\left\langle \dot{q}_k^{(0)}\right\rangle}\sin(\omega_k t)\right] = 0. \tag{4.24}$$

The two-point correlation function of the force is

$$\left\langle (-\zeta^{(0)}(t))(-\zeta^{(0)}(t'))\right\rangle = \frac{d}{dt}\frac{d}{dt'}\sum_k\sum_{k'}\bar{C}_k\bar{C}_{k'}\left[\left\langle q_k^{(0)}q_{k'}^{(0)}\right\rangle\cos(\omega_k t)\cos(\omega_{k'}t') + \frac{\left\langle q_k^{(0)}q_{k'}^{(0)}\right\rangle}{\omega_k\omega_{k'}}\sin(\omega_k t)\sin(\omega_{k'}t')\right], \tag{4.25}$$

which becomes, after doing the derivatives to $t$ and $t'$,

$$\sum_k\sum_{k'}\bar{C}_k\bar{C}_{k'}\omega_k\omega_{k'}\left[\left\langle q_k^{(0)}q_{k'}^{(0)}\right\rangle\sin(\omega_k t)\sin(\omega_{k'}t') + \frac{\left\langle q_k^{(0)}q_{k'}^{(0)}\right\rangle}{\omega_k\omega_{k'}}\cos(\omega_k t)\cos(\omega_{k'}t')\right]. \tag{4.26}$$

Now, using the initial conditions, and performing the sum over $k'$, this reduces to

$$\begin{aligned}\left\langle(-\zeta^{(0)}(t))(-\zeta^{(0)}(t'))\right\rangle =& k_BT\sum_k \frac{\bar{C}_k^2}{m_k}\left[\sin(\omega_k t)\sin(\omega_k t')+\cos(\omega_k t)\cos(\omega_k t')\right]\\ =& k_BT\sum_k \frac{\bar{C}_k^2}{m_k}\cos[\omega_k(t-t')]\\ =& 2k_BT\int_0^\infty \frac{d\omega}{\pi}\bar{J}(\omega)\omega\cos[\omega(t-t')],\end{aligned} \tag{4.27}$$

which indeed coincides with the memory kernel in Eq. (4.22). Thus, the fluctuation-dissipation theorem holds for linear-velocity coupling.

Coming back to the equation of motion Eq. (4.22), to evaluate the frequency integral in the friction term (last term on the left-hand side), we first perform two successive partial time-integrations for the friction term,

$$\begin{aligned}&2\int_0^t dt'\int_0^\infty \frac{d\omega}{\pi}\omega\bar{J}(\omega)\cos\left[\omega(t-t')\right]\dot{Q}(t')\\ &\quad= 2\int_0^t dt'\int_0^\infty \frac{d\omega}{\pi}\bar{J}(\omega)\sin\left[\omega(t-t')\right]\ddot{Q}(t') - \int_0^\infty \frac{d\omega}{\pi}\bar{J}(\omega)\sin(\omega t)\dot{Q}(0)\\ &\quad= -2\int_0^t dt'\int_0^\infty \frac{d\omega}{\pi}\frac{\bar{J}(\omega)}{\omega}\cos\left[\omega(t-t')\right]\dddot{Q}(t') + \int_0^\infty \frac{d\omega}{\pi}\frac{\bar{J}(\omega)}{\omega}\ddot{Q}(t)\\ &\quad\quad -\int_0^\infty \frac{d\omega}{\pi}\frac{\bar{J}(\omega)}{\omega}\cos(\omega t)\ddot{Q}(0) - \int_0^\infty \frac{d\omega}{\pi}\bar{J}(\omega)\sin(\omega t)\dot{Q}(0).\end{aligned} \tag{4.28}$$

The $\dddot{Q}$-term, i.e. the change in acceleration, is called the 'jerk'. We also recognize that the second term exactly cancels the counterterm in Eq. (4.22). Then, we assume the superohmic bath

$$\bar{J}(\omega) = \begin{cases}\lambda\omega & \text{if } \omega<\Omega\\ 0 & \text{if } \omega>\Omega\end{cases}, \tag{4.29}$$

where the diffusion coefficient is denoted by $\lambda$ to avoid confusion with the interpretation of the viscosity $\eta$ of a material in terms of spring constants $C_k$. The generalized Langevin

equation becomes

$$M\ddot{Q}(t) + V'[Q] - 2\lambda \int_0^t dt' \int_0^\Omega \frac{d\omega}{\pi} \cos\left[\omega(t-t')\right] \ddot{Q}(t') = -\bar{\zeta}^{(0)}(t), \tag{4.30}$$

where we included both $t = 0$ boundary terms, depending on $\dot{Q}(0)$ and $\ddot{Q}(0)$ into the fluctuation force, similar to what we have done before. Analogous to Eq. (3.40), we have

$$\bar{\zeta}^{(0)}(t) = \frac{d}{dt} \sum_k \bar{C}_k \left( \left[ q_k^{(0)} - \frac{\bar{C}_k}{m_k \omega_k} \dot{Q}(0) - \frac{\bar{C}_k}{m_k \omega_k^2} \ddot{Q}(0) \right] \cos(\omega_k t) + \frac{\dot{q}_k^{(0)}}{\omega_k} \sin \omega_k t \right). \tag{4.31}$$

which does not alter the fluctuation-dissipation theorem if we take the ensemble average with respect to bath *and* interaction, as in Eq. (3.41).

Now, we can use the exact same steps as in Eq. (3.37) to evaluate the integral over $\omega$ and find the Dirac-delta distribution; hence

$$M\ddot{Q}(t) + V'[Q] - 2\lambda \dddot{Q}(t) = -\bar{\zeta}^{(0)}(t), \tag{4.32}$$

As we have mentioned before, it is important to note, that the 'ohmic' bath we assumed in Eq. (4.29) does not coincide with the ohmic bath of the original Caldeira-Leggett model, since the coupling constants are different for these two cases. Indeed, expressed in terms of the original model it is superohmic. Specifically, using Eq. (A.7) from the Appendix A.1,

$$J(\omega) = \omega^2 \bar{J}(\omega) \propto \omega^3, \tag{4.33}$$

and hence the bath is cubically superohmic.

There is an important analogy here with the research done by Barone and Caldeira, who use the Caldeira-Leggett model for cubic baths to describe the dissipation of an electron interacting with its own radiation field [4]. Classically, such an electron is described by the Abraham-Lorentz equation,

$$-\frac{2e^2}{3c^3}\dddot{Q} + M^*\ddot{Q} + V'[Q] = f^{(0)}, \tag{4.34}$$

with the fluctuation force given by Eq. (3.16) for $\omega_k = ck$, for wavenumber $k$ and speed of light $c$—the dispersion relation for the photon. The Abraham-Lorentz equation has important problems of its own. For example, pre-acceleration, where the acceleration at time $t$ depends on the value of the radiation force at earlier times $t'$, which is, therefore, a memory effect.

Whereas the goal of Section 3 was to reproduce the Langevin equation in the classical limit using the closed description of the Caldeira-Legett model, Barone and Caldeira reproduce the Abraham-Lorentz equation from first principles. They start with the

Lagrangian

$$\mathcal{L} = \mathcal{L}_S + \mathcal{L}_B + \mathcal{L}_I \tag{4.35}$$

where the system Lagrangian is generic as in (3.2), the bath consists of the electrodynamic field associated with the self-field of the electron

$$\mathcal{L}_B = \frac{1}{8\pi}\int d\vec{x}\left[\frac{1}{c}\frac{\partial\vec{A}}{\partial t} + \vec{\nabla}\phi\right]^2 - (\vec{\nabla}\times\vec{A})^2, \tag{4.36}$$

and the system-bath interaction is given by

$$\mathcal{L}_I = \int d\vec{x}\left[\frac{1}{c}\vec{J}\cdot\vec{A} - \rho\phi\right], \tag{4.37}$$

where $\vec{A}$ and $\phi$ are the vector and scalar potentials, and $\rho$ and $\vec{J}$ the charge and current densities. Note that there is no counterterm explicitly assumed in this model.

By changing to the Hamiltonian formalism, writing the expressions in terms of conjugated momenta of the coordinates $Q$ and $\vec{A}$, and assuming a superohmic cubic spectral density of the form (4.33) they are able to derive the equation of motion

$$-\lambda\dddot{Q} + M^*\ddot{Q} + V'[Q] = f(t), \tag{4.38}$$

for

$$\lambda = \frac{2e^2}{3c^3} \tag{4.39}$$

and with the renormalized mass[32] given by

$$M^* = M + \frac{2\lambda\Omega}{\pi}, \tag{4.40}$$

for the bare electron charge $e$, bare electron mass $M$, and speed of light $c$. Here, we also see the dissipation term in proportional to the jerk, which is a direct consequence of the low-frequency behavior of the spectral distribution in a cavity [11, p. 109].

The merit of having written down the Lagrangian (4.35) in terms of the fundamental constants of electrodynamics is that Barone and Caldeira can now estimate how large the cut-off-dependent terms in the equations of motion are. The cut-off itself is given by

$$\Omega = \frac{2\pi c}{r_0}, \tag{4.41}$$

where $r_0$ is the characteristic electronic dimension. It is the classical electron radius in the classical limit, while it is the deBroglie wavelength of the electron in the quantum

[32]The renormalized mass has the usual interpretation of a mass renormalization in terms of the screening of the bare electron mass by the one-loop-and-higher Feynman diagrams of the electron propagator—which is simply what the electron self-interaction in quantum-electrodynamical language is.

case. The effective mass depends on the cut-off $\Omega$, but since the numerical values in Eq. (4.40) are known, we can conclude $M^* \sim M$.

Coming back to our result Eq. (4.32), we see that it has exactly the same form as the Abraham-Lorentz equation. However, where Caldeira and Barone assumed a very specific electrodynamical model to derive the Eq. (4.38), for our result we did not assume any fundamental physics. Hence, in our case, this could be seen as a self-interaction of quite a general particle—as long as the coupling is not too strong.

Furthermore, Barone and Caldeira note that the "counterterm is not imposed as in the formulation of the quantum Brownian motion [...]" [4, p. 58], since the counterterm appears naturally from the microscopic set-up of the model. This remark is important, since in our model we have also not include a counterterm as in Eq. (3.5) for quantum Brownian motion. We did included a counterterm to the Lagrangian that, in the linear-velocity coupling case, is proportional to the square of the velocity. Since this canceled a term in Eq. (4.28), this gives us an equation of motion (4.32) without mass renormalization.

### 4.2.3 Lévy flights: A non-polynomial coupling

Another way to let the terms with direct memory vanish is to assume that the second derivative of the coupling is very small compared to the other terms in the Langevin equation 4.14, i.e.

$$F''[\dot{Q}] \sim 0. \tag{4.42}$$

This simplifies the generalized Langevin equation (4.14) considerably,

$$\begin{aligned} M\ddot{Q}+V'[Q] + 2\int_0^t dt' \int_0^\infty \frac{d\omega}{\pi}\omega\tilde{J}(\omega)\cos\left[\omega(t-t')\right] F'[\dot{Q}(t)]F[\dot{Q}(t')] \\ \approx -\zeta^{(0)}(\dot{Q}(t);t) + 2\int_0^\infty \frac{d\omega}{\pi}\frac{\tilde{J}(\omega)}{\omega}F'[\dot{Q}(t)]^2\ddot{Q}(t). \end{aligned} \tag{4.43}$$

Note that Eq. 4.42 does not necessarily imply that we must choose the linear-velocity case of the previous section, for which it is trivially satisfied. This is where we establish a connection with Lévy flights in ultracold atoms such as we described in Section 2.4. To this end we intend to reproduce Marksteiner, Ellinger and Zoller's friction force that we saw in Section 2.4:[33]

$$\frac{\dot{Q}}{1+\left(\frac{\dot{Q}}{v_0}\right)^2} \tag{4.44}$$

where $v_0$ is a proportionality constant that contains the mass of the Brownian particle

[33] We do not have to be careful in equating physical momentum and mass×velocity.

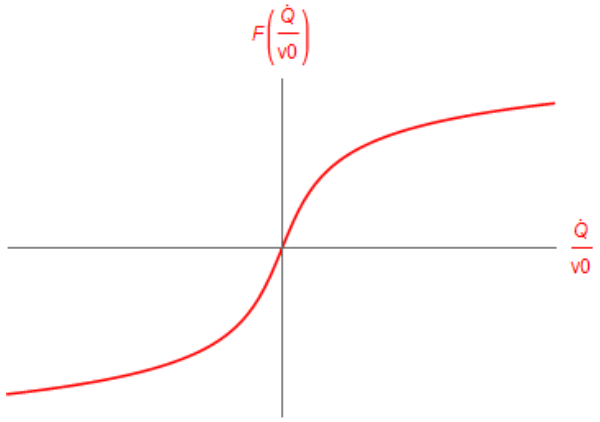


Figure 12: The coupling function of Eq. (4.44).

and the specifics of the physical set-up, e.g. the experimental properties of the laser during Sisyphus cooling. It turns out that we can choose

$$F[\dot{Q}] = \operatorname{sgn}\left(\frac{\dot{Q}}{v_0}\right) v_0 \sqrt{\log\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]}, \tag{4.45}$$

where the sgn-function is defined as

$$\operatorname{sgn}(x) = \begin{cases} -1 & \text{if } x < 0 \\ 0 & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases} \tag{4.46}$$

and is put in to ensure both a smooth transition of the first derivative at $\dot{Q} = 0$ and a unique value for $F[\dot{Q}]$ for every value of $\dot{Q}$. See Figure 12 for a sketch of the coupling 4.45.

To see the connection to the force 4.44, we must calculate the derivative of this coupling term. It is

$$F'[\dot{Q}] = \operatorname{sgn}\left(\frac{\dot{Q}}{v_0}\right) v_0 \frac{\dot{Q}}{\sqrt{\log\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]}\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]} = \frac{\dot{Q}}{F[\dot{Q}]\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]} \tag{4.47}$$

We then obtain for the force term in the Langevin equation (4.43)

$$F[\dot{Q}]F'[\dot{Q}] = \frac{\dot{Q}}{1+\left(\frac{\dot{Q}}{v_0}\right)^2}, \tag{4.48}$$

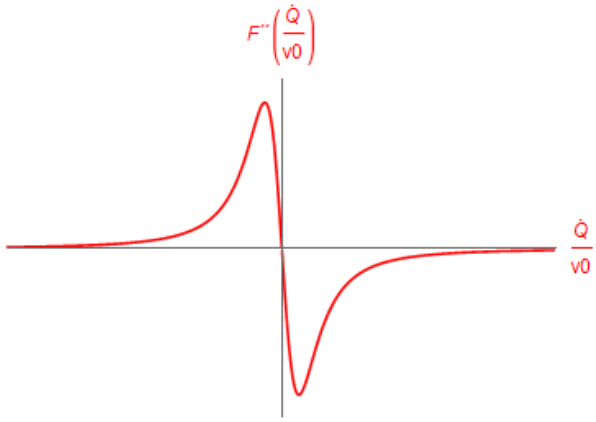


Figure 13: The second derivative of the coupling function as given in Eq. (4.49). One observes that for both limits, the low-velocity limit $\dot{Q} \to 0$ and the high-velocity limit $\dot{Q} \to \infty$, this vanishes. Hence, the approximation in Eq. (4.42) is justified.

which coincides with Eq. (4.44).

Of course, we must justify that our approximation Eq. (4.42) is correct. The second derivative of Eq. (4.45) is

$$F''[\dot{Q}] = \operatorname{sgn}\left(\frac{\dot{Q}}{v_0}\right)\frac{1}{v_0}\frac{1}{\left[1+(\frac{\dot{Q}}{v_0})^2\right]\sqrt{\log\left[1+(\frac{\dot{Q}}{v_0})^2\right]}}\left\{-\frac{\dot{Q}^2}{v_0\left[1+(\frac{\dot{Q}}{v_0})^2\right]\log\left[1+(\frac{\dot{Q}}{v_0})^2\right]}-\frac{2\dot{Q}^2}{\left[1+(\frac{\dot{Q}}{v_0})^2\right]}+1\right\} \tag{4.49}$$

In the low-velocity limit, $\dot{Q} \ll v_0$, this becomes

$$F''[\dot{Q}] \approx -\operatorname{sgn}\left(\frac{\dot{Q}}{v_0}\right)\frac{3}{2}\frac{\dot{Q}}{v_0^2} \tag{4.50}$$

to leading order in $\dot{Q}/v_0$. In the high-velocity limit, $\dot{Q} \gg v_0$, we have

$$F''[\dot{Q}] \approx -\operatorname{sgn}\left(\frac{\dot{Q}}{v_0}\right)\frac{\left[1+2\log(\frac{\dot{Q}}{v_0})\right]}{2\sqrt{2}\left[\log(\frac{\dot{Q}}{v_0})\right]^{3/2}}\frac{v_0}{\dot{Q}^2}. \tag{4.51}$$

to leading order in $v_0/\dot{Q}$. Thus, in both the low-velocity limit and the high-velocity limit our approximation (4.42) holds. This is also easily seen in the sketch of the second derivative in Figure 13.

The generalized Langevin equation (4.43) becomes

$$\begin{aligned} M\ddot{Q}+V'[Q]+2\int_0^t dt'\int_0^\infty \frac{d\omega}{\pi}\tilde{J}(\omega)\omega\cos\left[\omega(t-t')\right]\frac{\dot{Q}(t')}{1+\left(\frac{\dot{Q}(t')}{v_0}\right)^2} \\ \approx -\zeta^{(0)}(\dot{Q}(t);t)+2v_0^2\int_0^\infty \frac{d\omega}{\pi}\frac{\tilde{J}(\omega)}{\omega}\frac{\dot{Q}(t)^2}{\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]^2\sqrt{\log\left[1+\left(\frac{\dot{Q}(t)}{v_0}\right)^2\right]}}\ddot{Q}(t). \end{aligned} \tag{4.52}$$

Assuming $\tilde{J}(\omega)=\lambda\omega$, one has,

$$\begin{aligned} M\ddot{Q}+V'[Q]+2\lambda\int_0^t dt'\int_0^\Omega \frac{d\omega}{\pi}\omega^2\cos\left[\omega(t-t')\right]\frac{\dot{Q}(t')}{1+\left(\frac{\dot{Q}(t')}{v_0}\right)^2} \\ \approx -\lambda v_0\frac{\dot{Q}}{\sqrt{\log\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]}\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]}\dot{f}^{(0)}((t);t)+\frac{2v_0^2\Omega}{\pi}\frac{\dot{Q}(t)^2}{\left[1+\left(\frac{\dot{Q}}{v_0}\right)^2\right]^2\sqrt{\log\left[1+\left(\frac{\dot{Q}(t)}{v_0}\right)^2\right]}}\ddot{Q}(t). \end{aligned} \tag{4.53}$$

Like we have seen before, we can now perform two partial integrations in $t'$ in order to perform the frequency integral. Among the many terms that will be generated as such will be the jerk-terms $\dddot{Q}$ and $\ddot{Q}^2$-terms, as we have seen in Eq. (4.14) as well.

In the low-velocity limit the coupling Eq. (4.45) reduces to

$$F[\dot{Q}]\approx \operatorname{sgn}\left(\frac{\dot{Q}}{v_0}\right)v_0\sqrt{\left(\frac{\dot{Q}}{v_0}\right)^2}=\operatorname{sgn}\left(\frac{\dot{Q}}{v_0}\right)|\dot{Q}|=\dot{Q}. \tag{4.54}$$

Thus, in the low-velocity limit, this coincides with the self-interaction equation (4.34) we found in Section 4.2.2.

We have also seen that the approximation Eq. (4.42) holds in both limits. Nevertheless, for more moderate velocities, we are not that safe. There, $F''$ cannot be neglected. Therefore, it will be important to search for a cross-over behavior between the high-velocity Lévy dynamics and the linear-velocity limit.

As a final remark, it seems to us that the fluctuation-dissipation theorem in the high-velocity Lévy limit breaks down. Nevertheless, this is to be expected, since for superdiffusive behavior the central-limit theorem is broken—as we indicated in Section 2.4. An insightful paper by Costa, Morgado, Lima and Oliviera, shows where exactly the theorem fails for 'fast' superdiffusion [12].

## 4.3 Conclusion

In this chapter, we modified the original Caldeira-Leggett model as it was build up in Chapter 3. The change is in the interaction between the system and the bath; whereas before their coupling was of the coordinate-coordinate type, we choose a coupling general in the velocity of the system to the coordinates of the bath particles. The counterterm was adjusted accordingly. Employing the knowledge of the Caldeira-Leggett model of the previous chapter, such as using the spectral density, absorbing the spurious drift terms, and using the equipartition theorem in the classical limit, we were able to derive the *modified* generalized Langevin equation (4.14). Nevertheless, due to terms generated by the time derivative of the Euler-Lagrange equations, the result is much more involved than the original generalized Langevin equation (3.53). Most prominently, the extra terms are due to the existence of the second derivative of the coupling function $F''[\dot{Q}]$. The system has velocity-dependent multiplicative noise, as well as memory, for all choices of the spectral density. A numerical investigation of Eq. (4.14) is left for the Outlook.

Under the approximation $F''[\dot{Q}] \sim 0$, we find a much more tractable modified Langevin equation. Two realizations of the coupling were worked out. First, for the linear-velocity case, the approximation holds trivially, and we derive the equation of motion Eq. (4.32). Without assuming any fundamental physical picture, this equation bears exact resemblance–at least in form–to the Abraham-Lorentz equation of an electron interacting with its own radiation field. In addition, because of the counterterm in our model, we do not find a mass renormalization. Making the analogy with the work of Caldeira and Barone, who assumed a fundamental electrodynamical Lagrangian to derive the Abraham-Lorentz equation. Having expressed their results in terms of fundamental constants, they are able to estimate how large the cut-off-dependent terms in their equation of motion are. For fundamental models, we suggest a similar approach to deal with the cut-off dependent terms.

The second coupling we looked at as aimed at deriving a force Eq. (2.61) from the work of Marksteiner, Ellinger and Zoller, which gives rise to Lévy flights in Sisyphus cooling, as explained in Section 2.4. It turns out that the choice Eq. (4.45) gives exactly this expression. This was the original motivation of modifying the Caldeira-Leggett model to velocity-dependent coupling forces in the first place. In the low-velocity limit, this model reduces to the linear-velocity model and hence returns the Abraham-Lorentz equation. We have also shown that the approximation $F'' \sim 0$ holds in the low- and high-velocity limits. However, further research should be undertaken to interpolate in between these extremes, where the approximation fails and memory effects start playing a larger role. This will involve a numerical investigation, which we will leave to the Outlook.

Furthermore, the choice for the spectral density throughout this chapter has been to assume it to be linear in the frequency. However, one must stay vigilant to the ambiguous term 'ohmic bath' in this case, since the spectral density is determined by the coupling

constants and these coupling constants physically differ for every different choice of $F[\dot{Q}]$. In our case, we found, through Eq. (4.33), that the spectral density in terms of the $\bar{C}_k$ constants $\bar{J} \propto \omega$ corresponds to a cubically superohmic $J \propto \omega^3$ in terms of the original spring constants $C_k$.

# 5 Extending the quantum model

> I was inspired by the remarks in these books [of Heitler and Dirac]; not by the parts in which everything was proved and demonstrated carefully and calculated, because I couldn't understand those very well. At the young age what I could understand were the remarks about the fact that this doesn't make any sense, and the last sentence of the book of Dirac I can still remember, "it seems that some essentially new physical ideas are here needed." So, I had this as a challenge and an inspiration. I also had a personal feeling, that since they didn't get a satisfactory answer to the problem I wanted to solve, I don't have to pay a lot of attention to what they did do.
>
> —Richard P. Feynman, *Nobel Lecture* [22]

## 5.1 Feynman-Dirac quantization: the sum over all paths

The goal of this chapter is to construct a quantum version of the extended Caldeira-Leggett Lagrangian in terms of the general velocity coupling that we have used in the previous chapter. We will use the path-integral to calculate the propagator for the Lagrangian (4.1). From there, we go to the Euclidean version of the density operator. Since we are only interested in the particle of interest, we use the reduced density matrix strategy, by integrating out the bath particles from the full density matrix, leaving us with an effective dynamics for the system of interest only.

This calculation is a long and tedious one. Instead of starting from the most difficult path integral, we will work towards the path integral of the Lagrangian (4.1) for the general-velocity coupling by solving the forced harmonic oscillator problem separately. Hence, we will start by setting up the path-integral formulation and the evaluation of the free particle in Section 5.1.1 and derive the result for the driven harmonic oscillator in Section 5.1.2. In Section 5.1.3, we will employ the Wick-rotated functional-integral method to evaluate the path integral for our modified Caldeira-Leggett Lagrangian in terms of the general-velocity coupling. This procedure is analogous to the path integral of the original Caldeira-Legget model, such that we will not repeat much of the same steps by deriving the original quantum model explicitly, but we will point out differences in the derivation along the way. With our result for the general-velocity coupling Larangian, we will obtain an effective action by tracing out the harmonic oscillator degrees of freedom of the bath, as we will see in Section 5.2. This effective action can be seen as one of the original contributions of this thesis.

It turns out that we do not have to assume restictions for the general-velocity coupling all the way through path-integral quantization, leaving us with a equally general quantum model. From the effective action obtained in this way, we can investigate particular couplings from the general result, as we will do in Section 5.3; we will confine our scope to discussing the physical interpretations of three specific couplings: the coordinate-coordinate coupling of the original Caldeira-Leggett model, to compare our

results with; the linear-velocity case, which gave us the Abraham-Lorentz equation in Section 4.2.2; and the coupling of Eq. (4.45), which gave rise to a force responsible for Lévy flights in Sisyphus cooling in Section 4.2.3.

### 5.1.1 The free particle

For completeness, we will first formulate the path-integral representation of quantum mechanics.[34] Starting from the Hamiltonian representation, we can derive the path integral from Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \hat{\mathcal{H}}\left|\Psi(t)\right\rangle, \tag{5.1}$$

for a quantum state $|\Psi\rangle$ and Hamiltonian $\mathcal{H}$, with solutions[35]

$$\left|\Psi(t)\right\rangle = \exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}t\right)\left|\Psi(0)\right\rangle. \tag{5.3}$$

Using the completeness relation, we insert a complete set of basis states of position $x'$, this reads

$$\left\langle x \,|\, \Psi(t)\right\rangle = \int_{-\infty}^{\infty} dx' \left\langle x\right| \exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}t\right)\left|x'\right\rangle \left\langle x' \,|\, \Psi(0)\right\rangle, \tag{5.4}$$

which is equivalent to writing (suppressing the boundaries of the integral for brevity)

$$\Psi(x,t) = \int dx' K(x,t;x',0)\Psi(x',0), \tag{5.5}$$

with

$$K(x,t;x',0) = \left\langle x\right| \exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}t\right)\left|x'\right\rangle. \tag{5.6}$$

This is the so-called 'kernel', or 'propagator'; it encodes the dynamics of the quantum system. It can be interpreted as evolving the state at position $x'$ and time $t = 0$ to another state at position $x$ and time $t$.

The idea now, is to break up the time-evolution from the initial state $|\Psi(0)\rangle$ to the

[34] The following derivation is partly based on [68, pp. 109–123], [36] and [11].

[35] We restrict ourselves to Hamiltonians with no explicit time-dependence. If the Hamiltonian would be varying in time, the formal time-ordered solution to Eq. (5.1) reads

$$\left|\Psi(t)\right\rangle = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_0^t dt'\hat{\mathcal{H}}(t')\right)\left|\Psi(0)\right\rangle, \tag{5.2}$$

for the time-ordering operator $\mathcal{T}$, which has to be included, since the Hamiltonian does not commute with itself at different times.

final state $|\Psi(t)\rangle$ into discrete steps. First, if we envision an auxiliary time $0 < t_1 < t$, Eq. (5.3) becomes

$$|\Psi(t)\rangle = \exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}(t-t_1)\right)\exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}t_1\right)|\Psi(0)\rangle\,, \tag{5.7}$$

which, in the spacetime coordinate representation, is equivalent to

$$\Psi(x,t) = \int dx' \int dx'' K(x,t;x'',t_1)K(x'',t_1;x',0)\Psi(x',0). \tag{5.8}$$

This shows the semigroup property [36, p. 4] of kernels:

$$K(x,t;x',t') = \int dx'' K(x,t;x'',t'')K(x'',t'';x',t'). \tag{5.9}$$

If we now extend this property to decompose the evolution into $N$ time intervals $\Delta t = t/N$, we can write for a very general Hamiltonian with kinetic part $\hat{T}$ and potential $\hat{V}$ that

$$\exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}t\right) = \left[\exp\left(-\frac{i}{\hbar}(\hat{T}+\hat{V})\Delta t\right)\right]^N. \tag{5.10}$$

Now, using the Baker-Hausdorff approximation formula, this becomes

$$\left[\exp\left(-\frac{i}{\hbar}\hat{T}\Delta t\right)\exp\left(-\frac{i}{\hbar}\hat{V}\Delta t\right) + \frac{\left[\hat{T},\hat{V}\right]}{\hbar^2}(\Delta t)^2\right]^N. \tag{5.11}$$

In the continuum limit $\Delta t \to 0$, or, equivalently, $N \to \infty$, we obtain the exact relation

$$\exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}t\right) = \lim_{N\to\infty}\left[\hat{U}(\Delta t)\right]^N, \tag{5.12}$$

for the evolution operator

$$\hat{U}(\Delta t) = \exp\left(-\frac{i}{\hbar}\hat{T}\Delta t\right)\exp\left(-\frac{i}{\hbar}\hat{V}\Delta t\right). \tag{5.13}$$

This allows us to write the kernel, using the semi-group property (5.9) for $N$ discrete steps in time, as

$$K(x_N,t;x_0,0) = \lim_{N\to\infty}\left(\prod_{k=1}^{N-1}\int_{-\infty}^{\infty} dx_k\right)\langle x_{k+1}|\exp\left(-\frac{i}{\hbar}\hat{T}\Delta t\right)|x_k\rangle\exp\left(-\frac{i}{\hbar}V(x_k)\Delta t\right) \tag{5.14}$$

where we have renamed the initial and final coordinates $x_0$ and $x_N$ so that we can

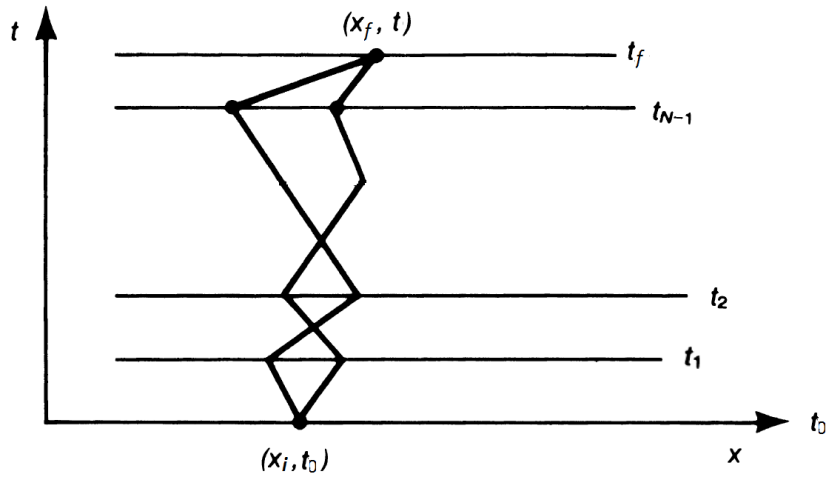


Figure 14: A depiction of multiple paths through spacetime from initial position $x_i$ at time $t_0$ to a final position $x_f$ at time $t$ in $N$ steps of discretized time. This is possible due to the semigroup property of Eq. (5.9). Picture (modified) extracted from [68, p. 117].

include them into the sum. See Figure 14 for a depiction of this procedure. The potential has been taken out of the expectation value as it is diagonal in the coordinate $x_j$.

For future reference (to simplify the calculation for the kernel of the harmonic oscillator), we need the propagator for the *free particle*,

$$\mathcal{H}_{\mathrm{FP}} = \frac{\hat{p}^2}{2m}, \tag{5.15}$$

with momentum eigenstates (with a continuous spectrum for eigenvalues $p$),

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{i}{\hbar} xp\right). \tag{5.16}$$

We can use this to evaluate the propagator, which contains all the information about the eigenstates $\{|\psi_n\rangle\}$ and eigenenergies $E_n$, where $n$ counts the energy levels. Using the completeness of a general set of eigenstates, Eq. (5.6) becomes

$$K(x,t;x',0) = \sum_n \exp\left(-\frac{i}{\hbar} E_n t\right) \psi_n(x)\psi_n^*(x'). \tag{5.17}$$

In the case of the free particle,

$$K(x,t;x',0) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp \exp\left[-\frac{i}{\hbar}\left(\frac{p^2}{2m}t + (x-x')p\right)\right], \tag{5.18}$$

which, performing the Gaussian integral,[36] becomes

$$K(x,t;x',0) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(\frac{im(x-x')^2}{2\hbar t}\right), \tag{5.20}$$

which is the result for the free particle propagator.

Returning to Eq. (5.14) for general potential $\hat{V}$, and comparing to the case of the free particle, we can write for one matrix element

$$\langle x_{k+1}| \exp\left(-\frac{i}{\hbar}\hat{T}\Delta t\right) |x_k\rangle \exp\left(-\frac{i}{\hbar}V(x_k)\Delta t\right) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \exp\left[-\frac{i}{\hbar}\left(\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 - V(x_k)\right)\Delta t\right] \tag{5.21}$$

This results in the expression for the kernel

$$K(x_N,t;x_0,0) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \lim_{N\to\infty} \left(\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} \sqrt{\frac{m}{2\pi i\hbar\Delta t}} dx_k\right) \exp\left[-\frac{i}{\hbar}\sum_{k=0}^{N-1}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 - V(x_k)\Delta t\right]. \tag{5.22}$$

Eq. (5.22) is nothing else but a discretized version of the action,

$$S[x] = \int_0^t ds\mathcal{L}(s) = \int_0^t ds\left(\frac{1}{2}m\dot{x}^2 - V(x)\right), \tag{5.23}$$

and, hence, for initial coordinate $x_0 = x_i$ and final coordinate $x_N = x_f$, the kernel can be written as

$$K(x_f,t;x_i,0) = \int_{x_i}^{x_f} \mathcal{D}x \exp\left(\frac{i}{\hbar}S[x]\right), \tag{5.24}$$

where $\mathcal{D}x$ represents all possible paths $x(t)$ satisfying the boundary conditions.

Eq. 5.24 is the central objects in the so-called spacetime-approach to quantum mechan-

[36] In principle, we have to address the issue that the exponential is complex valued. Technically, then, the evaluation of the Gaussian integral should then be written as

$$\int_{-\infty}^{\infty} dx \exp\left(-i\alpha x^2\right) = \sqrt{\frac{\pi}{i\alpha}} = \sqrt{\frac{\pi}{\alpha}} \exp\left(-\frac{i\pi}{4}\right). \tag{5.19}$$

However, we will ignore this issue, and leave the factor $i$ in the coefficients.

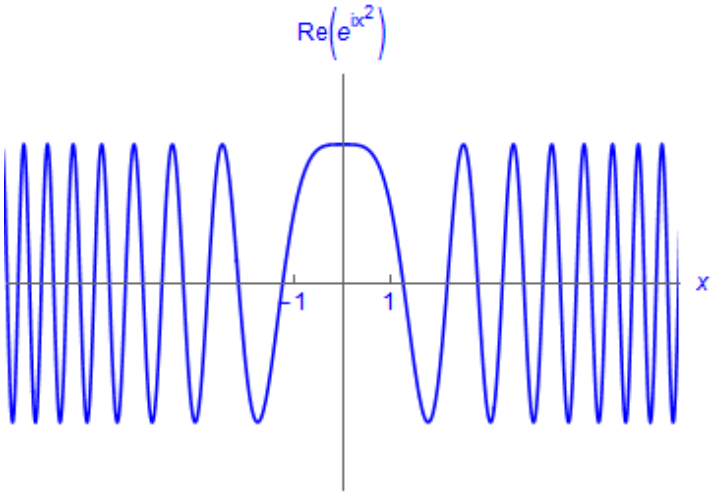


Figure 15: Perturbation theory around the classical path (here the extremum lies at $(x = 0)$ is justified, since the leading order of the action in the kernel (5.24) is quadratic. Hence, higher terms–the quantum fluctuations–will contribute less.

ics, as first formulated by Paul Dirac [14] and interpreted by Richard Feynman [18]. The interpretation is that a quantum state traverses each path satisfying the boundary conditions $x_i$ and $x_f$ through space with a weight $\exp(iS[x]/\hbar)$ corresponding to that path. Alternatively, this weight can be interpreted as the probability of finding the state traversing the corresponding path [21].

The classical path has the largest probability weight, since the action is minimal when it is evaluated for the classical path. If the potential is not quadratic in the position coordinate, exact results cannot be obtained. Quantum deviations from the classical action can then perturbatively found via the stationary phase approximation. The use of perturbation theory is justified, since the quantum fluctuations will always be small compared to the classical path, because the action is always quadratic to leading order—the linear terms vanish due to the equations of motion. Hence, the largest contribution to the kernel is Gaussian, and the largest contributions to the path integral come from the region where the coordinate is small—as depicted in Figure 15, where the real part of the complex Gaussian is plotted.

### 5.1.2 The driven harmonic oscillator

To expand on the merit of the path-integral method, let us calculate the result for the driven harmonic oscillator. This result will be necessary to successfully apply to functional-integral method of the next section. The Lagrangian is

$$\mathcal{L} = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 + xf(t), \tag{5.25}$$

for the force $f(t)$, which couples linearly to the coordinate and may be interpreted as an external field or an internal influence of the system on itself. The equation of motion is

$$m\ddot{x} + m\omega^2 x = f(t). \tag{5.26}$$

To calculate the propagator (5.24) for the driven harmonic oscillator, we have to calculate the action

$$\mathcal{S} = \int_0^t \left[\frac{1}{2}m\dot{x}^2(s) - \frac{1}{2}m\omega^2 x^2(s) + x(s)f(s)\right], \tag{5.27}$$

for every possible path between $x_i$ at $s = 0$ to $x_f$ at $s = t$. We now decompose the path into a classical path $x_{cl}$, corresponding to the extremal value of (5.27), and the quantum fluctuations $\xi(s)$ around this path

$$x(s) = x_{cl}(s) + \xi(s), \tag{5.28}$$

satisfying the boundary conditions

$$x_{cl}(0) = x_i, \qquad x_{cl}(t) = x_f, \tag{5.29}$$

$$\xi(0) = 0, \qquad \xi(t) = 0. \tag{5.30}$$

The action is decomposed accordingly,

$$\begin{aligned} S = &\int_0^t ds \left[\frac{1}{2}m\dot{x}_{cl}^2(s) - \frac{1}{2}m\omega^2 x_{cl}^2(s) + x_{cl}(s)f(s)\right] + \int_0^t ds \left[\frac{1}{2}m\dot{\xi}^2(s) - \frac{1}{2}m\omega^2\xi^2(s)\right] \\ &+ \int_0^t ds \left[\frac{1}{2}m\dot{x_{cl}}(s)\dot{\xi}(s) - \frac{1}{2}m\omega^2 x_{cl}(s)\xi(s) + \xi(s)f(s)\right]. \end{aligned} \tag{5.31}$$

The third part of this decomposition vanishes due to the equations of motion, which can be easily seen by partial integration

$$\int_0^t ds \left[m\dot{x}_{cl}\dot{\xi} - m\omega^2 x_{cl}\xi + \xi f(s)\right] = -\int_0^t ds \left[m\ddot{x}_{cl} + m\omega^2 x_{cl} - f(s)\right]\xi = 0, \tag{5.32}$$

due to Eq. (5.26). The second part is independent of the boundary values of the classical path and therefore encodes the entire quantum-mechanical contribution, while the first part is purely classical. We will focus on the classical part of the action first.

We have seen the solution to Eq. (5.26) before, as it is the same as the bath equation of motion (3.46) with solution (3.47), for $f(t) = \sum_k C_k F[Q]$. It was calculated in

Appendix C, with the general solution given in Eq. (C.25). The classical path, then, satisfying boundary conditions (5.29) is

$$x_{cl}(s) = x_f \frac{\sin(\omega s)}{\sin(\omega t)} + x_i \frac{\sin[\omega(t-s)]}{\sin(\omega t)} + \int_0^s du \frac{\sin[\omega(s-u)]}{m\omega} f(u) - \frac{\sin(\omega s)}{\sin(\omega t)} \int_0^t du \frac{\sin[\omega(t-u)]}{m\omega} f(u). \tag{5.33}$$

The classical action $S_{cl}$ can be calculated by plugging in the solution of the classical equation of motion Eq. (5.33) into the action and evaluating the integral over the auxiliary time $s$ explicitly. The calculation for the classical action can be found in Appendix D; the result is

$$\begin{aligned} S_{cl} = & \frac{m\omega}{2\sin(\omega t)} \left[ (x_i^2 + x_f^2)\cos(\omega t) - 2x_i x_f \right] \\ & + \frac{x_f}{\sin(\omega t)} \int_0^t ds \sin(\omega s) f(s) + \frac{x_i}{\sin(\omega t)} \int_0^t \sin[\omega(t-s)] f(s) \\ & - \frac{1}{m\omega \sin(\omega t)} \int_0^t dt \int_0^s du \sin(\omega u) \sin[\omega(t-s)] f(s) f(u). \end{aligned} \tag{5.34}$$

Now, we turn to the quantum fluctuations. After partial integration, the second term in Eq. (5.31) is

$$S_q = -\frac{1}{2} m \int_0^t ds \left[ \xi(s) \left( \frac{d^2}{ds^2} - \omega^2 \right) \xi(s) \right]. \tag{5.35}$$

We then expand the quantum path in terms of the orthogonal[37] eigenfunctions of the operator between brackets in Eq. (5.35),

$$\xi(s) = \sum_{n=1}^{\infty} a_n \xi_n(s), \tag{5.36}$$

with fixed endpoints $\xi_n(0) = \xi_n(t) = 0$. Solving, for eigenvalues $\alpha_n$, the equation $d^2/ds^2 + \omega^2 \xi_n = \alpha_n \xi_n$ gives eigenfunctions

$$\xi_n(s) = \sqrt{\frac{2}{t}} \sin\left(\frac{\pi n s}{t}\right) \tag{5.37}$$

and

$$\alpha_n = -\left(\frac{\pi n}{t}\right)^2 + \omega^2. \tag{5.38}$$

[37] The eigenfunctions form an orthogonal basis, since the operator $d^2/ds^2 + \omega^2$ is selfadjoint.

The quantum action becomes

$$S_q = \frac{1}{2}m\sum_n \left(\left(\frac{\pi n}{t}\right)^2 - \omega^2\right) a_n^2. \tag{5.39}$$

After the expansion Eq. (5.36), the kernel (5.24) becomes

$$K(x_f,t;x_i,0) = \mathcal{J}\exp\left(\frac{i}{\hbar}S_{cl}\right)\prod_{n=1}^{\infty}\int_{-\infty}^{\infty} da_n \exp\left[\frac{im}{2\hbar}\left(\frac{\pi n^2}{t} - \omega^2\right)a_n^2\right], \tag{5.40}$$

where $\mathcal{J}$ is the Jacobian for transformation (5.36). We can find the Jacobian explicitly, but, following the shortcut of Feynman & Hibbs [21], we can also compare with the result for the free particle by looking at the limit $\omega \to 0$, since the Jacobian itself is independent of $\omega$. Performing the Gaussian integral, keeping track of the $\omega$-dependence,

$$K(x_f,t;x_i,0) \propto \prod_{n=1}^{\infty}\left(1 - \frac{\omega^2 t^2}{\pi^2 n^2}\right)^{-1/2}\exp\left(\frac{i}{\hbar}S_{cl}\right) = \sqrt{\frac{\omega t}{\sin(\omega t)}}\exp\left(\frac{i}{\hbar}S_{cl}\right), \tag{5.41}$$

where only the proportionality with respect to $\omega$ has been taken into account. Now, for $\omega = 0$ the kernel should coincide with that of the free particle, in Eq. (5.20). Putting in the right prefactors, the result is

$$K(x_f,t;x_i,0) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega t)}}\exp\left(\frac{i}{\hbar}S_{cl}\right) \tag{5.42}$$

with the classical action given by Eq. (5.34). For $\omega \to 0$, this indeed gives Eq. (5.20).

### 5.1.3 Imaginary-time path integral: equilibrium reduced density matrix

It is possible to equate the equilibrium density matrix to the propagator (5.24) in imaginary time. The density matrix for a system at temperature $T = k_B/\beta$ is

$$\hat{\rho}(x,x') = \frac{1}{Z}\langle x|\exp\left(-\beta\hat{\mathcal{H}}\right)|x'\rangle, \tag{5.43}$$

for the partition function

$$Z = \langle x|\exp\left(-\beta\hat{\mathcal{H}}\right)|x\rangle \tag{5.44}$$

Comparing to the propagator in Eq. (5.6), we see that for $t = -i\hbar\beta$ they coincide—aside from the normalization factor. This is called the Wick rotation and we can express all our ingredients in terms of imaginary time. A general action, for example, after we

replace the auxiliary time $s$ by $-i\sigma$, reads

$$S^{\mathrm{E}}[x] = \int_0^{\hbar\beta} d\sigma \left[\frac{1}{2}m\left(\frac{dx}{d\sigma}\right)^2 + V(x)\right], \tag{5.45}$$

the so-called Euclidean action.[38]

We now recognize that the equilibrium density matrix, can be expressed as

$$\hat{\rho}(x,x') = \langle x|\exp\left(-\beta\hat{\mathcal{H}}\right)|x'\rangle = \frac{1}{Z}\int_{\bar{x}(0)=x'}^{\bar{x}(\hbar\beta)=x} \mathcal{D}\bar{x}(\sigma)\exp\left(-\frac{1}{\hbar}S^{\mathrm{E}}[\bar{x}(\sigma)]\right). \tag{5.46}$$

We now want to write the full density matrix of a composite model of system of interest and and bath, such as we have seen throughout Chapters 3 & 4. Schematically, we have split such Lagrangians into parts of the system $S$, the environment (or bath) $B$, their interaction $I$ and a counterterm $C.T.$, such that

$$\mathcal{L} = \mathcal{L}_S(Q) + \mathcal{L}_B(q_k) + \mathcal{L}_I(Q,q_k) + \mathcal{L}_{C.T.}(Q), \tag{5.47}$$

for system variable $Q$ and environmental degrees of freedom $q_k$, for $k \in \{1,2,...,N\}$. The density matrix for such a system, according to Eq. (5.46), reads

$$\hat{\rho}(Q,q_i,Q',q_i') = \frac{1}{Z}\int_{Q'}^{Q}\mathcal{D}\bar{Q}(\tau)\left(\prod_{k=1}^{N}\int_{q_k'}^{q_k}\mathcal{D}\bar{q_k}(\tau)\right)\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\mathcal{L}^{\mathrm{E}}(\bar{Q}(\tau),\bar{q}_i(\tau))\right], \tag{5.48}$$

where $\tau =$ is an auxiliary Euclidean time variable. The boundaries of the path integrals run from $\bar{Q}(0) = Q'$ to $\bar{Q}(\hbar\beta) = Q$ and $\bar{q_k}(0) = q_k'$ to $\bar{q_k}(\hbar\beta) = q_k$. Hence, variables with 'bars' denote possible variables of the boundary conditions.

For most practical purposes, we are uninterested in the environmental degrees of freedom, or, at least, wholly ignorant about it. Therefore, we perform the trace over the variable $q_i$, i.e. we integrate over all possible initial conditions of the bath particles, leaving us with the *reduced density matrix* $\hat{\rho}_R$. Mathematically,

$$\hat{\rho}_R(Q,Q') = \frac{1}{Z}\int_{Q'}^{Q}\mathcal{D}\bar{Q}(\tau)\left(\prod_{k=1}^{N}\int_{-\infty}^{\infty}dq_k(\tau)\right)\left(\prod_{k=1}^{N}\oint\mathcal{D}\bar{q_k}(\tau)\right)\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\mathcal{L}^{\mathrm{E}}(\bar{Q}(\tau),\bar{q}_i(\tau))\right], \tag{5.49}$$

where the environmental path integral is only over closed paths, since the trace only

[38] This offers some help for the physical interpretation of dynamics in imaginary time. Effectively, the Wick rotation simply inverts the potential, which offers some physical intuition.

picks out the diagonal elements of a matrix, i.e. only the closed paths for which $q_k := \bar{q}_k(0) = \bar{q}_k(\hbar\beta)$ contribute.

We will have to evaluate all these integrals separately. Let us first separate the $Q$-dependent parts of the Lagrangian from the $q_i$-dependent parts by using Eq. (5.47) and writing (dropping the argument $\tau$ for brevity)

$$\hat{\rho}_R(Q,Q') = \frac{1}{Z_{BI}} \int_{Q'}^{Q} \mathcal{D}\bar{Q}\mathcal{F}(\bar{Q}) \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left(\mathcal{L}_S^{\mathrm{E}}(\bar{Q}) + \mathcal{L}_{C.T}^{\mathrm{E}}(\bar{Q})\right)\right], \tag{5.50}$$

for the so-called influence functional

$$\mathcal{F}(\bar{Q}) = \prod_{k=1}^{N} \frac{\mathcal{F}_k(\bar{Q})}{Z_k}, \tag{5.51}$$

where

$$\mathcal{F}_k(\bar{Q}) = \int_{-\infty}^{\infty} dq_k \oint \mathcal{D}\bar{q}_k \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left(\mathcal{L}_B^{(k)}(\bar{q}_k) + \mathcal{L}_I^{(k)}(\bar{Q},\bar{q}_k)\right)\right], \tag{5.52}$$

which contains all contributions of the bath variables. The superscript $(k)$ indicates this is the Lagrangian *per* bath constituent, instead of the sum over all. $Z_{BI}$ is the partition function taking into account only the bath and interaction Lagrangians; $Z_k$ is the partition function of a single bath particle. Keeping track of these normalization factors, we see that we can relate it to the full partition function $Z$ as

$$Z = Z_{BI} \times \prod_{k=1}^{N} Z_k. \tag{5.53}$$

The influence functional (5.51), as the name might give away, describes the influence of the bath on the system of interest. First introduced first by Feynman and Vernon [19], it is possible to separate the $Q$-dependent part from the $q_i$-dependent part which is what makes the influence-functional method so successful.

For the time evolution of the composite system, we have assumed that, initially, the system and the environment are uncorrelated, i.e. their $t = 0$-density matrices factorize:

$$\hat{\rho}(Q, q_i; t=0) = \hat{\rho}_{S+C.T.}(Q; t=0) \times \hat{\rho}_B(q_i; t=0) \tag{5.54}$$

For more general initial conditions, see [28] for the free particle, [62] in the case of the damped harmonic oscillator, and [27] for a completely general approach.[39]

[39] The separability condition for the initial state of the composite system bears significant resemblance to Boltzmann's 'Stoßzahlansatz' in his 'derivation' of the second law of thermodynamics [72].

## 5.2 Obtaining the effective action for general-velocity coupling

In this section we will derive the propagator for the modified Caldeira-Leggett Lagrangian in terms of general-velocity coupling, using the functional-integral approach of the previous section. The goal is to write down the quantum version of the entire system, after which we extract only the information of the system of interest. Mathematically, this will entail evaluating the path integral and the regular integrals in Eq. (5.52). For the modified Caldeira-Leggett Lagrangian Eq. (4.1), we have the corresponding Euclidean expressions (replacing $t$ by $-i\hbar\beta$),[40]

$$S_0^E[Q] = \int_0^{\hbar\beta} d\tau \left( \frac{1}{2} M\dot{Q}^2 + V(Q) + \sum_{k=1}^{N} \frac{\tilde{C}_k^2}{2m_k\omega_k^2} F[\dot{Q}]^2 \right), \tag{5.55}$$

$$S_B^E[q_k] = \frac{1}{2} \int_0^{\hbar\beta} d\tau \sum_{k=1}^{N} m_k \left( \dot{q}_k^2 + \omega_k^2 q_k^2 \right), \tag{5.56}$$

$$S_I^E[q_k, Q] = \int_0^{\hbar\beta} d\tau \left( F[\dot{Q}] \sum_{k=1}^{N} \tilde{C}_k q_k \right), \tag{5.57}$$

where we have combined the action of the system with the counterterm and renamed it $S_0^{\mathrm{E}}$, since this only depends on the system of interest. The 'dots' denote derivatives with respect to imaginary time.

Now, we have to evaluate the influence functional per oscillator of Eq. (5.52),

$$\mathcal{F}_k(Q) = \int_{-\infty}^{\infty} dq_k \oint \mathcal{D}\bar{q}_k \exp\left[ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left( \frac{1}{2} m_k \left( \dot{q}_k^2 + \omega_k^2 q_k^2 \right) + F[\dot{Q}] \sum_{k=1}^{N} \tilde{C}_k q_k \right) \right]. \tag{5.58}$$

But this is precisely the path-integral calculation of the driven harmonic oscillator as we have seen in Section 5.1.2; the result was given by Eq. (5.42). We only have to replace $x$ by $q_k$, give the bath-parameters an index $k$, and replace the driving force $f(t)$ by our coupling function $\tilde{C}_k F[\dot{Q}(t)]$.

$$\mathcal{F}_k(Q) = \sqrt{\frac{m_k\omega_k}{2\pi i\hbar \sin(\omega_k t)}} \int_{-\infty}^{\infty} dq_k \exp\left( -\frac{1}{\hbar} S_{cl}^{(k)} \right) \tag{5.59}$$

The classical action was given in Eq. (5.34); for closed paths $q_k := q_i = q_f$, it simplifies

[40] From here on, we will drop the 'bars'.

to

$$S_{cl}^{(k)} = \frac{m_k\omega_k}{\sin(\omega_k t)} q_k^2 \left[\cos(\omega_k t) - 1\right] + \frac{\tilde{C}_k q_k}{\sin(\omega_k t)} \int_0^t ds \left(\sin(\omega_k s) + \sin[\omega_k(t-s)]\right) F[\dot{Q}(s)]$$
$$- \frac{\tilde{C}_k^2}{m_k\omega_k \sin(\omega_k t)} \int_0^t ds \int_0^s du \sin(\omega_k u) \sin[\omega_k(t-s)] F[\dot{Q}(s)] F[\dot{Q}(u)]. \tag{5.60}$$

In Euclidean time, we can make the replacements $\cos(\omega_k t) \to \cosh(\hbar\beta\omega_k)$; $\sin(\omega_k t) \to -i\sinh(\hbar\beta\omega_k)$; and, changing the auxiliary time variables and their boundaries (using Greek letters for imaginary times), the Euclidean classical action per oscillator reads

$$S_{cl}^{(k)\mathrm{E}} = \frac{m_k\omega_k}{\sinh(\omega_k t)} q_k^2 \left[\cosh(\hbar\beta\omega_k) - 1\right] + \frac{\tilde{C}_k q_k}{\sinh(\hbar\beta\omega_k)} \int_0^{\hbar\beta} d\tau \left(\sinh(\omega_k \tau) + \sinh[\omega_k(\hbar\beta - \tau)]\right) F[\dot{Q}(\tau)]$$
$$- \frac{\tilde{C}_k^2}{m_k\omega_k \sinh(\hbar\beta\omega_k)} \int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \sinh(\omega_k \sigma) \sinh[\omega_k(\hbar\beta - \tau)] F[\dot{Q}(\tau)] F[\dot{Q}(\sigma)]. \tag{5.61}$$

In order to perform the Gaussian integral in Eq. (5.59), we have to complete the square. This calculation is found in Appendix E. The result is

$$S_{cl}^{(k)\mathrm{E}} = \frac{m_k\omega_k}{\sinh(\omega_k t)} \left[\cosh(\hbar\beta\omega_k) - 1\right] \left[q_k - q_k^*\right]^2 - \frac{\tilde{C}_k^2}{2m_k\omega_k} \int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau - \sigma) F[\dot{Q}(\tau)] F[\dot{Q}(\sigma)], \tag{5.62}$$

for

$$\mathcal{G}_k(\tau) = \frac{\cosh\left[\omega_k\left(\frac{\hbar\beta}{2} - \tau\right)\right]}{\sinh\left(\frac{\hbar\beta\omega_k}{2}\right)}, \tag{5.63}$$

which has the important property of being periodic:

$$\mathcal{G}_k(\hbar\beta - \tau) = \mathcal{G}_k(\tau). \tag{5.64}$$

We can now do the Gaussian integral in the influence functional per bath constituent Eq. (5.59)–in Euclidean time–by making a constant shift $q_n \to q_n + q_n^*$, with unit

Jacobian,

$$\mathcal{F}_k(Q) = \sqrt{\frac{m_k\omega_k}{2\pi\hbar\sinh(\hbar\beta\omega_k)}}\int_{-\infty}^{\infty} dq_k \exp\Big\{-\frac{1}{\hbar}\frac{m_k\omega_k}{\sinh(\omega_k t)}\left[\cosh(\hbar\beta\omega_k)-1\right]q_k^2 + \frac{1}{\hbar}\frac{\tilde{C}_k^2}{2m_k\omega_k}\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau-\sigma)F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)]\Big\}. \tag{5.65}$$

Performing the integral,

$$\mathcal{F}_k(Q) = \frac{1}{\sqrt{2(1-\cosh(\hbar\beta\omega_k))}}\exp\left[\frac{1}{\hbar}\frac{\tilde{C}_k^2}{2m_k\omega_k}\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau-\sigma)F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)]\right]. \tag{5.66}$$

Now, using that $\sqrt{2(1-\cosh(\hbar\beta\omega_k))} = \sqrt{2(2\sinh^2(\hbar\beta\omega_k))} = 2\sinh^2(\hbar\beta\omega_k)$, which is precisely the inverse partition function for a single harmonic oscillator, as it should be. Hence,

$$\mathcal{F}_k(Q) = Z_k \exp\left[\frac{1}{\hbar}\frac{\tilde{C}_k^2}{2m_k\omega_k}\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau-\sigma)F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)]\right]. \tag{5.67}$$

The total influence integral is, then,

$$\mathcal{F}_k(Q) = \prod_{k=1}^{N}\frac{1}{Z_k} = \exp\left[\frac{1}{\hbar}\sum_{k=1}^{N}\frac{\tilde{C}_k^2}{2m_k\omega_k}\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau-\sigma)F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)]\right]. \tag{5.68}$$

The bath particles are now successfully integrated out. Their presence is seen through the double integral and the occurrence of the forces $F$. This term contains non-local interactions. That is to be expected, since the interactions that are mediated by the bath particles–here seen in the presence of the $F$-functions–are not explicit anymore, due to integrating out the bath coordinates. In other words, the dynamics of the bath is invisible, but its influence on the dynamics of the Brownian system of interest is not.

Using Eq. (2.32), we can write the reduced matrix,

$$\hat{\rho}_R(Q,Q') = \frac{1}{Z_{BI}} \int_{Q'}^{Q} \mathcal{D}Q \exp\left[-\frac{1}{\hbar}\left(S_0^E[Q] - \sum_{k=1}^{N} \frac{\tilde{C}_k^2}{2m_k\omega_k} \int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau-\sigma) F[\dot{Q}(\tau)] F[\dot{Q}(\sigma)]\right)\right], \tag{5.69}$$

where we recognize the effective action

$$S_{\text{eff}}^E = \int_0^{\hbar\beta} d\tau \left(\frac{1}{2}M\dot{Q}^2 + V(Q) - \sum_{k=1}^{N} \frac{\tilde{C}_k^2}{2m_k\omega_k^2} F[\dot{Q}]^2\right) + \sum_{k=1}^{N} \frac{\tilde{C}_k^2}{2m_k\omega_k} \int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau-\sigma) F[\dot{Q}(\tau)] F[\dot{Q}(\sigma)], \tag{5.70}$$

where we have written $S_0^E$ in terms of the system action and the counterterm action, again.

Let us focus on the last term, which is entirely induced by the bath. Following Feynman's lectures on statistical mechanics [23, p. 83] in the case of the linear coupling, we will define $F[\dot{Q}(\sigma)]$ to be a periodic function outside of the integral domain $0 \leq \sigma \leq \hbar\beta$ such that $F[\dot{Q}(\sigma + \hbar\beta) = F[\dot{Q}(\sigma)]$. Then, we take the boundaries to infinity $\int_0^{\hbar\beta} d\sigma \to \int_{-\infty}^{\infty} d\sigma$. Using the symmetry property (5.64), we can write for the bath-induced term

$$-\sum_{k=1}^{N} \frac{\tilde{C}_k^2}{2m_k\omega_k} \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \mathcal{G}_k(\tau-\sigma) F[\dot{Q}(\tau)] F[\dot{Q}(\sigma)]. \tag{5.71}$$

Since we work in the relaxation time approximation, we want to use only the dominant term of the function $\mathcal{G}_k$. For very long times $T = t_b - t_a \to \infty$, we write

$$\lim_{T\to\infty} \mathcal{G}_k(\tau-\sigma) = \lim_{T\to\infty} \frac{e^{\frac{T}{2}} e^{-\omega_k|\tau-\sigma|} + e^{-\frac{T}{2}} e^{\omega_k|\tau-\sigma|}}{e^{\frac{T}{2}} + e^{-\frac{T}{2}}} = e^{-\omega_k|\tau-\sigma|}, \tag{5.72}$$

where we have changed the dependence on the difference $\tau - \sigma$ to a dependence on the absolute difference $|\tau - \sigma|$, since this difference is always positive on the interval $0 \leq \sigma \leq \hbar\beta$ and this should not change when extending to an infinite domain.

The bath-induced term in the effective action becomes,

$$-\sum_{k=1}^{N} \frac{\tilde{C}_k^2}{2m_k\omega_k} \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma e^{-\omega_k|\tau-\sigma|} F[\dot{Q}(\tau)] F[\dot{Q}(\sigma)]. \tag{5.73}$$

Now, to separate local from non-local terms, we complete the square,

$$-\frac{1}{2}[F[\dot{Q}(\tau)] - F[\dot{Q}(\sigma)]]^2 = -\frac{1}{2}F^2[\dot{Q}](\tau) - \frac{1}{2}F^2[\dot{Q}](\sigma) + F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)], \tag{5.74}$$

such that the bath-induced term can be written as

$$\frac{1}{2}\sum_{k=1}^{N}\frac{\tilde{C}_k^2}{4m_k\omega_k}\int_0^{\hbar\beta}d\tau\int_{-\infty}^{\infty}d\sigma e^{-\omega_k|\tau-\sigma|}\left\{\Big[F[\dot{Q}(\tau)]-F[\dot{Q}(\sigma)]\Big]^2-\Big[F^2[\dot{Q}(\tau)]+F^2[\dot{Q}(\sigma)]\Big]\right\}. \tag{5.75}$$

Due to the periodic symmetry of the coupling functions and the exponential, by interchanging the integration variables of one of them, the last two terms simply add. Hence, the second part of Eq. (5.75) becomes

$$-\sum_{k=1}^{N}\frac{\tilde{C}_k^2}{4m_k\omega_k}\int_0^{\hbar\beta}d\tau\int_{-\infty}^{\infty}d\sigma e^{-\omega_k|\tau-\sigma|}F^2[\dot{Q}(\sigma)]. \tag{5.76}$$

To evaluate the integral over $\sigma$, we first split the domain into a part where $\sigma<\tau$ and a part where $\sigma>\tau$,

$$\int_{-\infty}^{\sigma}d\sigma e^{-\omega_k(\tau-\sigma)}F^2[\dot{Q}(\sigma)]+\int_{\sigma}^{\infty}d\sigma e^{+\omega_k(\tau-\sigma)}F^2[\dot{Q}(\sigma)]=\frac{2F^2[\dot{Q}(\sigma)]}{\omega_k}, \tag{5.77}$$

which exactly cancels the contribution from the counterterm, as can easily be seen by consulting Eq. (5.70). Hence, the only contribution from the bath-induced term we are left with is a purely non-local (it only depends on differences) term

$$S^E_{\text{non-local}}[Q(\tau)]=\frac{1}{2}\sum_{k=1}^{N}\frac{\tilde{C}_k^2}{4m_k\omega_k}\int_0^{\hbar\beta}d\tau\int_{-\infty}^{\infty}d\sigma e^{-\omega_k|\tau-\sigma|}\Big[F[\dot{Q}(\tau)]-F[\dot{Q}(\sigma)]\Big]^2. \tag{5.78}$$

We now use the (by now) familiar procedure of the spectral density of Eq. (3.24) to write the discrete sum over the oscillators $k$ into an continuous integral over frequency $\omega$. Remember, our coupling constants $\tilde{C}_k$ for the velocity-coupling do not coincide with the spring constants $C_k$. Specifically,

$$\sum_{k=1}^{N}\frac{\tilde{C}_k^2}{4m_k\omega_k}e^{-\omega_k|\tau-\sigma|}=\frac{1}{2\pi}\int_0^{\infty}\tilde{J}(\omega)e^{-\omega|\tau-\sigma|}, \tag{5.79}$$

such that the effective action (5.70) becomes

$$S^E_{\text{eff}}=\int_0^{\hbar\beta}d\tau\left(\frac{1}{2}M\dot{Q}^2+V(Q)+\frac{1}{4\pi}\int_0^{\hbar\beta}d\tau\int_{-\infty}^{\infty}d\sigma\int_0^{\infty}d\omega\tilde{J}(\omega)e^{-\omega|\tau-\sigma|}\Big[F[\dot{Q}(\tau)]-F[\dot{Q}(\sigma)]\Big]^2\right) \tag{5.80}$$

This is one of the main results of this thesis. For ohmic dissipation,[41]

$$\tilde{J}(\omega) = \lambda\omega, \tag{5.81}$$

one finds for the bath-induced term, after partial integration in $\omega$,

$$S^E_{\text{non-local}}[Q(\tau)] = \frac{\lambda}{4\pi}\int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \int_0^{\Omega} d\omega e^{-\omega|\tau-\sigma|}\frac{\Big[F[\dot{Q}(\tau)] - F\dot{Q}(\sigma)]\Big]^2}{|\tau-\sigma|}. \tag{5.82}$$

and, completing the integral over $\omega$ for $\Omega \to \infty$,

$$S^E_{\text{non-local}}[Q(\tau)] = \frac{\lambda}{4\pi}\int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \frac{\Big[F[\dot{Q}(\tau)] - F\dot{Q}(\sigma)]\Big]^2}{|\tau-\sigma|^2}. \tag{5.83}$$

This term is entirely induced by the bath. It is analogous to the famous 'Caldeira-Leggett'-term, as we have mentioned in Eq. (3.65), but it is much more general. In our case, the coupling is not linear, but entirely general and in terms of velocity. If we would have started out with a coordinate-coordinate coupling and counterterm such as in the original Caldeira-Leggett model, the result would be exactly Eq. (5.80) with $F$ replaced by $Q$.

The final result for the Euclidean effective action is

$$S^E_{\text{eff}}[Q(\tau)] = \int_0^{\hbar\beta} d\tau \left\{\frac{1}{2}M\dot{Q}^2 + V(Q)\right\} + \frac{\lambda}{4\pi}\int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \frac{\Big[F[\dot{Q}(\tau)] - F[\dot{Q}(\sigma)]\Big]^2}{|\tau-\sigma|^2}. \tag{5.84}$$

Eq. (5.80) in general, or Eq. (5.84) for baths with $\tilde{J} \propto \omega$ in particular, can be seen as a starting point for further research. To indicate some possibilities, we will now look at several specific choices for this coupling to make a connection to the specific choices made in Chapter 4, namely the non-polynomial coupling we have used in Section 4.2.3 and its low-velocity limit, the linear-coupling case, as we saw in Section 4.2.2.

## 5.3 Specific choices for the velocity coupling

In Chapter 4, the most important results were those for a linear-velocity coupling and a non-polynomial coupling (4.45). The linear-velocity case gave rise to a equation of motion analogous to the Abraham-Lorentz equation of a self-interacting electron. For the coupling in Eq. (4.45), we saw that this resulted in an expression equivalent to that of Lévy flights in ultracold-atom experiments. Since the former is the low-velocity limit of the latter, we will start with the non-polynomial coupling (4.45) in Section 5.3.1,

[41] Ohmic dissipation in the sense that the spectral density in terms of $\tilde{C}_k$ is linear in $\omega$.

reducing to the linear-velocity case in Section 5.3.2.

The goal of these sections is to mostly to indicate further research. In particular for the non-polynomial coupling (4.45) through numerical research has to be done, as we will come back to in the outlook. In the linear-velocity case, we find a result for the quantum effective action, Although specific calculations can be done using this effective action (for example, calculating its decoherence properties for two Gaussian distributed quantum states), we will provide a physical interpretation for this effective action—corresponding to the physics of the corresponding classical Abraham-Lorentz equation.

### 5.3.1 Quantum Lévy flights in ultracold atoms

Combining previous results, namely the general effective action of Eq. (5.84) and the coupling found in Section 4.2.3 to reproduce to the force term by Marksteiner, Ellinger and Zoller, Eq. (4.45), we find an effective action that represents the quantum version of this force,

$$S_{\text{eff}}[Q(\tau)] = \int_0^{\hbar\beta} d\tau \left\{ \frac{1}{2} M\dot{Q}^2 + V(Q) \right\} + \frac{\lambda}{4\pi} \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \frac{1}{|\tau-\sigma|^2} \left\{ \sqrt{\log\left[1+\left(\frac{\dot{Q}(\tau)}{v_0}\right)^2\right]} - \sqrt{\log\left[1+\left(\frac{\dot{Q}(\sigma)}{v_0}\right)^2\right]} \right\}, \tag{5.85}$$

Although it is clear that the path integral has to be evaluated numerically, which can then also be used to calculate decoherence properties, we will leave this as a point for further research. However, in the low-velocity limit, where the coupling becomes linear in velocity, the effective action becomes easier to interpret.

### 5.3.2 The low-velocity limit: resisting acceleration

The result Eq. (5.85) is very similar to the results obtained by Caldeira & Leggett [11, p. 149–150] for the coordinate-coordinate coupling of Chapter 3. Following the same steps–using the equilibirum denisty operator, tracing out the bath and writing the effective action as a local and a non-local part–they find the effective action

$$S_{\text{eff}}[Q(\tau)] = \int_0^{\hbar\beta} d\tau \left\{ \frac{1}{2} M\dot{Q}^2 + V(Q) \right\} + \frac{\eta}{4\pi} \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \frac{[Q(\tau)-Q(\sigma)]^2}{|\tau-\sigma|^2}, \tag{5.86}$$

as we already mentioned in the conclusion of Chapter 3. Here, the bath is assumed to be ohmic,

$$J(\omega) = \sum_k \frac{C_k^2}{m_k \omega_k} \delta(\omega_k - \omega) = \eta\omega. \tag{5.87}$$

The last term in Eq. (5.86) is called the Caldeira-Leggett term and it describes a bath-induced effective potential that is non-local, since it only depends on the relative position of the Brownian system at different times. It is interpreted as friction, because for successive times close together, i.e. $|\tau - \sigma| \sim 0$, this non-local term diverges unless the relative distance of the particle at different times, $Q(\tau) - Q(\sigma)$, also tends to zero. Hence, it is energetically favorable for the particle to resist displacement; which is exactly what friction does.

Turning to our results, in the low-velocity limit, $\dot{Q} \ll v_0$, using the Taylor expansion of Eq. (4.54) we find that the non-polynomial coupling of the previous section, Eq. (5.85), reduces to

$$S_{eff}[\bar{Q}(\tau)] = \int_0^{\hbar\beta} d\tau \left\{ \frac{1}{2} M \dot{Q}^2 + V(Q) \right\} + \frac{\lambda}{4\pi} \int_0^{\hbar\beta} d\tau \int_{-\infty}^{\infty} d\sigma \frac{\left[ \dot{Q}(\tau) - \dot{Q}(\sigma) \right]^2}{|\tau - \sigma|^2}. \tag{5.88}$$

Again, the second term is non-local, since it exclusively depends on the relative velocity of the Brownian system at different times. The interpretation of this *modified Caldeira-Leggett term* can be made in the same way as for the original term. For successive times close together, i.e. $|\tau - \sigma| \sim 0$, this term diverges unless the relative velocity of the Brownian system at different times, $\dot{Q}(\tau) - \dot{Q}(\sigma)$, also tends to zero. Hence, it is energetically much better for the particle to resist acceleration, and we can interpret this bath-induced effect as that of *inertia* on top of the mass $M$ in the local part of the action.

There are two points to be made about this comparison to the original Caldeira-Leggett model and the linear-velocity model. First, to derive Eq. (5.88), we assumed an ohmic bath in terms of the coupling constant $\tilde{C}_k$. As we pointed out throughout Chapter 4, and explicitly in Eq. (4.33), this corresponds to a cubically superohmic spectral density in terms of the spring constants $C_k$ of the original Caldeira-Leggett model. Second, the previous point implies that, as we saw in Section 4.2.2, the classical equation of motion corresponding to Eq. (5.88) is the Abraham-Lorentz equation (4.38) we derived in Section 4.2.2.

## 5.4 Conclusion

In this chapter we have discussed the path-integral formulation of quantum mechanics, deriving the well-known propagators for the free particle and the forced harmonic oscillator. Most of the tedious work went into deriving the classical action for the forced harmonic oscillator, which we have rearranged to Appendix D. Doing this cal-

culation separately, made the evaluation of the influence functional for the modified Caldeira-Leggett Lagrangian Eq. (4.1) more accessible.

The goal of this chapter was to derive a quantum effective action for a completely general coupling of the velocity of a Brownian system to the coordinates of the environment. In Section 5.2, by using the influence-functional method of Feynman and Vernon in the Euclidean-time path-integral formalism and tracing out the bath coordinates, we found the effective action we were after. The result, before assuming a specific spectral density, is Eq. (5.80). For $\tilde{J}(\omega) \propto \omega$, gives a final result Eq. (5.84), which seems to be of the same form as the original Caldeira-Leggett term; this was to be expected, since the path integral over the system coordinate $Q$ is not performed in this procedure.

The final result can be seen as a starting point for further research. It is a collection of different models, where each model is specified by a particular coupling. We have looked at two such models, drawn from Chapter 4, namely the coupling (4.44) that we used to make a connection with the results of Marksteiner, Ellinger and Zoller in the case of Lévy flights in Sisyphus cooling, and its low-velocity limit: the linear-velocity coupling case, which resulted in the Abraham-Lorentz equation. Unfortunately, the expression (5.85) does not allow for a straightforward analytical evaluation, and hence the path integral over $Q$ should be performed numerically. In the case of the coupling linear in velocity, however, a clear physical interpretation is found. Analogous to the interpretation of friction in the original Caldeira-Leggett term (5.86), the modified Caldeira-Leggett term in Eq. (5.88) is that of inertia. In other words, the result of the bath-induced effective dynamics is that the Brownian system resisting acceleration (on top of Newtonian inertia).

For further calculation, one should specify a particular from for the external potential $V(Q)$. In that case, one can, in principle, determine the effective dynamics of the system of interest by performing the path integral over all paths $Q(\tau)$. In the original Caldeira-Leggett model, only the models $V(Q) \propto Q^n$ for which $n \in \{0, 1, 2\}$ result in expressions that can be analytically evaluated. Especially, for a harmonic potential, $V(Q) \propto Q^2$, the original Caldeira-Leggett model results in seminal model to describe decoherence (the dissipation of entanglement as described in Section 2.2), where an exact localization rate can be calculated for two initially Gaussian-distributed wave-packets. The analysis of the analogous model for the effective action of the general-velocity coupling in Eq. (5.80), will be left to further research, as we will come back to in the Outlook.

# 6 Conclusion & Outlook

The goal of this thesis was twofold. On the one hand, to construct a closed Lagrangian model that could reproduce Lévy motion. The motivation for this was largely to account for a closed description of Lévy flights during Sisyphus cooling. On the other hand, to quantize such a system using path-integral quantization. We choose to search for these goals by modifying the Caldeira-Leggett model to general velocity-dependent coupling. With this choice, we left other possibilities behind. For example, trying to construct a stochastic Schrödinger equation in the style of Kostin [40] and Nelson [63], using a modified quantization scheme [13], or entering the Lindblad formalism [47].

We discussed the theory of Brownian motion from the point of view of Einstein's diffusion and the velocity-dependent Langevin equation. In the relaxation time approximation, i.e. when all important timescales are larger than the collision time $\tau$, we could safely assume white noise correlations, avoiding the Itô-Stratonovich dilemma.

In Chapter 3, we have developed the Caldeira-Leggett model, and showed the derivation of the Langevin equation in the classical limit. We also proved its internal consistency by showing that it satisfies the fluctuation-dissipation theorem for all choices of the spectral density $J(\omega)$. This offered an *a posteriori* justification of the model.

Chapter 4 contained our first original contributions. By writing the Lagrangian (4.1), we modified the interaction between the system and the bath. Before, their coupling was of the coordinate-coordinate type. Now, we choose a coupling general in the velocity of the system, while still coupled to the coordinates of the bath particles. The counterterm is adjusted accordingly. The resulting *modified* generalized Langevin equation was (4.14). Compared to the generalized Langevin equation (3.53) for general-coordinate coupling, there are extra terms due to the existence of the second derivative of the coupling function $F''[\dot{Q}]$. The system has velocity-dependent multiplicative noise, as well as memory, for all choices of the spectral density.

Under the approximation $F''[\dot{Q}] \sim 0$, we have worked out two realizations of the coupling function $F[\dot{Q}]$. First, for the linear-velocity case, the approximation holds trivially and we derive the equation of motion Eq. (4.32). Without assuming any fundamental physical picture, this equation bears exact resemblance–at least in form– to the Abraham-Lorentz equation of an self-interacting electron. Since we also changed the counterterm in our model, we do not find a mass renormalization, since the new counterterm adds precisely that amount of mass to the kinetic part of the system of interest.

It is important to bear in mind that we found this under the assumption that the spectral density $\bar{J}$ is linear in the frequency, and that this corresponds to an ohmic bath in terms of coupling constants $\bar{C}_k$, but that for coupling constants $C_k$, the bath is cubically superohmic, $J \propto \omega^3$. Hence, the term 'ohmic bath' is ambiguous when one does not explicitly specify the dimension of the coupling constants.

For the occurrence of Lévy flights in ultracold-atoms experiments like Sisyphus cooling,

as was discussed in Section 2.4, we were able to reproduce the force Eq. (4.44) from the work of Marksteiner, Ellinger and Zoller [56], which gives rise to Lévy flights. Here, individual atoms in a cooling atom cloud exhibit Lévy flights as a result of the recoil caused by spontaneous photon emission. It turns out that the choice Eq. (4.45) gives exactly this expression. This was the original motivation of modifying the Caldeira-Leggett model to velocity-dependent coupling forces. We also point out that, in the low-velocity limit, this model reduces to the linear-velocity model and hence returns the (form of the) Abraham-Lorentz equation. We have also shown that the approximation $F'' \sim 0$ holds in the low- and high-velocity limits, but further research should be undertaken to interpolate in between these extremes, where the approximation fails and memory effects start playing a larger role. This will involve a numerical investigation.

In Chapter 5 we have discussed the path-integral formulation of quantum mechanics and used the Feynman-Vernon influence-functional method in Euclidean time to integrate out the bath particles and derive an effective action for our modified Lagrangian (4.1). The result, for a bath ohmic in terms of coupling constants $\tilde{C}_k$, the final result is given by Eq. (5.84). It has the same form as the original Caldeira-Leggett term.

This final result should be seen as a starting point for further research. It is a collection of different models, where each model is specified by a particular coupling. We have looked at the same models as before, the linear-velocity case and the Lévy-flight case. The expression for the Lévy-flight case, Eq. (5.85), does not allow for a straightforward analytical evaluation, and hence the path integral over $Q$ should be performed numerically. In the low-velocity limit, this case reduces to the linear-velocity coupling. Analogous to the interpretation of friction in the original Caldeira-Leggett term (5.86), the modified Caldeira-Leggett term in Eq. (5.88) is that of inertia. The classical equation of motion corresponding to this, is, again, the Abraham-Lorentz equation (4.34).

In addition to the above-mentioned numerical work to be done for several results, one can also look at the decoherence properties of the Lévy-flight coupling and/or the linear-velocity coupling case. For further calculation, one should specify a particular form for the external potential $V(Q)$. In that case, one can, in principle, determine the effective dynamics of the system of interest by performing the path integral over all paths $Q(\tau)$.

One more remark is in place concerning a possible general velocity-coupling Caldeira-Leggett *Hamiltonian* and pursue the search for the generalized Langevin equation from there, as worked out in Appendix F. This approach looks very interesting on account of the absence of $\ddot{Q}$-terms due the equivalence of time derivatives of momentum $\dot{P}$ and the external potential, as given by Hamilton's equation (F.2). This is promising, since the external potential is an experimental handle one can work with in the lab. At the same time, it reduces the complexity of the generalized Langevin equation of the velocity-coupling method, as given in Eq. (4.14), by transforming acceleration terms into derivatives of the external potential, resulting in Eq. (F.10).

# Appendices

## A Canonical transformation of the Caldeira-Leggett Lagrangian

Instead of using the Caldeira-Leggett Lagrangian as in Eq. (3.10) one can write it without the counterterm and with a coordinate-velocity coupling with strength $\bar{C}_k$ instead of a coordinate-coordinate coupling with strength $C_k$, like

$$\mathcal{L} = \frac{1}{2}M\dot{Q}^2 - V(Q) + \frac{1}{2}\sum_{k=1}^{N} m_k(\dot{q}_k^2 - \omega_k^2 q_k^2) + Q\sum_{k=1}^{N}\bar{C}_k\dot{q}_k, \tag{A.1}$$

The canonical momenta of the bath particles are

$$p_i = \frac{\partial\mathcal{L}}{\partial\dot{q}_i} = m_i\dot{q}_i + \bar{C}_i Q. \tag{A.2}$$

The corresponding Hamiltonian, via the well-known Legendre transformation, becomes

$$\mathcal{H} = \frac{P^2}{2M} + V(Q) + \sum_{k}^{N}\left[\frac{(p_k - \bar{C}_k Q)^2}{2m_k} + \frac{1}{2}m_k\omega_k^2 q_k^2\right]. \tag{A.3}$$

Following [61], we perform a canonical transformation to the bath constituents

$$p_i \to m_i\omega_i q_i \qquad\qquad q_i \to -\frac{p_i}{m_i\omega_i}, \tag{A.4}$$

which is canonical because it preserves the Poisson bracket:

$$1 = \{q_i, p_i\}_{P.B.} \to -\{p_i/\cancel{m_i\omega_i}, \cancel{m_i\omega_i}q_i\}_{P.B.} = 1. \tag{A.5}$$

The Hamiltonian is transformed to

$$\mathcal{H} = \frac{P^2}{2M} + V(Q) + \sum_{k}^{N}\left[\frac{p_k^2}{2m_k} + \frac{1}{2}m_k\omega_k^2 q_k^2\right] - Q\sum_{k}^{N}\bar{C}_k\omega_k q_k + \frac{1}{2}Q^2\sum_{k}^{N}\frac{\bar{C}_k^2}{m_k}, \tag{A.6}$$

which coincides, after writing the Lagrangian through the inverse Legendre transformation, with the original Caldeira-Leggett model (3.10), for

$$\bar{C}_k = \frac{C_k}{\omega_k}, \tag{A.7}$$

which makes dimensional sense as the time-derivative in the inverse frequency units cancel each other.

# B Laplace transformations

The Laplace transform is similar to the Fourier transform; the former turns a complex function into a function of a complex variable, while the latter creates a complex function of a real variable. In physics, the Laplace transformation can be conveniently employed to switch between the time-domain and the frequency-domain (extended as a complex variable). The Laplace transformation of a function $f(t)$, in the domain $t > 0$, is defined as

$$\tilde{f}(l) = \mathfrak{L}\{f(t)\}(l) = \int_0^\infty dt\ f(t)e^{-lt}, \tag{B.1}$$

where $l$ is some auxiliary variable, which must be transformed away at the end of a calculation. As an example, we can take the transform of the function $g(t) = e^{-at}$, resulting in

$$\tilde{g}(l) = \mathfrak{L}\{e^{-at}\} = \int_0^\infty dt\ e^{-(l+a)t} = \frac{1}{l+a} \tag{B.2}$$

The Laplace transformation has some important properties, notably for solving partial differential equations. It is a linear operator: $\mathfrak{L}\{af(t)\} = a\mathfrak{L}\{f(t)\}$; and it turns *derivatives into multiplication*: $\mathfrak{L}\{f'(t)\} = l\mathfrak{L}\{f\} - f(0)$. We can, for instance, solve the decay equation $dN/dt = -\lambda N$ by using the Laplace transformation on both sides,

$$\begin{aligned} \mathfrak{L}\{\dot{N}(t)\} &= \mathfrak{L}\{-\lambda N(t)\} \\ l\mathfrak{L}\{N(t)\} - N(0) &= -\lambda\mathfrak{L}\{N(t)\} \\ \rightarrow \mathfrak{L}\{N(t)\}(l) &= \frac{N(0)}{l+\lambda}. \end{aligned} \tag{B.3}$$

Then, applying the inverse transformation,

$$\begin{aligned} N(t) &= \mathfrak{L}^{-1}\{\mathfrak{L}\{N(t)\}(l)\} \\ &= \mathfrak{L}^{-1}\{\frac{N(0)}{l+\lambda}\} \\ &= N(0)\mathfrak{L}^{-1}\{\frac{1}{l+\lambda}\} \\ &= N(0)e^{-\lambda t}, \end{aligned} \tag{B.4}$$

where in the last step the Eq. (B.2) is used. It is often the most convenient to recognize Laplace transformations of standard functions in this way. However, this is not always possible. In that case, the calculation becomes more involved, and one must invoke the

inverse transformation via the so-called Fourier-Mellin integral (or Bromwich integral):

$$f(t) = \mathfrak{L}^{-1}\{F(l)\}(t) = \frac{1}{2\pi i} \lim_{T\to\infty} \int_{\delta+iT}^{\delta-iT} dl F(l) e^{lt}, \tag{B.5}$$

where $\delta$ is a (small) real number that prevents the contour from hitting the poles.

The Laplace transform also satisfies the convolution theorem, i.e. it turns a convolution,

$$g(t) \star h(t) := \int_0^t d\tau \; g(t-\tau) g(\tau) \tag{B.6}$$

into a multiplication,

$$\begin{aligned} \mathfrak{L}\{g(t) \star h(t)\} &= \int_0^t d\tau \int_0^\infty dt \; g(t-\tau) h(\tau) e^{-lt} \\ &= \int_0^\infty dv \; e^{-lu} g(v) \int_0^\infty du \; e^{-lv} h(u) \\ &= \tilde{g}(l)\tilde{h}(l), \end{aligned} \tag{B.7}$$

where in the second line we performed a change of variables $t = u + v$, $\tau = v$. The inverse convolution theorem then reads

$$\mathfrak{L}^{-1}\{\tilde{g}(l)\tilde{h}(l)\} = g(t) \star h(t). \tag{B.8}$$

# C Solving the driven harmonic oscillator differential equation

The driven harmonic oscillator equation is

$$m\ddot{x}(t) + kx(t) = F(t), \tag{C.1}$$

where $F(t)$ is a general force function, and $m$ and $k$ are constant. An example of such a system is the mass-spring system undergoing friction due to its environment. To solve it, we will need to find the homogeneous solution and a particular solution. The *un*driven, or homogeneous, harmonic oscillator equation is

$$m\ddot{x}(t) + kx(t) = 0, \tag{C.2}$$

which has solutions

$$x_h(t) = A\sin(\omega t) + B\cos(\omega t), \tag{C.3}$$

for $\omega^2 = k/m$ and constants $A$ and $B$, which can be found by specifying initial conditions for position and velocity.

The *driven* harmonic oscillator Eq. (C.1) is harder to solve. If we had a particular solution $x_p$, we can construct all the other solutions by adding it to the homogeneous solution (C.3) and then find the constants $A$ and $B$ via the initial conditions,

$$x(t) = x_h(t) + x_p(t) = A\sin(\omega t) + B\cos(\omega t) + x_p(t). \tag{C.4}$$

However, the force function $F(t)$ has a general form on which the particular solution heavily depends. To meet ends, we can use the linearity of the left-hand side of Eq. (C.1) and write down a superposition of simple solutions

$$m\frac{d^2}{dt^2}\left[x_1(t) + x_2(t)\right] + k\left[x_1(t) + x_2(t)\right] = \tilde{F}_1(t) + \tilde{F}_2(t), \tag{C.5}$$

where each component satisfies the separate differential equations

$$m\ddot{x}_1(t) + kx_1(t) = \tilde{F}_1(t) \tag{C.6}$$

$$m\ddot{x}_2(t) + kx_2(t) = \tilde{F}_2(t). \tag{C.7}$$

Thus, we can *choose* a simple set of $\tilde{F}$s and write $x_p(t)$ as a (weighted) sum of these simpler solutions. The simplest $\tilde{F}(t)$, arguably, is a delta distribution

$$\tilde{F}(t) = \delta(t). \tag{C.8}$$

This means there is no force at $t < 0$ nor at $t > 0$; there is only one 'kick' at $t = 0$ after which the system starts to oscillate. Consistent with this, we restrict ourselves to the retarded Green function, which is equivalent to assuming causality. Since there is no force after the kick, the solution will again be like the homogeneous solution of Eq. (C.3); hence

$$x(t) = \left\{ \begin{array}{ll} 0 & \text{if } t < 0 \\ \tilde{A}\sin(\omega t) + \tilde{B}\cos(\omega t) & \text{if } t > 0 \end{array} \right\}. \tag{C.9}$$

This almost solves the problem, it leaves us only with finding the correct 'junction' condition to make sure the solution is continuous at $t = 0$. Looking at the equation

$$m\ddot{x} + kx = \delta(t) \tag{C.10}$$

and integrating around the point $x = 0$

$$\int_{t=-\epsilon}^{t=+\epsilon} dt\left[m\ddot{x}(t) + kx(t)\right] = \int_{t=-\epsilon}^{t=+\epsilon} dt\delta(t) \tag{C.11}$$

leads to

$$m\left[\dot{x}(\epsilon)-\dot{x}(-\epsilon)\right]+\mathcal{O}(\epsilon)=1, \tag{C.12}$$

Assuming the second term is small because of

$$\|\int_{t=-\epsilon}^{t=+\epsilon} x(t)\| \leq \max\|x(t)\| 2\epsilon, \tag{C.13}$$

we can close the gap from both sides, $\epsilon \downarrow 0^+$ and $\epsilon \uparrow 0^-$, and obtain, at leading order

$$m\dot{x}(t=0^+)-m\dot{x}(t=0^-)=1. \tag{C.14}$$

According to Eq. (C.9) we have $\dot{x}(t=0^-)=0$ and $\dot{x}(t=0^-)=1/m$. Also, because Eq. (C.13) ensures that

$$\lim_{\epsilon\to 0}\int_{t=-\epsilon}^{t=+\epsilon} dt\dot{x}(t)=0, \tag{C.15}$$

we can conclude that

$$\lim_{\epsilon\to 0}\int_{t=-\epsilon}^{t=+\epsilon} dt\dot{x}(t)=\lim_{\epsilon\to 0}\left[x(\epsilon)-x(-\epsilon)\right]=0, \tag{C.16}$$

such that

$$x(t=0^+)=0=x(t=0^-). \tag{C.17}$$

Now, we can determine the $\tilde{A}$ and $\tilde{B}$ from (C.9) at $t=0$ and find that

$$\tilde{B}=0 \quad , \quad \tilde{A}=\frac{1}{m\omega}, \tag{C.18}$$

leading us, finally, to

$$x_p(t)=\frac{\sin\omega t}{m\omega}. \tag{C.19}$$

From here we can straightforwardly write Eq. (C.1) as a weighted sum of linear differential equations. First, it is possible to construct the arbitrary force $F(t)$ using the simple solution just obtained,[42]

$$F(t)=\int_{t'=-\infty}^{\infty} dt' F(t')\delta(t-t'), \tag{C.20}$$

where $F(t')$ plays the role of a weight of the delta distribution around each point $t'$.

[42] We can imagine that any bijective function is made of delta functions with appropriate weights.

Since the delta function at $t' = t$ has strength $F(t')$ instead of unity, we simply multiply the solution Eq. (C.19) with $F(t')$. Also, we should account for the delta functions at $t < t'$, but not for those at $t > t'$, since due to our causality assumption they have not yet influenced the system. Thus, for *an arbitrary fluctuation force* the particular solution is

$$x_p(t) = \int_{t'=-\infty}^{\infty} dt' F(t') \frac{\sin\left[\omega(t-t')\right]}{m\omega}, \tag{C.21}$$

We can check this by calculating the first and second derivatives of $x_p(t)$,

$$\frac{d}{dt} \int_{t'=-\infty}^{\infty} dt' F(t') \frac{\sin\left[\omega(t-t')\right]}{m\omega} = \left[ F(t') \frac{\sin\left[\omega(t-t')\right]}{m\omega} \cancelto{0}{} \right]_{t'=t} + \int_{t'=-\infty}^{\infty} dt' F(t') \frac{\cos\left[\omega(t-t')\right]}{m} \tag{C.22}$$

and

$$\begin{aligned} m\frac{d^2 x_p(t)}{dt^2} &= \frac{d^2}{dt^2} \int_{t'=-\infty}^{\infty} dt' F(t') \frac{\sin\left[\omega(t-t')\right]}{\omega} = \frac{d}{dt} \int_{t'=-\infty}^{\infty} dt' F(t') \cos\left[\omega(t-t')\right] \\ &= \left[F(t') \cos\left[\omega(t-t')\right]\right]_{t'=t} - \int_{t'=-\infty}^{\infty} dt' F(t') \sin\left[\omega(t-t')\right] \\ &= F(t) - \omega \int_{t'=-\infty}^{\infty} dt' F(t') \sin\left[\omega(t-t')\right], \\ &= F(t) - m\omega^2 x_p(t), \end{aligned} \tag{C.23}$$

which shows that (C.21) indeed satisfies (C.1)

$$\frac{d^2 x_p(t)}{dt^2} + \omega^2 x_p(t) = \frac{F(t)}{m}. \tag{C.24}$$

To find all possible solutions, we add the homogeneous solution,

$$x(t) = A\sin(\omega t) + B\cos(\omega t) + \frac{1}{m\omega} \int_{t'=-\infty}^{t} dt' F(t') \sin\left[\omega(t-t')\right]. \tag{C.25}$$

For general initial conditions $x(t=0) = x_0$ and $\dot{x}(t=0) = \dot{x}_0$:

$$x(t) = x_0 \sin(\omega t) + \frac{\dot{x}_0}{\omega} \cos(\omega t) + \frac{1}{m\omega} \int_{t'=-\infty}^{t} dt' F(t') \sin\left[\omega(t-t')\right]. \tag{C.26}$$

# D Classical action of the driven harmonic oscillator

We start with the action for the driven harmonic oscillator of mass $m$, frequency $\omega$, and fluctuation force $f(t)$,

$$S[x] = \int_0^t ds \left[\frac{1}{2}m\dot{x}^2(s) - \frac{1}{2}m\omega^2 x^2(s) + x(s)f(s)\right]. \tag{D.1}$$

Here, we will compute its classical result, i.e. the value for the path $x_{cl}$ which extremizes the numerical value of this functional as given by Hamilton's principle. This is a *boundary value* problem, with boundaries $x_{cl}(s=0) = x_i$ and $x_{cl}(s=t) = x_f$, while also satisfying the equations of motion

$$m\ddot{x}_{cl} + m\omega^2 x = f(s). \tag{D.2}$$

The classical path, using the general solution to the equations of motion Eq. (C.25), is

$$\begin{aligned} x_{cl}(s) = x_f \frac{\sin(\omega s)}{\sin(\omega t)} + x_i \frac{\sin[\omega(t-s)]}{\sin(\omega t)} + \int_0^s du \frac{\sin[\omega(s-u)]}{m\omega} f(u) \\ - \frac{\sin(\omega s)}{\sin(\omega t)} \int_0^t du \frac{\sin[\omega(t-u)]}{m\omega} f(u). \end{aligned} \tag{D.3}$$

satisfying for the boundary constraints in Eq. (D.2). One can check this by explicit differentiation

$$\begin{aligned} \frac{d^2 x_{cl}(s)}{ds^2} =& -\omega^2 \left( x_f \frac{\sin(\omega s)}{\sin(\omega t)} + x_i \frac{\sin[\omega(t-s)]}{\sin(\omega t)} \right) \\ &+ \frac{\omega}{m\omega}\frac{d}{ds}\left( \cancelto{0}{\sin[\omega(s-s)]} + \int_0^s du \cos[\omega(s-u)] f(u) - \frac{\cos(\omega s)}{\sin(\omega t)} \int_0^t du \sin[\omega(t-u)] f(u) \right) \\ =& (-\omega^2)\left( x_f \frac{\sin(\omega s)}{\sin(\omega t)} + x_i \frac{\sin[\omega(t-s)]}{\sin(\omega t)} \right) + \frac{(-\omega^2)}{m\omega} \int_0^s du \sin[\omega(s-u)] f(u) \\ &- (-\omega^2)\frac{\sin(\omega s)}{\sin(\omega t)} \int_0^t du \sin[\omega(t-u)] f(u) + \frac{f(s)}{m} \\ =& -\omega^2 x_{cl}(s) + \frac{f(s)}{m}, \end{aligned} \tag{D.4}$$

showing that it satisfies Eq. (D.2).

The classical action $S_{cl}$ can be calculated by plugging in the solution of the classical equation of motion into the action and evaluating the integral over the auxiliary time $s$ explicitly. To simplify beforehand, we partially integrate Eq. (D.1) to obtain

$$\begin{aligned} S_{cl} &= \int_0^t ds \left[\frac{1}{2}m\left(\ddot{x}_{cl}^2 + \omega^2 x_{cl} - \frac{f(s)}{m}\right)x_{cl}\right] + \frac{1}{2}m\left[\dot{x}_{cl}(s)x_{cl}(s)\right]_{s=0}^{s=t} \\ &= \frac{1}{2}m\dot{x}_{cl}(t)x_{cl}(t) - \frac{1}{2}m\dot{x}_{cl}(0)x_{cl}(0) + \int_0^t ds x_{cl}(s)f(s), \end{aligned} \tag{D.5}$$

where the equations of motion (D.2) were used to go from the first to the second line. Explicit calculation leads to

$$\dot{x}_{cl}(0) = \frac{\omega x_f}{\sin(\omega t)} - \omega x_i \frac{\cos(\omega t)}{\sin(\omega t)} - \frac{1}{m\sin(\omega t)}\int_0^t ds \sin[\omega(t-s)]f(s) \tag{D.6}$$

and

$$\begin{aligned} \dot{x}_{cl}(t) &= \omega x_f \frac{\cos(\omega t)}{\sin(\omega t)} - \frac{\omega x_i}{\sin(\omega t)} + \frac{1}{m}\int_0^t du \cos[\omega(t-u)]f(u) - \frac{\cos(\omega t)}{m\sin(\omega t)}\int_0^t du \sin[\omega(t-u)]f(u) \\ &= \omega x_f \frac{\cos(\omega t)}{\sin(\omega t)} - \frac{\omega x_i}{\sin(\omega t)} + \frac{1}{m\sin(\omega t)}\int_0^t ds \sin(\omega s)f(s), \end{aligned} \tag{D.7}$$

where, in the last line, we changed the auxiliary time variable from $u$ to $s$ and used the trigonometric relation that

$$\cos[\omega(t-u)] - \sin[\omega(t-u)]\cos(\omega t)\sin(\omega t)^{-1} = \sin(\omega u)\sin(\omega t)^{-1}. \tag{D.8}$$

Now, we have all the ingredients to evaluate Eq. (D.5)

$$\begin{aligned} S_{cl} =& \frac{m\omega}{2}\frac{x_f(x_f\cos(\omega t) - \cancel{x_i})}{\sin(\omega t)} + \frac{x_f}{2\sin(\omega t)}\int_0^t ds\sin(\omega s)f(s) - \frac{m\omega}{2}\frac{x_i(\cancel{x_f} - x_i\cos(\omega t))}{\sin(\omega t)} \\ &+ \frac{x_i}{2\sin(\omega t)}\int_0^t ds\sin[\omega(t-s)]f(s) + \frac{1}{2\sin(\omega t)}\int_0^t dsx_f\sin(\omega s)f(s) \\ &+ \frac{1}{2\sin(\omega t)}\int_0^t dsx_i\sin[\omega(t-s)]f(s) + \frac{1}{m\omega}\int_0^t ds\int_0^s du\sin[\omega(s-u)]f(u)f(s) \\ &- \frac{1}{m\omega}\int_0^t ds\int_0^s du\frac{\sin(\omega s)}{\sin(\omega t)}\sin[\omega(t-u)]f(u)f(s). \end{aligned} \tag{D.9}$$

Observe that the second term and the fifth term simply add, as do the fourth and sixth terms. For the final two terms, we can use another (similar) simplifying trigonometric relation

$$\sin[\omega(t-u)] - \sin[\omega(t-u)]\sin(\omega t)\sin(\omega t)^{-1} = \sin(\omega u)\sin(\omega t)^{-1}, \tag{D.10}$$

which gives us the final result for the classical action of the driven harmonic oscillator:

$$\begin{aligned} S_{cl} =& \frac{m\omega}{2\sin(\omega t)}\left[(x_i^2 + x_f^2)\cos(\omega t) - 2x_ix_f\right] \\ &+ \frac{x_f}{\sin(\omega t)}\int_0^t ds\sin(\omega s)f(s) + \frac{x_i}{\sin(\omega t)}\int_0^t \sin[\omega(t-s)]f(s) \\ &- \frac{1}{m\omega\sin(\omega t)}\int_0^t ds\int_0^s du\sin(\omega u)\sin[\omega(t-s)]f(s)f(u). \end{aligned} \tag{D.11}$$

# E Completing the square for the influence functional

To perform a Gaussian integral, we will need to complete the square for bath variable $q_k$ in Eq.(5.61). We can write the action as

$$\begin{aligned} S_{cl}^{(k)\mathrm{E}} =& \frac{m_k\omega_k}{\sinh(\omega_k t)}\left[\cosh(\hbar\beta\omega_k)-1\right]\left[q_k-q_k^*\right]^2 - \frac{m_k\omega_k}{\sinh(\hbar\beta\omega_k)}\frac{1}{\cosh\hbar\beta\omega_k-1}\frac{C_k^2}{2m_k\omega_k}\Big\{\{... \\ &... \int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \sinh(\omega_k\tau)\sinh\left[\omega_k(\hbar\beta-\sigma)\right] + \sinh(\omega_k\sigma)\sinh\left[\omega_k(\hbar\beta-\tau)\right] + ... \\ &... + \sinh(\omega_k\tau)\sinh(\omega_k\sigma)\sinh\left[\omega_k(\hbar\beta-\tau)\right]\sinh\left[\omega_k(\hbar\beta-\tau)\right]\Big\}F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)]\Big\} \\ &- \frac{C_k^2}{m_k\omega_k\sinh(\hbar\beta\omega_k)}\int_0^{\hbar\beta} d\tau\int_0^{\tau} d\sigma\sinh(\omega_k\sigma)\sinh[\omega_k(\hbar\beta-\tau)]F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)], \end{aligned} \tag{E.1}$$

where

$$q_k^* = \frac{C_k}{2m_k\omega_k}\int_0^{\hbar\beta} d\tau\left(\frac{\sinh(\omega_k\tau)+\sinh[\omega_k(\hbar\beta-\tau)]}{\cosh(\hbar\beta\omega_k)}\right)F[\dot{Q}(\tau)]. \tag{E.2}$$

The second term in Eq. (E.1) (comprising the two lines in the middle) is $q_n^{(0)}$, which has to be subtracted in order to complete the square; note that a factor 2 results from adjusting the range of the $\sigma$-integral from $\{0,\hbar\beta\}$ to $\{0,\tau\}$. the last term is unchanged with respect to Eq. (5.61).

Then, we add the terms appearing under the double integrals in Eq. (E.1). To do this, we use the following non-trivial trigonometric relation[43]

$$\begin{aligned} &\frac{1}{2\sinh(a)\left[\cosh(a)-1\right]}\Big\{\left[\sinh(x)\sinh(y)+\sinh(a-x)\sinh(a-y)\right]+ \\ &\left[\sinh(x)\sinh(a-y)+\sinh(y)\sinh(a-x)\right]\Big\}+\frac{\sinh(a-x)\sinh(y)}{\sinh(a)} = \quad \frac{\cosh\left[a/2-x+y\right]}{2\sinh(a/2)}, \end{aligned} \tag{E.3}$$

for $a=\hbar\beta\omega_k$, $x=\omega_k s$ and $y=\omega_k u$.

[43] It seems to me that there should be an elegant way to show why this holds. However, the only way I have found is by using Euler's formula and work out the algebra in terms of exponentials, which is a bit long-winded. In any case, it is easily checked with the aid of a computer program.

The result, then, is

$$S_{cl}^{(k)\mathrm{E}} = \frac{m_k\omega_k}{\sinh(\omega_k t)}\left[\cosh(\hbar\beta\omega_k)-1\right]\left[q_k-q_k^*\right]^2 - \frac{C_k^2}{2m_k\omega_k}\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma \mathcal{G}_k(\tau-\sigma)F[\dot{Q}(\tau)]F[\dot{Q}(\sigma)], \tag{E.4}$$

for

$$\mathcal{G}_k(\tau-\sigma) := \frac{\cosh\left[\omega_k\left(\frac{\hbar\beta}{2}-(\tau-\sigma)\right)\right]}{\sinh\left(\frac{\hbar\beta\omega_k}{2}\right)}. \tag{E.5}$$

# F General momentum-coupling in the Hamiltonian picture

We write down the Hamiltonian of a closed system of harmonic oscillators coupled to a generic system through a general momentum-coupling term.

$$\mathcal{H} = \frac{P^2}{2M} + V(Q) + \frac{1}{2}\sum_{k=1}^{N}\left(\frac{p_k^2}{m_k} + m_k\omega_k^2 q_k^2\right) + F(P)\sum_{k=1}^{N} C_k q_k. \tag{F.1}$$

We do not include a counterterm. One can think about the incorporation of a counterterm discussing the physics of the model and possible potential shifts. For the point we want to make here, we do not need to discuss the difference between models with or without counterterms.

The Hamilton equations are,

$$\dot{P} = -\frac{\partial\mathcal{H}}{\partial Q} = -\frac{\partial V}{\partial Q}, \tag{F.2}$$

$$\dot{Q} = \frac{\partial\mathcal{H}}{\partial P} = \frac{P}{M} - \frac{\partial F(P)}{\partial P}\sum_k C_k q_k, \tag{F.3}$$

$$\dot{p}_i = -\frac{\partial\mathcal{H}}{\partial q_i} = -m_i\omega_i^2 q_i + C_i F(P), \tag{F.4}$$

$$\dot{q}_i = \frac{\partial\mathcal{H}}{\partial p_i} = \frac{p_i}{m_i}, \tag{F.5}$$

which leads to the following set of second-order differential equations,

$$M\ddot{Q} = -V'(Q) + M\frac{\partial^2 F(P)}{\partial P^2}\frac{\partial V}{\partial Q}\sum_k C_k q_k - M\frac{\partial F(P)}{\partial P}\sum_k C_k\dot{q}_k \tag{F.6}$$

$$m_i\ddot{q}_i = -m_i\omega_i^2 q_i + C_i F(P) \tag{F.7}$$

The (now familiar) driven harmonic oscillator equation for the bath has solution,

$$q_i(t) = f^{(0)}(t) + \frac{C_i}{m_i\omega_i}\int_0^t dt' \sin[\omega_i(t-t')]F[P(t')], \tag{F.8}$$

and its first derivative,

$$\dot{q}_i(t) = \dot{f}^{(0)}(t) + \frac{C_i}{m_i}\int_0^t dt' \cos[\omega_i(t-t')]F[P(t')] + \frac{C_i}{m_i\omega_i}\left[\cancelto{0}{\sin[\omega_i(t-t')]}F[P(t')]\right]^{t'=t}. \tag{F.9}$$

The generalized Langevin equation becomes,

$$\begin{aligned} M\ddot{Q} + V'(Q) = MV'(Q)F''[P(t)]\sum_k C_k\left\{f_k^{(0)}(t) + \frac{C_k}{m_k\omega_k}\int_0^t dt' \sin[\omega_k(t-t')]F[P(t')]\right\} \\ -MF'[P(t)]\sum_k C_k\left\{\dot{f}_k^{(0)}(t) + \frac{C_k}{m_k}\int_0^t dt' \cos[\omega_k(t-t')]F[P(t')]\right\}. \end{aligned} \tag{F.10}$$

Integrating by parts the Sine term (second term on the RHS), we obtain

$$\begin{aligned} M\ddot{Q} + V'(Q) =& MV'[Q(t)]F''[P(t)]f^{(0)}(t) - MF'[P(t)]\dot{f}^{(0)}(t) \\ &- MV'[Q(t)]F''[P(t)]\sum_k \frac{C_k^2}{m_k\omega_k^2}\int_0^t dt' \cos[\omega_k(t-t')]F'[P(t')]\dot{P}(t') \\ &+ MV'[Q(t)]F''[P(t)]\left[\sum_k \frac{C_k^2}{m_k\omega_k^2}\cos[\omega_k(t-t')]F[P(t')]\right]_{t'=0}^{t'=t} \\ &- MF'[P(t)]\sum_k \frac{C_k^2}{m_k}\int_0^t dt' \cos[\omega_k(t-t')]F[P(t')], \end{aligned} \tag{F.11}$$

where it is not helpful to add the two cosine terms due their mismatch of the coefficients of $\omega_i$. Evaluating the boundaries, and invoking the equation of motion $\dot{P}(t) = -V'[Q(t)]$

we find

$$\begin{aligned} M\ddot{Q} + V'[Q(t)] =& MV'[Q(t)]F''[P(t)]f^{(0)}(t) - MF'[P(t)]\dot{f}^{(0)}(t) \\ &+ MV'[Q(t)]F''[P(t)]\sum_k \frac{C_k^2}{m_k\omega_k^2}\Big\{\int_0^t dt' \cos[\omega_k(t-t')]F'[P(t')]V'[Q(t')]F[P(t) \\ &- \cos[\omega_k t]F[P(0)]\Big\} - MF'[P(t)]\sum_k \frac{C_k^2}{m_k}\int_0^t dt' \cos[\omega_k(t-t')]F[P(t')], \end{aligned} \tag{F.12}$$

which can be written as

$$\begin{aligned} M\ddot{Q} + V'[Q(t)] =& M\xi^{(0)}[Q(t),P(t);t] - M\zeta^{(0)}[Q(t),P(t);t] \\ &+ M\int_0^t dt' \mathcal{K}_1[Q(t'),P(t');t] \\ &+ MV'[Q(t)]F''[P(t)]\gamma(0)F[P(t)] \\ &- M\mathcal{K}_2^{(0)}[Q(t),P(t');t] \\ &- M\int_0^t dt' \mathcal{K}_3[P(t),P(t')], \end{aligned} \tag{F.13}$$

for the *multiplicative* fluctuation forces

$$\xi^{(0)}[Q(t),P(t);t] = V'[Q(t)]F''[P(t)]f^{(0)}(t), \tag{F.14}$$

and

$$\zeta^{(0)}[Q(t),P(t);t] = F'[P(t)]\dot{f}^{(0)}(t), \tag{F.15}$$

the memory-functions

$$\mathcal{K}_1[Q(t),Q(t'),P(t'),P(t');t] = V'[Q(t)]F''[P(t)]\gamma_1(t-t')F'[P(t')]V'[Q(t')], \tag{F.16}$$

$$\mathcal{K}_2^{(0)}[Q(t),P(t');t] = V'[Q(t)]F''[P(t)]\gamma_1(t)F[P(0)], \tag{F.17}$$

$$\mathcal{K}_3[P(t),P(t')] = F'[P(t)]\gamma_2(t-t')F[P(t')] \tag{F.18}$$

where, analogous to the original Caldeira-Leggett approach, we have defined

$$\gamma_1(t-t') = \Theta(t-t')\sum_k \frac{C_k^2}{m_k\omega_k^2}\cos[\omega_k(t-t')], \tag{F.19}$$

and

$$\gamma_2(t-t') = \Theta(t-t') \sum_k \frac{C_k^2}{m_k} \cos[\omega_k(t-t')], \tag{F.20}$$

where the Heaviside step-function is put in by hand to ensure causality, i.e. events at times $t' > t$ do not influence at earlier times $t' < t$. The multiplicative fluctuation force in Eq. (F.15) satisfies the fluctuation-dissipation theorem in the same way as in Eq. (4.27).

This approach seems to be very promising on account of the absence of $\ddot{Q}$-terms due the equivalence of time derivatives on the momentum and the external potential, ensured by the equation of motion (F.2).

Despite these promising features, however, it is not straightforward to find a suitable Lagrangian that gives rise to this Hamiltonian. The physical problem is caused by the fact that when velocity couples to position, the simple relation $P = M\dot{Q}$ fails and the canonical momentum differs from the physical momentum of the system.

Mathematically this problem translates in the failure to find a invertible relation between the coupling function $F[P]$ in the Hamiltonian picture with its counterpart $F[\dot{Q}]$ in the Lagrangian picture. Demanding invertibility will put constraints on the generality of $F[\dot{Q}]$, leaving only even powers for a polynomial representations of it.

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