Quantum Dissipation:
A Tale in Three Acts

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The present report is an introduction to the quantum theory of dissipative systems. Dissipation is modeled by a linear coupling of the system coordinate to a collection of harmonic oscillators. This model is then treated in an imaginary time path integral formalism. The averaging over the harmonic oscillator degrees of freedom, often called 'integration of the bath', yields an effective action that completely describes the systems coupling to the environment. The remainder of the report then illustrates the physical effects of dissipation in the case of tunneling from a metastable state and in a double well potential. It is found that dissipation generally suppresses the quantum effects of tunneling and interference.

I. INTRODUCTION

Quantum mechanics has been hugely successful since its development in the beginning of the 20th century and is in excellent agreement with experiments. Nevertheless, at least one major issue remains: Many effects of quantum mechanics, such as e.g. interference, are not observed in our classical, macroscopic world. If quantum mechanics truly is a fundamental theory, it must provide an explanation as to why these effects are not observed in macroscopic contexts. Moreover, the classical limit must be derivable from the underlying quantum theory. The resulting task in the sixties was thus to find a way to maintain the validity of quantum mechanics macroscopically. A way to approach this problem is to couple the quantum system of interest to an environment.

When people first started to model the environment with extra terms in the Hamiltonian the challenge was to effectively deal with these more complicated Hamiltonians in the standard operator formalism. More effective attempts were made by using Richard Feynman's path integral formulation of quantum mechanics [1]. Feynman himself developed, together with his doctoral student Frank Vernon, an effective treatment of systems coupled to an environment with a *real time path integral* method in 1963 [2]. Twenty years later Caldeira and Leggett [3] presented a method to treat a system coupling to an environment in an *imaginary time path integral* approach, which simplified several calculations.

Since then this formulation has proven very useful to describe the behavior of a system coupled to an environment. A few examples are: a metastable state within a cubic potential (decay), oscillations within a double well potential and a treatment of dissipation for two level systems (Spin-Boson problem). The latter is of special interest in the quickly evolving field of quantum computation where one exploits quantum effects to develop new computing techniques. But most importantly, quantum dissipation gives explanations for the lack of quantum effects in our macroscopic, classical world.

We have structured our discussion of quantum dissipation into a four-course composition. The first section is focussed around describing dissipation in the quantum mechanical formalism. Its aim is to formulate the problem and present the Caldeira-Leggett model which we will use throughout the remainder of the report. In the second section we show how the path integral formalism provides a natural setting in which the effects of an environment on a quantum system can be explored. Following these two theoretical sections, we will apply the formalism to the problem of metastable decay and the double well potential in the third section. To conclude we will briefly review the principal results of this discussion and provide you with an outlook as well as a guide to the literature. We hope the topic may fascinate you as much as it fascinated ourselves and wish you 'bon appétit'!

II. INCLUDING DISSIPATION INTO QUANTUM MECHANICS

As an amuse-bouche, we will briefly review the classical treatment of dissipation. The entrée is then formed by the description of dissipation in a quantum mechanical framework along the lines of Caldeira and Leggett [4]. In essence, we will learn that dissipation can be modelled by coupling the system of interest to a collection of independent harmonic oscillators, which we call the 'heat bath' or for short 'bath'[1]. Even though such a description suggests that we need to know the microscopic properties of each oscillator, it will turn out that we can describe the bath phenomenologically with the help of a spectral density function.

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[1] We use the terms environment, bath and heat bath synonymously.

A. What is Dissipation?

Before we can include dissipation into the formalism of quantum mechanics, we must first define more precisely what this term means. In this paper we will understand dissipation as loss of energy to environmental degrees of freedom, that is degrees of freedom in which we are not directly interested. To form an idea of how a phenomenon like this could be integrated into quantum mechanics, it pays off to first review its classical treatment. In classical physics we describe dissipative effects with an equation of motion akin to

$$M\ddot{q} + \frac{\mathrm{d}V}{\mathrm{d}q} + \eta\dot{q} = 0, \tag{1}$$

where q is the generalized system coordinate, M a mass parameter and η a damping parameter. The dissipation is encoded in this equation through the third term, which depends linearly on the generalized velocity. Such an equation of motion can describe a damped pendulum or an RLC circuit for instance. If we add a fluctuating force $\xi(t)$ to the right side of this equation it can be used to model not only the damped average motion of a system but also fluctuations around it. This generalized, stochastic equation is known as *Langevin equation* [5] and is used for example to describe Brownian motion or thermal noise in a resistor. It is important to note that the inclusion of dissipation in this equation is purely phenomenological. There is no mention of the microscopic mechanisms that produce the friction or fluctuations. They are hidden in η and $\xi(t)$ respectively. This allows us to treat dissipation without knowing the microscopic details of all the interactions that produce it.

To find a quantum mechanical description of dissipation one needs to take more care. A major difficulty is that the quantum mechanical formalism ensures energy conservation if the Hamiltonian is not explicitly time dependent. Several approaches have been developed to circumvent this problem. A particularly successful and quite general approach began with the seminal work of Caldeira and Leggett [4] and has proven fruitful for numerous theoretical investigations on the effect of an environment on a quantum mechanical system. We will focus our discussion on this approach, which is known as the *Caldeira-Leggett Model*.

B. The Caldeira-Leggett Model

1. The Main Idea

In the Caldeira-Leggett model one looks at the total system which includes the environment and the system of interest as shown in Figure (1). The total system is described quantum mechanically with a time independent Hamiltonian, so the total energy is conserved. As a model for the bath we choose a collection of N quantum harmonic oscillators which are not coupled to each other.

This choice makes sense for two reasons. The first reason is a practical one. A harmonic oscillator is one of the few systems that can be treated analytically in quantum mechanics and will greatly simplify calculations later on. The second reason is physical. If the temperature of the heat bath is not too high, that is if the energy in the heat bath is sufficiently 'dilute' that each individual environmental degree of freedom carries just a slight amount of energy, we can approximate these degrees of freedom locally around their potential minimum. Such an approximation leads to harmonic oscillators at leading order. Finally, we choose the coupling between the system and
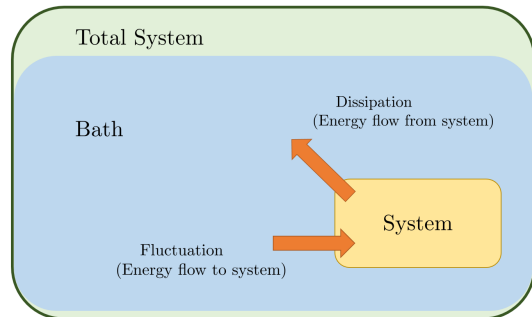

Figure 1. Illustration of the Caldeira-Leggett Model. The total system (system + bath) is described quantum mechanically and the energy of the total system is conserved. The environment (bath) is modeled as a collection of harmonic oscillators that are not coupled to each other. A linear coupling between system and environment enables energy transfer.

the bath to be linear in both the system and the bath coordinates. This comes again mainly from a practical consideration: as we will learn for a linear coupling we can integrate out the individual bath coordinates [2]. One can then write down the *Caldeira-Leggett Hamiltonian* as follows

$$\mathcal{H}_{CL} = \underbrace{\frac{p^2}{2M} + V(q)}_{\mathcal{H}_S} + \underbrace{\sum_{i=1}^{N}\left(\frac{p_i^2}{2m_i} + \frac{m_i}{2}\omega_i^2 x_i^2\right)}_{\mathcal{H}_B}$$
$$- \underbrace{q\sum_{i=1}^{N}c_i x_i + q^2\sum_{i=1}^{N}\frac{c_i^2}{2m_i\omega_i^2}}_{\mathcal{H}_{SB}}. \tag{2}$$

In this expression q, p are the generalized system coordinate and momentum, M is a mass parameter and x_i, p_i are the generalized coordinates and momenta of the individual harmonic oscillators in the bath. The m_i and ω_i specify the properties of each bath mode and the c_i

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[2] In fact, to carry out the 'integration of the bath' it is sufficient for the coupling to be linear in the bath coordinates only, but the resulting expressions become more tedious to work with. We will not pursue this approach further.

are coupling constants. Note that the bath Hamiltonian is the sum of N independent harmonic oscillators, as described above. The system-bath interaction is contained in the $\mathcal{H}_{\text{SB}}$ part of the Hamiltonian. This consists of a bilinear coupling between the system and the oscillator modes (first term) and a counter term (second term) that is added to prevent a renormalization of the system potential V. If it were not present, the coupling to the oscillators would shift the extremum of the potential. It is important to note that this counter term does not couple the coordinates q and x_i.

2. The Classical Limit

To see that the Hamiltonian (2) produces the familiar effects of dissipation and fluctuation in our system, we have to convince ourselves that the equations of motion from this Hamiltonian reduce to the Langevin equation in the classical limit. We start with the Heisenberg equation of motion $\frac{\mathrm{d}A}{\mathrm{d}t} = (i/\hbar)[\mathcal{H}, A]$ to find the equations of motion for the operators q and x_i,

$$\text{System E.O.M} \quad M\ddot{q} + \frac{\mathrm{d}V}{\mathrm{d}q} + q\sum_i \frac{c_i^2}{m_i\omega_i} = \sum_i c_i x_i \tag{3}$$

$$\text{Bath E.O.M} \quad \ddot{x}_i + \omega_i^2 x_i = \frac{c_i}{m_i}q \tag{4}$$

Note that the bath equations of motion (4) are those of a driven harmonic oscillator. If we assume q to be given, we can formally solve these equations for given initial conditions[3]. Doing so and plugging the solution for $x_i(t)$ into the system equation of motion (3) yields

$$M\ddot{q} + \frac{\mathrm{d}V}{\mathrm{d}q} + \int_0^t \mathrm{d}s\,\gamma(t-s)\dot{q}(s) = \xi(t), \tag{5}$$

where the damping kernel γ is defined as

$$\gamma(t) = \sum_i^N \frac{c_i^2}{m_i\omega_i^2}\cos(\omega_i t) \tag{6}$$

and the function $\xi(t)$ represents a fluctuating force that depends on the initial conditions of the bath and system coordinates. The equilibrium expectation value of this fluctuating force vanishes [6].

Up to now we have worked with finitely many bath modes. If for example the system is also a harmonic oscillator, we can use a normal mode representation to convince ourselves that the system will return to its initial state after a possibly long, but finite, amount of time. More generally, this phenomenon is known as *Poincaré Recurrence* and leads to trouble if we want to actually describe dissipation [6]. Luckily, there is a way around this problem. We can assume a continuous distribution of bath modes and take the limit $N \to \infty$.

In order to make the above description useful even if we do not have a microscopic model of our bath it is convenient to define the spectral density of bath modes

$$J(\omega) \equiv \frac{\pi}{2}\sum_i \frac{c_i^2}{m_i\omega_i}\delta(\omega - \omega_i). \tag{7}$$

This spectral density is a phenomenological quantity that contains information about the bath modes and their coupling to the system and is sufficient to characterize the heat bath [6]. In practice, one works by specifying a choice for the spectral density $J(\omega)$ without explicitly giving all c_i, ω_i and m_i. An important spectral density, with which we will work with throughout this paper, is the so called *ohmic* density $J(\omega) = \eta\omega$. Note that a truly ohmic bath is not physical, since an integration over all bath modes would lead to an infinite amount of energy contained in the bath. In practice, to evade this so called UV-catastrophe one defines a cut-off frequency after which the functional dependence of the spectral density drops to 0 quickly.

Having defined the spectral density we rewrite the damping kernel as

$$\gamma(t) = \frac{2}{\pi}\int_0^\infty \mathrm{d}\omega\,\frac{J(\omega)}{\omega}\cos(\omega t). \tag{8}$$

For ohmic damping we can evaluate this damping kernel and find $\gamma(t) = 2\eta\delta(t)$. Inserting this in Eq. (5) we find the operator equation of motion for strictly ohmic dissipation

$$M\ddot{q} + \frac{\mathrm{d}V}{\mathrm{d}q} + \eta\dot{q} = \xi(t). \tag{9}$$

The form of this equation is equivalent to Langevin's equation. Indeed, with the use of *Ehrenfest's Theorem* we see that the Caldeira-Leggett Hamiltonian reproduces the phenomenological equation of motion describing dissipation (1) in the classical limit. This is an indication that the Caldeira-Leggett Hamiltonian allows us to generalize dissipation to a quantum system.

3. In a Nutshell

Before we proceed and learn how to effectively work with this formalism, let us pause a moment to recapitulate what we have learned. The essential idea of the

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[3] The solution is

$$x_i(t) = x_i(0)\cos(\omega_i t) + \frac{p_i(0)}{m_i\omega_i}\sin(\omega_i t) + \int_0^t \mathrm{d}s\,\frac{c_i}{m_i\omega_i}\sin(\omega_i(t-s))q(s).$$

Caldeira-Leggett model is that we couple the system to an environment represented by quantum harmonic oscillators. The physics of dissipation and fluctuation is then obtained from an energy flow between the system and bath. We saw that due to *Poincaré Recurrence* it makes sense to assume a continuous distribution of bath modes, which we describe phenomenologically by the spectral density. This is useful because it frees us from having to specify the properties of each environmental degree of freedom individually. Finally, we convinced ourselves that we can recover the *Langevin equation* in the classical limit. Of course not every dissipative system can be described by such a Hamiltonian, but this model gives a good effective description for a wide variety of systems, and maybe equally important, it allows for analytical treatment.

III.   QUANTUM DISSIPATION WITHIN THE PATH INTEGRAL FORMALISM

We now come to the first main course. In this section we will study the time evolution of density matrix elements of an arbitrary system coupled to an environment at thermal equilibrium. As a result we will be able to express these matrix elements through the so called *effective action* $\mathcal{S}_{\text{eff}}$ which contains all the information about the environment.

$$\rho_\beta(q, q') = \frac{1}{Z} \int \mathcal{D}\bar{q} \exp\left[-\frac{1}{\hbar}\mathcal{S}_{\text{eff}}[\bar{q}]\right] \qquad (10)$$

This is one of the principal results of the formalism introduced by Caldeira and Legget in 1981 [4] and will be derived below in the path integral formalism in *imaginary time*. The special thing to note is that the effective action is *independent* of the coordinates x_i of the individual oscillators in the bath. The reason for this is that the formula arises from an averaging process over all the bath modes which is known in the literature as *integration of the bath*. Also note that in contrast to the previous section, in which we worked within the operator formalism of quantum mechanics, in the path integral formalism we deal with scalar functions instead.

A.   Introduction to the Formalism

Before we actually start to work with dissipation let us introduce some concepts[4] starting with the *density matrix*. As we know from thermodynamics, the probability

to find a system in the n-th energy eigenstate in thermal equilibrium[5] is given by

$$\mathbb{P}_n = \frac{1}{Z_\beta}e^{-\beta E_n} \qquad (11)$$

where Z_β denotes the system partition function and $\beta = (k_B T)^{-1}$ with k_B the Boltzmann constant and T the temperature. The partition function is defined as $Z_\beta = \text{tr}\left(e^{-\beta H}\right)$. In analogy we define the density matrix of a system in thermal equilibrium as

$$\rho_\beta(q, q') = \frac{1}{Z_\beta}\langle q\,|\exp\left(-\mathcal{H}\beta\right)|\,q'\rangle. \qquad (12)$$

and state that the probability of a system being in state $|q\rangle$ at time t is given by $\rho_\beta(q, q, t)$.[6] From previous chapters of this proseminar we know that the above matrix element can be obtained by performing a Wick rotation. We then called this modified path integral imaginary time path integral and find

$$\rho_\beta(q, q', t) \;=\; \frac{1}{Z_\beta} \int_{\bar{q}(0)=q}^{\bar{q}(t)=q'} \mathcal{D}\bar{q} \exp\left(-\frac{1}{\hbar}\mathcal{S}^E[\bar{q}]\right). \qquad (13)$$

Here we use barred variables ($\bar{q}$) to represent paths. A path evaluated at a certain time corresponds to a certain value of the associated variable (e.g. $\bar{q}(t) = q$). $\mathcal{S}^E$ denotes the euclidean action obtained from the classical action by performing a Wick rotation. The euclidean action can be found by inverting the potential (i.e. $V \mapsto -V$) which leads to

$$\mathcal{S}^E = \int d\tau\, \mathcal{L}^E(q, \dot{q}, \tau) = \int d\tau\,(T + V) \qquad (14)$$

with $\mathcal{L}$ the euclidean Lagrangian, T the kinetic energy and V the potential energy. Note that the effective action equals to the imaginary time integral over the Hamiltonian (2).

B.   Formulation of the Problem

Knowing the density matrix for every time is equivalent to knowing the time evolution of the system. From the Hamiltonian (2) we can directly obtain the euclidean action:

$$\mathcal{S}^E[\bar{q}, \{\bar{x}_i\}] = \mathcal{S}_{\text{S}}^E[\bar{q}] + \mathcal{S}_{\text{B}}^E[\{\bar{x}_i\}] + \mathcal{S}_{\text{SB}}^E[\bar{q}, \{\bar{x}_i\}] \qquad (15)$$

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[4] We do not claim to provide an extensive introduction. To get a thorough understanding of the involved concepts a study of the literature is highly advised. Interested readers are referred to [7] and references therein.

[5] It turns out that beeing in thermal equilibrium does not constrain our system in any way since this is only a statistical condition. Furthermore, it is a requirement for our environment to be in thermal equilibrium.

[6] Note that this is even true if $|q\rangle$ does not represent the energy eigenbasis. In fact we will use $|q\rangle$ as a position eigenstate.

with[7]

$$\mathcal{S}_{\text{S}}^{E}[\bar{q}] = \int_{0}^{\hbar\beta} d\tau \left[\frac{M}{2} \dot{\bar{q}}^{2} + V(\bar{q}) \right] \quad (16)$$

$$\mathcal{S}_{B}^{E}[\{\bar{x}_{i}\}] = \int_{0}^{\hbar\beta} d\tau \sum_{i=1}^{N} \frac{m_{i}}{2} \left(\dot{\bar{x}}_{i}^{2} + \omega_{i}^{2}\bar{x}_{i}^{2} \right) \quad (17)$$

$$\mathcal{S}_{\text{SB}}^{E}[\bar{q}, \{\bar{x}_{i}\}] = \int_{0}^{\hbar\beta} d\tau \left[-\bar{q} \sum_{i=1}^{N} c_{i}\bar{x}_{i} + \bar{q}^{2} \sum_{i=1}^{N} \frac{c_{i}^{2}}{2m_{i}\omega_{i}^{2}} \right]. \quad (18)$$

Besides plugging this action into (13) we have to integrate over the coordinates of the system (q) and the bath ones ($\{x_{i}\}$)[8]. This leads to a density matrix for the total system

$$W_{\beta}(q, \{x_{i}\}, q', \{x'_{i}\}) = \quad (19)$$

$$\frac{1}{Z_{\beta}} \int_{\bar{q}(0)=q}^{\bar{q}(\hbar\beta)=q'} \mathcal{D}\bar{q} \int_{\bar{x}_{i}(0)=x_{i}}^{\bar{x}_{i}(\hbar\beta)=x'_{i}} \{\mathcal{D}\bar{x}_{i}\} \exp\left(-\frac{1}{\hbar} \mathcal{S}[\bar{q}, \{\bar{x}_{i}\}] \right).$$

Since we only care about the behaviour of our system, the time evolution of the bath is not of interest for us. Furthermore we do not want to be forced to choose the bath explicitly to get a density matrix element for our system. Somehow we have to deal with these degrees of freedom. The most convenient way is to average them out, i.e. we take the expected influence of each bath oscillator on the system. This procedure is called tracing out, which means one takes the trace over the bath coordinates to get to the so called reduced density matrix of a system

$$\rho_{\beta}(q, q', t) = \text{tr}_{\text{B}}(W_{\beta}(q, \{x_{i}\}, q', \{x'_{i}\}, t)).$$

We may write the trace as an integral over all possible values of x_{i} for each bath oscillator. Translated into the path integral formalism we obtain for (13)

$$\rho_{\beta}(q, q', t) = \frac{1}{Z_{\beta}} \int_{\bar{q}(0)=q}^{\bar{q}(\hbar\beta)=q'} \mathcal{D}\bar{q} \int_{-\infty}^{\infty} \{dx_{i}\}$$

$$\times \oint_{\bar{x}_{i}(0)=x_{i}}^{\bar{x}_{i}(\hbar\beta)=x_{i}} \{\mathcal{D}\bar{x}_{i}\} \exp\left(-\frac{1}{\hbar} \mathcal{S}[\bar{q}, \{\bar{x}_{i}\}] \right). \quad (20)$$

The circled integral indicates a closed integration. An important remark here, since we are taking the trace over the bath degrees of freedom, we are only considering closed paths (i.e. paths with the same initial and final value). We aim to perform these integrations for arbitrary systems, but first we will reformulate the problem

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[7] From now on we will drop the label E for euclidean.
[8] Whenever we use brackets {} we mean a set of variables.

in a more structured way. The reduced density matrix can be rewritten in a more compact form as

$$\rho_{\beta}(q, q', t) = \frac{1}{Z} \int \mathcal{D}\bar{q} \exp\left(-\frac{1}{\hbar} \mathcal{S}_{S}[\bar{q}] \right) F[\bar{q}]. \quad (21)$$

Here Z stands for the partition function of only our system and $\mathcal{S}_{S}$ is the system action (16). Additionally we introduced the influence functional $F[\bar{q}]$ which represents the influence of the environment on the system. We can decompose it in the form

$$F[\bar{q}] = \prod_{i=1}^{N} \frac{1}{Z_{i}} F_{i}[\bar{q}] \quad (22)$$

with Z_{i} the partition function of a single bath oscillator and $F_{i}[\bar{q}]$ the influence of a single oscillator. The influence of a single oscillator explicitly reads as

$$F_{i}[\bar{q}] = \int dx_{i} \oint \mathcal{D}\bar{x}_{i} \exp\left(-\frac{1}{\hbar} \mathcal{S}_{i}[\bar{q}, \bar{x}_{i}] \right) \quad (23)$$

and

$$\mathcal{S}_{i}[\bar{q}, \bar{x}_{i}] = \int_{0}^{\hbar\beta} d\tau \frac{m_{i}}{2} \left[\dot{\bar{x}}_{i}^{2} + \omega_{i}^{2} \left(\bar{x}_{i} - \frac{c_{i}}{m_{i}\omega_{i}^{2}} \bar{q} \right)^{2} \right] \quad (24)$$

The problem of finding the density matrix of an arbitrary system is now reduced to determining the influence functional $F[\bar{q}]$, which is known as the *integration of the bath*.

C. Integration of the Bath

First of all one has to deal with the paths appearing in the action (24). We recall that these paths $\bar{x}_{i}$ have to be closed as a consequence of taking the trace. After a periodic continuation we can think of them as being periodic functions and expand them in a Fourier series. We do the same also for the paths $\bar{q}$ even though these paths do not have to be periodic. Consequently this derivation of the density matrix elements only holds for the diagonal elements where the periodicity condition also holds for $\bar{q}$. However, these will be the only restriction needed in the further discussion. The Fourier expansions read

$$\bar{x}_{i}(\tau) = \sum_{n} x_{i,n} e^{i\nu_{n}\tau} \quad (25)$$

$$\bar{q}(\tau) = \sum_{n} q_{n} e^{i\nu_{n}\tau} \quad (26)$$

with $\nu_{n} = \frac{2\pi}{\hbar\beta} n$. Since $\bar{x}_{i}(\tau)$ represents a real function (path) it holds that $x_{i,-n} = x_{i,n}^{*}$. Inserting these Fourier expansions into (24) leads to:

$$\mathcal{S}_{i} = \hbar\beta \sum_{n} \frac{m_{i}}{2} \left[\nu_{n}^{2}|x_{n}|^{2} + \omega_{i}^{2} \left| x_{n} - \frac{c_{i}}{m_{i}\omega_{i}^{2}} q_{n} \right|^{2} \right]. \quad (27)$$

Here we have used that $\int_0^{\hbar\beta} d\tau\, e^{i\tau(\nu_n + \nu_{n'})} = \hbar\beta\delta_{n,-n'}$, due to the orthogonality of $e^{i\nu_n\tau}$. The ν_n^2 factor results from the derivative and one observes that $|x_n|^2 = x_{i,n} \cdot x_{i,-n}$. Similarly the second term in the sum of (27) is obtained since the period of $\bar{q}(\tau)$ has to be the same as the one of $\bar{x}_i(\tau)$. Next we perform a *semi-classical approximation*.

$$S_i(\bar{x}_i) = S_i(\bar{x}_i^{\text{cl}}) + \frac{1}{2}\bar{y}_i \left.\frac{\partial^2 S_i}{\partial\bar{x}_i^2}\right|_{\bar{x}_i = \bar{x}_i^{\text{cl}}} \bar{y}_i \qquad (28)$$

$\bar{x}_i^{\text{cl}}$ denotes the classical path and $\bar{y}_i$ is a perturbation around the classical path. The action has a stationary point at this path, which is why the first functional derivative does not appear in (28). Since the action (24) is at most quadratic in $\bar{x}_i$ the above expression is not an approximation but rather correct. Deriving the Euler-Lagrange equations for our Lagrangian [9] leads to

$$\ddot{\bar{x}}_i - \omega_i^2 \bar{x}_i = -\frac{c_i}{m_i}\bar{q}. \qquad (29)$$

Inserting the Fourier series Ansatz leads to a relation between the Fourier series coefficients of $x_{n,i}$ and q_n.

$$x_{n,i}^{\text{cl}} = \frac{c_i}{m_i(\nu_n^2 + \omega_i^2)}q_n \qquad (30)$$

With $\bar{x}_i = \bar{x}_i^{cl} + \bar{y}_i$ which directly translates to the same statement for the Fourier series coefficients, we are able to express (27) trough the classical path and the perturbation.

$$S_i[\bar{x}_i^{\text{cl}} + \bar{y}_i, \bar{q}] = \qquad (31)$$
$$\hbar\beta \sum_n \frac{c_i^2}{2m_i}|q_n|^2 \left(\frac{1}{\omega_i^2} - \frac{1}{\nu_n^2 + \omega_i^2}\right) + \hbar\beta \sum_n \frac{m_i}{2}\omega_i^2|y_n|^2.$$

This equation can be found after performing some algebra and neglecting all terms linear in y_n since we already know from (28) that they have to sum up to zero. The first sum corresponds to the classical action and the second to the perturbation around the classical path respectively. Additionally having replaced the bath coordinates x_i trough system coordinates q, the only thing that we are left to deal with is the perturbation term

$$S_{\text{int}} = \hbar\beta \sum_i \sum_n \frac{c_i^2}{2m_i}|q_n|^2 \left(\frac{1}{\omega_i^2} - \frac{1}{\nu_n^2 + \omega_i^2}\right) \qquad (32)$$

$$S_{\text{pert}} = \hbar\beta \sum_i \sum_n \frac{m_i}{2}\omega_i^2|y_n|^2. \qquad (33)$$

Recalling that the c_i are the coupling constants, if we set these constants to zero this means that the bath is not coupled to the system at all, i.e. there is no influence of

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[9] The Lagrangian is the integrand in (24).

the bath on the system. Going back to (21) we see that if the bath has no influence on the system, the influence functional $F[\bar{q}]$ has to reduce to one. Since $S_{\text{int}} = 0$ for $c_i = 0$ the action in (23) reduces to $S = S_{\text{pert}}$ which is independent of q. This allows us to do the integration in (23) over S_{pert} independently of the choice of the system. Furthermore this solution is already known, Z_i is just the partition function of a harmonic oscillator. Consequently the perturbation part of the influence equals to the product of the bath oscillator partition functions, i.e. the integration over the perturbation part cancel with the product of the partition functions.

We have now arrived at an expression for the influence functional

$$F[\bar{q}] = \prod_{i=1}^N \int dx_i \oint \mathcal{D}\bar{x}_i \exp\left(-\frac{1}{\hbar}S_{int}\right) \qquad (34)$$

which is only dependent on the interaction action S_{int}. Unfortunately the interaction action is not in a simple form yet. Our aim is to express it as a function of the path $q(\tau)$ in a compact form. As the next step we do the "reverse" Fourier series expansion, i.e. we plug in the definition of the Fourier series coefficients into our action. They are defined as

$$q_n = \frac{1}{\hbar\beta}\int_0^{\hbar\beta} d\tau e^{-i\nu_n\tau}q(\tau). \qquad (35)$$

Using the Fourier series from the delta function and defining a function $K(\tau)$

$$\delta(\tau - \tau') = \frac{1}{\hbar\beta}\sum_n e^{i\nu_n(\tau - \tau')} \qquad (36)$$

$$K(\tau) = \sum_i \frac{c_i^2}{m_i\hbar\beta}\sum_n \frac{e^{i\nu_n\tau}}{\nu_n^2 + \omega_i^2} \qquad (37)$$

we may rewrite (32) as

$$S_{\text{int}} = \sum_i \frac{c_i^2}{2m_i\omega_i^2}\int_0^{\hbar\beta} d\tau q(\tau)^2$$
$$- \int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau d\tau' K(\tau - \tau')q(\tau)q(\tau'). \qquad (38)$$

Realizing that

$$\int_0^{\hbar\beta} d\tau\, K(\tau) = \frac{1}{2}\sum_i \frac{c_i^2}{m_i\omega_i^2} \qquad (39)$$

allows us to rewrite S_{int} as

$$S_{\text{int}} = \qquad (40)$$
$$\frac{1}{4}\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau d\tau' K(\tau - \tau')(q(\tau) - q(\tau'))^2.$$

Basically we are now done; we have succeeded in finding a compact expression for the system-environment interaction action. The difference of a system coupled to

external degrees of freedom compared with an isolated one, is given by a modification of the action within the path integral approach. In the coupled case, the action is defined as [10]

$$\mathcal{S}_{\text{eff}} = \mathcal{S}_{\text{S}} + \mathcal{S}_{\text{int}}. \tag{41}$$

The form of the interaction action (40) gives rise to an interesting feature of coupled systems. The double time integral within the definition of this action leads to a so called *non-local term*. But what does it mean for a term being *non-local*?

When studying a system, one approach is to do a semi-classical approximation, where we fluctuate around a classical path. Applying the Euler- Lagrange equations to obtain the classical path results in general to

$$M\ddot{q}(\tau) = \tag{42}$$
$$\frac{\partial}{\partial q}V(q(\tau)) + \frac{1}{2}\int_0^{\hbar\beta} \mathrm{d}\tau'\, K(\tau-\tau')(q(\tau) - q(\tau')).$$

The solution for the classical path at a certain time depends on the solutions at later or earlier times, since the second time derivative of q directly depends of the integration over one whole period of q. We call this integration appearing in the Euler-Lagrange equation a non- local term. Physically speaking we see *self interaction* of the system. Earlier states affect states at later time and vice versa. This self interaction is realized trough the coupling to an environment which serves as an energy reservoir. This means energy may flow from the system to the environment and then re-excite the system at later times. It is also possible that energy flows from the environment to the system right at the start[11].

The only thing that we still need to treat in (40) is the function $K(\tau)$ since it is directly dependent on the oscillator frequencies, their masses and coupling constants. In most cases one is not able to model these constants directly. Therefore we again make use of the spectral density introduced in (7). Instead of modeling every single oscillator, we think of them as if they where distributed according to the spectral density $J(\omega)$. A relation between $K(\tau)$ and $J(\omega)$ would simplify our problem substantially. Observing that the second sum in the definition of $K(\tau)$ (37) can be considered as an Fourier series expansion, we have

$$K(\tau) = \frac{1}{2}\sum_i \frac{c_i^2}{m_i\omega_i} \cdot \frac{\cosh\left(\omega\left[\frac{\hbar\beta}{2} - |\tau - \tau'|\right]\right)}{\sinh\left(\omega\frac{\hbar\beta}{2}\right)} \tag{43}$$

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[10] In the uncoupled case, $\mathcal{S}_{\text{int}}$ is just zero.

[11] This case would then be the opposite of dissipation. Although we aim to discuss dissipation we include this process of excitation when we talk about quantum dissipation generally. In our diagram in Figure 1 such processes are indicated by the *fluctuation* arrow.

here we now recognize that replacing the sum with $J(\omega)$ and subsequent integration over ω yield to the exact expression for $K(\tau)$.

$$\mathcal{S}_{\text{int}}^E = \frac{1}{4\pi}\int_0^{\hbar\beta}\int_0^{\hbar\beta}\mathrm{d}\tau\mathrm{d}\tau' \tag{44}$$
$$\times \int_0^\infty \mathrm{d}\omega J(\omega)\frac{\cosh\left(\omega\left[\frac{\hbar\beta}{2} - |\tau - \tau'|\right]\right)}{\sinh\left(\omega\frac{\hbar\beta}{2}\right)} \cdot (q(\tau) - q(\tau'))^2$$

This is the most general form for the interaction action for such an environment. Considering ohmic damping $J(\omega) = \eta\omega$ one can actually perform the integration over ω analytically and obtain

$$\mathcal{S}_{\text{int}} = \tag{45}$$
$$\frac{\eta}{4\pi}\int_0^{\hbar\beta}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{d}\tau'\left(\frac{\pi}{\hbar\beta}\right)^2\frac{(q(\tau) - q(\tau'))^2}{\sin^2\left(\frac{1}{\hbar\beta}|\tau - \tau'|\right)}.$$

Which finally enables us to write the density matrix elements in the desired form as

$$\boxed{\rho_\beta(q,q') = \frac{1}{Z}\int\mathcal{D}\bar{q}\exp\left[-\frac{1}{\hbar}\mathcal{S}_{\text{eff}}[\bar{q}]\right].} \tag{46}$$

This section not only presented a way to calculate the density matrix elements, it also showed how to characterize coupled systems through an effective action $\mathcal{S}_{\text{eff}} = \mathcal{S}_S + \mathcal{S}_{\text{int}}$ with

$$\mathcal{S}_{\text{eff}}[\bar{q}] = \int_0^{\hbar\beta}\mathrm{d}\tau\left[\frac{M}{2}\dot{\bar{q}}^2 + V(\bar{q}) + \right.$$
$$\left.\frac{\eta}{4\pi}\int_0^{\hbar\beta}\mathrm{d}\tau'\left(\frac{\pi}{\hbar\beta}\right)^2\frac{(\bar{q}(\tau) - \bar{q}(\tau'))^2}{\sin^2\left(\frac{\pi}{\hbar\beta}|\tau - \tau'|\right)}\right] \tag{47}$$

for ohmic systems. It is quite remarkable that it is possible to condense the complex process of exchanging energy between a system and an environment with infinitely many degrees of freedom in such a concise way. But even more surprising is the fact that the above derivation is completely general for every potential and it is non- perturbative. Furthermore we saw that coupling a system to an environment leads to a non-local term and therefore enables self interaction.

IV. APPLICATIONS OF THE FORMALISM

In the previous section we have learned that coupling to a bath of harmonic oscillators can be treated within the path integral formalism by adding an extra term, the interaction term $\mathcal{S}_{\text{int}}$, to the action. We now turn our attention to the physics that arises from this modified action. More specifically, we will look at the cubic and quartic potentials discussed in previous chapters of this proseminar and see how the interaction action affects the system's behavior.

A. Decay from a Metastable State

As a first example, we investigate tunneling from a metastable state under the influence of ohmic damping. The principal goal of this example is to find the decay rate Γ in a semi-classical approximation and to compare it with the decay rate in the case of no damping.

Our metastable system is modeled by a cubic potential of the form,

$$V(q) = \frac{27}{4}V_0 \left(\frac{q}{a}\right)^2 \left(1 - \frac{q}{a}\right) \tag{48}$$

where a is the width and V_0 the height of the potential barrier.
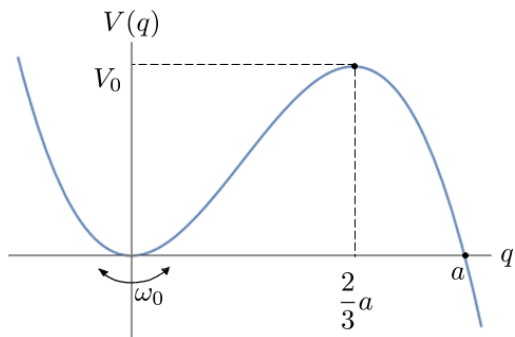
Figure 2. Cubic potential with a potential barrier of width a and height V_0. The frequency of small oscillations around the metastable minimum at $q = 0$ is $\omega_0 = \sqrt{27V_0/(Ma^2)}$.

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For later convenience we define ω_0 as the frequency of small oscillations around the metastable minimum at the origin.

In the previous chapter it was shown that the decay rate of such a cubic system is given by

$$\Gamma \equiv \frac{2\,\mathrm{Im}(E)}{\hbar} \propto A\exp\left(-\frac{\mathcal{S}_{\text{eff}}[q_b]}{\hbar}\right). \tag{49}$$

Here q_b was the so called *bounce solution* of the Euclidean equations of motion that was associated with a negative eigenvalue of the fluctuation operator and A is the fluctuation determinant of this solution. It is this negative eigenmode that gives rise to the imaginary part in the energy after an analytic continuation and hence this solution is responsible for the decay of the system[12]. Using this result, we devise the following plan of attack for our problem:

1. Find the effective action of the system and the Euclidean equations of motion that follow from it.

2. Solve the Euclidean equations of motion to find the modified bounce solution $q_b(\tau)$.

3. Calculate the bounce action $\mathcal{S}_{\text{eff}}[q_b]$ to obtain the exponential factor in the decay rate Γ.

Let us start with the first step. To simplify calculations and make the physics more visible, we make the following assumptions:

- **Ohmic environment:** $J(\omega) = \eta\omega$. This is the simplest spectral density for a bath. It is also one of the few cases that can be treated analytically. The physical interpretation of such an environment was discussed in detail in section I.

- **Zero Temperature $T = 0$:** This is equivalent to taking the limit $\beta \to \infty$ and allows us to work with Fourier transforms instead of Fourier Series. We will relax this condition at the end of the section.

Using these two assumptions, we find that the effective (Euclidean) action with ohmic damping (47) takes the form

$$\mathcal{S}_{\text{eff}}[\bar{q}] = \int_{-\infty}^{\infty} d\tau \left[\frac{M}{2}\dot{\bar{q}}^2 + V(\bar{q})\right.$$
$$\left. + \frac{\eta}{4\pi}\int_{-\infty}^{\infty} d\tau' \left(\frac{\bar{q}(\tau) - \bar{q}(\tau')}{\tau - \tau'}\right)^2\right]. \tag{50}$$

From here we can already draw an important qualitative conclusion. The interaction term in Eq. (50) is positive definite. Thus in the small damping limit ($\eta \to 0$), where the classical bounce trajectory q_b is not changed to first order in η, the damped action is always larger than the undamped action [13]. This means that the decay rate Γ is exponentially suppressed, compared to the undamped case. In fact, this holds quite generally at low temperatures and we can say as a rule of thumb that coupling to an environment *exponentially suppresses quantum tunneling* [3].

Let us proceed with our calculation. To find the decay rate in a semi-classical approximation we must find the classical paths, that is the stationary points, of the effective action. Using the Euler-Lagrange equations, we find the Euclidean equation of motion for the classical paths $q(\tau)$ [14]

$$M\ddot{q} = V'(q) + \frac{\eta}{2\pi}\fint_{-\infty}^{\infty} d\tau' \frac{q(\tau) - q(\tau')}{(\tau - \tau')^2}. \tag{51}$$

The bar in the integral signifies that it is to be understood as Cauchy principal value. This integro-differential

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[12] For an excellent treatment of the undamped problem with instanton methods see also [7] and [8].

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[13] Later we will see that this holds for any η.

[14] For readability we have dropped the subscript cl and the bar for this example.

equation is difficult to solve and has to be treated numerically in general. But we can nonetheless learn about some of the relevant physics by taking the limits $\eta \to 0$ or $\eta \to \infty$. In the subsequent paragraph we will concentrate on the latter case and only state the underdamped limit for comparison at the end. We refer to literature for a more detailed treatment of the former case [9]. This concludes the first step of our plan.

1. Overdamped limit ($\eta \to \infty$)

In the overdamped limit we can expand q perturbatively in $1/\eta$ and look at the leading order for a first approximation. We also assume that $V_0 \sim \eta$, such that we do not lose the effect of the potential altogether. In this regime we find at leading order in η,

$$\mathcal{O}(\eta): \quad 0 = V'(q) + \frac{\eta}{\pi} \fint_{-\infty}^{\infty} \mathrm{d}u \, \left. \frac{\partial q}{\partial \tau} \right|_u \frac{1}{u - \tau} \qquad (52)$$

Here the integral term from Eq. (51) has been rewritten using the fundamental theorem of calculus and a change of the integration order, after which the $\mathrm{d}\tau'$ integration can be performed explicitly.

To find the nontrivial (bounce) solution of this differential equation we note that the integral term is nothing but a convolution. So after inserting our potential and taking the Fourier transform of Eq. (52) we find an equation for $\hat{q}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\tau \, q(\tau) \exp(i\omega\tau)$ in Fourier space[15]

$$0 = M\omega_0^2 \left[\hat{q}(\omega) - \frac{3}{2} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \hat{q}(\omega')\hat{q}(\omega - \omega') \right] + \eta|\omega|\hat{q}(\omega). \tag{53}$$

This equation can be solved by the Ansatz[16]

$$\hat{q}(\omega) = \hat{q}_0 \exp\left(-\frac{|\omega|}{\omega_b} \right). \tag{54}$$

Explicitly inserting this Ansatz into Eq. (53) yields the parameters $\hat{q}_0$ and ω_b. With an inverse Fourier transform we find that the overdamped bounce action in (imaginary) time is given by

$$q_b(\tau) = \frac{(4/3)a}{1 + (\omega_b\tau)^2} \tag{55}$$

$$\omega_b = \frac{\omega_0}{\gamma} \tag{56}$$

$$\gamma = \frac{\eta}{M\omega_0}, \tag{57}$$

---

[15] We used the relations $\widehat{1/\tau} = i\pi\,\mathrm{sgn}(\omega)$, $\widehat{\partial_\tau q} = -i\omega\hat{q}$ and the convolution theorem.

[16] One can guess this Ansatz for example from asymptotic considerations of Eq. (51) from which it follows that $q \sim 1/\tau^2$ for $|\tau|$ large. This fall-off hints at a Lorentzian line shape and thus one could try a Lorentzian Ansatz for $q(\tau)$. Hearteningly, our Ansatz is just the Fourier transform of a Lorentzian.

where we have defined the dimensionless damping parameter γ and the bounce frequency ω_b. Let us take a moment to dwell on this solution and look at the physics it encapsulates.
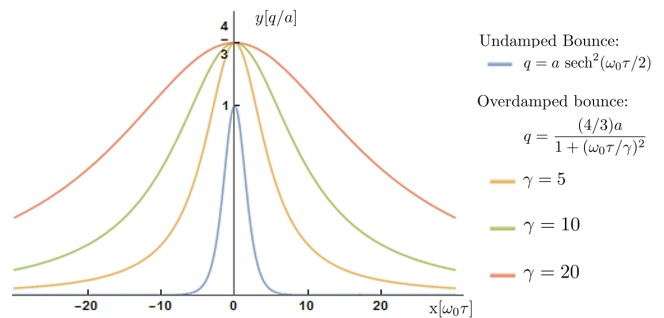
First of all we see that the overdamped bounce

Figure 3. The undamped bounce (blue) is plotted versus the bounce solution in the overdamped limit for various damping strengths γ. Two features are especially salient. The overdamped bounce goes higher up and is wider than its undamped counterpart. An explanation is given in the text. Note that strictly speaking these solutions become exact only in the limit where $\gamma \to \infty$ so that the height of the overdamped bounce would increase continuously from 1 to 4/3 as we increase γ.

solution has a Lorentzian shape with a 'temporal' width of $\tau_b \equiv \omega_b^{-1} = \gamma\omega_0^{-1}$. Since the overdamped limit corresponds to $\gamma \gg 1$ this means that the bounce takes much longer to complete than in the undamped case, where it had a width of $\tau_0 = \omega_0^{-1}$. In a WKB picture the particle spends more time under the barrier and so we expect the tunneling rate to be decreased accordingly. This is in line with our qualitative inspection of Eq. (50).

Secondly, we note that the modified bounce solution has a higher peak in the Euclidean potential than its undamped equivalent. What could be the physical reason for this behavior? A possible explanation arises when we look at the potential in 'normal' time, where the particle now appears to tunnel to lower energies. Hence it loses energy as it goes through the barrier. This energy is transferred to the ohmic heat bath to which our particle is coupled. Thus we learn that in the presence of a finite damping, there is a loss of energy during tunneling.

Now that we have found the modified bounce solution, we can carry out the final step in our plan of attack. We can calculate the bounce action to obtain the exponential factor in the decay rate. With some persistence one can solve the integrals in Eq. (50) for $q_b(\tau)$ and arrive at the bounce action

$$\mathcal{S}_{\mathrm{eff}}[q_b] = \frac{4\pi}{9}\eta a^2. \tag{58}$$

Using Eq. (49) we can then immediately obtain the decay rate Γ. We see that the tunneling rate is exponentially suppressed by a factor proportional to the

damping strength η and the width under the barrier a squared. It is striking that this factor is independent of the height of the potential. Note that our qualitative inspection of Eq. (50), which was done for small η, also holds true in the overdamped case: Tunneling is exponentially suppressed in the damping strength as we couple our system to the environment. This observation can be seen as one of the arguments[17] why we never encounter quantum tunneling in our everyday life. Since macroscopic objects like stones or cats are so strongly coupled to their environment their tunneling rate is infinitesimally small.

A nice second interpretation of this result can be given in terms of the formal quantum theory of measurement. A well-known feature of this theory is that any measurement of a quantum system projects its state on an eigenfunction of the measured observable. In our case we can view the environment as measurement device that repeatedly performs position measurements on our system. This localizes the particle and thereby suppresses quantum tunneling. Such an understanding can be made more quantitative, as is done for example in Ref. [3].

2. Overdamped limit at finite temperature

After having calculated the zero temperature case explicitly, it is instructive to see how the results change for nonzero temperature. The main difference and also difficulty in the calculation is that we now have to calculate a bounce trajectory which is periodic in imaginary time with period $\hbar\beta = \hbar/k_B T$. The interaction term in the action is then given by Eq. (47). Renormalizing the mass and the height of the potential [10], one can massage the effective action to take the form

$$\mathcal{S}_{\text{eff}}[\bar{q}] = \int_0^{\hbar\beta} \mathrm{d}\tau \left[\frac{M}{2}\dot{\bar{q}}^2 + V(\bar{q}) + \right.$$
$$\left. \frac{\eta}{4\pi} \int_{-\infty}^{\infty} \mathrm{d}\tau' \left(\frac{\bar{q}(\tau) - \bar{q}(\tau')}{\tau - \tau'} \right)^2 \right]. \quad (59)$$

This looks familiar and indeed the structure of this effective action is equivalent to the effective action in the zero temperature limit. The small but important difference between the two situations is that the finite temperature bounce has to fulfill periodic boundary conditions. This case is treated best by expanding q_b in a Fourier Series. With analogous arguments to the zero temperature limit, such an approach leads to the set of equations

$$0 = M\omega_0^2 \left[q_n - \frac{3}{2}\sum_{n'\in\mathbb{Z}} q_{n-n'}q_n \right] + \eta|\omega_n|q_n, \quad (60)$$

where q_n is the n-th Fourier coefficient and $\omega_n = 2\pi/\hbar\beta$. We have one such equation for each Fourier mode $n \in \mathbb{Z}$. Note the similarity of this equation to Eq. (53).

With the Ansatz $q_n = q_0 \exp(-b|n|)$ we find the parameters

$$q_0 = \frac{4\pi}{3}\frac{\omega_0}{\hbar\beta}\gamma \quad (61)$$

$$\tanh(b) = \frac{2\pi}{\hbar\beta}\frac{1}{\omega_0}\gamma = \frac{T}{T_0} \quad (62)$$

$$T_0 \equiv \frac{\hbar\omega_0}{2\pi k_B \gamma} \quad (63)$$

with the *crossover temperature* T_0. The origin of the name is that the temperature T_0 marks a division between two regimes. For $T \to T_0$ we have $b \to \infty$ and so $q_b(\tau) \equiv q_0$. This disappearance of the bounce type motion signifies a regime change. As we increase the temperate to the crossover temperature, thermal activation across the barrier becomes more and more important and ultimately overtakes quantum tunneling as the main decay channel. As we increase the temperature, the exchange of energy between system and bath leads to a phase transition when T is of the order of T_0.

By plugging this into the action one finds in the overdamped limit $\gamma \to \infty$ [11],

$$\mathcal{S}_{\text{eff}}[q_b, T] = \frac{4\pi}{9}\eta a^2 \left[1 - \frac{4}{3}\left(\frac{T}{T_0}\right)^2 + \dots \right]. \quad (64)$$

We find that for small T the first corrections to the action come at $\mathcal{O}(T^2)$ and are negative, which means they will increase the decay rate[18].

3. Underdamped limit at finite temperature

For completeness we will state the result for weak coupling to the environment. Once again, one resorts to a perturbative treatment around the undamped bounce via an expansion in order of η and employs a Fourier series expansion to treat the finite temperature case [9]. After some algebra one arrives at the expression

$$\mathcal{S}_{\text{eff}}[q_b, T] = \frac{36}{5}\frac{V_0}{\omega_0}\left[1 + \gamma\left\{ \frac{45\zeta(3)}{\pi^3} \right.\right.$$
$$\left.\left. - \frac{5}{2\pi}\left(\frac{T}{T_0}\right)^2 - \frac{\pi}{12}\left(\frac{T}{T_0}\right)^4 + \dots \right\} + \mathcal{O}(\eta^2) \right]. \quad (65)$$

---

[17] Another argument is that the tunneling rate for massive objects is already small.

[18] Heuristically one could guess this by the following argument. At low temperature corrections appear because the bounce has to have a period $\hbar\beta$. For the overdamped case we found $q_b(\tau) \sim 1/\tau^2$ and so we expect the temperature corrections to appear at leading order with $\Delta\mathcal{S}(T) \propto T^2$.

In this expression the crossover temperature T_0 is defined as $T_0 = \hbar\omega_0/(2\pi k_B)$[19]. Again the first correction due to the damping is proportional to $\gamma V_0/\omega_0 = (2/27)\ \eta a^2$, which is independent of the height of the potential. The first temperature corrections also come at $\mathcal{O}(T^2)$, as in the strong coupling limit. Note also that as $\gamma \to 0$ the standard undamped solution is recovered. The obtained values for the effective action in both the over- and underdamped limits are summarized in Table I.
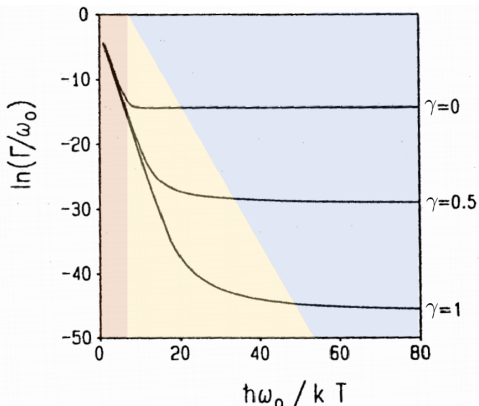
Figure 4. Arrhenius plot for the decay rate Γ of a metastable state as a function of inverse temperature. The system is coupled to an ohmic environment and curves are shown for three values of the coupling parameter γ. The different regimes are roughly indicated by background colors (red - thermal activation, yellow - crossover, blue - quantum tunneling). The plot is adapted from [11].

4. Summary of results for the damped metastable system

In this first example we focused on the effects that coupling to an environment has on the decay of a metastable system. To conclude, let us briefly summarize the main points.

1. At zero temperature coupling to an (ohmic) environment suppresses quantum tunneling exponentially with the damping strength η and the width under the barrier a squared. The suppression is independent of the height of the potential.

2. The bounce solution in the dissipative case was found to have a higher peak in the Euclidean potential than the undamped bounce. This characterizes the loss of energy during tunneling in the presence of coupling to an environment.

3. As T approaches the crossover temperature T_0 (which depends on the coupling parameter γ), there is a phase transition from a regime where quantum tunneling is the primary decay channel (low temperatures) to a regime where thermal activation is the main decay mechanism.

An illustration of the combined effects thermal activation and quantum tunneling is shown in the *Arrhenius plot* in Figure 4. The red shaded region corresponds to the limit where thermal activation is mainly responsible for the decay. Here temperatures are high compared to the crossover temperature and the decay rate shows the typical exponential (Boltzmann) dependence on inverse temperature. The crossover regime, where quantum tunneling and thermal activation interact to produce a more complicated dependence, is roughly given by the yellow region. In the blue region the curves flatten out, indicating that temperature independent quantum tunneling takes over as the primary decay mechanism. Note that with increased damping strength the crossover from the thermal to the quantum regime becomes less distinct.

B. Qualitative Results of dissipation within the double well potential

In this section we will present the effect of coupling a particle in a double well potential to an ohmic environment.[20] All presented results and figures in this section are adapted from [12]. In Figure 5 the double well po-
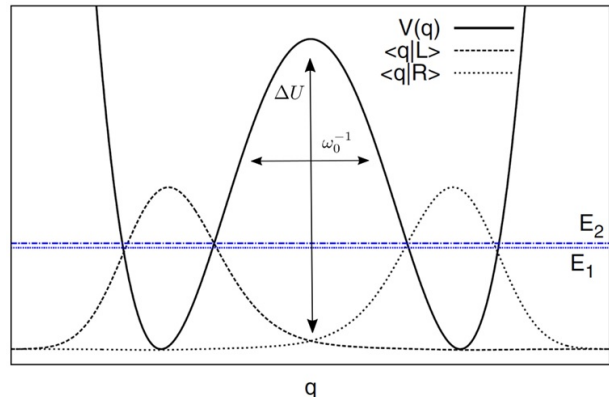

Figure 5. Symmetric double-well potential, the first two energy levels (horizontal lines) and localized states
$|L/R\rangle = (|E_1\rangle \pm |E_2\rangle)/\sqrt{2}$.

tential with its lowest two energy levels is shown. The height of the wall is chosen to be ΔU and the width

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[19] In general the crossover temperature depends on the coupling to the environment. The all-order expression is $T_0(\gamma) = \frac{\hbar\omega_0}{2\pi k_B}(\sqrt{\gamma^2/4+1} - \gamma/2)$.

[20] Actually the environment is not purely ohmic. To make the system physical we introduce an exponential cut-off. $J(\omega) = \eta\omega \exp(-\omega/\omega_c)$ with $\omega_c \gg \omega_0$.

Table I. Results for the cubic potential coupled to an ohmic environment. The effective actions for the different coupling limits are presented. Terms of order $\mathcal{O}(\eta^2)$ in the weak coupling and $\mathcal{O}(1)$ in the strong coupling limit have been neglected.

	Weak coupling limit $(\eta \to 0)$	Strong coupling limit $(\eta \to \infty)$
$T = 0$		
Bounce $q_b(\tau)$	$a \operatorname{sech}^2\left(\frac{\omega_0}{\tau}\right)$	$\frac{(4/3)a}{1 + (\omega_0\tau)^2}$
Action $\mathcal{S}_{\text{eff}}[q_b, T = 0]$	$\frac{36}{5}\frac{V_0}{\omega_0} + \frac{24\,\zeta(3)}{\pi^3}\eta a^2$	$\frac{4\pi}{9}\eta a^2$
$T \geq 0$:		
Crossover Temp. T_0	$T_0 = \frac{\hbar\omega_0}{2\pi k_B}$	$T_0 = \frac{\hbar\omega_0}{2\pi k_B}\frac{1}{\gamma}$
Action $\mathcal{S}_{\text{eff}}[q_b, T]$	$\frac{36}{5}\frac{V_0}{\omega_0} + \frac{8}{15}\eta a^2\left[\frac{45\zeta(3)}{\pi^3} - \frac{5}{2\pi}\left(\frac{T}{T_0}\right)^2 - \frac{\pi}{12}\left(\frac{T}{T_0}\right)^4 + \ldots\right]$	$\frac{4\pi}{9}\eta a^2\left[1 - \frac{4}{3}\left(\frac{T}{T_0}\right)^2 + \ldots\right]$

scales with ω_0^{-1} according to $V(q) = \frac{M^2\omega_0^4}{64\Delta U}q^4 - \frac{M\omega_0^2}{4}q^2$. The states $|L\rangle$ and $|R\rangle$ are position eigenstates according to a *discrete variable representation* (DVR).

1. Discrete Variable Representation

In the limit of low temperature one can argue that a system is constrained to the lowest few energy eigenstates, since the probability of finding it without excitations in higher energy states decreases exponentially. For our purpose, let us consider the lowest n energy eigenstates, hence our now truncated Hilbert space is defined as $H = \operatorname{span}\{|E_1\rangle, |E_2\rangle, \ldots |E_{n-1}\rangle, |E_n\rangle\}$. In the following section we will investigate the tunneling rate between the left and right well and therefore it is important to know the position eigenstates. Having a n dimensional Hilbert space implies that we have n position eigenstates ($|Q_i\rangle$) such that within this Hilbert space a particle can only be localized at n discrete positions (Q_i). The position operator in the energy basis reads as $q_{ij} = \langle E_i|\hat{q}|E_j\rangle$. Diagonalizing leads to the eigenfunctions and the corresponding positions as eigenvalues.

2. Double-Doublet System

For the following discussion we apply a DVR considering the lowest four energy eigenstates. The *double-doublet* system is shown in Figure 6. It is called so, since it consists of four energy levels distributed in two groups of two levels. This motivates us to define frequencies corresponding to the energy gaps. $\Omega_0 = \frac{\omega_4 + \omega_3}{2} - \frac{\omega_2 + \omega_1}{2} \approx 0.82\omega_0$, $\Omega_1 = \omega_4 - \omega_3 \approx 0.12\omega_0$ and $\Omega_2 = \omega_2 - \omega_1 \approx 0.004\omega_0$. Here ω_i corresponds to the i-th energy level E_i according to $E_i = \hbar\omega_i$. Applying the DVR and diagonalizing the position operator leads to the position eigenstates presented in Figure 7. Two of them are located within the left well and the other two in the right
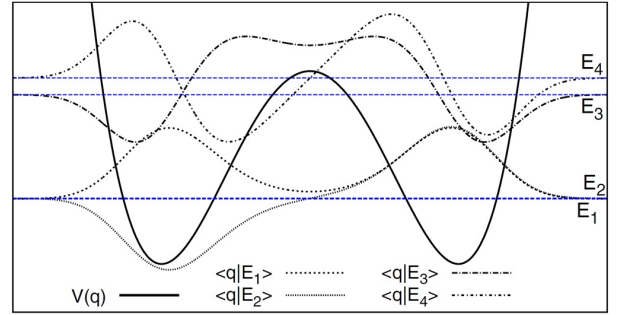

Figure 6. The double-doublet system. Dashed lines correspond to the energy eigenstates. The blue lines indicate the corresponding energy levels. Two groups consisting of two energy levels can be observed.

one. Compared to Figure 5 where a two level system (TLS) is considered we now have two positions per well which allows intra well motion. The time evolution of the
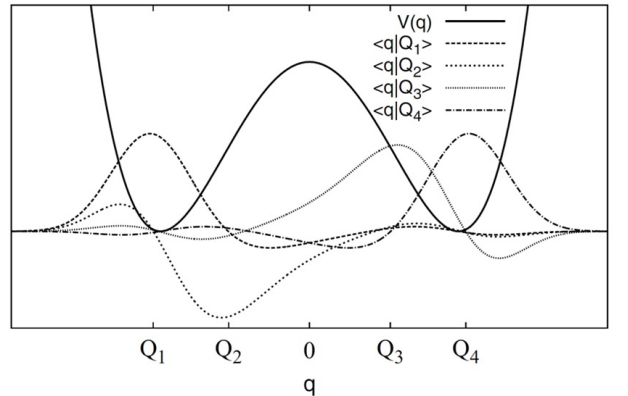

Figure 7. The double-doublet system. Dashed lines correspond to the position eigenstates according to the DVR with the lowest four energy eigenstates.

double-doublet system without any dissipative effects is

shown in Figure 8. Initially the particles location is set to be $|Q_1\rangle$, i.e. it is located in the left well. Figure 8 then shows the probability that the particle is found in the left well after a certain time. The main oscillation is given by the fluctuations between the first two energy levels with frequency Ω_2. This is not surprising since the probability densities should be the highest for these two (lowest energy) states. A second oscillation occurs due to the energy gap within the upper group with frequency Ω_1 in Figure 8. There is actually a third oscillation, but the resolution is not high enough to display it. This oscillation happens at much faster time scales with frequency Ω_0. We call all these oscillations *coherent oscillations.* This reflects that phase information is conserved over a certain time interval. Physically the different energy eigenstates begin to interfere and as a result the particle tunnels from the left well to the right well and back again with some determined constant frequency. In this case without dissipation, these oscillations will go on forever.
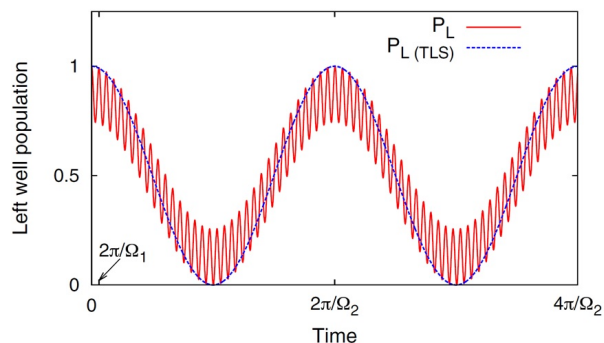

Figure 8. The free system is initially in the state $|Q_1\rangle$. The blue curve corresponds to the TLS whereas the red one corresponds to the four-level system.

3. Dissipation

Until now we have used the imaginary time path integral formalism to calculate density matrix elements. Without introducing the real time path integral formalism[21] in full detail, let us give some of its key features. Instead of calculating the density matrix directly, Feynman and Vernon expressed its time evolution through the propagator and calculated it with real time path integrals. Within our four-level system the time evolution of the propagator is given as

$$\rho_{q,q'}(t) = \sum_{q_0,q_0'=Q_1}^{Q_4} G(q,q',t_f;q_0,q_0',t_0)\rho_{q_0,q_0'}(t_0). \quad (66)$$

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[21] The real time path integral formalism was introduced in 1963 by Feynman and Vernon [2]. For a proper derivation of the following statements, we refer the reader there and to [12].

Here the propagator can be understood as a product of two single propagators since we have to consider the evolution of both, q and q'. Such a propagator is given by

$$G(q_f,q_i,t_f,t_0) = \int_{\bar{q}(t_0)=q_i}^{\bar{q}(t_f)=q_f} \mathcal{D}\bar{q} \exp\left(\frac{i}{\hbar}\mathcal{S}[\bar{q}]\right). \quad (67)$$

The total propagator is then found to be

$$G(q,q',t_f;q_0,q_0',t_0) = \quad (68)$$
$$\int_{\bar{q}(0)=q_0}^{\bar{q}(t)=q} \int_{\bar{q}(0)=q_0'}^{\bar{q}(t)=q'} \mathcal{D}\bar{q}\,\mathcal{D}\bar{q}' \exp\left(\frac{i}{\hbar}\mathcal{S}[\bar{q},\bar{q}']\right),$$

with $\mathcal{S}[\bar{q},\bar{q}'] = \mathcal{S}[\bar{q}] - \mathcal{S}[\bar{q}']$. But what is a path in the DVR for this double path integral? Figure 9 illustrates this nicely. As we have discretized, a path is no more a smooth function $\bar{q}(\tau)$, but rather it consists of a sequence of coordinates $\{(q',q)_i\}$ and times $\{t_i\}$ indicating that the position of the particle changes at time t_i from position $(q',q)_i$ to $(q',q)_{i+1}$. The measure $\int_{\bar{q}(0)=q_0}^{\bar{q}(t)=q} \int_{\bar{q}(0)=q_0'}^{\bar{q}(t)=q'} \mathcal{D}\bar{q}\,\mathcal{D}\bar{q}'$
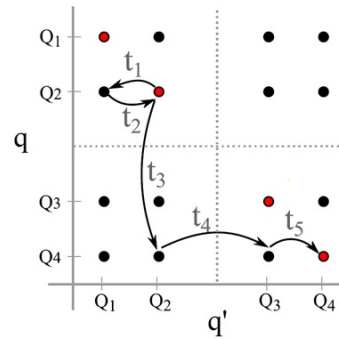

Figure 9. Example of a path with five transitions within the DVR.

then reduces to the sum

$$\sum_{n=0}^{\infty} \sum_{\text{paths}_n} \int_{t_0}^{t_f} dt_n \int_{t_0}^{t_n} dt_{n-1} \ldots \int_{t_0}^{t_2} dt_1 \ldots \quad (69)$$

where n is the number of transitions and $\sum_{\text{paths}_n}$ is the sum over all possible path configurations. This allows us to calculate this path integral numerically. Of course one needs to make some additional approximations such as e.g., considering the number of transitions to be less than a fixed integer N. In Figure 10 the analogue of Figure 8 is shown, but now including dissipation. The temperature is set to be very low and the coupling very weak. For more detailed phase information and the approximations made to obtain these results we refer the reader to [12]. The oscillations remain the same. But as expected they get damped, similarly to a damped harmonic oscillator. In Figure 11 the same plot is shown, but now for stronger coupling. Again there are two visible oscillations but in this case they flatten out much faster. We still talk about coherent oscillations, since there exists a time interval where the particle tunnels from the left
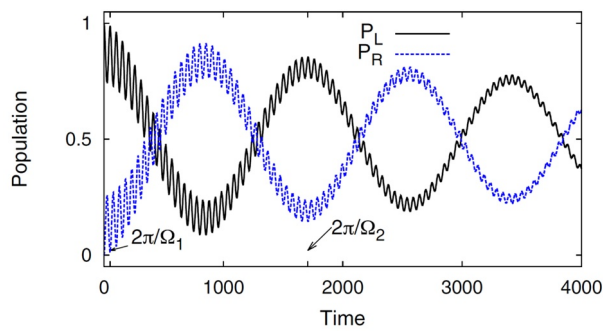
Figure 10. Time evolution of the populations for very low coupling and very low temperature. The black line corresponds to the probability that the particle is in the left well and the blue line to the right.

to the right and back again (on average). If we define the coherence time as the length of the time interval over which phase information is (on average) predictable we may state that stronger coupling leads to shorter coherence times. But what is the influence of temperature?
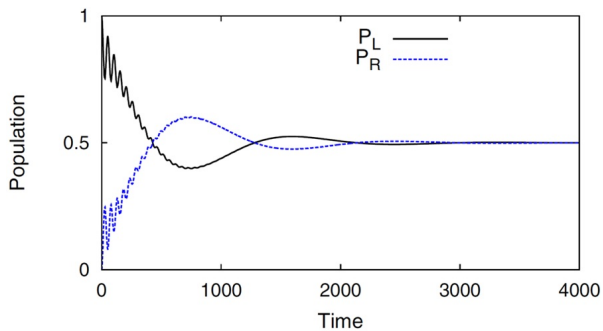

Figure 11. The same as in Figure 10 but now with stronger coupling.

Figure 12 shows the occupation probabilities for all four position eigenstates. In Figures 8, 10 and 11 we plotted in each case the sum $\rho_{11} + \rho_{22}$ i.e. the probability that the particle is in the left well. Instead here, we are able to look at oscillations between position states within the wells. First of all, there is no oscillation seen between the wells, but there is an oscillation within the left well. The coherence time in this case is very short compared to those from Figures 10 and 11. In the right well there is no oscillation at all. How did this process of flattening out happen so fast if the coupling is high enough that the particle could not tunnel coherently to the right? The solution is thermal excitations, since the bath has finite temperature it is possible that it excites our particle. Afterwards it may tunnel or just jump to the right if it gained enough energy.
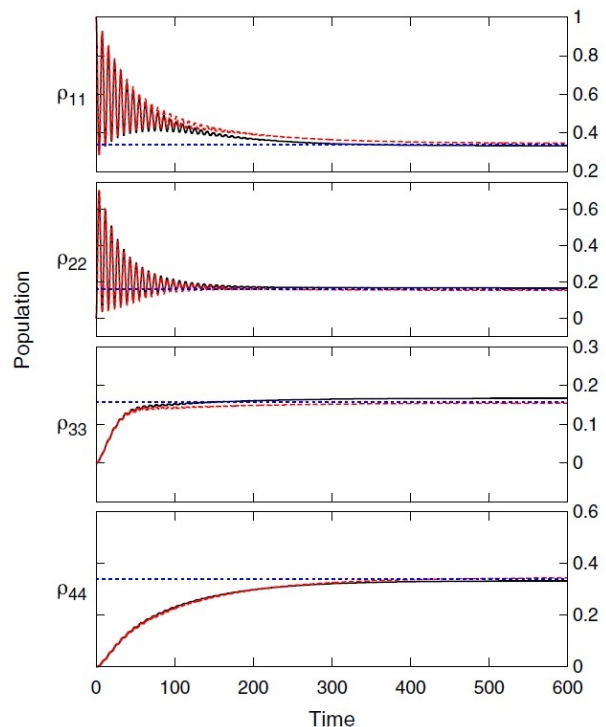

Figure 12. Occupation probabilities for all four position eigenstates (red line). The blue line indicates the solutions of Figures 10 and 11 at $t = \infty$. In this case we take intermediate temperature and strong coupling. The particle oscillates within the left well but there are no oscillations seen in the right one.

V.   CONCLUSION

To bring our discussion of dissipative quantum systems to an end we take a brief look back at the main themes of this report.

We have learned that an environment can be modeled in quantum mechanics by adding a linear coupling to a bath of harmonic oscillators to the Hamiltonian. It then turned out that the path integral formulation of quantum mechanics provides a powerful setting to explore this extended Hamiltonian. When we averaged over the bath oscillator modes to find an effective description of our system we found that the intricate interaction between system and environment amounted to adding the compact, additional term $\mathcal{S}_{\text{int}}^{E}$ to the total system action. This additional term in the action is the main result of this discussion.

To develop an intuition of some of the physics contained in this action, we looked at a metastable and a double well potential. These illustrated dissipative quantum tunneling and the loss of phase coherence respectively. Two results specifically stand out. For the first problem we demonstrated that environmental coupling exponentially suppresses quantum tunneling. In the second problem we found that by exchanging energy with the surrounding heat bath, the system can lose its phase

coherence and hence its quantum mechanical character. We may therefore conclude that in both cases dissipation makes the system more classical in the sense that it suppresses the purely quantum effects of tunneling and interference.

In our brief survey we only touched on small part of this broad field of research and highlight some of the guiding principles. For readers interested in learning more about dissipative quantum systems and their role in the loss of quantum coherence we especially recommend references [3] and [13].

VI. AUTHOR CONTRIBUTIONS AND ACKNOWLEDGEMENTS

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