Dissipative Spin Systems

in Non-Ohmic Environments:

Real-Time Path Integral

Monte Carlo Simulations

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Introduction

The purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules.

N. Metropolis et al., 1953 [43]

The above citation is taken from a paper of Nicholas Metropolis and co-workers who developed the famous Metropolis sampling. This algorithm is on the heart of Monte Carlo (MC) simulations and innumerable physicists have benefited from it since then [44, 45]. However, the formulation is maybe a bit strong. As the opinion about when to indicate an electronic computing machine as “fast” slightly changed within the last six decades, the sentence would probably mean that we were able to completely solve condensed matter physics now, in the year 2014. This is indeed not the case and maybe, it should be mentioned that this statement was restricted to classical statistics and two-body interactions. Still, the soft exaggeration does not weaken the tribute to the authors. MC simulations are today an indispensable tool in numerous divisions of physics [63], chemistry, and even areas that seem to have nothing in common with natural sciences. Although not all of them work with the sampling method that was presented in this paper, it still started a development that was completely unpredictable by the authors and their coevals in the 1950s.

In this work, we make use of this old, but not old-fashioned methodology in order to investigate dynamical problems in a certain area of condensed matter physics. This is quantum dissipation [1, 2], a field that started to evolve in the 1980s, apart from some pioneer works in the preceding decades [13, 14, 21]. Its theoretical backbone are the so-called system-plus-reservoir models, mainly the famous Caldeira-Leggett model [12]. Quantum dissipation is inspired by the insight that neither theorists, nor experimentalists can disregard the interaction of a system with its environment – both on the macroscopic and the microscopic scale. There is no system in the world, except from the universe as a whole, that is fully isolated from its surrounding. Therefore, dissipation is an inherent phenomenon even in the quantum world.
When leaving atomic scales towards mesoscopic devices, there are a lot of realizations where the laws of quantum mechanics are still valid. During the last years, experimental groups succeeded in designing solid state structures of growing complexity that are dominated by quantum mechanics [16, 17, 18, 32, 33, 34, 35]. These many-body systems form the bridge between the atomic and the macroscopic world. High-resolution spectroscopic methods enable us to study the dynamics of very small structures on time intervals of femtoseconds [19]. Therefore, realistic theoretical models for such systems become more and more important.

As in most of these systems only a small number of states is involved, the models behind must start from tight-binding systems, or, to be more precise, artificial atoms or spin systems. The main focus in this work is laid on the spin-boson model (SBM) [20, 21] which couples a spin-1/2 or two-level system (TLS) to a continuously distributed set of non-interacting harmonic modes. The simple underlying idea is justified by its wide applicability in several fields of modern physics [1]. Going beyond a single TLS, we extend the SBM towards the interacting spins model (ISM), consisting of two spins that can interact directly and couple to the same environment. Its name is not established, but we use it as a working terminus.

When dealing with system-plus-reservoir models, the properties of the reservoir are of primary importance. A common choice are the so-called Ohmic reservoirs, which were studied with a plethora of methods within the last decades [1, 2, 20]. Therefore, we can claim that spin-1/2 systems in contact with these surroundings are widely understood.

However, this is not true for other bath spectra. Especially the sub-Ohmic baths have been attracting increased attention for a couple of years, basically motivated by the occurrence of a second order quantum phase transition [97, 98, 99, 105, 106]. Next to the equilibrium properties, also investigations into the dynamics witnessed a boost of activities, thereby bringing up the hitherto unresolved question about the quantum-to-classical or coherent-incoherent transition in the deep sub-Ohmic range [110, 112, 114]. Similar issues are treated for the ISM in this work. Here, we additionally focus on effects that are on the heart of quantum information, such as spin-spin entanglement and decoherence-free subspaces. Motivated by devices that couple single quantum dots to photonic band-gap materials [132, 133], we also study the dynamics of a spin-1/2 system interacting with a gapped bosonic spectrum.

Investigating the dynamics of such models is possible either by discretizing the bath spectrum and taking into account a computationally very expensive number of degrees of freedom [80, 109], or by making use of path integrals (PIs) [10, 11]. Although PIs seem to be rather strange and needlessly complicated objects at first sight, they still have their right to exist. In fact, they form the modern language of quantum mechanics and there are more than a few problems that would be completely intractable, if we did not know about PIs [4, 5]. The PI approach runs into a formalism that fully eliminates the bath degrees of freedom [22, 23], resulting in a couple of different methods which make use of that [71, 111].

Nevertheless, all these approaches have different limitations and are restricted to certain areas of parameter space. The only method that yields numerically exact results for all parameters is our Path Integral Monte Carlo (PIMC) which evaluates dynamical quantities.
by making use of the ideas of Metropolis. Here, physics meets methodology and all the key words from the title are brought together: Real-time PIMC for dissipative spin systems is a computational method that determines the exact spin dynamics in all parameter regions and thereby demonstrates its power in comparison to other approaches, especially for non-Ohmic environments.

The only restriction we have is that the determination of quantum dynamics with PIs goes hand in hand with a horrible interference of single paths. Therefore, the statistical error bars grow exponentially with the simulated system time. This is known as the dynamical sign problem, limiting our investigations to intermediate times. However, we also present a scheme that allows for diminishing this problem in certain parameter ranges.

This work is divided into two parts. First, we treat the physical (Chap. 1) and the numerical (Chap. 2) background. Chap. 1 gives a short introduction into the field of quantum dissipation in general. We sketch the underlying basics and the difficulties that arise. Special emphasis is laid on the SBM and its dynamical properties. Finally, we describe the way from the SBM to the ISM and discuss some features that are connected with the latter. In Chap. 2, we present the Metropolis algorithm from the very beginning and discuss some restrictions and pitfalls, especially the notorious sign problem [49]. We explain in detail, how the Metropolis technique is applied to our models and how the sign problem is soothed within our approach [54]. It was tried to make a compromise between understandability on the one hand and clearness on the other hand. Although the literature concerning the used approaches could fill libraries, the reader should be able to understand all important contents out of these chapters.

All the results are captured in the second part, consisting of Chaps. 3 to 6. Let us skim them briefly. Chaps. 3, 4, and 5 involve the SBM with regard to different environmental spectra. In Chap. 3, we deal with Ohmic reservoirs, which are used as a test-bed for an approximative scheme named Chain PIMC (CH-PIMC). This method allows us to partially circumvent the sign problem for a variety of parameters, which sticks the connection to Chap. 4. Here, we study the efficiency of CH-PIMC for the more complicated sub-Ohmic reservoirs. Of particular importance is the fact that our numerical approach is able to shed light on regions of sub-Ohmic parameter space that cannot be reached by other non-approximative methods. We are therefore able to answer the questions outlined above. The surprising results are supported by analytical calculations and were confirmed qualitatively by other groups in the meantime [113]. In Chap. 5, we investigate the time evolution of a TLS that couples to a reservoir with a spectral gap, motivated by devices that couple semiconductor quantum dots to the gapped electromagnetic spectrum of a photonic crystal. Chap. 6 finally studies different effects that appear for the ISM, where both Ohmic and sub-Ohmic reservoirs are involved. The presence of a second spin opens the door for fascinating quantum effects, especially the mystery of entanglement, that has been confusing physicists since the early days of quantum mechanics [136, 137].

As already told, the big advantage of our PIMC method is its wide applicability in parameter space. This is the basis for a variety of interesting outcomes that are presented in this work.
In general, we will see that the bath is not always disturbing – instead, it often turns out to be a source of knowledge and understanding. This can be seen as the general message of this work. Some important findings were published in Refs. [65, 66, 67].

In the following, we work with natural units,

\[ h = 1, \quad k_B = 1. \]
Part I

THEORY AND METHODOLOGY
Chapter 1

Dissipative Quantum Mechanics

As briefly outlined in the introduction, the rules of quantum mechanics can be studied on mesoscopic length scales. The coupling to surrounding degrees of freedom, ranging from electromagnetic excitations [33, 36] to mechanical modes [32], becomes inevitably involved into the dynamics. Allowing quantum mechanics to leave the nano-world is metaphorically expressed in the 80-years old picture of Schrödinger’s cat, i.e. an atomic system that gets entangled with a macroscopic object [137]. Physicists all around the world are in the act of translating this picture into real experiments [35]. By doing so, they are unavoidably confronted with decoherence and dissipation.

Describing dissipation in quantum mechanics is a non-trivial task. Whenever working with a time-independent many-particle Hamiltonian, energy is conserved and there seems to exist no possibility to include dissipative effects that are characterized by a flow of energy from the system to its surrounding. The way out are so-called system-plus-reservoir models that treat the system of interest and the large environment in one total Hamiltonian. This way, conservation of energy is valid for the total system and we can apply all tools we know from quantum and statistical mechanics.

Before tackling these models, let us start with something that is common knowledge in physics. The first time when dissipation occurs in classical mechanics is typically the damped harmonic oscillator, whose position $X(t)$ fulfills the simple differential equation

$$M\ddot{X}(t) + M\gamma\dot{X}(t) + M\omega^2 X(t) = 0.$$  \hspace{1cm} (1.1)

We have a particle of mass $M$, that is subject to phenomenological Stokes friction $-M\gamma\dot{X}(t)$ and moves in a parabolic potential. There are a lot of possibilities of how to generalize Eq. (1.1): First, we can drive the harmonic oscillator by adding a time-dependent external force $F(t)$ to the right hand side. When this force is generated by environmental fluctuations, it has to fulfill some statistical relations, which we will see below. Second, we can introduce friction “with memory” by replacing $\gamma\dot{X}(t) \rightarrow \int_0^t dt'\gamma(t - t')\dot{X}(t')$. Then, the frictional medium keeps in mind the particle’s velocity $\dot{X}(t')$ at prior times $t' < t$. These two extensions lead us to a stochastic equation that will be derived below in a more systematic way out of a system-plus-reservoir model [1, 2].
If this is done, the road to quantum dissipation is treded. We can quantize the classical Hamilton function and arrive at a Hamiltonian that contains system, reservoir and interaction between them – this is the famous Caldeira-Leggett model (CLM) [12]. Assuming the system to have only two states (two-level system, TLS) [3], we straightforwardly get the spin-boson model (SBM), which is the physical heart of the main part of this work. Its generalization to a system of two interacting TLSs is named interacting spins model (ISM). All these issues will be handled during this chapter.

1.1 The Caldeira-Leggett model

The fundamental difficulty of friction in quantum mechanics was already brought up in the introducting sentences: Conservation of energy seems to avoid dissipative effects. Therefore, we include the macroscopically large environment into the total Hamiltonian. The most common choice for the interaction is linear in force and quadratic in energy. This leads us to the well-established CLM, which is an archetypical example of a system-plus-reservoir model and was originally proposed by Ullersma in 1966 [13]. In this first section, we describe the CLM in classical terms and then turn to the quantum mechanical case [1].

1.1.1 Classical and quantum dynamics

We should clarify one thing in the very beginning: The coupling of the system to a linear superposition of a vast number of bath coordinates ensures that the range of the model goes far beyond a collection of harmonic modes. A fundamental relation of statistics, the central limit theorem, predicates that the sum of a large number of random variables is distributed according to a Gaussian, independent of the single distribution functions. In terms of full counting statistics, this means that only the second cumulant, corresponding to the variance, is of relevance. Therefore, also systems with non-harmonic modes can be modeled in this way. This is what lends a certain universality to the CLM.

The underlying physical picture is quite simple: One has a system, given by \( H_S(P, X) = \frac{P^2}{2M} + U(X) \), a bath \( H_B \) consisting of a large number of non-interacting modes and a coupling term \( H_I \),

\[
H = H_S + H_I + H_B. \tag{1.2}
\]

The environmental degrees of freedom are characterized by their masses \( m_\alpha \) and frequencies \( \omega_\alpha \),

\[
H_B = \sum_\alpha \left( \frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} x_\alpha^2 \right), \tag{1.3}
\]

while the interaction term is linear in the system's and the modes' displacement with indi-
vidual coupling parameters $c_{\alpha}$,

$$H_I = -X \sum_{\alpha} c_{\alpha} x_{\alpha} + X^2 \sum_{\alpha} \frac{c_{\alpha}^2}{2m_{\alpha} \omega_{\alpha}^2}. \quad (1.4)$$

Metaphorically spoken, we look at a particle that is coupled to the surrounding degrees of freedom via springs and moves in a 1D-potential. The first term in Eq. (1.4) is the virtual interaction, while the latter is a counter term that avoids a potential renormalization. Its necessity becomes obvious, when one searches for the equilibrium position of the i'th oscillator for fixed $X$, given by

$$\frac{\partial V(x_i)}{\partial x_i} = -c_i X + m_i \omega_i^2 x_i \quad \text{with potential} \quad V(x_i) = -Xc_i x_i + m_i \omega_i^2 x_i^2/2.$$ 

In the potential minimum, this expression must vanish. So, the oscillator's potential energy at the global minimum reads

$$V(x_{eq}^i) = -c_i^2 X^2 / 2m_i \omega_i^2$$

and depends on the particle's position $X$. This dependence is dropped by adding the renormalization term. The sum of interaction and bare environment can hence be written as

$$H_B + H_I = \sum_{\alpha} \left[ \frac{p_{\alpha}^2}{2m_{\alpha}} + \frac{m_{\alpha} \omega_{\alpha}^2}{2} \left( x_{\alpha} - \frac{c_{\alpha}}{m_{\alpha} \omega_{\alpha}^2} X \right)^2 \right]. \quad (1.5)$$

It is important to mention that the microscopic model parameters $m_{\alpha}$, $\omega_{\alpha}$ and $c_{\alpha}$, although they are independent of each other, affect the system’s dynamics only in a special combination: The whole bath influence can be led back to the spectral density $I(\omega)$,

$$I(\omega) := \frac{\pi}{2} \sum_{\alpha} \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}} \delta(\omega - \omega_{\alpha}), \quad (1.6)$$

where a detailed derivation of this dependence is sketched in App. B. $I(\omega)$ becomes a smooth function in the limit of quasi-continuously distributed modes. This is of particular importance, when we want to ensure a basic property of dissipation: If the periods of any finite number of modes have a lowest common multiple, they fix the Poincaré recurrence time that is the time scale on which the total system reproduces its dynamics. For a continuous bath spectrum, this time is infinite and the model is able to describe a net flow of energy to the surrounding, as it should be the case for our purpose.

Making use of the classical Hamiltonian equations of motion, the dynamics is given by

$$\dot{P} = -U'(X) + \sum_{\alpha} \left( c_{\alpha} x_{\alpha} - \frac{c_{\alpha}^2}{2m_{\alpha} \omega_{\alpha}^2} X \right),$$

$$\dot{X} = \frac{P}{M},$$

$$\dot{p}_{\alpha} = -m_{\alpha} \omega_{\alpha}^2 x_{\alpha} + c_{\alpha} X,$$

$$\dot{x}_{\alpha} = \frac{p_{\alpha}}{m_{\alpha}}. \quad (1.7)$$

Integration of Eqs. (1.7) ends up in a stochastic equation, known as the generalized Langevin equation (GLE),

$$M \ddot{X}(t) + M \int_0^t dt' \gamma(t-t') \dot{X}(t') + U'(X(t)) = \xi_B(t), \quad (1.8)$$
that is governed by the damping kernel
\[ \gamma(t) := \frac{1}{M} \sum_{\alpha} \frac{c_{\alpha}^2}{m_\alpha \omega_{\alpha}^2} \cos(\omega_{\alpha} t) = \frac{2}{\pi M} \int_0^\infty d\omega \frac{I(\omega)}{\omega} \cos(\omega t) \] (1.9)

and the stochastic force
\[ \xi_B(t) := \sum_{\alpha} c_{\alpha} \left( x_{\alpha}(0) - \frac{c_{\alpha}}{m_\alpha \omega_{\alpha}^2} X(0) \right) \cos(\omega_{\alpha} t) + \frac{p_{\alpha}(0)}{m_\alpha \omega_{\alpha}} \sin(\omega_{\alpha} t) \] (1.10)

So, all the microscopic parameters merge in the time-dependent functions \( \gamma \) and \( \xi_B \) that can be interpreted as a friction and a fluctuating random force. As the velocity \( X(t') \) at prior times \( t' < t \) affects the dynamics at time \( t \), memory effects are included. Clearly, the absolute value of \( \gamma(t) \) should approach zero for \( t \to \infty \), but the way it decays (e.g., exponentially or algebraically) can influence the physics dramatically. Special types of friction do not include any memory, \( \gamma(t) \propto \delta(t) \), and are called time-local or Markovian. For causality reasons, \( \gamma(t < 0) \) does not contribute in the equation of motion.

Eq. (1.8) is a stochastic differential equation, in which the bath force \( \xi_B(t) \) acts as an external driving and is nothing but a Gaussian random variable that fulfills
\[ \langle \xi_B(t) \rangle = 0 \]
\[ \langle \xi_B(t)\xi_B(t') \rangle = Mk_B T \gamma(t-t'). \] (1.11)

Note that \( \xi_B \) is related to the damping kernel by its auto-correlation function by (1.11). As it connects dissipation to a random driving force, it is one example for a fluctuation-dissipation theorem: The noise of the environment is the reason that the system transfers energy to its surrounding. The average in Eq. (1.11) is done by a simple phase space integral with density
\[ \rho_B(\{x_{\alpha}(0), \{p_{\alpha}(0)\}) = Z^{-1} \exp \left\{ -\beta \sum_{\alpha} \left[ \frac{p_{\alpha}(0)^2}{2m_\alpha} + \frac{m_\alpha \omega_{\alpha}^2}{2} \left( x_{\alpha}(0) - \frac{c_{\alpha}}{m_\alpha \omega_{\alpha}^2} X(0) \right)^2 \right] \right\}, \] (1.12)

\( Z \) being the normalization, i.e., the bath sum of states. It becomes clear from Eq. (1.12), how the terminus “stochastic” must be understood: Eq. (1.8) in itself is purely deterministic. However, the initial conditions of the bath degrees of freedom cannot be fixed, but instead follow this Gaussian distribution. The solution of the GLE is thus already given by (1.11). As all correlations containing the bath force at three or more times, e.g. \( \langle \xi_B(t)\xi_B(t')\xi_B(t'') \rangle \), can be led back on the average \( \langle \xi_B(t) \rangle \) and the auto-correlation \( \langle \xi_B(t)\xi_B(t') \rangle \) for a Gaussian ensemble, we do not require any further information but (1.11) to solve the problem.

We now turn to the quantum mechanical description by canonically quantizing Eq. (1.2) and using the standard Liouville-von Neumann time evolution. Similar to the classical case, we can break down the effect of the whole surrounding onto the spectral density. Due to its harmonic structure, the bath can be integrated out exactly via path integrals (PIs) [22]. This is referred to the Feynman-Vernon formalism [23]. We leave with a functional dependence on the system paths, the so-called influence functional (IF).
1.1. THE CALDEIRA-LEGGETT MODEL

The Feynman-Vernon approach in itself is exact. The only price we have to pay is that we lose the whole information about the detailed bath state, conserving nothing but its effect on the system. To keep things easier, we just mention some basic results in this section and refer for details to App. B, where the main steps concerning the derivation of the IF are sketched for a TLS with factorizing initial state. The latter is an assumption that is already contained in the subsequent results, so the initial density matrix containing the sum of states $Z$ reads

$$W(0) = \rho_S(0)W_B(0) = \rho_S(0)Z^{-1}e^{-\beta H_B} \quad \text{with}$$

$$Z = \text{Tr}_B(e^{-\beta H_B}) = \prod_{\alpha} \left[ 2 \sinh \left( \frac{\omega_\alpha \beta}{2} \right) \right]^{-1}. \quad (1.13)$$

with $\text{Tr}_B$ denoting the trace over the bath. $\rho_S$ is the bare system’s density and underlies no further assumptions. In the beginning, the bath is in thermal equilibrium with itself. Writing down the time evolution, it is possible to perform the trace over the bath degrees of freedom. The remainder is called reduced dynamics. One finally arrives at the IF, which enters the action by a factor $\exp(-\Phi_{CLM}[X, X'])$ and reads

$$\Phi_{CLM}[X, X'] = \int_0^t dt' \int_0^{t''} dt'' [X(t'') - X'(t'')] \cdot [L(t' - t'')X(t'') - L^*(t' - t'')X'(t'')]$$

$$+ i \Lambda_{cl} \int_0^t dt'[X^2(t') - X^2(t'')], \quad (1.14)$$

$L^*$ denoting complex conjugation. Instead of the Langevin kernel, we use the auto-correlation function or influence kernel\footnote{$L'$ and $L''$ denote real and imaginary part of $L$.}

$$L(t) = L'(t) + iL''(t) := \langle \xi_B(t)\xi_B(0) \rangle$$

$$= \frac{1}{\pi} \int_0^\infty d\omega \ I(\omega) \left[ \coth \left( \frac{\omega \beta}{2} \right) \cos(\omega t) - i \sin(\omega t) \right], \quad (1.15)$$

which is connected to the latter via $L''(t) = \frac{M}{2} \frac{d}{dt} \gamma(t)$. $\Lambda_{cl}$ is the so-called classical reorganization energy,

$$\Lambda_{cl} := \frac{1}{\pi} \int_0^\infty d\omega \frac{I(\omega)}{\omega}, \quad (1.16)$$

to be discussed in Subsec. 1.2.3. $X(t')$ and $X(t'')$ are the forward and backward paths on the Keldysh contour, respectively. So, Eq. (1.14) contains interactions of the path $X(t')$ with $X'(t'')$ at earlier times $t'' < t'$ and vice versa, but also local (last term) and non-local interactions of $X$ and $X'$ with themselves. The last contribution in Eq. (1.14) stems from the counter term in Eq. (1.4).

It is easy to see that the relative coordinate $X - X'$ couples in a bilinear way via $L'$, whereas $L''$ links $X - X'$ to the sum coordinate $X + X'$. The factor containing $L'$ describes classical fluctuations, as it suppresses paths with $X \neq X'$. This coincides with the fact that it is
real-valued and depends on temperature. By contrast, the term with $L''$ is a pure phase factor that describes quantum fluctuations and leads to interference of different paths.

One often works with the twice-integrated bath auto-correlation function $Q(t)$ instead of $L(t)$,

$$Q(t) = \frac{1}{\pi} \int_0^\infty d\omega \frac{I(\omega)}{\omega^2} \left[ \coth \left( \frac{\omega \beta}{2} \right) [1 - \cos(\omega t)] + i \sin(\omega t) \right].$$  \hfill (1.17)

The integration constants are fixed by $Q(0) = 0$ and $\dot{Q}(0) = i \Lambda_{cl}$.

### 1.1.2 The spectral density

As noted above, it is the spectral density $I(\omega)$ that contains the whole bath influence on the system, next to its temperature. It is therefore suitable to classify some properties of this important quantity. A standard choice for the bath dissipation is the so-called Ohmic friction, where $I(\omega)$ increases linearly with $\omega$, but with a smooth or sharp cut-off at a finite frequency $\omega_c$, that is required to avoid divergencies. Also from the physical point of view, many-body systems require a large-frequency cut, such as the Debye frequency for phonons in crystals [7]. Widely used is a cut-off that damps out the high-energetic modes exponentially. The spectral density then reads

$$I(\omega) = 2\pi \alpha \omega e^{-\frac{\omega}{\omega_c}}$$  \hfill (1.18)

with the dimensionless dissipation strength $\alpha$. It is called Ohmic because the corresponding friction kernel entering the GLE is

$$\gamma(t) = \frac{4\alpha}{M} \frac{\omega_c}{1 + \omega_c^2 t^2} \frac{\omega_c}{\omega_c \to \infty} \frac{4\pi \alpha}{M} \delta(t),$$  \hfill (1.19)

leading to the equations of motion of an Ohmic resistor in an electromagnetic circuit. So, Markovian dynamics is gathered from Ohmic baths with $\omega_c \to \infty$ in the classical range. A generalization is introduced by a power-law spectrum,

$$I(\omega) = 2\pi \alpha \omega_c^{1-s} \omega^s e^{-\frac{\omega}{\omega_c}}.$$  \hfill (1.20)

For $s < 1$ ($s > 1$), we call the damping sub-Ohmic (super-Ohmic). The first case will be of great importance in Chaps. 4 and 6. Therefore, we want to give a short hint to the problems that arise here. It is obvious that the coupling of the system to the lower energetic bath modes is enhanced compared to the Ohmic case. Calling in mind Heisenberg’s uncertainty relation,

$$\Delta E \Delta t \gtrsim h,$$  \hfill (1.21)

we learn that virtual excitations with small energies are long-ranged in time. This can be also seen from the damping kernel, that reads

$$\gamma(t) = \frac{4\alpha}{M} \frac{\omega_c}{(1 + \omega_c^2 t^2)^{\frac{s}{2}}} \Gamma(s) \cos[s \arctan(\omega_c t)].$$  \hfill (1.22)
and decays as $t^{-s}$ in the sub-Ohmic case, compared to $\gamma(t) \propto t^{-2}$ for Ohmic damping\(^2\). This is what makes sub-Ohmic damping complicated both in physical and computational sight. Every approach that neglects correlations at times that are larger than some finite cut-off time runs the risk of eliding important physical effects in this regime.

We end this section with a brief remark on the noise characteristics in the classical case. Fourier transforming the time-dependent bath fluctuations given by $L(t)$, we arrive at the so-called power spectrum $S(\omega)$. This is a characteristic quantity for any type of noise and appears also in signal processing and electronics. In our case, it is defined by \([1]\)

\[
S(\omega) := \int_{-\infty}^{\infty} dt \langle \xi_B(t)\xi_B(0) \rangle \cos(\omega t) = 2T \frac{I(\omega)}{\omega},
\]

as $\langle \xi_B(t)\xi_B(t') \rangle = MT\gamma(t-t')$ in the classical limit. So, Ohmic friction is connected to a frequency-independent power spectrum called white noise, whereas the deep sub-Ohmic case $s \to 0$ corresponds to famous $1/f$ or pink noise.

This is actually the CLM in a nutshell. In the following, we want to focus on tight-binding Hamiltonians, i.e. systems with discrete degrees of freedom. The SBM and the ISM are only two out of many representatives.

\section{1.2 The spin-boson model}

The dissipative formalism studied in the previous section is now used to describe quantum mechanical systems that can only have two different states. As the $z$-component of a spin-$1/2$ particle is an archetypical example, we often refer to spins. When coupling the spin to an environment in the same way as in the Caldeira-Leggett formalism, we achieve the SBM \([20]\), which is presented right now. Although this model is nothing but a simple version of the CLM, it was “discovered” by Blume, Emery and Luther \([21]\) more than a decade before Caldeira and Leggett presented their model.

\subsection{1.2.1 Experimental relevance}

Systems consisting of only two quantum states are omnipresent in modern physics. Well-known examples are atoms that show Rabi oscillations when interacting with a periodic field, Rydberg atoms, electron transfer in a plethora of chemical reactions and tunneling between molecular configurations, where ammoniac ($\text{NH}_3$) is one famous representative. There are even examples in particle physics, such as strangeness oscillations of neutral K mesons \([20]\). The most important application are of course quantum bits (qubits), that may have the potential to start a new revolution in computer science and therefore belong to the most studied systems in today’s physics \([6, 25, 26]\). We note in passing that the TLS is often

\(^2\text{In this case, the cosine term gives a factor } (1 + \omega^2c^2t^2)^{-1/2}.\)
motivated by truncation of an asymmetric quartic potential, where temperature is so small that only the ground states in each single well contribute.

Several types of qubits base on the Josephson effect [28]. One example consists of a superconducting ring, that is interrupted by an external magnetic flux, a so-called rf SQUID (radio-frequency superconducting quantum interference device). The barrier bears an Ohmic resistance \( R \) and acts as a capacitor \( C \), while the ring structure accounts for a self-inductance \( L \). One can show that the total flux \( \phi = \phi_{\text{ext}} + LI \) follows the equation of motion [1]

\[
C \ddot{\phi} + \frac{\dot{\phi}}{R} + \frac{\partial V(\phi)}{\partial \phi} = 0,
\]

where the potential term \( V(\phi) \) is

\[
V(\phi) = \frac{1}{2L}(\phi - \phi_{\text{ext}})^2 - E_J \cos \left( \frac{2\pi \phi}{\phi_0} \right).
\]

Here, \( E_J = I_c \hbar/2e \) is the Josephson energy with critical current \( I_c \) and \( \Phi_0 = \hbar/2e \) is the flux quantum. In the domain \( L > \phi_0^2/4\pi^2E_J \), the flux can be trapped in one or several local minima. This way, the system can tunnel between different “localized” states. While this forms a so-called flux qubit, similar devices may realize charge qubits. Closely related to the latter is a very promising candidate, the so-called transmon [29]. Its main advantage is its weak sensitivity against charge noise, allowing for coherence times on the order of 100\( \mu \)s, compared to \( 1 - 2\mu \)s for other charge qubits.

As we do not know any physical system that lives in its own world and does not communicate with the surrounding, dissipation is always present. This justifies the embedding of our TLS into a bosonic reservoir and directly leads us to the SBM. For impressive technological progress within the last years, see e.g. [30, 31, 32, 33, 34, 36]. Other examples are quantum tunneling of defects in crystals and of light particles in metals (see [1] and references therein), TLSs in glasses [37], and electron transfer in chemistry [38]. Further realizations are mentioned in Secs. 3.1, 4.1, and 5.1.

In the following, we summarize some results for the free TLS, that can easily be found analytically, before we turn to the dissipative model. A part of the discussion concentrates on how the environmental variables are integrated, where most of the calculations are postponed to the appendix. Finally, we spend some words on the non-interacting blip approximation (NIBA) which is a well-established analytic theory for the SBM dynamics.

### 1.2.2 The free two-level system

A system that can only take two different states lives in a two dimensional Hilbert space. In analogy with an electronic spin, we label the corresponding localized states with \( |+1\rangle \) and \(|-1\rangle \). The Hamiltonian of this simple TLS expressed in the language of Pauli matrices

\[^3\text{Notice that the connection between the state and the corresponding matrix elements is defined via the eigenvalues of the } \sigma_2 \text{ Pauli matrix, so e.g. the matrix element } \langle -1|A|-1 \rangle \text{ of any observable } A \text{ corresponds}\]
reads

\[ H_{TLS} = \frac{1}{2} \begin{pmatrix} \epsilon & -\Delta \\ -\Delta & -\epsilon \end{pmatrix} = \frac{\epsilon}{2}\sigma_z - \frac{\Delta}{2}\sigma_x, \]  

(1.26)

where \( \epsilon \) is a bias and \( \Delta \) the tunnel matrix element between the sites \([3]\). The system’s eigenvalues are

\[ E_{\pm} = \pm \frac{1}{2} \sqrt{\epsilon^2 + \Delta^2} \]  

(1.27)

and have the form of hyperbolas when plotted as a function of \( \epsilon \) for constant \( \Delta \neq 0 \). The effect that both curves do not meet in the unbiased case \( \epsilon = 0 \) is called avoided crossing and is a consequence of tunneling: Even if the \( \sigma_z \) eigenstates are degenerated, the TLS eigenstates differ by an energy of \( \Delta \).

For the dynamics, the system is initially prepared in an arbitrary pure state \( |\psi\rangle \) with density

\[ \rho_0 = |\psi\rangle \langle \psi| = \frac{1}{2} \left( 1 + \sum_{\nu=x,y,z} P_{\nu}(0)\sigma_{\nu} \right), \]  

(1.28)

where the initial values must be chosen such that Eq. (1.30) is fulfilled. With \( H^2 = \frac{1}{4}(\epsilon^2 + \Delta^2)\mathbb{1} \), we can easily calculate the propagator \( e^{-iHt} \) that determines the operator dynamics, \( \sigma_i(t) = e^{iHt}\sigma_ie^{-iHt} \). The time-dependent expectation values \( P_{\nu}(t) \equiv \langle \sigma_{\nu}(t) \rangle \) therefore read

\[
\begin{align*}
P_x(t) &= P_x(0)\frac{\Delta^2 + \epsilon^2 \cos(\Omega t)}{\Omega^2} - P_y(0)\frac{\epsilon}{\Omega} \sin(\Omega t) + P_z(0)\frac{\epsilon \Delta}{\Omega^2} [\cos(\Omega t) - 1], \\
P_y(t) &= P_z(0)\frac{\epsilon}{\Omega} \sin(\Omega t) + P_y(0)\cos(\Omega t) + P_z(0)\frac{\Delta}{\Omega} \sin(\Omega t), \\
P_z(t) &= P_z(0)\frac{\epsilon \Delta}{\Omega^2} [\cos(\Omega t) - 1] - P_y(0)\frac{\Delta}{\Omega} \sin(\Omega t) + P_z(0)\frac{\epsilon^2 + \Delta^2 \cos(\Omega t)}{\Omega^2},
\end{align*}
\]  

(1.29)

where \( \Omega = \sqrt{\Delta^2 + \epsilon^2} \). We distinguish between the populations \( (1 \pm P_z(t))/2 \) and the coherences \( P_x(t) \) and \( P_y(t) \). The latter can also be gained by the relation \( P_y(t) = -\frac{\Delta}{\Omega} \frac{dP_z}{dt} \), which follows immediately from Heisenberg’s equation of motion and holds also in the dissipative case. At all times, the expectation values fulfill the Bloch sphere equation

\[ P_x(t)^2 + P_y(t)^2 + P_z(t)^2 = 1 \]  

(1.30)

that holds for a pure state, \( \text{Tr}(\rho^2) = 1 \), and turns into \( \sum_{\nu} P_{\nu}(t)^2 < 1 \) for mixed ensembles. This is particularly the case when the surrounding modes get involved into the dynamical evolution, so that Eq. (1.30) is only valid at \( t = 0 \).

### 1.2.3 Dissipative model and reduced dynamics

From now on, dissipation is included in the spirit of the CLM. The displacement operator \( X \), that couples to the stochastic force \( \xi_B \), cf. Eq. (1.10), is replaced by \( -\sigma_z/2 \), so that to the entry \( A_{22} \).
the localized states refer to the positions $\pm 1/2$. Due to $\sigma^2_z = 1$, the counter term is just a constant and can be dropped. The spin-boson (SB) Hamiltonian then reads

$$H_{SB} = H_{TLS} + H_I + H_B = \frac{\epsilon}{2}\sigma_z - \frac{\Delta}{2}\sigma_x + \frac{1}{2}\sum_\alpha c_\alpha x_\alpha + \sum_\alpha \left( \frac{p^2_\alpha}{2m_\alpha} + \frac{m_\alpha \omega^2_\alpha}{2} x^2_\alpha \right). \quad (1.31)$$

With this, we can motivate the reorganization energy defined in (1.16). This quantity appears in Marcus theory, a description for electron transfer in donor-acceptor systems at high temperatures, cf. Sec. 3.1. It can easily be interpreted by taking a look at the interaction part in Eq. (1.31) for the classical model. Depending on the spin’s position, the potential surfaces of the bath modes have their minima at $x_\alpha = \pm c_\alpha/2m_\alpha \omega^2_\alpha$. When the particle is transferred to the other site, the corresponding rearrangement of the mode’s displacement causes an energy shift of $\Delta E = \sum_\alpha \frac{c^2_\alpha}{2m_\alpha \omega^2_\alpha}$, which is equal to (1.16).

In the following, we will see that the dissipative part can be reduced to a very compact functional dependence, which is the IF. Authors often avoid its detailed derivation in textbooks. This is why we investigate some time and give a few more steps of the derivation in App. B.

The expectation value of any observable $\sigma_\nu$ ($\nu = x, y, z$) in the dissipative model is given by

$$\langle \sigma_\nu(t) \rangle = \text{Tr} \left[ W(0)e^{iH_{SB}t}\sigma_\nu e^{-iH_{SB}t} \right] \quad (1.32)$$

with $t$ being the system time. We restrict the discussion to an initial density matrix that factorizes the TLS and the environmental part,

$$W(0) = \rho_0 Z^{-1}e^{-\beta H_B} \quad (1.33)$$

with $\rho_0$ from (1.28). All further steps for the factorized preparation can be found in App. B. We note in passing that another kind of initial preparation, which can be treated exactly with PIs, are the so-called correlated initial preparations. Here, one starts with a density $\sum_{\lambda,\nu} c_{\lambda\nu}\sigma_\lambda e^{-\beta H_{SB}} \sigma_\nu$, where $H_{SB}$ is the full Hamiltonian and $c_{\lambda\nu}$ are coefficients which must be chosen such that the density is Hermitian and normalized. However, correlated initial preparations require an additional PI in imaginary time and are less instructive from the physical point of view. As we only deal with real-time PI’s, they are of no relevance in this work. Therefore, the corresponding contributions that would appear were dropped in Eq. (1.14).

After discretizing the double PI and eliminating the surrounding degrees of freedom, we end up with an expression of the form (2.8) for the dynamics of any SB observable, where the IF $\Phi^{SB}[\zeta, \eta]$ reads in its continuous version

$$\Phi^{SB}[\zeta, \eta] = \int_0^t dt' \int_0^{t'} dt'' \zeta(t') [L(t' - t'') \zeta(t'') + iL''(t' - t'') \eta(t'')]. \quad (1.34)$$

Here, we insert the auto-correlation function $L(t)$ defined in Eq. (1.15) and the center-of-mass and relative coordinates

$$\eta := \frac{\sigma + \sigma'}{2}, \quad \zeta := \frac{\sigma - \sigma'}{2}. \quad (1.35)$$
As a last step, we want to include the effect of a shifted environment, i.e., a bath that is equilibrated with respect to the position \( \mu \neq 0 \). One therefore has to do the replacement
\[
e^{-\beta H_B} \rightarrow e^{-\beta (H_B - \frac{\mu}{2} \xi_B)} = e^{-\beta (H_B - \frac{\mu}{2} \sum \alpha c_{\alpha} x_{\alpha})}.
\]
(1.36)

\( \mu = 0 \) means that the bath is initially located in the Landau-Zener region, i.e., exactly between the TLS eigenstates. Of course, we could have done the whole IF derivation with initial bath state (1.36) instead of \( e^{-\beta H_B} \). Actually, it is physically more instructive to choose another way. Equilibration with respect to the position \( \mu \) means that the system coordinates are held fixed at \( \zeta(t) = 0 \) and \( \eta(t) = \mu \) for \( -\infty < t < 0 \). Therefore, we replace the integration borders of the IF 0, ..., \( t \) by \( -T, ..., t \). The values for \( t < 0 \) are inserted as described. Performing the limit \( T \rightarrow \infty \), we get \( \Phi_{SB} \rightarrow \Phi_{SB} + \Phi_{\text{shift}} \) with the additional contribution
\[
\Phi_{\text{shift}}[\zeta] = -i \mu \int_0^t dt' \zeta(t') \dot{Q}''(t').
\]
(1.37)

Note that, in general, \( \mu \) does not have to be an eigenvalue of \( \sigma_z \). However, next to the situation \( \mu = 0 \) (to which we refer as the standard preparation), the value \( \mu = P_z(0) \) (called shifted or polarized preparation) is the most relevant one in physical sense. It can easily be realized in charge systems: By applying a strong electric field for \( t < 0 \), the system can be pushed in one of the \( \sigma_z \) eigenstates, so that the bath adjusts to this fixed spin position. If the field is switched off, the total system evolves out of a factorized state with shifted bath and the TLS reserving in the corresponding \( \sigma_z \) eigenstate. Therefore, this initial setting is used in most of our simulations.

Let us have a brief look at the matrix elements of the free TLS propagators that enter the action as an independent factor next to the IF, see Eq. (2.8). In discretized form, \( K_{\sigma_{j+1}, \sigma_j} \) reads after making use of Trotter’s formula
\[
K_{\sigma_{j+1}, \sigma_j} = \langle \sigma_j | e^{-iH_{TLS} t} | \sigma_{j+1} \rangle \approx e^{-i \frac{\epsilon}{2} \sigma_{j+1}^z} \langle \sigma_j | e^{i \frac{\Delta \sigma_{x}}{2} \sigma_{x}^\tau} | \sigma_{j+1} \rangle.
\]
(1.38)

As the bias part \( \epsilon \sigma_z / 2 \) acts on an eigenstate, it can be split from the tunneling part. Collecting these factors from all Trotter steps at both forward and backward path, one clearly sees that all terms containing the bias \( \epsilon \) merge in a factor
\[
\exp \left( -i \frac{\epsilon}{2} \int_0^t dt' [\sigma(t') - \sigma'(t')] \right) = \exp \left( -i \epsilon \int_0^t dt' \zeta(t') \right).
\]
(1.39)

This term can be easily understood from the physical point of view: In an off-diagonal state with \( \sigma = -\sigma' \), forward and backward path differ by an energy \( \epsilon \), which leads to accumulation of a phase difference during time evolution. If we compare Eq. (1.39) to Eq. (1.37), we see that the initial bath displacement enters the action in the same way as a time-dependent bias of size \( -\mu \dot{Q}''(t) \) [73] ⁴.

⁴Assuming a time-dependent \( \epsilon(t) \) from the very beginning makes things more complicated, because then, the propagation requires a time-ordered product. However, the calculation still results in the factor (1.39).
CHAPTER 1. DISSIPATIVE QUANTUM MECHANICS

The basics of our model are now sketched. Before discussing in long terms, how to implement all this in the computer, we present a perturbative analytical treatment that ought to serve as a reliable reference for our Path Integral Monte Carlo (PIMC) simulations and discuss the technical details in Chap. 2.

1.2.4 The non-interacting blip approximation

The NIBA is a widely established theory [116, 118, 119] and although its simplifications seem to be very rough, it yields qualitatively and in several parameter regimes even quantitatively fine results. We first sketch a formal exact solution of the SBM and then introduce the approximations that lead to the NIBA equations of motion. The discussion is limited to the case of the initial preparation \( \rho(0) = |+1\rangle\langle +1| \), although this theory has been extended to non-diagonal initial preparations [122]. Finally, we discuss the limits in which NIBA is expected to work.

Our starting point is the time evolution of the reduced density matrix,

\[
\rho_{\sigma_j,\sigma'_j}(t) = \rho_{\sigma_j,\sigma'_j}(0) + \int_{\sigma(0)=1}^{\sigma(t)=\sigma_j} D\sigma \int_{\sigma'(0)=1}^{\sigma'(t)=\sigma'_j} D\sigma' A[\sigma]A^*[\sigma']B[\sigma]B^*[\sigma']e^{-\Phi^{ex}[\sigma,\sigma']}.
\] (1.40)

\( A \) is the part that contains the tunneling matrix element \( \Delta \), \( B \) includes the effect of the bias and \( \Phi^{ex} \) is the exact IF, formulated in sum and difference coordinates \( \chi/\xi := (\sigma \pm \sigma')/2 \)

\[
\Phi^{ex}[\xi,\chi] = \int_0^t dt' \int_0^{t'} dt'' \dot{\xi}(t') \left[ Q'(t' - t'')\dot{\chi}(t'') + iQ''(t' - t'')\dot{\chi}(t'') \right].
\] (1.41)

The sum and difference paths \( \chi \) and \( \xi \) read

\[
\chi(t) = \sum_{j=0}^{2n} \chi_j \Theta(t - t_j), \quad \xi(t) = \sum_{j=1}^{2n} \xi_j \Theta(t - t_j).
\] (1.42)

The \( t_j \) are the flip times where the spin changes its direction either on the forward or on the backward path. Obviously, Eq. (1.41) differs from the original one (1.34) by a twofold partial integration. Notice that the bath shift factor (1.37) is already included in Eq. (1.41) for \( \mu = P_z(0) = 1 \). If one wants to study different bath preparations, one has to insert a time-dependent bias of size \( (\mu - 1)\dot{Q}''(t) \) in the factor \( B \). Time-ordering requires \( t_0 = 0 \leq t_1 \leq ... \leq t_{2n} \leq t \). The \( \chi \)'s and \( \xi \)'s are not independent of each other; we thus have

\[
\chi_0 = 1, \quad \chi_{2j+1} = -\chi_{2j}, \quad \xi_{2j} = -\xi_{2j-1}.
\] (1.43)

Clearly, the \( \chi_j,\xi_j \in \{-1,1\} \) are not the values of the coordinate \( \chi(t),\xi(t) \) after a certain number of flips, but the change in the related coordinate compared to the situation before the flip. The set of paths in (1.42) measure the diagonal elements, because they start and end in a diagonal state, \( \xi(0) = \xi(t) = 0 \). For the off-diagonal operators \( \sigma_x \) and \( \sigma_y \), one has to sum over paths with an odd number of flips.
With this parametrization, the multitude of paths is scanned by a convoluted integration over the flip times and a sum over all possible values of the intermediate \( \chi \)'s and \( \xi \)'s. Due to (1.43), only half of them are independent. We rename the free values with \( \chi_{1...n}, \xi_{1...n} \) and perform the PI via
\[
\sum_{n=1}^{\infty} \int_0^t \mathcal{D}\{t_j\} \sum_{\{\chi_i,\xi_i\}} \equiv \sum_{n=1}^{\infty} \int_0^t dt_{2n} \int_0^{t_{2n}} dt_{2n-1} ... \int_0^{t_2} dt_1 \sum_{\chi_{1...n}=\pm1, \xi_{1...n}=\pm1} \sum_{\tau_{2n}} .
\] (1.44)

A convenient indication is to name the diagonal states with \( \chi(t) = \pm 1, \xi(t) = 0 \) sojourns and the off-diagonal ones with \( \xi(t) = \pm 1, \chi(t) = 0 \) blips. Apparently, the time intervals spent in a sojourn (blip) are \( s_j = t_{2j+1} - t_{2j} \) \( (\tau_j = t_{2j} - t_{2j-1}) \). The IF term containing \( Q'(t) \) suppresses the blip times exponentially with increasing coupling. This is important for truncating the following analytical expression.

The double integral of the IF can be easily evaluated to
\[
\Phi^{ex} = \sum_{j=1}^{n} \left[ S_j - i \sum_{k=0}^{j-1} \xi_j X_{jk} \chi_k \right] + \sum_{j=2}^{n} \sum_{k=1}^{j-1} \xi_j \Lambda_{jk} \xi_k .
\] (1.45)

where
\[
\Lambda_{jk} = \text{Re} \left[ Q(t_{2j} - t_{2k-1}) + Q(t_{2j-1} - t_{2k}) - Q(t_{2j} - t_{2k}) + Q(t_{2j-1} - t_{2k-1}) \right] \\
X_{jk} = \text{Im} \left[ Q(t_{2j} - t_{2k-1}) + Q(t_{2j-1} - t_{2k}) - Q(t_{2j} - t_{2k}) + Q(t_{2j-1} - t_{2k+1}) \right] \\
S_j = \text{Re} \left[ Q_{2j} - Q_{2j-1} \right]
\] (1.46)

for \( k > 0 \). The terms \( X_{j0} \) depend on the choice of the environment’s initial preparation. In the following, we are only interested in the shifted bath preparation, corresponding to \( t_0 \rightarrow \infty \). Intra-blip interaction is stored in the \( S_j \), while \( \Lambda(X) \) describes the interaction of blips with earlier blips (sojourns). The summation over the sojourn coordinates \( \chi_{1...n-1} \) can now be performed exactly. This leads to a formally exact solution for \( P_z(t) \) [116],
\[
P_z(t) = 1 + \sum_{n=1}^{\infty} \int_0^t \mathcal{D}\{t_j\} \left( -\frac{\Delta^2}{2} \right)^n \sum_{\xi_{j}=\pm1} \left[ F_n^{(+)} B_n^{(s)} - F_n^{(-)} B_n^{(a)} \right].
\] (1.47)

Here, we recognize a factor \( i\Delta \) for each spin flip. Numerous quantities were defined that contain the dissipative and biasing effects (we restrict to the non-driven case \( \epsilon = \text{const.} \)):
\[
B_n^{s/a} = \frac{\cos \left( \epsilon \sum_{j=1}^{n} \xi_j \tau_j \right)}{\sin \left( \epsilon \sum_{j=1}^{n} \xi_j \tau_j \right)} \\
F_n^{(+/-)} = G_n \frac{\cos(\phi_{0n})}{\sin(\phi_{0n})} \prod_{k=1}^{n-1} \cos(\phi_{kn}) \\
G_n = \exp \left[ -\sum_{j=1}^{n} S_j - \sum_{j=2}^{n} \sum_{k=1}^{j-1} \xi_j \xi_k \Lambda_{jk} \right] \\
\phi_{kn} = \sum_{j=k+1}^{n} \xi_j X_{jk} .
\] (1.48)
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Figure 1.1: The figure shows the NIBA approximations in the IF. The system is in a blip state if $|\xi| = 1$ and in a sojourn state otherwise. While interblip terms $S_i$ are conserved, the blip-blip interaction $\Lambda$ is thrown away. Further, the blip-sojourn interaction $X$ is neglected, except for the neighbor term $X_{i,i-1}$.

$s/a$ label the symmetry/antisymmetry with respect to the sign of $\epsilon$. Clearly, Eq. (1.47) is impossible to be evaluated numerically. Therefore, one has to start with approximations now. The blip times are suppressed compared to the sojourn times, when the system couples strongly to the bath, $s_j \gg \tau_j$. Furthermore, the interaction between two time intervals decreases, when their distance increases. For these reasons, one neglects the whole blip-blip interaction $\Lambda$, except for the intrablip terms $S$, and the interaction $X$ of blips with earlier sojourns, except the nearest neighbor term. This is sketched in Fig. 1.1. The IF contribution then shrinks to

$$\Phi_{\text{NIBA}} = \sum_{j=1}^{n} S_j - i \sum_{j=0}^{n} \xi_j X_{j,j-1} \chi_{j-1}$$

where $X_{j,j-1} \approx Q''(\tau_j)$. This seems to be a very rude approximation, but its predictions will still be very useful. The steps up to now were only sketched to give the reader a feeling of the idea behind and of the “roughness” of the approximation. For all the further steps including improved approaches, we refer to the extensive literature [1, 116, 118, 119]. The equation of motion for populations $P_{z,\text{NIBA}}$ finally reads

$$\frac{dP_{z,\text{NIBA}}(t)}{dt} = -\int_{0}^{t} dt' \left[ K_a(t-t') + K_s(t-t') P_{z,\text{NIBA}}(t') \right],$$

with kernels

$$K_s(t) = \Delta^2 e^{-Q'(t)} \cos(\epsilon t) \cos [Q''(t)]$$

$$K_a(t) = \Delta^2 e^{-Q'(t)} \sin(\epsilon t) \sin [Q''(t)].$$

(1.51)

For details concerning numerical implementation, see Ref. [123]. An alternative derivation can be found in [117]. We also sketch the result for $P_{x,\text{NIBA}} [120, 121, 122]$,

$$P_{x,\text{NIBA}}(t) = \int_{0}^{t} dt' \left[ K_{s,x}(t-t') - K_{a,x}(t-t') P_{z,\text{NIBA}}(t') \right],$$

(1.52)

where

$$K_{a,x}(t) = \Delta e^{-Q'(t)} \cos(\epsilon t) \sin [Q''(t)]$$

$$K_{s,x}(t) = \Delta e^{-Q'(t)} \sin(\epsilon t) \cos [Q''(t)].$$

(1.53)
Take note of the fact that \( P_N^{\text{NIBA}}(t) \) is just a time integral over \( K_{N,x}^s \) in the case of a symmetric TLS. Again, \( P_y^{\text{NIBA}}(t) \) can be determined via \( P_y^{\text{NIBA}}(t) = -\frac{1}{\Delta} \frac{d}{dt} P_z^{\text{NIBA}}(t) \).

As already indicated, the NIBA results increase in accuracy, when the system-bath coupling or the temperature increase. This is easy to understand as the Gaussian term \( \exp \left( -\sum_j S_j \right) \) suppresses the blip times and makes the approximation work better. As it is easy to show, NIBA also gives the correct result for vanishing dissipation, at least for \( \epsilon = 0 \). Therefore, it fails especially in the intermediate regime.

### 1.3 Model for interacting spins

After having explained the physics of the SBM in detail, we want to extend the model towards a system that consists of two spins \( A \) and \( B \), which interact with each other and couple to the same environment. Whereas a lot of methodology can be adopted, we still get insight into complete new physics.

Models of this type are of fundamental interest in a variety of fields. One application is exciton transfer in biomolecules, a field, that has been attracting enormous attention within the last few years due to its fundamental role it plays in nature [140]. In addition, such models are of substantial importance in some fields that are even more prospering: This is quantum information and quantum optics [25, 26, 27]. Here, interacting qubits, realized e.g. by trapped ions, Rydberg atoms, or superconducting solid-state devices are the fundamental entities for quantum computation [6]. As both the progress during the last years and the potential for future developments in the overall field of quantum optics are tremendous, it was not surprising that the 2012 Nobel Prize in Physics was awarded to French physicist Serge Haroche and American physicist David Wineland for their pioneer works on light-matter interaction of atoms in cavities.

#### 1.3.1 The free system

One possibility to make these spins interact is a coupling term that contains the \( \sigma_x \) operators, thereby arriving at the bare Hamiltonian \( H_{2\text{TLS}} \)

\[
H_{2\text{TLS}} = \frac{\epsilon_A}{2} \sigma_z^A - \frac{\Delta_A}{2} \sigma_x^A + \frac{\epsilon_B}{2} \sigma_z^B - \frac{\Delta_B}{2} \sigma_x^B - J \sigma_x^A \sigma_x^B.
\]  

The parameters in Eq. (1.54) are bias asymmetries \( \epsilon_{A/B} \), tunnel matrix elements \( \Delta_{A/B} \) (where both bias and tunnel coupling might be different for the two spins) and coupling \( J^5 \).

The system lives in a four-dimensional Hilbert space, where we introduce the orthogonal

\[\sigma_z^A \rightarrow \sigma_z^A \otimes 1^B.\]  

\[\sigma_z^A \rightarrow \sigma_z^A \otimes 1^B.\]
basis states

\[ |1\rangle = |+1+1\rangle, \quad |2\rangle = |+1-1\rangle, \quad |3\rangle = |-1+1\rangle, \quad |4\rangle = |-1-1\rangle. \tag{1.55} \]

The states on the right hand side refer to \( \sigma_z \) eigenstates of the single spins, so, e.g. \(|+1-1\rangle\) actually means that spin \( A \) is in state \(|+1\rangle\) and \( B \) in state \(|-1\rangle\). We keep on using the notation that calls spin \( A \) first. Writing the whole stuff in matrix form, we arrive at

\[
H_{2\text{TLS}} = \begin{pmatrix}
\epsilon_A + \epsilon_B & -\Delta_B & -\Delta_A & -J \\
-\Delta_B & \epsilon_A - \epsilon_B & -J & -\Delta_A \\
-\Delta_A & -J & \epsilon_A + \epsilon_B & -\Delta_B \\
-J & -\epsilon_A & -\epsilon_B & -\Delta_A
\end{pmatrix}. \tag{1.56}
\]

We only get compact analytical expressions for the \( 4 \times 4 \) propagator \( K(t) = e^{-iH_{2\text{TLS}}t} \) in some special cases. In general, \( K(t) \) is evaluated numerically. We prepare the system in a product state of the subsystems,

\[
\rho(0) = \rho^A(0) \otimes \rho^B(0), \tag{1.57}
\]

where each one is in any state on the surface of the Bloch sphere, i.e.

\[
\rho^{A/B}(0) = \frac{1}{2} \left( 1 + \sum_{\nu=x,y,z} P^A/B(0) \sigma^{A/B}_\nu \right). \tag{1.58}
\]

with \( \sum_{\nu} (P^A/B)^2 = 1 \) for a pure state. This way, the spins are not entangled in the beginning – neither with the bath, nor with each other.

However, the non-existence of entanglement between the spins is not indispensable. For this purpose, we introduce another set of initial preparations that are characterized by a maximal entanglement between both spins. These are the four Bell states \cite{135}, that we label according to an established convention,

\[
|\Psi^-\rangle = \frac{1}{\sqrt{2}} (|2\rangle - |3\rangle), \quad |\Psi^+\rangle = \frac{1}{\sqrt{2}} (|2\rangle + |3\rangle) \\
|\Phi^-\rangle = \frac{1}{\sqrt{2}} (|1\rangle - |4\rangle), \quad |\Phi^+\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |4\rangle). \tag{1.59}
\]

Hence, the initial density is given by a pure (but entangled) state, e.g. \( \rho(0) = |\Psi\rangle\langle\Psi| \). We do not want to go into further details concerning the Bell states and their relevance. Instead, we refer to Subsec. 6.4.2, where they will reappear.

Now, what are the observables of interest? Being Hermitian \( 4 \times 4 \) matrices, one clearly sees that we end up with 16 observables, four of them diagonal and twelve of them off-diagonal ones. Due to conservation of probability, only three of the former are independent. In order to go through them in a systematic way, we divide them into four categories: The first contains the populations with both spins being in a diagonal state. In addition, we have
four observables that refer to non-diagonal states for both spins, another four with spin \( A \) being diagonal and spin \( B \) off-diagonal, and finally four where the situation is vice versa.

Let us start with the populations. We ask for the probability of the system to be in the state \( |\nu\rangle \in \{|1\rangle, |2\rangle, |3\rangle, |4\rangle\} \) according to the basis (1.55). Then, the matrix representation \( A \) of the observable is simply diagonal with \( A_{ii} = 1 \) and \( A_{jj} = 0 \) for \( j \neq i \).

Things become slightly different for the other observables. Choosing twelve off-diagonal matrices is not unique. Therefore, we define six \( \sigma_x \)- and six \( \sigma_y \)-like observables. This is illustrated for the off-diagonal elements 12 and 21, determined by the matrices \( \sigma_x,_{12} \) and \( \sigma_y,_{12} \):

\[
\sigma_{x,12} = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix} \equiv \frac{1_A + \sigma_z^A}{2} \otimes \sigma_x^B
\]

\[
\sigma_{y,12} = \begin{pmatrix}
0 & -i & 0 & 0 \\
i & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix} \equiv \frac{1_A + \sigma_z^A}{2} \otimes \sigma_y^B. \quad (1.60)
\]

The matrices \( \sigma_{x/y,13}, \sigma_{x/y,14}, \sigma_{x/y,23}, \sigma_{x/y,24} \) and \( \sigma_{x/y,34} \) are defined in complete analogy.

It is straightforward to check, how one would extract the observables for a single spin, \( \sigma_x \equiv 1_A \otimes \sigma_x^B \), as an example. Writing \( 1_A = (1_A + \sigma_z^A)/2 + (1_A - \sigma_z^A)/2 \), we see that the corresponding \( 4 \times 4 \) matrix is \( \sigma_{x,12} + \sigma_{x,34} \).

We would like to get a first feeling for the dynamics of the free system and show some plots for different parameters in Fig. 1.2. Here and in the remainder, we use \( \Delta_A \) as an energy and inverse time scale. The six panels show the population dynamics for a system with initial density \( \rho(0) = |1\rangle\langle 1| = \text{diag}(1,0,0,0) \).

Let us start the discussion with a system of unbiased, uncoupled, and identical spins (\( \epsilon_A = 0, J = 0, \Delta_A = \Delta_B \), upper left panel). Tunneling causes oscillations between the states \( |1\rangle \) and \( |2\rangle \), \( |3\rangle \) and \( |4\rangle \) (\( \Delta_B \)), \( |1\rangle \) and \( |3\rangle \), \( |2\rangle \) and \( |4\rangle \) (\( \Delta_A \)), respectively. So, the system oscillates from \( |1\rangle \) to \( |4\rangle \) and the other way round, thereby degrading states \( |2\rangle \) and \( |3\rangle \) to intermediate stations, that are less populated at average.

Increasing \( J \) up to \( 0.5\Delta_A \) and keeping the other parameters constant causes a direct coupling between \( |1\rangle \) and \( |4\rangle \) (upper middle). By this, each state couples to all the others with the same magnitude. Henceforth, the dynamics is nothing but a back and forth oscillation between the initially occupied state \( |1\rangle \) and the others. The latter, however, have the same values at all times and therefore do not exchange population among each other.

Things change, when \( J \) becomes larger than \( \Delta_{A/B}/2 \) (\( J = 2\Delta_A \), upper right panel). Then, the interplay between states \( |1\rangle \) and \( |4\rangle \) dominates. For \( J \gg \Delta_A, \Delta_B \), the populations \( P_1 \) and \( P_4 \) shows a beat with envelope frequency \( \Delta_A = \Delta_B \) and a frequency of shrouded oscillations that grows \( \propto J \).
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Figure 1.2: The panels show the free dynamics of the populations with different tunnel couplings, interactions $J$, and biases $\epsilon^{A/B}$. The system is initially prepared in the state $|1\rangle$. See text for details.

In the lower left panel, we return to $J = 0.5\Delta_A$ and decrease $\Delta_B$ down to $0.5\Delta_A$. While the populations of states $|3\rangle$ and $|4\rangle$ remain the same, the interplay between $|1\rangle$ and $|2\rangle$ changes: In the very beginning, the population flow towards $|2\rangle$ is suppressed compared to the prior situations. Evolving a bit further in time, $P_2$ grows beyond $P_3$ and $P_4$, because the population flows from these two states towards $|2\rangle$. After a short dip of $P_2$, $P_4$ starts to decrease, whereas $P_2$ increases towards its maximal value 1.

The opposite case, $\Delta_B = 2\Delta_A$, can be seen in the lower middle panel. In the beginning, we observe a strong flow from $|1\rangle$ to $|2\rangle$, resulting in a fast increase of $P_2$. Then, $|2\rangle$ starts again to lose population and runs towards its maximum after passing a local minimum. This dynamics takes place faster than in the case right before.

In the last example, we assign again the same values to $\Delta_A$ and $\Delta_B$, keep $J = 0.5\Delta_A$, but introduce a bias $\epsilon_A = 2\Delta_A$. In general, one can ascertain that the populations of states $|3\rangle$ and $|4\rangle$ are suppressed compared to the unbiased case. This is of course what we would
expect. In addition, a fast frequency is imprinted on the dynamics of $P_1$ and $P_2$. As it grows with increasing $\epsilon$ while its amplitude decreases, the whole system reduces to an effective TLS with oscillation frequency $\Delta_B$ in the limit of a very large bias (not shown).

Conclusively, the mixture of different frequencies expresses itself in a complex back and forth between different states. By putting such a framework into a bosonic bath, one ought to create a system that shows multifarious physics.

1.3.2 The dissipative model

We switch on dissipation and couple both spins to the same bath. The system-bath interaction is introduced in a familiar way, i.e. the position operator $X = -(\sigma^A_z + \sigma^B_z)/2$ couples to the stochastic bath force,

$$H_{ISM} = H_{TLS} + \sum_\alpha \left[ \frac{m_\alpha \omega_\alpha^2}{2} \left( x_\alpha + \frac{c_\alpha}{m_\alpha \omega_\alpha^2} \frac{\sigma^A_z + \sigma^B_z}{2} \right)^2 + \frac{p_\alpha^2}{2m_\alpha} \right]$$

$$= H_{TLS} + \frac{\sigma^A_z + \sigma^B_z}{2} \sum_\alpha c_\alpha x_\alpha + \sum_\alpha \left( \frac{m_\alpha \omega_\alpha^2}{2} + \frac{p_\alpha^2}{2m_\alpha} \right) + \sum_\alpha \frac{c_\alpha^2}{2m_\alpha \omega_\alpha^2} \left( \frac{\sigma^A_z + \sigma^B_z}{2} \right)^2,$$

(1.61)

The IF is basically governed by replacing $\eta \to \eta^A + \eta^B$ and $\zeta \to \zeta^A + \zeta^B$ in (1.34) and adding the counter term contribution, cf. Eq. (1.14). Contrarily to the SBM, the latter must not be dropped, as its absence would cause a static interaction between spins $A$ and $B$. This corresponds to friction forces that do not depend on the particle’s velocity in the language of classical Langevin equation. Throwing away the constant parts $(\sigma^A_z)^2$, we arrive at

$$\Phi_{ISM}[\zeta^{A/B}, \eta^{A/B}] = \int_0^t dt' \int_0^{t'} dt'' [\zeta^A(t') + \zeta^B(t')] \left\{ L'(t' - t'') \left[ \zeta^A(t'') + \zeta^B(t'') \right] + iL''(t' - t'') [\eta^A(t'') + \eta^B(t'')] \right\} - i2\mu \int_0^t dt' [\zeta^A(t') + \zeta^B(t')] \dot{Q}''(t')$$

$$+ i\Lambda_d \int_0^t dt' [\eta^A(t') \zeta^B(t') + \zeta^A(t') \eta^B(t')]$$

(1.62)

The parameter $\mu$ is given by the average value of the spin sum coordinates for $t < 0$, i.e.

$$\mu = \frac{\eta^A(t < 0) + \eta^B(t < 0)}{2}. \quad (1.63)$$

It is obvious that the subsystems $A$ and $B$ are coupled even in the case $J = 0$. The bath causes non-Markovian interactions between the spins according to terms of the form $\zeta^A(t') L'(t' - t'') \zeta^B(t'')$ and $\zeta^A(t') L''(t' - t'') \eta^B(t'')$. This way, there might be the possibility of creating entanglement, even if the spins do not interact directly. Notice that the SBM cannot be recovered by simply dropping the coupling term in $H_{ISM}$. Indirect interaction transferred by the surrounding is always present and removing the responsible terms by hand
would lead to the physically completely different situation of each spin coupling to its own bath.

The presented model is only one theoretical realization for a system of interacting TLSs. However, the way to couple system and bath linearly is a well-established choice and technically straightforward. All the PI methods can be applied similarly. We will actually see that an arrangement of two spins and a bath gains insight into a variety of new quantum mechanical effects.
Chapter 2

Path Integral Monte Carlo for Spin Systems

From the physical point of view, we have collected the whole inputs to analyze the spin dynamics. Remind that we did not do any approximation – up to now, the whole procedure is exact. Fortunately, this is also true for the numerical implementation that is presented right now: The Path Integral Monte Carlo (PIMC) method is known to yield numerically exact results for the dynamics of the spin-boson model (SBM) and the interacting spins model (ISM).

Now, what about this computational method that is mentioned in the chapter title? The terminus “Monte Carlo” (MC) may remind the reader to gambling and to formula 1. Indeed, MC simulations have one thing in common with each of these associations: They work with randomness and they require very fast machines, actually. But there exist substantial differences: In contradiction to gambling in the casino, we do not need good luck and the machines we work with are computers rather than V8 fuel engines.

As the power of computers has been growing exponentially with a doubling time of 18 months due to Moore’s law (which was stated in 1965!), we are treading a very promising way. This has led to the paradox situation that MC becomes more and more important in physics, the further its hour of birth lies in the past. The fields of applicability seem to be endless. A plethora of different MC techniques is used in nearly all divisions of physics and chemistry, but also in mathematics, biology, finance, economics, and even traffic simulations and meteorology. Ranging from questions such as how to create a random number generator [47, 48] to the full range of nuisances with modeling, implementation and debugging, a large variety of interesting problems is included [44, 45]. Surely, MC simulations caused myriad scientists quite a headache during the last decades.

In this chapter, we derive the main ingredients for the implementation. First, we give a short introduction into the technique of MC simulation in general, but with a special focus on so-called Metropolis sampling and the dynamical sign problem that appears in quantum dynamics [49]. Then, we show how the path integral (PI) expressions are discretized and
observables are extracted, before we mention some details that are important for the implementation. Finally, we inspect the difficulties on the way from the SBM to the ISM.

2.1 What is Monte Carlo?

One could define MC simulations as the totality of computational methods that try to calculate measurable properties by usage of random numbers. However, although it is a supporting pillar in the total concept, results do fortunately not depend on randomness in the end. We know from elementary mathematics that random can be systemized quantitatively by introducing distribution functions.

These functions play a basic role in Metropolis sampling, as sequences of coordinate values are generated according to a given distribution. We first present the underlying algorithm, before we try to visualize the unspeakable dynamical sign problem, which is a consequence of quantum mechanical interference.

2.1.1 Metropolis algorithm

The Metropolis algorithm was developed in 1953 by Metropolis et al. [43] and is the fundament of so-called importance sampling. Its basic idea is on the heart of thermodynamics. Any thermalized many-body system jumps between a huge variety of different states on the microscopic level, called microstates. Performing a summation over all of them or determining their sequence would be a completely hopeless attempt for typical particle numbers in the order of $10^{23}$. But as we are only interested in averages and fluctuations of macrostates, we do not care about any single microscopic realization.

We know from statistical physics that the very most part of possible states does not contribute significantly to the phenomenological state. This is what importance sampling makes use of. Instead of performing an average over all possibilities, thereby including all the states that are completely negligible, Metropolis algorithm shows how to select the important states and to get a correct result within some error bars.

This rather thermodynamical motivation should not mislead the reader over the fact that typical systems to be studied are mesoscopic in the following sense: The number of involved degrees of freedom is much too large to be treated on the level of single particle equations, but also much smaller than the number of particles in thermodynamic systems.

Metropolis algorithm works as follows: Suppose we deal with a system of $q$ degrees of freedom $x_1, \ldots, x_q$. We assume these variables to be in the microscopic state 1, labeled by $x^{(1)}_{1, \ldots, q}$, and called a configuration. $x_{1, \ldots, q}$ correspond to positions and momenta, as long as we work within Hamiltonian mechanics. In the canonical ensemble, the probability $p_1$ to be in this state depends only on its energy $H$,

$$p_1 \propto \exp \left[ -\beta H \left( x^{(1)}_{1, \ldots, q} \right) \right] = \exp \left[ -\beta H^{(1)} \right].$$

(2.1)
The factor $e^{-\beta H}$ plays the role of our *MC weight*. Now, we change one or several variables randomly and arrive at the state 2, that is labeled by $x_1^{(2)}, ..., x_q^{(2)}$ and occurs with a probability

$$p_2 \propto \exp \left[ -\beta H \left( x_1^{(2)}, ..., x_q^{(2)} \right) \right] = \exp \left[ -\beta H^{(2)} \right]. \quad (2.2)$$

Figure 2.1: This flowchart sketches the single steps in the Metropolis algorithm. Starting from an equilibrated configuration, we perform a flip and accept the new configuration with a certain probability. After a couple of flips, the quantity $A$ is evaluated with the current configuration. Repeating this procedure again and again, we can calculate a statistical estimator for $A$ in the end.

If $p_2 > p_1$, we accept the new configuration 2 and throw away the old one 1. If the opposite is the case, $p_1 > p_2$, we accept the configuration 2 with a probability $p_2/p_1$ that is given by the energy difference, $\exp \left[ -\beta \left( H^{(2)} - H^{(1)} \right) \right]$ in the canonical case. One such random modification including the decision upon its acceptance is called a *MC move* or *flip*, whereas a sequence of $q$ MC moves is a *MC step*. The number of MC steps between two accumulations (see below) is labeled with $r$. Clearly, the “size” of one flip influences the acceptance ratio. Both too frequent and too rare approval can cause problems, either with regard to ergodicity, or because of extreme spreading in configuration space with the consequence of large error bars. A rule of thumb is to perform the flips such that only some few percent are accepted.

The acceptance probability does also depend sensitively on temperature: Decreasing $\beta$ leads again to increased spreading, as long as the order of magnitude of the energy difference between consecutive microstates remains the same. This problem can be circumvented by choosing the acceptance probabilities differently, e.g. with the *Glauber sampling* for spin lattices [44]. We do not want to go into details, but rather mention that any acceptance probability is suitable, if it fulfills the *detailed balance relation*,

$$p(\vec{x}_n)w(\vec{x}_n \to \vec{x}_m) = p(\vec{x}_m)w(\vec{x}_m \to \vec{x}_n), \quad (2.3)$$
where \( w(\vec{x}_n \rightarrow \vec{x}_m) \) labels the transition rate for a change from state \( \vec{x}_n \) to \( \vec{x}_m \). It is obvious that the choice \( w(\vec{x}_n \rightarrow \vec{x}_m) = \frac{1}{\tau_0} \min[1, p(\vec{x}_m)/p(\vec{x}_n)] \) satisfies Eq. (2.3){\footnote{\( \tau_0 \) is introduced for dimensional reasons and has the meaning of a characteristic time scale for the jumps.}}. This relation, however, is nothing but the requirement for stationarity of the simple master equation

\[
\frac{dp(\vec{x}_n)}{dt} = \sum_m \left[ p(\vec{x}_n)w(\vec{x}_n \rightarrow \vec{x}_m) - p(\vec{x}_m)w(\vec{x}_m \rightarrow \vec{x}_n) \right].
\] (2.4)

Thus, MC sampling is a large Markov chain, where all possible configurations \( \vec{x}_n \) take the role of system states that change into each other with rates \( w(\vec{x}_n \rightarrow \vec{x}_m) \). The defining property for Markov chains is that the state \( i + 1 \) depends only on the state \( i \). It is needless to say this is valid for Metropolis sampling.

Now we know, how the random flipping is performed, but how do we actually calculate the value of an observable? The flipping procedure is repeated again and again. After one or several MC steps, the current configuration is \textit{accumulated} or \textit{sampled}, which means that the observable of interest, call it \( A \), is evaluated with the present values of \( x_1, \ldots, x_q \). The sampled configurations should not be correlated and therefore, it is a non-trivial task to determine the number of MC steps one should perform between two accumulations. For a detailed consideration, we refer to the literature [44, 45]. The way how this question is answered for our simulations is dealt within Sec. 2.2.

Still, Metropolis algorithm is neither restricted to the canonical ensemble, nor to thermodynamics in general. From the theoretical point of view, we can calculate every quantity that is determined by

\[
A = \int dx_1 \ldots dx_q A(\vec{x})p(\vec{x}),
\] (2.5)

regardless, if the multiple integration scans phase space, the possible paths of a quantum trajectory or anything else. The only requirements are that the number of degrees of freedom does not exceed a computationally treatable limit and that the function \( p(\vec{x}) \) fulfills the conditions of a good MC weight, i.e. it is

- real-valued and positive,
- normalized,
- and suppresses most parts of the integration area exponentially.

Then, the MC estimator for \( A \) reads

\[
A \approx \bar{A} = \frac{1}{N} \sum_{i=1}^N A(\vec{x}^{(i)}),
\] (2.6)

where the \( \vec{x}^{(i)} \) are configurations distributed according to the MC weight \( P \). \( N \) is the number of accumulations. It can be useful to include a factor \( f(\vec{x})/f(\vec{x}) \) where the numerator is
attached to the MC weight and the denominator to the sampled quantity. Thus, $A$ reads

$$
\bar{A} = \frac{1}{N} \sum_{i=1}^{N} \frac{A(\vec{x}^{(i)})}{f(\vec{x}^{(i)})},
$$

(2.7)

with $\vec{x}^{(i)}$ distributed according to $P(\vec{x})f(\vec{x})$.

The problem of how to deal with an unnormalized distribution is solved quite easily: We just divide the right hand side of Eq. (2.7) by $N^{-1} \sum_{i} 1/f(\vec{x}^{(i)})$, so that the observable $A$ is replaced by a unity operator. Things become difficult when one wants to have a MC estimator for the sum of states $Z = \sum_{n} e^{-\beta E_{n}}$, corresponding to the normalization of the unnormalized MC weight $e^{-\beta E_{n}}$. Then, one has to resort to an algorithm by Wang and Landau, in which both spin configurations and temperature are flipped [46].

### 2.1.2 The dynamical sign problem

The heart of MC is, as stated above, of thermodynamical nature. In analogy, we could say that its main difficulty is of quantum mechanical nature, at least, when we want to simulate the dynamics instead of equilibrium values. The origin of this dynamical sign problem is the propagator $e^{-iHt}$ that determines the time evolution of any quantum mechanical system. As the exponent increases linearly with time, the sign problem grows exponentially with $t$. Its combating is typically a main challenge for everybody who studies quantum dynamics with MC methods.

This problem is already visible in the structure of PIs: One sums over all paths that connect two different points in space-time, whereas every path is weighted with a phase factor $\exp(iS[q]/\hbar)$, $S$ being the classical action functional. So, paths that are far away from the classical one and therefore have large action are not suppressed as it would be the case for PIs of thermodynamic ensembles. Instead, they run around the unit circle in the complex plane. The question why this can work at all is answered by fundamental principle of interference: Most of the paths annihilate each other and we remain with a reasonable result.

The scaling of the sign problem with system time is illustrated in Fig. 2.2. We plot the signal-to-noise ratio (STN ratio) $P_{z}/\Delta P_{z}$ for a measurement of $\sigma_{z}$ with arbitrary bath parameters. One can clearly see the exponential increase of noise. The slope in the log-plot depends on the individual parameters, but the exponential nature is universal. In this case, the red line shows a fit with $STN \propto e^{-0.225t}$. The number of accumulations is $N = 2^{27}$ for all simulations.

To get a further imagination of the sign problem’s magnitude, we show some point clouds in the complex plane in Fig. 2.3. These points are the single contributions to $P_{z}(0.1\Delta^{-1})$, in one case for a free and biased system and in the other one for an unbiased system with dissipative coupling to a sub-Ohmic bath. Each point refers to a special path that is reached during the sampling. Even by taking a closer look at the values, there is no evidence at all that the imaginary part goes to zero at average, but the real part does not. This is what
forces us to sample a huge number of paths, typically on the order of $2^{25} \ldots 2^{30}$. Notice that the absolute values of the points are much larger in the non-dissipative case, meaning that the error bars are much larger than for the dissipative system. It will become clear in Sec. 2.2.1, why dissipation helps us to soothe the sign problem.

There are several ideas, how to get the sign problem better under control in dynamical systems [49]. However, none of them is a cure-all. In this work, we present two ways of repressing this problem for our models: One of them is rather technical, but of general purpose (see also App. D); the other one is motivated physically and applies only in certain parameter regimes (see Chap. 3).

### 2.2 Monte Carlo simulation for the spin-boson model

This section merges the physical contents of Sec. 1.2 with the algorithmic tools we have learned in the preceding section [40]. A lot of calculations and technical details are outsourced to the appendix, in avoidance of an interruption of the flow of reading. As systems with continuous degrees of freedom are completely intractable by the presented method, we focus on tight-binding systems with finite-dimensional Hilbert spaces. In this section, we deal with the SBM and sketch the difficulties that arise for a model with two spins in Sec. 2.3.

Let us spend some words on the history of implementation of spin-boson (SB) dynamics. The first work using PIMC was published in 1983 by Behrman et al. [50]. In the following years, it was mainly Chandler, Mak, and Egger, who improved the approach by using so-called stationary-phase MC techniques [49, 51, 52, 53]. All these early works focused on...
2.2. MONTE CARLO SIMULATION FOR THE SPIN-BOSON MODEL

Figure 2.3: The point clouds illustrate the dramatic influence of the dynamical sign problem. Each point contributes to the expectation value $P_z(0.1\Delta^{-1})$ for a free system with bias (left) and a dissipative system with sub-Ohmic bath. Both dissipation and bias shift the values from the real axis to the complex plane. The points seem to spread completely irregularly and it is not at all visible that the real part has a finite average within error bars, but the imaginary part does not. Notice that the average is $P_z(0.1\Delta^{-1}) \approx 1$ in both cases. The limiting circles and the patterns occur for reasons that are not important here.

Later, Egger and Mak developed a way to half the configuration space by eliminating the center-of-mass coordinate [54]. Here, the focus was directed on the dynamics of the diagonal SB observables that evolve out of non-equilibrium states. The code we use in this work grounds on their ideas, continuing several works of Mühlbacher, Escher, and Ankerhold on the SBM and related systems [59, 60, 61, 62]. In addition, Mühlbacher and Egger introduced the multilevel blocking algorithm that tries to soothe the sign problem in a different way [39, 56, 57, 58].

The following issues build the main methodological progress in this work:

- measurement of the off-diagonal two-level system (TLS) observables,
- the possibility to prepare the TLS in an arbitrary initial state,
- basing on the preceding two points: the implementation of an approximative scheme named Chain Path Integral Monte Carlo (CH-PIMC), see Chap. 3,
- the implementation of band-gap reservoirs, see Chap. 5,
- and the extension to a model of interacting spins that couple to an environment, see Secs. 1.3, 2.3, and Chap. 6.
2.2.1 Discretization and MC weight

In order to avoid breaking the golden thread, we skip some analytic calculations and limit ourselves on writing down the main formulae, before we turn our attention on their practical implementation. In Apps. B to D, we discretize the PI expression that is valid for any SB observable $\sigma_\nu \ (\nu = x, y, z)$ at time slice $i \equiv (i - 1)\tau$ and reads

$$P_{\nu,i} = \sum_{\eta_1, \ldots, q} \rho_0(\eta_1, \zeta_1) \left[ \prod_{j=1}^{q} KK_{\eta_j, \eta_{j+1}}(\zeta_j, \zeta_{j+1}) \right] \exp \left[ -\Phi^{SB} \right] M_{\nu,i} \tag{2.8}$$

expressed in the coordinates (1.35). $q$ is the so-called Trotter number, labeling the number of intervals of length $\tau = t/q$, in which the time is divided. The PI is discretized by a summation over all intermediate spins with $\zeta_{q+1} = 0$, $\eta_j$ and $\zeta_j$ being the values of relative and center-of-mass coordinates, respectively. Now, what do all these new symbols stand for? First, we have the discretized influence functional (IF), cf. Eq. (1.34),

$$\Phi^{SB} = \sum_{j=2}^{q} \zeta_j \sum_{k=2}^{j-1} \Lambda_{j-k \zeta_k} + \zeta_1 \sum_{j=1}^{q} \Lambda_j^{(1)} \zeta_j + \sum_{j=2}^{q} \zeta_j \sum_{k=2}^{j-1} X_{j-k \eta_k}$$

$$+ i\eta_1 \sum_{j=2}^{q} X_j^{(1)} \zeta_j + i\mu \sum_{j=1}^{q} X_j^{(\mu)} \zeta_j, \tag{2.9}$$

with all the quantities given in Eqs. (B.15)$^2$. The original structure of the continuous IF is clearly visible. Further, the combined propagator that contains the evolution of the free system from time step $i$ to $i+1$ for both forward and backward path is introduced$^3$,

$$KK_{\eta_j, \eta_{j+1}}(\zeta_j, \zeta_{j+1}) = K(\sigma_{j+1}, \sigma_j)K^*(\sigma_j', \sigma_{j+1})|_{\sigma, \sigma' \rightarrow \eta, \zeta}. \tag{2.10}$$

We will learn right below, why these objects are defined as functions of $\zeta$, but with the $\eta$’s as matrix indices. One can assure oneself easily that they have dimension $(2 - |\zeta_j|) \times (2 - |\zeta_{j+1}|)$ for fixed $\zeta$’s. The only place where the observable and the time step at which it should be determined enters, is the measurement operator, $M_{\nu,i}$, which is discussed in App. C.

As already mentioned, the trick to decrease the sign problem is to eliminate the center-of-mass coordinates. For this purpose, we freeze the relative coordinates $\zeta$ and perform the $\eta$ sums exactly, which corresponds to a q-fold matrix product of the $KK$’s that arise by modification of the combined propagators, Eq. (2.10). Here, we are only interested in the result. The derivation is sketched in App. D. We arrive at

$$P_{\nu,i} = \sum_{\zeta_1, \ldots, q, \eta_{q+1}} \exp \left[ -i\mu \varphi^{(\mu)} \right] \exp \left[ -w(\zeta_1, \ldots, q) + w^{od}(\zeta_1, \ldots, i) \right] \sum_{\eta_1} \left[ \prod_{j=1}^{q} \overline{KK}^j(\zeta_j, \ldots, q) \right]_{\eta_1, \eta_{q+1}} \tag{2.11}$$

$^2$Do not mix them up with the terms for the non-interacting blip approximation, cf. Eqs. (1.46).

$^3$The $\eta$’s take the values 0 and $\pm 1$. In the implementation, the indices of the $KK$ matrices run from 1 to $2 - |\zeta_{j+1}|$. In this case, the translation between the values of the matrix indices and the $\eta$’s is trivial. We therefore always use $\eta_{j+1}$ as indices, but keep in mind that the implementation works just the other way round.
Not only the quantum fluctuations part of the IF, but also the initial density \( \rho_0 \) and the measurement operator \( M_{\nu,i} \) are absorbed in the \( \overline{KK} \)'s. These matrices as well as the detailed structure of the functions \( \varphi^{(\nu)} \), \( w \), and \( w^{\text{od}} \) can be viewed in Eqs. (D.2) and (D.3).

Up to now, the presented approach has not been connected to any computational realization. At least theoretically, one could try to calculate Eq. (2.11) exactly. This is of course only possible for small Trotter numbers \( q \lesssim 10 \). On intermediate time scales, a typical Trotter number of \( q = 80 \) would already lead to a \( 2 \cdot 3^{80} \approx 10^{38} \) addends, each one consisting of a product of \( q \) matrices – the whole procedure for only one measured value \( P_{\nu,i} \)!

Needless to say that this is a completely hopeless endeavor. Therefore, we have to reduce these \( 10^{38} \) constituents to the ones that give a significant contribution to the PI. Here, Metropolis importance sampling comes into play. We thus have to find an appropriate MC weight.

The properties a MC weight should have were discussed above. Luckily, we can split off a part in Eq. (2.11) that fulfills exactly these main constraints: The factor \( \exp(-w) \) is very helpful, because it suppresses a huge part of the totality of configurations exponentially. Especially for strong friction and large temperatures, the \( \zeta \)'s are pushed towards zero and the sampled paths have only a few time steps with \( \zeta_j = \pm 1 \). All simulations indeed show that the error bars become smaller and smaller, when the system-bath coupling \( \alpha \) or the temperature increase.

However, the effect of this factor decreases for small \( \alpha \) and even vanishes for a free TLS. So, we have to take care that we still get the error bars under control in the small coupling regime. Therefore, we paste a factor \( K(\zeta_1,...,\eta_{q+1})/K(\zeta_1,...,\eta_{q+1}) \) and do it the way that is described in Sec. 2.1: We add the numerator to the MC weight and the denominator to the quantity we want to evaluate. The function \( K \) reads

\[
K(\zeta_1,...,\eta_{q+1}) = \prod_{j=0}^{\lfloor q/N \rfloor} |KK^N|_j
\]

(2.12)

where the brackets denote the next smaller integer. We introduced the real-valued matrices

\[
|KK^N|_j = \begin{cases} |KK_1 \cdots KK_{\text{mod}(q,N)}|, & j = 0 \\ |KK_{N(j-1)+1+\text{mod}(q,N)} \cdots KK_{Nj+1+\text{mod}(q,N)}|, & j \geq 1 \end{cases}
\]

(2.13)

with the combined propagator \( KK_i \) from Eq. (2.10). On the right hand side, the operation is in fact a matrix product. Further, \( \text{mod}(q, N) \) is the modulo function. If \( \text{mod}(q, N) = 0 \), the \( j = 0 \) part is lapsed. Eq. (2.13) means that we multiply blocks of \( N \) \( KK \) matrices (including a “rest block” of length \( \text{mod}(q, N) \) at the beginning of the chain), take the absolute value of each entry and multiply the resulting real valued matrices. The choice of \( N \) is ambiguous: On the one hand, larger \( N \) decreases the CPU time slightly, but on the other hand it blows up the virtual memory. This is because the \( KK \) matrices are calculated for frozen \( \zeta \)'s and so the whole combinatorics of possible \( \zeta \) paths must be stored. In our code, we work with \( N = 4 \).
This factor reduces the number of contributing paths for arbitrary \( \alpha \). The complete MC weight then reads

\[
W_{MC} = K(\zeta_{1,\ldots,q}, \eta_{q+1}) \exp[-w(\zeta_{1,\ldots,q})]
\] (2.14)

The current values \( \zeta_{1,\ldots,q}, \eta_{q+1} \) are called a spin path or spin chain in the following. Note that the MC weight must be normalized. Therefore, we divide the accumulated expressions by the norm of (2.14). This is simply done by inserting the measurement operator 1 into (2.8).

### 2.2.2 Structure of the code

These contents form the computational backbone of the program, that is implemented with fortran90. In order to get a detailed understanding, we continue with sketching a couple of important details.

In the beginning, one has to do a lot of preparation and book-keeping. After defining the variables, reading the input parameters, allocating the arrays, etc., one proceeds with calculating the discretized bath elements defined in App. B. This can be skipped, if there already exist data of a prior simulation in the current directory that can be continued.

After preparing the spin chain in its initial state and performing some equilibration moves (see Sec. 2.2.3), we proceed with sampling. This main part of the program is just a do loop with a total of \( \mathcal{N} \) cycles, \( \mathcal{N} \) denoting the number of accumulations that must be a power of 2 for a reason that will become clear in an instant. Within this loop, we have another loop that runs from 1 to \( r \cdot q \), where \( q \) is the Trotter number. The parameter \( r \) denotes the number of MC steps and is chosen such that \( (1 - P)^r \leq 0.5 \), \( P \) being the total acceptance probability, that is determined by simply counting accepted and rejected flips.

![Diagram](image.png)

Figure 2.4: This diagram visualizes the main steps that are processed in the program. See text for explanation.

In each cycle of the outer loop, the accumulation procedure is performed once by calling a subroutine that evaluates the observables with the current spin path. Here, we mainly
have to initialize the $\tilde{K}$ matrices, calculate their product and apply all the measurement operators. This is just brute-force implementation of the contents of App. D.

Each time, when $k/16$ of the total number of accumulations are finished, all relevant data are written in a file, from which they can be read when either the program stops because of a technical problem or the data of a finished simulation are used as the first part of a new one with higher number of accumulations. This is just to avoid data loss and to diminish the problem of limited CPU time for single jobs. In the grid system that is used for our simulations, a job is aborted after seven days. In a few cases, this is not enough to push the error bars satisfactorily. Therefore, the results of a simulation with $N = 2^n$ that runs, say, six days, can be used as the first half of another simulation with the same parameters, but a total of $N = 2^{n+1}$, requiring another six CPU days.

If all the $N$ cycles are processed, we ask for the number of so-called MC segments. If the program is told to simulate more than one segment, the simulation starts again in the beginning, but with modified initial preparation. The idea is to create a chain of single elements where each element is an independent simulation. A detailed explanation can be found in Sec. 3.2.

After having finished the loop with $N$ cycles for all MC segments, all the data to create the output are collected. Before doing so, we call a subroutine that calculates the error bars. Then, $P_{\pm 1}$ and $P_{x,y,z}$ is determined for $q$ time steps, yielding $10 \cdot q + 2$ different observables as each quantity – including the normalization – carries both real and imaginary part. All the real parts are written in text files while the imaginary parts are only evaluated in order to check that they are close to zero. Next, the von Neumann entropy is governed from $P_{x/y/z}$, see Sec. 3.3. In addition, we collect some data concerning the MC statistics, before the program is finished.

### 2.2.3 Further details

We end this section by spending some words on the initial spin chain, the way how the error bars are calculated, and how CPU time depends on discretization and physical parameters.

**Choice of initial spin chain**

Before we can start flipping and sampling, we have to set the spin chain in an initial state. It is common wisdom that the first samples of a MC chain with random initial setting must be thrown away, because the system needs some time to run from the initial configuration towards the region that gives an appreciable contribution \[44\] – which corresponds to reaching the steady state in the master equation (2.4). If we simply choose a random spin configuration, it takes little imagination to realize that we are very likely to start in a region with exponentially small MC weight. Fortunately, we do not start in a random configuration and therefore do not have to care about the question, how many initial samples we have to drop.
CHAPTER 2. PATH INTEGRAL MONTE CARLO FOR SPIN SYSTEMS

Figure 2.5: The plot shows the portion of groups of paths that are classified by their number of sites \( n \) where \( \zeta_j \neq 0 \). As they are highly degenerated for growing \( n \), the zero path is already the dominant single path when dissipation is absent. Increasing coupling and temperature suppresses the non-zero paths exponentially. The dissipation is of Ohmic type.

Taking a closer look to our MC weight (see Eq. (2.14)) leads us to the insight that dissipation constricts the configuration space and pushes the system towards the single path with \( \zeta_j = 0 \), \( j \in [1; q] \), which we call the zero path. But the same is true for the non-dissipative case, which can be seen from Fig. 2.5. For some MC simulations with Ohmic bath and different dissipation parameters, all sampled paths are sorted according to the number of sites on which \( \zeta_j \) is non-zero, choosing \( q = 50 \) Trotter steps in total. Note that the number of possible paths that are non-zero at \( n \) sites and zero at \( 50 - n \) is binomially distributed, i.e. \( \binom{50}{n} 2^n 1^{50-n} \), which is on the order of \( 10^{23} \) for \( n = 33 \) but equals 1 if \( n = 0 \). Nevertheless, the zero path contributes nearly one percent even in the absence of dissipation and is the clearly dominant path for rather small coupling (\( \alpha = 0.3, T = 0 \)). Further increase of \( \alpha \) and \( T \) suppresses the totality of non-zero paths even more.

For higher temperatures, the sampled path happens to differ from the zero path only rarely and we regain (quasi-)classical physics: One definite path gives the very largest contribution and plays the role of a classical trajectory. This clearly justifies that we begin the simulation by setting the system into the zero path and performing only some 1000 equilibration steps (which typically cost a few seconds of CPU time) to play it safe.

By doing so, we solve another problem that is connected to the MC weight. We know from Sec. 2.2.1 that there is a factor \( K(\zeta_1, \ldots, \zeta_q, \eta_{q+1}) \) in the denominator of the sampled quantity. For paths with extremely small weight, it may happen that we get an arithmetic exception, because we divide by zero. This problem would occur regularly, if one dealt with 200 or more Trotter steps and chose a random initial path. In contrast, it is extremely unlikely that we will ever reach these regions, when we start with the classical zero path. As we
know, Metropolis algorithm is proven to be ergodic, but luckily not on the time scales of our simulations. Otherwise, we would still reach these small $W_{MC}$ regions and run the risk of getting zero denominators.

**The standard deviation**

We have seen that the dynamical sign problem makes life difficult. However, another problem that appears in all Metropolis sampling procedures is *correlation of subsequent configurations*. This actually influences the way how to calculate the error bars.

We call in mind that one MC step contains a total of $q$ trial flips. Therefore, within a MC step, each single site has the chance to be flipped once at average. Let the acceptance probability be on the order of one percent. Then, it is obvious that two spin chains are still highly correlated, when $q$ trial moves are performed in between, but 99 percent of them are rejected. The only reliably working way to reduce these correlations is mentioned above: We perform $r$ steps instead, the actual value of $r$ depending on the acceptance ratio.

However, the correlations also enter the error bar determination. In our implementation, we use an approach that allows to estimate error bars for correlated data in a very elegant way. In general, a physical observable given by $\langle A \rangle = \int d\vec{x} \, p(\vec{x}) A(\vec{x})$ with an exact, but unknown density $p(\vec{x})$ is connected to a variance of

$$\sigma^2(m) = \langle m^2 \rangle - \langle m \rangle^2 = \frac{1}{N} \left[ \gamma_0 + 2 \sum_{j=1}^{N-1} \left( 1 - \frac{j}{N} \right) \gamma_j \right]$$

(2.15)

with estimator $m = N^{-1} \sum_{j=1}^{N} x_j$ and correlation coefficients $\gamma_{ij} \equiv \gamma_{|i-j|} = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle$. These $\gamma$'s inhibit us from determining the error bars efficiently. We follow a scheme invented by Flyvbjerg and Petersen and refer to their article for further details [64]. The idea is to build $n$ levels for every single observable, where $n$ is connected to the total number of samples via $N = 2^n$. From the first to the second level, the data set $x_1, ..., x_N$ is transformed to a set of half the size by defining

$$x'_i = \frac{1}{2} (x_{2i-1} + x_{2i}), \quad 1 \leq i \leq \frac{N}{2}.$$  

(2.16)

The same is done from the $i$th to the $i+1$st level, ending up with a single value at the last level. It is straightforward to show that $\sigma^2(m) = \sigma^2(m')$. In the work of Flyvbjerg and Petersen, the authors develop a blocking scheme that reminds on methods of renormalization group. Within this scheme, the error bars are determined from level to level and all correlations are canceled, in the sense that they are simply kept out of calculations. Clearly, this scheme does not allow for reducing the MC flips between two measurements, but it makes the error calculation rather easy compared to Eq. (2.15).
The CPU time

Now, how does CPU time actually depend on the parameters? First of all, we have to clarify that the numerical costs for all the stuff which is processed in the beginning and the end of the program are completely negligible compared to flipping and accumulating. As the effort grows linearly with $q$ for the latter, but proportional to $q^2$ for the former, CPU time depends on Trotter number and accumulations like

$$h_{CPU} \propto N(\tilde{c}_1 q + \tilde{c}_2 q^2) = N(c_1 t + c_2 t^2), \quad (2.17)$$

when we assume the Trotter increment $\tau = t/q$ to be constant for a certain set of physical parameters. A fit onto the data in Fig. 2.2 gives $\tilde{c}_1 \approx 0.13$ and $\tilde{c}_2 \approx 0.005$, meaning that the quadratic part, i.e. the flipping, dominates if $q \gtrsim 25$.

However, one aspect is completely missing up to now. Eq. (2.17) does not tell anything about the size of the error bars. We know from Fig. 2.2 and Eq. (2.15) that the STN ratio scales $\propto e^{-at}\sqrt{N}$, where $a$ is a function of the physical parameters. Requiring the noise to be pushed towards some constant size, we immediately get

$$h_{CPU} \propto e^{2at}(c_1 t + c_2 t^2). \quad (2.18)$$

Note that $N$ is hidden in the requirement for the size of the STN ratio: The number of accumulations must be large enough to push the error bars towards the desired level. In addition, the Trotter number $q$ must be chosen such that the dynamics converges: If there are no visible deviations for two simulations with $q_1$ and $q_2 > q_1$, the dynamics is assumed to be correct within the error bars. Therefore, both exponent $a$ and increment $\tau$ depend on the physical parameters.

The exact dependence can only be estimated in a qualitative way. Driving the system towards the classical limit by raising $\alpha$ and $T$ requires finer Trotter discretization and a higher number of MC steps $r$ (hidden in $c_2$) on the one hand, but suppresses the variety of contributing paths (i.e. smaller $a$ in Eq. (2.18)) on the other hand. As the former effects influence CPU time algebraically, but the latter does this exponentially, the numerical effort clearly decreases. Arguing with Eq. (2.17), we can say that we need much less accumulations to arrive at the same size of error bars in the quasi-classical limit. Note that the dependence of the noise on temperature is just the other way round as in a canonical ensemble, see Sec. 2.1. This is because the flipped coordinates of the spin system are not thermalized, as it is the case when one studies the equilibrium properties of many-body systems, i.e. the configurations distributed according to $\exp(-\beta H)$ with total Hamiltonian $H$.

For a few parameter sets, the restriction to less than seven days of CPU time is not at all sufficient. Therefore, we use a very simple form of “parallelization”: We run up to 16 simulations independently for the same parameters, thereby taking care that the random seed, i.e. the initialization of the random number generator, differs. In the end, we collect all results together, as if they were the outcome on one simulation. In a strict sense, this approach violates the fundamental principle of Markovianity. Our method consists of sticking
2.3 Extensions for the interacting spins model

When we build up the PIMC for the ISM, we luckily do not need to reinvent the wheel. Instead, we can recycle a lot of the methods from the previous section. Compared to the simple SBM, book-keeping becomes more complicated and the required CPU time increases, but conceptually, most things can be adopted. This should not hide the fact that the implementation is a lot of work, as it increases the bureaucratic complexity significantly.

So, what do we have to do? Introducing relative and center-of-mass coordinates for each of the spins, defining a combined propagator and discretizing the IF is basically the same as for the SBM. Luckily, even the derivation of measurement operators and the summation over the quasi-classical coordinate works similarly. All these technical steps are summarized in App. E.

Even choosing an appropriate MC weight is completely similar to the SBM. We split off the real part of the IF, \( \exp(-w^{ISM}) \), with

\[
w^{ISM}(\zeta_{1,...,q}) = \sum_{j=2}^{q} \sum_{k=2}^{j} (\zeta_j^A + \zeta_j^B) \Lambda_{j-k}(\zeta_k^A + \zeta_k^B) + (\zeta_1^A + \zeta_1^B) \sum_{j=1}^{q} \Lambda_{(1)}^j(\zeta_j^A + \zeta_j^B),
\]

Eq. (2.19)

cf. Eq. (E.12), multiply it with the numerator of the factor \( \prod_j |KK_N|_{ij}/\prod_j |KK_N|_{ij} \) (with new |KK_N| matrices according to the KK’s defined for the SBM) and generate spin chains that are distributed according to this MC weight after having eliminated the \( \eta^{A/B} \)'s. The denominator of the additional factor is again attached to the measured observable. Note that we still flip single \( \zeta \) values either of spin A or of spin B, and not the value of a collective coordinate.

The sign problem increases dramatically compared to the SBM. The reason herefore is mainly that the number of degrees of freedom doubled due to the second spin. In addition, the quasi-classical path with \( \zeta_j^A = \zeta_j^B = 0 \) is not that pronounced any longer. Sure, it is still the dominant single path, but the dissipative part (2.19) weights paths with \( \zeta_j^A = -\zeta_j^B \) equally. Likewise, a large spin-spin coupling \( J \) shifts the paths away from the diagonal, i.e. \( \zeta^{A/B} \neq 0 \).

Here, it is of course the free system’s part of the MC weight that is responsible for this additional spreading in the configuration space.

Increasing \( J \) such that it is the dominant energy scale, we arrive at the situation that the system resides in the off-diagonal states nearly as often as in the diagonal ones. An exemplaric simulation with Ohmic bath and parameters \( \alpha = 0.3 \), \( T = 0 \), \( J = 2\Delta \) and...
identical unbiased spins brings up that the system spends 39% of the simulation time in a state where both spins are diagonal, but 32% in a state where both spins are off-diagonal. For a coupling strength as large as $\alpha = 1$, these values change to 50% and 44%, proving that the states with one off-diagonal and one diagonal spin are extremely suppressed. This is perfectly coinciding with the preceding arguments.

For these reasons, we have to take care about the initial spin configuration. The zero path still carries the largest weight, but its dominance shrinks down extremely. We still choose it as the starting configuration, but enlarge the number of equilibrating MC steps to at least 10,000.

The increase of CPU time for a two-spin system compared to a single spin with same $q$ and $N$ is enormous. For the time that is spent with flipping, we must get at least a factor of 2, as one MC step now consists of $2q$ flips instead of $q$. The increase for updating the MC weight with larger $KK$ matrices ramps up this factor considerably. For the accumulation procedure, we have to deal with larger matrices on the one hand and a higher number of sampled observables on the other hand. In addition, the forth and back between the $\eta$ values and the matrix indices of the $KK$’s and $\tilde{K}\tilde{K}$’s requires an implemented function that is called very frequently during one accumulation procedure. Altogether, we end up with a factor of 10 in CPU time and even larger error bars for the same $q$ and $N$! The reader should therefore not be disappointed, when we have to restrict the system time to smaller values than for the SBM.

All the methodological stuff is now plowed through. We do not want to bore the reader with further details and refer to the appendix instead. With this, we close the first part of this work and proceed with the numerical results.
Part II

RESULTS
Chapter 3

Chain Path Integral Monte Carlo for Ohmic Baths

After having presented the most important parts of methodology and implementation, we now turn our attention to the results. We start with the spin-boson (SB) dynamics for an Ohmic bath as this is a standard choice for a broadband reservoir when describing dissipative systems.

Due to extensive theoretical work during the last decades with both numerical and analytical methods, the properties of the Ohmic spin-boson model (SBM) are well understood [1, 2, 15, 20]. Therefore, it is not so easy to reach uncharted waters. However, the ability to measure the off-diagonal dynamics enables us to develop a scheme that allows us to partially circumvent the dynamical sign problem in certain areas of parameter space. This is in itself just a technical improvement, but we will see that we also get some new physical insight out of that. We name our procedure Chain Path Integral Monte Carlo (CH-PIMC), as its basic idea is to build chains from single time segments. The main results were published in [66].

One of the central intentions is to border the regimes, where our method applies. After that, we attach a short section that discusses the dynamics of off-diagonal observables and the entropy of the reduced system. But first of all, we ought to justify the relevance of Ohmic damping. Here and in the following chapters, we work with the polarized bath preparation \( \mu = P_z(0) = 1 \), if not stated differently.

### 3.1 Motivation

The Ohmic spectral density is defined by

\[
I(\omega) = 2\pi \alpha \omega \exp\left(\frac{-\omega}{\omega_c}\right),
\]

(3.1)

\( \alpha \) labeling the dimensionless coupling strength and \( \omega_c \) the (soft) UV cut-off [1]. In Sec. 1.1, we mentioned its connection to Markovian dynamics for elevated temperatures. How-
ever, it is this regime that links the Ohmic SBM to another important theory dealing with charge transport in chemistry: This is famous Marcus theory for electron transport in donor-acceptor systems [38], a semi-classical rate description that was developed in the 1960’s and awarded with the 1992 Nobel Prize in Chemistry. It assumes a classical particle to move in the free energy surface

\[ F(\mathcal{E}, \sigma) = -\frac{\hbar e}{2} \sigma + \frac{1}{2\mu^2 \beta \langle (\Delta \mathcal{E})^2 \rangle \hbar \Lambda_{cl}} \left( \mu \mathcal{E} - \frac{\hbar \Lambda_{cl}}{2} \sigma \right)^2, \]  

where \( \mu \mathcal{E} \) is the polarization coordinate, given by the electron’s position and the dipole moment \( \mu \), and \( \langle (\Delta \mathcal{E})^2 \rangle \) is the variance of the polarization fluctuations. The relationship to the SBM comes from the variable \( \sigma = \pm 1 \), fixing, whether the electron moves in the donor (\( \sigma = -1 \)) or acceptor (\( \sigma = +1 \)) parabola, respectively. Dissipation is included via polarization fluctuations \( \langle \mathcal{E}(t) \mathcal{E}(0) \rangle = \frac{\hbar^2}{4} L(t) \). Further, \( \Lambda_{cl} \) is the classical reorganization energy, that was defined in Eq. (1.16). This way, analytical Marcus theory results can be compared to PIMC simulations [39].

However, the Ohmic model is also of importance in the quantum regime, \( T \to 0 \). It applies to impurities that interact with a background of normal conducting electrons, where a particle is coupled to virtual electron-hole pairs [1]. Although being in contact with a fermionic reservoir, these systems can effectively be treated by bosonic environments of Ohmic type. Of particular importance are magnetic impurities that can be described within the anisotropic Kondo model. The latter was shown to map on the Ohmic SBM by bosonization, respectively [41, 42].

Hence, the occurrence of a transition between a ferromagnetic and an anti-ferromagnetic phase in the anisotropic Kondo model has an analogon in the SBM. Indeed, a localized or self-trapped phase with \( P_z(t \to \infty) \neq 0 \) was already found in 1982 [68, 69]. The quantum phase transition is of Kosterlitz-Thouless type and occurs for system-bath couplings \( \alpha > \alpha_c = 1 \).

This can also be seen from a unitary transformation, where the bare tunnel matrix element \( \Delta \) is renormalized by a factor \( \eta \), determined by the self-consistent equation [108]

\[ \eta = \exp \left( -\frac{1}{2\pi} \int_0^\infty d\omega \frac{I(\omega)}{(\omega + \eta \Delta)^2} \right). \]  

For an Ohmic bath with sharp cut-off \( \propto \Theta(\omega_c - \omega) \), one finds \( \Delta_{\text{eff}} = \Delta (\Delta/\omega_c)^{\frac{1}{\alpha - 1}} \) which vanishes in the limit \( \alpha \to 1 \).

Further experimental implementations for an SBM in general are Cooper pair boxes, where a gate voltage controls a bias \( \epsilon \) and the Josephson energy corresponds to \( \Delta \). Coupling such a system to a long LC transmission line, one can achieve an Ohmic spectrum [83, 84]. Other practical realizations work with 1D Luttinger liquids [85] or atomic quantum dots coupled to a Bose-Einstein condensate [86].

The population dynamics of the Ohmic model is in fact best understood. At \( T = 0 \), the system is known to pass a transition from underdamped oscillations for \( \alpha < 0.5 \) to a monotonic decay in the opposite range. For a dynamical investigation, we are interested in the
twice-integrated auto-correlation function $Q(t)$

$$Q(t) = 2\alpha \left[ \log(1 + i\omega_c t) - \log \frac{\Gamma(\kappa + it/\beta)\Gamma(\kappa - it/\beta)}{\Gamma^2(\kappa)} \right],$$

where $\kappa = 1 + (\omega_c/\beta)^{-1}$. Classical fluctuations scale as $\text{Re}[L(t)] \propto 1/t^2$, while the imaginary (quantum) part decays faster, $\text{Im}[L(t)] \propto 1/t^3$. In the scaling limit $\omega_c \gg \Delta$ and for elevated temperatures, Markovian dynamics is regained. We have come to full circle, as the approximative scheme we present right now is in a way Markovian.

### 3.2 Idea and limits of Chain Path Integral Monte Carlo

As we already indicated in the chapter introduction, the idea behind CH-PIMC is to glue together several independent MC simulations. The parameters for all these single simulations are identical; they only differ in their initial preparation. We first present the basic principles and introduce the notation, before we discuss its applicability and explain a modification that allows to enlarge the accessible parameter range.

#### 3.2.1 Principles

The ability to measure the coherence dynamics gives us the full information of the TLS’s state at any time which is reachable by PIMC simulations. In addition, we can prepare the system in an arbitrary non-diagonal state, see Eq. (1.33). Combining these two circumstances leads us to the following idea: Why not simulate the TLS dynamics up to a system time $t_s$, take the values of the reduced density at $t_s$ and use them as initial preparation for a new simulation with time $t_s$, too? Connecting the data of both runs, we end up in one simulation ranging from 0 to $2t_s$. In theory, we can repeat this procedure again and again: The final values at $nt_s$ can fix the initial state for another simulation up to $(n+1)t_s$, finally arriving at $t = Nt_s$ (with $0 \leq n \leq N - 1$). We call $N$ the number of MC segments.

By doing so, we approximate the correct (and unknown) reduced density $\rho(t) = \text{Tr}_B[W(t)]$ by densities that are defined in single sections,

$$\rho(t) \approx \rho_n(t) = \text{Tr}_B[W_n(t)] \quad \text{for} \quad nt_s \leq t \leq (n+1)t_s. \quad (3.5)$$

The total densities are governed from

$$W_n(t) = \exp[-iH_{SB}(t-nt_s)] \rho_n(nt_s) \mathcal{Z}^{-1} e^{-\beta(H_B - \mu_n\xi_B)} \exp[iH_{SB}(t-nt_s)] \quad (3.6)$$

with stochastic force $\xi_B$ and adjusted bath shifts $\mu_n$, to be discussed below. The reduced densities are therefore defined inductively by their values at the matching points,

$$\rho_n(nt_s) = \rho_{n-1}(nt_s) \quad (3.7)$$

---

1The analytical form can be determined by performing the limit $s \to 1$ in Eq. (4.2).
with \( \rho_0(0) \equiv \rho_0 = |+1\rangle \langle +1 | \) if not declared differently.

Mathematically spoken, the discussion turns on the half-group property

\[
W(t + t_s) = \exp[-iH_S t_s] W(t) \exp[iH_S t_s] = \exp[-iH_S (t + t_s)] W(0) \exp[iH_S (t + t_s)]
\]

that always holds for the total density matrix \( W(t) \), but in general not for the reduced one. As the trace over the bath is already performed, we only know its effective impact on the system, but do not have any detailed information about its real state.

Let us first have a brief look at the advantages we expect. As the dynamical sign problem scales exponentially with the overall time \( t \), the computational benefit is enormous. Due to Eq. (2.18), the ratio of CPU times for similar size of error bars is

\[
\frac{h_{CPU}^{CH-PIMC}}{h_{CPU}^{PIMC}} = \frac{n e^{2a t_s} c_2 t_s^2}{e^{2a t_s} c_2 (n t_s)^2} = \frac{1}{n} e^{2a t_s (1-n)},
\]

thereby assuming the \( t^2 \)-term to dominate over the linear contribution. Fascinatingly, the gain is even a bit more than exponential!

However, the idea is too simple to be free of substantial problems. We always prepare system and bath in a factorizing state in the beginning of each new segment. This way, bath memory is cut and one would naively suppose that it gets inevitably lost. Still, we have recovered memory effects in a twofold manner: first, by adjusting the bath’s equilibrium position and second, by preparing the TLS in a state that lies inside the Bloch sphere.

Turning the Bloch sphere equation into an inequality means that the TLS remembers some bath influence from the past: The TLS is no longer in a pure state, which is a soft contradiction for a simple reason: \( \sum_{\nu=x,y,z} P^{2}_{\nu} < 1 \) means that the system is in a mixed state and gets entangled with the reservoir\(^2\). Still, we factorize both entities for the subsequent segments, thereby implicitly assuming no entanglement. In fact, we would not be physicists, if we did not try it although.

In order to move the bath a bit closer to the (unknown) state it had at the end of the prior segment, we can at least adjust the initial bath shift parameter \( \mu_n \) for the new segment. Assuming that the majority of bath modes is able to instantaneously follow the spin, we choose \( \mu_n = P_z(n t_S) \) for the \( n + 1 \)st segment. Later on, we will see that this is not always the best choice. Therefore, we treat the reservoir’s position\(^3\) as a variable quantity, where we restrict for simplicity to the cases “adjusted” (i.e. \( \mu_n = P_z(n t_s) \)) or “not adjusted” (\( \mu_n = P_z(0) \)) and skip the possibility to place \( \mu_n \) somewhere in between.

Before presenting first results, we should think a moment about when this method is expected to work. Clearly, this procedure is exact, if there is no coupling to the bath. This special

\(^2\)See also Subsec. 3.3 and the discussion of the von Neumann entropy. Strictly speaking, this quantity measures the system-bath entanglement only at \( T = 0 \) \([74]\).

\(^3\)Strictly speaking, the bath is not located at position \( \mu \), but its modes are equilibrated to \( \mu \), i.e. mode \( i \) sits at the position \( x_i = -\mu c_i/(2m_i \omega^2_i) \).
The figure shows the TLS dynamics from a single MC run up to $t = 8\Delta^{-1}$ in comparison with a CH-PIMC simulation consisting of 20 segments of length $2\Delta^{-1}$ (overall time $40\Delta^{-1}$). The latter are not only in perfect agreement with the analytical result (black lines), but also have error bars of symbol size, whereas the standard PIMC error bars are tremendous. A bias $\epsilon = \Delta$ is applied and the TLS starts to evolve from a non-diagonal state with $P_x(0) = 0.6$, $P_y(0) = 0$ and $P_x(0) = -0.8$.

It should be stressed that both standard PIMC and CH-PIMC simulations required a CPU time of approximately three days in this case. Two things jump to the eyes: First, the CH-PIMC coincides with the exact result over the whole time range. Second, the standard PIMC data spread horribly, whereas the error bars of CH-PIMC data are smaller than the symbol size. Trying to reach $t = 12\Delta^{-1}$ within one single run would be really hard work and $t = 20\Delta^{-1}$ would be nearly impossible. However, by usage of CH-PIMC, we can easily reach $t = 40\Delta^{-1}$ or even more. This illustrates drastically, what Eq. (3.9) wants to tell us.

Unfortunately, this huge gain cannot be assigned to the dissipative case. Here, every matching point is connected to a small error, that is partially conserved in the subsequent dynamics. For this reason, we first have to check the reliability of our method for weak to moderate damping. We can see from Fig. 3.2 that matching works fine far beyond the range in which master equations apply ($\alpha\Delta\beta \ll 1$, $T > \Delta$, [1]). Coinciding with these requirements, deviations between PIMC and CH-PIMC are only present for $T = 0.5\Delta$. The segment time is $t_s = 5\Delta^{-1}$. Increasing temperature above $2\Delta$, the inspected regime already starts to overlap...
with the region of incoherent motion, which is the next parameter region to be tested.

![Graph](image)

Figure 3.2: The CH-PIMC fully covers the regime where master equations apply \((T \gtrsim \Delta, \alpha < 0.1)\) and gives accurate results even far beyond \((\text{up to } \alpha = 0.4)\). PIMC and CH-PIMC data are labeled with the same color; we have \(t_s = 5\Delta^{-1}\). Deviations are only visible for the curve with \(T = 0.5\Delta\) and \(\alpha = 0.1\).

Here, we also expect CH-PIMC to give reliable results as quasi-classical dynamics is regained: Entanglement is strongly suppressed and the re-factorized initial state for the following segments seems to come very close to the truth. The picture behind is a classical one: We assume the oscillator parabola to follow the spin instantaneously and the system to live on the diagonal of the density matrix, i.e. \(|P_x|, |P_y| \ll 1\).

In Fig. 3.3, we see that the incoherent relaxation is reproduced perfectly for temperatures \(T \gtrsim \Delta\). However, small kinks occur when \(T\) approaches zero. Simulating such large segment lengths with PIMC is only possible because temperature and dissipation are very large and the spectrum is Ohmic.

As the coupling strength that is necessary to overdamp the dynamics decreases down to \(\alpha \lesssim 0.1\) when \(T > 2\Delta\), the regimes of master equations and incoherent relaxation overlap. Therefore, CH-PIMC is always reliable for these temperatures, independent of the coupling strength. For smaller temperatures, we see deviations from exact PIMC, when the coupling decreases. In summary, temperature is the main indicator to determine whether the method works or not.

### 3.2.2 Adjustment of the off-diagonal quantities

Our simulations suggest that the CH-PIMC works, if \(T \gtrsim \Delta\). Next, we pose the question, if we can actually enlarge the region of applicability. For this purpose, we search for an idea
Figure 3.3: The CH-PIMC works fine in the incoherent Ohmic range. The exponential relaxation towards $P_z(t \to \infty) = 0$ is only affected for very small temperatures.

to smoothen the population dynamics, thereby explicitly allowing jumps in $P_x$ and $P_y$. As a consequence, Eqs. (3.5) and (3.7) are no longer valid for the off-diagonal elements from now on. This method is named modified CH-PIMC and works as follows. We change the off-diagonal quantities at the matching point, i.e.

$$
\begin{align*}
P_{x,(n)}(nt_s) &= P_{x,(n-1)}(nt_s) + \delta P_x, \\
P_{y,(n)}(nt_s) &= P_{y,(n-1)}(nt_s) + \delta P_y, \\
P_{z,(n)}(nt_s) &= P_{z,(n-1)}(nt_s),
\end{align*}
$$

with $\delta P_{x,y}$ adjusted such that the kinks in $P_z(t)$ vanish. The last equation guarantees the continuity of $P_z$, whereas we learn from the second that also $\dot{P}_z = -\Delta P_y$ is continuous, as long as $\delta P_y = 0$. Our observations ought to show, if this indeed gives the best matching. The optimization criterion is to minimize the curvature $k_l$ at the matching point, which reads in discretized form

$$
\begin{align*}
k_l(nt_s) &= \frac{P_z(nt_s + l\tau) + P_z(nt_s - l\tau) - 2P_z(nt_s)}{l^2\tau^2}.
\end{align*}
$$

Here, $l$ is an integer that selects the points which enter the calculation of the curvature: $l = 1$ for example means that $k$ is just determined by the matching point and its nearest neighbors; $l = 2$ chooses instead the next nearest neighbors, and so forth. Clearly, the correct value for $k$ would be given by a non-integer $l \to 0$. However, as long as the Trotter slicing is much smaller than the time scales on which the TLS dynamics takes place, we can choose $l \lesssim 5$ in order to get a reasonable result.

The reason for introducing this additional degree of freedom is the following. We suppose that a perfect overall matching is governed from a good matching at the first time steps – at
least if memory is not too long-ranged. So, the task is to prevent the dynamics from making jumps within a few Trotter steps after the matching point, corresponding to a small value of the curvature around \( n t_s \). We limit the discussion to chains with two segments, henceforth.

When plotting the absolute value of \( k_l \) for fixed \( l \) as a function of \( \delta P_x \) and \( \delta P_y \), we clearly see the form of a V-shaped valley, where \(|k_l|\) reaches a minimum along a straight line within the \( \delta P_x-\delta P_y \) plane (not shown). The latter can be determined easily by fitting the data onto the function

\[
f(\delta P_x, \delta P_y) = A|\delta P_y - M \cdot \delta P_x - T| + B.
\]

The fit parameters \( A \) and \( B \) are cast away, while \( M \) and \( T \) give slope and \( \delta P_y \)-axis intercept of the linear function \( \delta P_y(\delta P_x) \). Drawing all the lines for \( 1 \leq l \leq 5 \) gives us a unique result: All of them meet close to one single point (see the left panel in Fig. 3.4). Reading off the \( \delta P_{x,y} \) values of the intersection obviously gives us the point where the average curvature of the connected segments at \( n t_s \) is minimized and the curve is “as smooth as possible”.

Our approach is therefore a mixture between trial and error and strict determination. One has to simulate a certain amount of curves with different \( \delta P_x \) and \( \delta P_y \) so that the fit procedure works fine. Then, it is straightforward to distinguish the point in the \( \delta P_x-\delta P_y \) plane that corresponds to perfect matching. Fig. 3.4 illustrates its capability. In the left panel, we see the straight lines extracted from the fit onto the 3D-plot \(|k_l|(\delta P_x, \delta P_y)\), where the colors encode different \( l \) (see caption). We can clearly see the intersection at \((\delta P_x, \delta P_y) \approx (-0.02, 0.08)\), which is only misled by the black line. The corresponding dynamics is shown in the right panel and demonstrates good agreement on the short-time scale. Marginal deviations for longer times are due to the fact that temperature was chosen close to the border of applicability: All our simulations reveal this modified PIMC to work for \( T \gtrsim 0.5\Delta \) in the incoherent domain.

Fig. 3.5 shows that the CH-PIMC still fails in the coherent low-T regime \((\alpha = 0.3, T = 0)\), even if we modify the off-diagonal observables. Although the dynamics is regained on the first few Trotter steps, it clearly drifts away from the correct result afterwards. In contradiction to theoretical predictions, we find \( \delta P_y \neq 0 \). This has to do with the way how the bath is adapted at the matching points and will be discussed in more detail in Sec. 4.2.

Although this modification may seem a bit artificial, it contains some interesting physical messages. The purpose is to smoothen the dynamics of the diagonal part of the density matrix by manipulating the off-diagonal elements. We can conclude that, at least in certain parameter ranges, one can effectively reproduce the influence of the bath memory onto the \( P_z \) dynamics. In all simulations, we have \( P_z(t) > 0 \) (not shown), so that \( \delta P_z < 0 \) (which is always the case for the perfect matching) actually reduces the coherences between the \( \sigma_z \) eigenstates. So, very roughly spoken, suppressing the coherence between the two spin states is in a way equivalent to conserving the non-local bath effects, as long as we only glance at the dynamics of the diagonal elements.
Figure 3.4: (left) Trying to minimize the curvature at the matching point by varying \( \delta P_x \) and \( \delta P_y \) gives straight lines in the \( \delta P_x - \delta P_y \) plane, that meet close to the point of perfect matching. Colors refer to \( l = 1 \) (black), \( l = 2 \) (blue), \( l = 3 \) (green), \( l = 4 \) (red) and \( l = 5 \) (orange). (right) The exact dynamics (black) is best reproduced by the darker blue line. Parameters are \( \alpha = 0.8 \) and \( T = 0.5\Delta \).

### 3.3 Coherence and entropy dynamics

We now present some results for the \( P_x \) dynamics, also including an excursion to entropy and system-bath entanglement. At \( T = 0 \) and for \( \alpha > 0.5 \), the non-interacting blip approximation (NIBA) yields an analytical result for the saturated \( P_x \) dynamics,

\[
\langle P_x^{\text{NIBA}} \rangle_\beta \equiv P_x^{\text{NIBA}}(t \to \infty) = \int_0^\infty dt' K_{s,x}(t') = \frac{\Delta}{\omega_c} \frac{1}{2\alpha - 1},
\]

where \( K_{s,x} \) is the integral kernel from (1.53). This expression can only be valid when \( \omega_c \gg \Delta \) and \( \alpha \) is not close to 1/2. Otherwise, the constraint \( |P_x(t)| \leq 1 \) is violated. However, as long as this requirement is fulfilled, NIBA turns out to be a very accurate description, as is shown in Fig. (3.6). The result in itself is not surprising. When dissipation increases, coherences are more and more suppressed. It is exactly this regime, where NIBA gives also fine predictions for \( P_z(t) \).

We skip further plots for \( T > 0 \), as this does not show any unexpected tendencies: Thermal fluctuations suppress the coherences even more and guide the system towards the classical range, where the density matrix is almost diagonal. For example, at \( T = 3\Delta \) and \( \alpha = 1 \), the \( P_x \) equilibrium value is pushed to \( \langle P_x \rangle_\beta \approx 0.08 \); for \( T = 10\Delta \) and \( \alpha = 1.6 \) even down to \( \langle P_x \rangle_\beta \approx 0.03 \).

Instead, we return to the quantum regime at \( T = 0 \). Here, the dynamics shows first classical signatures as it becomes overdamped for \( \alpha > 0.5 \), while localization occurs beyond \( \alpha_c = 1 \). Correspondingly, both crossovers are visible in the equilibrated values of the von Neumann entropy \( S \), at least in the scaling limit \( \omega_c \gg \Delta \).

Let us study this observable in more detail. According to Eq. (1.28), the reduced density
matrix reads
\[
\rho = \frac{1}{2} \begin{pmatrix}
1 + P_z & P_x - i P_y \\
P_x + i P_y & 1 - P_z
\end{pmatrix}.
\] (3.14)

Its eigenvalues are easily calculated to
\[
\lambda_{1/2} = p_\pm = \frac{1}{2} \left( 1 \pm \sqrt{P_x^2 + P_y^2 + P_z^2} \right).
\] (3.15)

Performing the trace in the eigenbasis of \( \rho \), one immediately finds (\( k_B = 1 \))
\[
S = -p_+ \log p_+ - p_- \log p_-.
\] (3.16)

Due to \( 0 \leq p_\pm \leq 1 \), \( S \) is limited to the range [0; log 2]. The von Neumann entropy does also serve as a measure of entanglement between TLS and bath, at least for \( T = 0 \) [74]. This is evident from the fact that the combination \( P_x^2 + P_y^2 + P_z^2 \) quantifies the purity of the spin state. However, a non-pure (mixed) state ought to be entangled with the environment in any way.

Obviously, it is not necessary to sample \( S \) as an own observable. Instead, we just calculate it from the \( P_\nu \) dynamics and determine the propagation of uncertainty. The error bars are then determined by
\[
\Delta S(P_x, P_y, P_z) = \frac{1}{2} \log \left( \frac{p_+}{p_-} \right) \sum_{\nu=x,y,z} P_\nu^2 \Delta P_\nu.
\] (3.17)

In recent NRG and Bethe ansatz works [76, 77, 78], it was found that the von Neumann entropy increases monotonically in the delocalized phase and reaches its maximal value at

Figure 3.5: Even the modified CH-PIMC does not work in the coherent range, when temperature is very small (\( \alpha = 0.3 \) and \( T = 0 \)).
Figure 3.6: We compare PIMC data for $P_x$ to the NIBA dynamics in the incoherent Ohmic regime at $T = 0$ for different couplings and cut-off frequencies. Deviations increase when $\alpha$ approaches the coherent-incoherent transition point $\alpha = 0.5$, at which the NIBA result (3.13) becomes unphysical.

$\alpha = \alpha_c$. In the scaling limit, this maximum is not a pronounced cusp but rather a plateau ranging from $\alpha = 0.5$ to $\alpha = \alpha_c$. In the localized phase $\alpha > 1$, $S$ decays rapidly towards zero.

Now, can we find hints to these equilibrium properties in the SB dynamics? Unfortunately, our inspection is limited to the delocalized regime: As the coherences saturate much faster than the populations, it makes sense to prepare the TLS in a fully off-diagonal state, $P_x(0) = 1, P_y(0) = P_z(0) = 0$. We thereby find nicely converging results for $\alpha < 1$. However, as $\langle P_z \rangle_\beta \neq 0$ in the opposite regime, the equilibrated state is much too far to be reachable for PIMC.

Fig. 3.7 illustrates the results. We use $\omega_c = 10\Delta$ or $20\Delta$ and vary the dissipation strength, thereby labeling the same $\alpha$ with the same color. In each case, the upper curve refers to the higher cut-off. Furthermore, the thick black line marks the upper border $\log 2$. We see that the plateau values increase for increasing $\alpha$ and $\omega_c$ and that the values culminate at $S = \log 2$: The curves for $\alpha = 0.7$ and $\alpha = 0.5$ ($\omega_c = 20\Delta$) almost touch the upper bound. Although this is also true for $\alpha = 0.4$, this curve shows a slight tendency to fall down again. This is because $P_x(t)$ decays from $P_x(0) = 1$ to a global minimum, from which it softly approaches its equilibrium value (not shown).

Our observations are, however, no direct hint to the localization transition as we skipped curves in the localized phase for the reason mentioned above. Nevertheless, the agreement in the delocalized phase is fine. Notice that such observations are only possible, when one has access to the full reduced density matrix with regard to both initial preparation and time...
Figure 3.7: Dynamics of the von Neumann entropy $S(t)$ for an Ohmic bath at $T = 0$ and an off-diagonal initial preparation ($P_x(0) = 1$, $P_y(0) = P_z(0) = 0$). Colors refer to different $\alpha$. The upper one of each pair of identically colored curves refers to $\omega_c = 20\Delta$, whereas the lower one has $\omega_c = 10\Delta$. The dynamics rapidly reaches the maximal value $\log 2$ beyond $\alpha = 0.5$.

3.4 Conclusions and outlook

What are the basic insights from this chapter? We find the CH-PIMC to work in the Ohmic regime if $T \gtrsim \Delta$. However, as $\hbar \beta$ can be interpreted as the time scale of the bath, it is no wonder that exactly this quantity marks the border: One could summarize in a simplifying way that our approximation does well, if the bare system is “not faster” than the bath. In addition, we learned that the modified CH-PIMC can reproduce the effects of the memory cut in an effective way for temperatures that go a bit below, i.e. $T \gtrsim 0.5\Delta$.

Concerning the outlook, we must concede that the PIMC for Ohmic reservoirs is rather exploited. Even if the CH-PIMC might be improved or if there were other ways to fight the sign problem in a more efficient way, it is rather unlikely that really new physics is found. Analogously, this first result chapter should be assessed in view of methodic improvements, i.e. the measurement of coherences and the CH-PIMC, and not with regard to the physical component.
Chapter 4

Sub-Ohmic Damping

A possible generalization to non-Ohmic broadband reservoirs was already mentioned in Chap. 1: One can choose a power-law spectrum with $I(\omega) \propto \omega^s$ and $0 < s < 1$, referred to as sub-Ohmic ($s > 1$ is named super-Ohmic). Although the latter is very common in experiments, e.g. for phonons in solids or exciton transfer in biomolecules [96], its physics is not so multifarious compared to the sub-Ohmic damping. For example, the super-Ohmic model is known to exhibit no phase transition. In contrast, the sub-Ohmic environment is not only of interest with regard to thermodynamics, but also in view of the effect of slow modes onto the dynamics.

The chapter is commenced by a motivation, discussing some theoretical background and the experimental relevance. We then turn our attention to the applicability of Chain Path Integral Monte Carlo (CH-PIMC), that was introduced in Chap. 3. Starting from this discussion, we first focus on those parts of the sub-Ohmic regime in which CH-PIMC works and study the decay dynamics therein, before we turn to the opposite range. In fact, our approach was the first to solve the problem of how the transition from quantum-coherent oscillation to quasi-classical overdamped dynamics takes place [112, 114]. Attention is invited to the fact that we will get very surprising results, which are confirmed analytically. Finally, we pose the question, whether it is possible to see signatures of the localization phase transition in the time evolution of the entropy.

4.1 Motivation

In general, dealing with sub-Ohmic dissipation is more challenging than Ohmic friction. Enhancement of low-frequency modes leads to a long-ranged interaction in time, which, in contrast to other numerical methods, fortunately does not bear any new methodical difficulties for the PIMC, but more complicated physics instead.

The sub-Ohmic spectral density reads

$$I(\omega) = 2\pi \alpha \omega_0^{1-s} \omega^s e^{-\frac{\omega}{\omega_0}}, \quad (4.1)$$
where $\alpha$ and $\omega_c$ are already known from the Ohmic bath and the parameter $s$ controls the strengthening of slow modes. For $s \to 1$, the Ohmic case is approached. Here, the low-energetic oscillators are less pronounced compared to the case $s \to 0$, which we name the *deep* sub-Ohmic regime.

There are several ideas of how to implement a sub-Ohmic spin-boson model (SBM) experimentally. One goes back to Shnirman et al. [87]. They propose a realization with a superconducting island that is subject to a gate voltage and interacts with a superconducting lead via Josephson junctions. In a certain limit, the system is effectively reduced to two charge states. This qubit carries a bias that is determined by the gate voltage and a tunneling amplitude that depends on the external flux through the ring formed by lead and island. The device is exposed to charge fluctuations causing $1/f$ noise, corresponding to a sub-Ohmic spectrum with $s \to 0$. Porras et al. [88] suggest to realize the same limit by addressing a single ion in a 2D Coulomb crystal by an off-resonant standing laser wave, where the collective mechanical modes act as the bath’s degrees of freedom.

In another work [89], it is shown that the exponent $s = 1/2$ can be realized by coupling a resistor-dominated RLC transmission line capacitively to two points of a mesoscopic metal ring. The latter is divided into a larger “arm” and a smaller “dot”, which is assumed to be occupied by $N$ or $N + 1$ electrons, thereby being truncated to a spin-1/2 system. We note in passing that recent progress in engineering environments for Cooper pair boxes may grant access to exponents $s < 1/2$ [90]. Further systems in which sub-Ohmic damping is expected to occur are ultra-slow glasses [37, 91], nanomechanical devices [92], and heavy fermions [93, 94].

Similar to the Ohmic case, the sub-Ohmic SBM separates into two phases with $P_z(t \to \infty) = 0$ (delocalized) and $P_z(t \to \infty) \neq 0$ (localized) at $T = 0$. But in contrast to the former, the transition is of second order for all values $0 < s < 1$ [97, 98, 99, 104, 105]. Originally, this localized phase was believed to occur at every finite $\alpha$ for all sub-Ohmic exponents [20]. Several works show that this transition accompanies a maximum of entanglement at $\alpha = \alpha_c$ [97, 105].

Again, it is the slow modes that cause this behavior. The localization can be best understood from a dynamical perspective. Suppose a TLS that is strongly coupled to a sub-Ohmic bath with polarized initial preparation, cf. Eq. (1.33). Allowing the system to evolve, the sluggish modes tend to prevent it from following its free counterpart ($\alpha = 0$) that oscillates between the $\sigma_z$ eigenstates. Thereby, the dissipative TLS is pulled towards its initial state, still favoring it over the opposite state when the dynamics is already saturated. Note that this picture is a bit misleading from the thermodynamical point of view, as the free energy surface splits into two equivalent minima one of which is preferred by the asymmetrically prepared spin.

Although most investigations focussed on equilibrium properties, the sub-Ohmic dynamics gained increased attention during the last years. In general, there are two classes of approaches to the SBM dynamics: One of them takes into account a finite number of bath modes and works with the full Hilbert space of system and reservoir, whereas the other
4.2 Chain Path Integral Monte Carlo in the sub-Ohmic regime

Can the CH-PIMC scheme help us also for sub-Ohmic baths? Reasonable doubts arise from the fact that any Markovian approach seems to be a completely hopeless endeavor, when

1^However, the authors of Ref. [110] see at least a first hint on the effect we observe in the deep sub-Ohmic range.

2^Relation (4.2) is easily proved by rewriting \( \coth (\omega \beta / 2) = (1 + e^{-\omega \beta})/(1 - e^{-\omega \beta}) \) and expanding the denominator with the geometric series. Note that the Hurwitz zeta functions in Eq. (4.2) are only converging for spectral exponents \( s > 2 \). Here, we have to get clear about the fact that the combination in which they appear in (4.2) converges for \( s > 0 \), when we collect all terms in one sum. This is of importance for the implementation.
the bath memory is even more long-ranged than in the Ohmic case. However, as already pointed out in Chap. 3, CH-PIMC captures parts of the bath memory and therefore cannot be indicated as “purely Markovian”.

Nevertheless, decreasing the spectral exponent does not allow us to hope that things become easier. The CH-PIMC is therefore not expected to work in the range of low temperatures, $T \lesssim 0.5\Delta$, where it fails already for Ohmic damping. We skip the discussion of the original approach presented in Sec. 3.2 and switch immediately to the modified CH-PIMC. Of course, the former is captured within the latter by simply setting $\delta P_x, \delta P_y = 0$.

Fig. 4.1 shows some results for both the “soft” and the deep sub-Ohmic regime ($s = 0.75$ and $s = 0.25$, respectively) with moderate temperature $T = \Delta$ and $\alpha > \alpha_c$ (where $\alpha_c$ is the critical coupling for the quantum phase transition). It is clearly visible that the matching works for $s = 0.75$, while it fails for $s = 0.25$. Obviously, the long-ranged bath memory can not be recast by changing the values of $P_x$ and $P_y$ for small $s$.

![Figure 4.1: The modified CH-PIMC works in the incoherent sub-Ohmic regime for exponents close to Ohmic damping ($s = 0.75$, $\alpha = 0.5$), whereas it fails in the deep sub-Ohmic range ($s = 0.25$, $\alpha = 0.1$). The other parameters are $T = \Delta$ and $t_s = 4\Delta^{-1}$.](image)

One comment concerning the adjustment of the initial bath state is necessary. For Ohmic dissipation, matching can be improved by changing the bath equilibrium position $\mu$ to $P_z(nt_s)$. In the sub-Ohmic regime, this adjustment indeed worsens the matching – which is again an artefact of sluggish modes. Therefore, the bath is always prepared in its original state $\mu_n = P_z(0)$ in the beginning of each new segment. This confusing observation is best understood: For sub-Ohmic damping, a significant part of the modes does not perform any dynamical response on the time scale $t_s$. As a consequence, the matching becomes worse when the whole bath including the slow modes is forced to a new equilibrium position $\mu_n \neq P_z(0)$. 
4.3. INCOHERENT REGIME AT T > 0

Further, we find that the theoretical prediction $\delta P_y = 0$ is perfectly fulfilled both in the Ohmic and the sub-Ohmic regime, but only if the bath is always located at its original position, $\mu_n = P_z(0)$. Any adjustment according to $\mu_n = P_z(nt_s)$ leads to $\delta P_y \neq 0$. Although disagreeing with our theoretical forecast, this feature is intriguing: Placing the bath at a position $\mu_n \neq P_z(0)$ leads to a kink in the dynamics. This is because the slow modes, that remain close to their initial positions for a rather long time, start to pull the spin and prevent it from oscillating back and forth. A non-zero $\delta P_y$ can compensate this effect as $P_y \propto \dot{P}_z$.

Without boring the reader with further data any longer, we summarize the question of applicability for sub-Ohmic baths by stating that CH-PIMC works, as long as $s \geq 0.5$, $T \gtrsim 0.5\Delta$ and $\alpha$ is large enough to overdamp the dynamics. Again, the system must not be “too quantum”, fixing a lower bound for both temperature and spectral exponent.

4.3 Incoherent regime at $T > 0$

The CH-PIMC can now be used to gain some insight into the equilibration rates at finite temperatures. Combining both PIMC types, we can cover large parts of the incoherent regime: For $T \lesssim 0.5\Delta$, the required Trotter discretization is so small that we can extract the decay rates from one single run, while the applicability of CH-PIMC enables us to scan the whole opposite regime, $T > 0.5\Delta$.

![Figure 4.2](image-url)  

**Figure 4.2:** The curves show how an exponential decay is fitted to PIMC (blue) and CH-PIMC (red) data after cutting the transient dip. The fitted exponentials are drawn in black.

In Fig. 4.2, we see a perfectly monotonic decay, which is characterized by one time constant after a short transient dip. The dynamics is plotted together with the fitted curves for two parameter sets. One of them is gained from a single run and the other one by CH-PIMC. For the latter, we choose the non-modified approach ($\delta P_{x,y} = 0$) and adjust the bath's
position. This seems to violate the borders that were set above. However, the procedure is still working: It is not so important to smoothen the curve at the matching point, as long as $t_s \gg t_{\text{dip}}$ (with $t_{\text{dip}}$ being the time scale on which the dip vanishes) and the dip amplitude is small.

Let us switch to the question of what we can learn from an analytical treatment in this regime. In the case of strong friction, the equation of motion of the non-interacting blip approximation (NIBA) for the symmetric TLS,

$$\frac{d}{dt} P_z(t) = - \int_0^t dt' K_s(t - t') P_z(t'),$$

with kernel (1.51), can be approximated by $P_z(t') \approx P_z(t)$, if we assume $K_s$ to decay much faster than $P_z$. Eq. (4.4) therefore reduces to a simple first-order differential equation to be solved by an exponential decay $P_z(t) = P_z(0)e^{-\Gamma t}$ with rate [20]

$$\Gamma = a_s \exp \left[-2\alpha b_s \Gamma(s - 1)\right] \quad \text{with}$$

$$b_s = 1 + 2(\omega_c \beta)^{1-s}[\zeta(s - 1, 1) - \zeta(s - 1, 1/2)],$$

$$a_s = \frac{\Delta^2}{2\omega_c} \left[ \frac{\pi(\omega_c \beta)^{1+s}}{2\alpha \Gamma(1 + s)\zeta(1 + s, 1/2)} \right]^{1/2}. \tag{4.5}$$

In Fig. 4.3, we compare the decay rates governed from Eq. (4.5) with those extracted from MC simulations. Both methods agree very well. Deviations are visible for small coupling and low temperatures. Here, the dynamics approaches the coherent regime and both the kernel

Figure 4.3: We see a comparison between analytical NIBA decay rates, Eq. (4.5), and rates extracted from MC simulations, cf. Fig. 4.2. This proves that, first, both approaches are in agreement, and secondly, the life times are really huge compared to the bare TLS time scale $\Delta^{-1}$.
approximation in the NIBA and the possibility to fit an exponential decay to the PIMC data become problematic. However, the exponential dependence on the coupling strength is apparent in the whole range.

4.4 Coherence behavior at $T = 0$

Next, we switch to $T = 0$ and study the spin dynamics for increasing system-bath coupling and $\mu = 1$, depending on the spectral exponent. We will see that, similar to the applicability of the CH-PIMC, the regime $s < 0.5$ plays a special role. What we expect, according to well-known results for Ohmic reservoirs, is that the system displays oscillations for weak coupling, that vanish more and more and turn into a monotone decay for increasing coupling – similar to the damped harmonic oscillator known from classical mechanics.

This phenomenon is called *decoherence* and is known to be quite universal for quantum systems that couple to broadband reservoirs [1, 2]. In general, decoherence means the destruction of superposition. Imagine a TLS that is prepared in a state $\alpha |0\rangle + \beta |1\rangle$ with $|0\rangle$ and $|1\rangle$ being eigenstates of the TLS Hamiltonian. The system will conserve the superposed state during time evolution, resulting in off-diagonal elements $|\rho_{ij}| \propto |\alpha\beta|$ in the density matrix. However, when the fluctuating forces of the environment come into play, coherences are about to vanish and the density matrix shrinks to a classical probability distribution with non-zero entries only on the diagonal.

![Coherent-incoherent transition at $T = 0$ for sub-Ohmic exponent $s = 0.75$. The purple line indicates the border $\alpha_{CI} \approx 0.20$, when we take the existence of a local minimum as a criterion for coherent dynamics.](image)

Now, what about decoherence in a sub-Ohmic SBM at $T = 0$? In fact, the question of
coherent-incoherent (CI) crossover was not completely solved until publication of our work [65]. In the regime $s \geq 0.5$, the transition was found to occur at $\alpha_{CI} \leq \alpha_c$ (with the critical $\alpha_c$ for the phase transition). However, statements concerning $s < 0.5$ were contradictory: While Wang et al. [114] supposed $\alpha_{CI} < \alpha_c$ for all sub-Ohmic exponents, Nalbach et al. [112] found $\alpha_{CI} > \alpha_c$, although they could not determine the exact values. Fortunately, our PIMC scheme is predestinated to solve problems of this type.

### 4.4.1 Investigation of the coherent-incoherent transition

We start at spectral exponents close to the Ohmic case. Fig. 4.4 shows the dynamics for $s = 0.75$ depending on $\alpha$. Obviously, the population makes the predicted transition to incoherent motion. As a criterion for coherent motion, we check, if $P_z(t)$ has one or several local minima, so that the purple line indicates the border between both regimes. We thus find $\alpha_{CI}(s = 0.75) \approx 0.20 < \alpha_c = 0.30$, which is in agreement with Ref. [112] and a NIBA estimation that is done below, see Eq. (4.6).

Analyzing the dynamics at $s = 0.5$ (Fig. 4.5), we obtain similar results: Except from an initial dip, that we do not get rid of even for ultra-strong dissipation (see also curves in Fig. 4.2), we observe that oscillations vanish when friction is strong. Using the existence of a further local maximum as a criterion, we get $\alpha_{CI}(s = 0.5) \approx 0.11$, which is again close to what was found in Ref. [112] and to Eq. (4.6). Here, we are at a special crossing point as $\alpha_c = 0.106 \approx \alpha_{CI}$: For $s > 0.5$, overdamped decay arises in the delocalized regime, as the phase border meets the CI-transition line. Below $s = 0.5$, one might expect the transition to occur in the localized phase, i.e. $\alpha_{CI} > \alpha_c$.

![Figure 4.5: Same as in Fig. 4.4, but for $s = 0.5$. As the transient dip is always present, we call the dynamics coherent, if oscillations appear behind the first minimum. The transition occurs at $\alpha_{CI} \approx 0.11$.](image-url)
However, the unimpressive transient dips in Fig. 4.5 are nothing but forerunners to what happens when $s$ is again decreased. Fig. 4.6 ($s = 0.25$) illustrates the astonishing results: For coupling strengths up to $\alpha = 0.1$, the oscillations are still present and become even faster. A zoom into the upper-left corner of the plot and a look at curves with even stronger friction up to $\alpha = 0.3$ (see inset, nearly 14 times the critical coupling $\alpha_c \approx 0.022$) confirms that the oscillations do not only survive, but also increase in frequency. This is validated by simulations with a maximal value $\alpha = 0.8$ ($\approx 37\alpha_c$, not shown)!

![Figure 4.6: Choosing a very small exponent $s = 0.25$, we see no transition to incoherent motion even for very strong damping (see inset: $\alpha = 0.3 \approx 14\alpha_c$).](image)

Further simulations show that $s = 0.5$ in fact seems to mark the border beyond which overdamped motion occurs. Even at $s = 0.48$, we see slight oscillations for coupling strengths that are much larger than the critical value $\alpha_c$ (not shown)!

Our findings are summarized in a phase diagram (Fig. 4.7), where we also depict the curve $\alpha_c(s)$ (purple), indicating the crossover to localization (data for $\alpha_c$ are taken from Ref. [97]). Note that the observed effect is not a phase transition in the sense of thermodynamics, because it has nothing in common with equilibrium properties. Instead, we can call this a dynamical phase. For long times, however, the oscillations always die out and by using the terminus “surviving”, we want to paraphrase that these features are visible at short to intermediate times, but for arbitrarily large coupling.

What does the phase diagram actually tell us? For $s > 0.5$, things develop exactly in the way one would expect: The oscillating dynamics for small $\alpha$ becomes overdamped and the system runs into a localized phase, if $\alpha$ is further increased. We can therefore distinguish the “phases” coherent-delocalized, incoherent-delocalized, and incoherent-localized. The latter is strictly bordered to the left, as there is no incoherent dynamics for $s < 0.5$. Therefore, the fourth “phase” (coherent-localized) at $0 < s < 0.5$ and $\alpha > \alpha_c(s)$ has no upper bound
Figure 4.7: Combining our findings on the coherent-incoherent transition and literature data for the localization transition [97], we can characterize the SBM at $T = 0$ by this phase diagram. The purple line for the transition to overdamped motion is given by Eq. (4.6) and agrees with PIMC data. For $s > 0.5$, localization occurs in the overdamped range, while we do not get rid of oscillations for $s < 0.5$ at even ultra-strong damping.

for strong coupling. Interestingly, this corresponds exactly to the regime where the so-called quantum-to-classical mapping for the the phase transition fails [100].

The borderline between coherent and incoherent motion in the diagram 4.7 is extracted from an analytical NIBA investigation. Calling in mind that the population for the symmetric TLS follows an equation with integral kernel $e^{-Q'(t)} \cos[Q''(t)]$, we expect the transition to occur when the decaying part $e^{-Q'(t)}$ wins over the cosine term. This depends on the time scales of oscillation and decay, respectively. We therefore search for the time $t_*$ when the cosine reaches its first zero, i.e. $Q''(t_*) = \pi/2$, and insert this value into $Q'(t)$. Damping ought to overcome oscillations if $Q'(t_*) > 1$, whereas we expect coherences in the opposite case. It turns out that the constraint $Q'(t_*) > 1$ cannot be fulfilled for $s < 0.5$, which is in perfect agreement with our results. For $s \geq 0.5$, the predicted transition line is given by

$$
\alpha_{CI}(s) \approx \frac{\pi}{4|\Gamma(s-1)| \cos(s\pi/2)} \left(\frac{\Delta}{\omega_c}\right)^{1-s}.
$$

Individual values are $\alpha_{CI}(s = 0.5) = 0.099$ and $\alpha_{CI}(s = 0.75) = 0.235$, which coincide with PIMC results. Furthermore, the Ohmic result $\alpha_{CI}(s = 1) = 0.5$ is exactly reproduced. This is once more a hint that NIBA yields even quantitatively good results in several parameter ranges.

However, the observation of oscillations in the population dynamics is in itself not a proof for quantum coherence. Therefore, we need some unmistakable evidence for the quantum nature. This is done by the curves in Fig. 4.8, where we see the von Neumann entropy $S(t)$ and the coherence $P_x(t)$ for $s = 0.25$, $T = 0$, and two different couplings. As the former is an established measure for entanglement at $T = 0$, the plots point out that the TLS and the
4.4. COHERENCE BEHAVIOR AT $T = 0$

Figure 4.8: This plot proves that the oscillations in the deep sub-Ohmic range are of quantum nature: First, the system becomes entangled with the reservoir, where entanglement is quantified by the von Neumann entropy (right axis). Secondly, the coherence $P_x(t)$ reaches large values and oscillates with maxima (minima) where $P_z(t)$ has minima (maxima). We have $s = 0.25$ and $T = 0$.

sub-Ohmic environment are correlated in a non-classical way. Further, the coherence $P_x(t)$ reaches quite large values and oscillates with the same frequency as $P_z(t)$, thereby passing minima, when $P_z(t)$ reaches maxima and vice versa. Therefore, we can definitely claim that what we observe are real quantum-mechanical coherences.

Up to now, we have interesting phenomena, but no physical picture behind. To get to the bottom of this feature, we study how these oscillations depend on the initial bath displacement. Fig. 4.9 shows the $P_z$ dynamics for a sub-Ohmic bath with $s = 0.25$, $\alpha = 0.1$, $T = 0$, and different bath shift parameters $\mu$. The basic message jumps to the eyes: Fast coherent oscillations clearly depend on the initial equilibration position of the bath modes. While we still observe them for $\mu = 0.8$, they are already reduced to one single hollow for $\mu = 0.5$ and disappear more or less, when the bath is initially placed in the Landau-Zener region ($\mu = 0$).

4.4.2 The limit $s \to 0$

The limit $s \to 0$ is perfect for getting insight from an analytical treatment. It is only one further step to arrive at the root of the matter: One has to remember that a bath displacement of $\mu$ enters the action functional in the same way as a time-dependent bias of size $-\mu \text{Im}[\dot{Q}(t)]$ does. In the limit $s \to 0$, we have for $T = 0$

$$Q_0(t) \approx -\kappa_s \left[ s + (s - 1) \omega_c e^{i\frac{\pi}{2} (1-s)} \right],$$

$$\dot{Q}_0(t) \approx \kappa_s (1-s) \omega_c e^{i\frac{\pi}{2} (1-s)} \approx i \frac{2 \alpha \omega_c}{s}, \quad (4.7)$$
Figure 4.9: Shifting the bath from the polarized preparation ($\mu = 1$) towards the Landau-Zener region ($\mu = 0$) leads to a soft die-out of the fast oscillations ($s = 0.25$, $\alpha = 0.1$). This can be understood from the equivalence of a polarized bath with a time-dependent bias that becomes quasi-static for $s \to 0$.

with $\kappa_s = 2\alpha|\Gamma(s-1)| \approx 2\alpha/s$. We see that $\dot{Q}_0(t)$ is time-independent within our approximation and grows linearly with $\alpha$. In addition, it is inversely proportional to $s$ – a dependence that is examined below. Notice that the approximative result for $\dot{Q}_0''$ is nothing but the classical reorganization energy $\Lambda_{cl}$. So, the bias is quasi-static and its size is given by $\Lambda_{cl}$. A detailed investigation shows that this contribution clearly prevails all other terms in the influence functional. Therefore, we can roughly map the system onto a free TLS that is subject to a large bias and does not feel the dissipative influence of the surrounding. Instead, the whole dynamics is dictated by the effect of the initial setting. Calling in mind the bare TLS’s population dynamics, Eq.(1.29), we find for a biased system with $P_z(0) = 1$

$$P_z(t) = \frac{\epsilon^2 + \Delta^2 \cos(\sqrt{\Delta^2 + \epsilon^2}t)}{\Delta^2 + \epsilon^2}.$$  \hspace{1cm} (4.8)

By simply setting $\epsilon = 2\alpha\omega_c/s \gg \Delta$, we end up with oscillations of frequency $\approx \epsilon$.

The same result is hidden in the NIBA. Its equation of motion reads in Laplace space

$$\hat{P}_z(\lambda) = \frac{1}{\lambda + \hat{K}(\lambda)},$$  \hspace{1cm} (4.9)

where the initial condition $P_z(0) = 1$ is already inserted. We are interested in the poles of $\hat{P}_z(\lambda)$, i.e. the zeros of $\lambda + \hat{K}(\lambda)$, corresponding to decay rates (real parts) and frequencies (imaginary parts). Being linear in time, $\hat{K}(\lambda)$ can be calculated with standard rules,

$$\hat{K}(\lambda) = \Delta^2 e^{\kappa_s} \frac{\lambda - \rho_s'}{(\lambda - \rho'_s)^2 + (\rho''_s)^2}$$  \hspace{1cm} (4.10)
with \( \rho_s = \omega_c \kappa_s (s - 1) \exp[i(1 - s)\pi/2] \). Calculation of the zeros of \( \lambda + \hat{K}(\lambda) \) leads to the cubic equation
\[
\lambda^3 - 2\lambda^2 \rho_s' + \lambda \left[ (\rho_s')^2 + (\rho_s'')^2 + \Delta^2 e^{s\kappa_s} \right] - \Delta^2 \rho_s' e^{s\kappa_s} = 0.
\] (4.11)

For \( s \to 0 \), \( \rho_s' \) becomes small compared to \( \rho_s'' \). We therefore neglect the constant term as well as \( (\rho_s')^2 \) in the linear term and find the roots
\[
\lambda_1 = 0,
\lambda_{2/3} = \rho_s' \pm i\sqrt{(\rho_s'')^2 + \Delta^2 e^{s\kappa_s}}.
\] (4.12)

\( \lambda_1 \) assigns the localization, where \( P_z(t \to \infty) \) is given by its residue. Actually, \( \lambda_{2/3} \) are more important for our purpose, as they contain the decay rate \( \gamma_s \) and the effective frequency \( \Omega_s \),
\[
\gamma_s(\alpha) = \rho_s' = 2\alpha \omega_c \Gamma(s) \cos[(1 - s)\pi/2] \approx \pi \alpha \omega_c
\]
\[
\Omega_s(\alpha) = \sqrt{(\rho_s'')^2 + \Delta^2 e^{s\kappa_s}} \approx \rho_s'' \approx \frac{2\alpha \omega_c}{s},
\] (4.13)

which is the same result as in our previous considerations. It is worthwhile to mention that the effective frequency is inversely proportional to \( s \), but the decay rate \( \gamma \) is independent of \( s \). Notice that the observed oscillations are purely bath-induced: In expression (4.13), there is no dependence on \( \Delta \). Instead, the bath modes cause a bias that exceeds all other energy scales.

Figure 4.10: The effective frequency gained from analytical considerations (Eq. (4.13)) coincides with a fit onto PIMC data when \( s \) approaches zero, whereas \( s = 0.25 \) is quantitatively not convincing.

One further comment should avoid misunderstandings: We always talk about the low-frequency modes causing this effect and the reader may wonder, why there occurs a factor
ωc in Eq. (4.13). The solution of this seemingly disagreement is trivial: The factor ωc is nothing but an artefact from the factor ωc1−s in the definition of the sub-Ohmic spectral density, Eq. (1.6), and is not related to fast modes in any way.

We conclude this subsection with a comparison of these investigations with numerical data. Fig. 4.10 shows a plot of the effective frequency Ωs(α), using the square root expression in Eq. (4.13) and the frequency fitted to the MC data. Unless the deviations for s = 0.25 are obvious, the ratio of both frequency values approaches 1 for decreasing s and increasing α.

### 4.4.3 Robustness of the oscillations

The choice of the bath properties seems to be quite special, although the initial preparation is comparatively easy to realize for charge systems. It is thus manifest to have a closer look on the sensitivity of the observed oscillations onto several distortions. First, we want to check the robustness against thermal fluctuations. Second, we examine the dependence on both low and high frequency cut-offs.

It is common wisdom in mesoscopic physics that high temperatures destroy coherences and drive a system towards the classical domain. In general, thermal perturbations should rush the sluggish modes and therefore reduce their ability to resist an adjustment to the spin position for such a long time.

![Graph](image)

Figure 4.11: Sub-Ohmic coherences are disturbed by thermal noise. In this plot, we choose s = 0.1, α = 0.1 and a polarized bath preparation. Here, coherent patterns disappear for $T \gtrsim 0.8\Delta$.

Fig. 4.11 shows that this picture is indeed correct, where we have α = 0.1 for a rather small exponent (s = 0.1). We observe that temperature has to be quite large in order to
4.4. COHERENCE BEHAVIOR AT T = 0

destroy coherences: The patterns vanish for \( T \gtrsim 0.8\Delta \) and we still see coherent structures for \( s = 0.05, \alpha = 0.1 \), and a temperature that is larger than the bare system’s frequency, \( T = 1.5\Delta \) (not shown)! Clearly, this behavior preserves as long as the reorganization energy dominates all the other terms. Therefore, decreasing \( s \) makes the system more inert against thermal fluctuations. This could be of particular interest for an experimental verification: If such a small \( s \) can be implemented in the lab, this device is expected to be very resistant against thermal noise. By contrast, coherences are about to vanish, if \( T \gtrsim 0.2\Delta \) at \( s = 0.25 \) and \( \alpha = 0.1 \).

Finally, let us have a brief look at the question of how the cut-off scheme changes things. We therefore take again a bath with the above parameters, \( s = 0.25, \alpha = 0.1 \), and \( T = 0 \). Clearly, manipulations in the high-frequency characteristics are expected to cause only soft changes: It should not make a qualitative difference, if we choose an exponential or a sharp ultra-violet (UV) cut-off, as it is often used in renormalization group techniques,

\[
I_{UV}(\omega) = I(\omega)\Theta(\omega_c - \omega). \tag{4.14}
\]

Contrarily, the infra-red (IR) cut at \( \omega_l \),

\[
I_{IR}(\omega) = I(\omega)\Theta(\omega - \omega_l), \tag{4.15}
\]

is expected to cause a significant difference. Fig. 4.12 confirms our supposition. The curves that use a sharp cut-off lie very close to the ones with exponential cut-off, whereas the single

\[\text{Figure 4.12: The cut-off type (sharp or exponentially) does not influence the behavior significantly. For both cut-off schemes, the size of } \omega_c \text{ enters only in the predicted way. However, even a very soft modification of the low-frequency modes makes the coherences vanish. We have } s = 0.25, \alpha = 0.1, \text{ and } T = 0.\]

Contrarily, the infra-red (IR) cut at \( \omega_l \),

\[
I_{IR}(\omega) = I(\omega)\Theta(\omega - \omega_l), \tag{4.15}
\]
Figure 4.13: The figure shows the dynamics of the von Neumann entropy for $s = 0.75$, $T = 0$ and different $\alpha$. On the depicted time scale, maximal entropy is reached for $\alpha = 0.24$, but the slopes of the curves suggest that the coupling strength that corresponds maximal $S$ lies somewhere above, probably close to $\alpha = 0.28$. This gives a hint to the quantum phase transition.

curve with a very soft IR cut ($\omega_l = 0.05\Delta$) gets rid of coherences except from the first hollow. Maybe the reader wonders, why the oscillations vanish, although the majority of slow modes is still present. However, as the reorganization energy is the relevant scale, we see from $\Lambda_{cl}(\omega_l = 0.05\Delta) \approx 0.71 \Lambda_{cl}(\omega_l = 0)$ that this seemingly soft IR-cut is in fact dramatic!

### 4.5 Entropy and phase transition

It was mentioned that the quantum phase transition towards a localized phase is attended by a maximum of the von Neumann entropy $S$, defined in Eq. (3.16). We want to check whether this transition can also be seen in the dynamical evolution. The limiting factor is once again the sign problem that prevents us from long simulation times.

Before we turn the attention to the PIMC results, let us briefly discuss, why this behavior occurs. As $\langle P_y \rangle_{\beta} = 0$, $S$ is a function of $\langle P_z \rangle_{\beta}^2 + \langle P_x \rangle_{\beta}^2$. For small coupling, we are in the delocalized regime with $\langle P_z \rangle_{\beta} = 0$, but large coherences, $\langle P_x \rangle_{\beta} \to 1$. This can be seen from the canonical result $\langle P_x \rangle_{\beta} \approx \text{Tr}(\sigma_x e^{-\beta H_0}) = \tanh(\beta \Delta/2)$, which is valid for $\alpha \to 0$. In the opposite (localized) range, coherences are suppressed, but $\langle P_z \rangle_{\beta}$ converges rapidly to 1$^3$. This way, we have $[\langle P_x \rangle_{\beta}^2 + \langle P_z \rangle_{\beta}^2]^{1/2} \to 1$ in both limits, so that the entropy is pushed

---

$^3$Strictly speaking, we have $\langle P_z \rangle_{\beta} = 0$ in thermal equilibrium, because none of the sites is preferred for a symmetric system. However, at the phase transition, the free energy surface splits into two equivalent minima for $\alpha > \alpha_c$, similar to Ginzburg-Landau theory. In NRG studies, one gets $\langle P_z \rangle_{\beta} \neq 0$ by applying a
Figure 4.14: Same as in Fig. 4.13, but for spectral exponent $s = 0.25$ and a non-diagonal initial preparation, $P_x(0) = 0.8, P_z(0) = 0.6$. These data suggest a value $\alpha_c \approx 0.025$. Due to the small coupling, pushing the error bars is much more expensive than in Fig. 4.13.

Towards zero. Clearly, $S$ must reach its maximal value for $S$ somewhere in between [97, 105].

Fig. 4.13 shows the entropy dynamics for $s = 0.75$, $T = 0$ and various coupling strengths. The curves for $\alpha \leq 0.2$ rise very fast and reach their maximum values in the interval $t = 2.5, ..., 4$. This is the regime of coherent oscillations. When increasing $\alpha$ such that the dynamics becomes overdamped, the entropy shows a monotonic increase over the full time range of the plot. As the values are not saturated, one cannot uniquely determine a value that corresponds to maximal entropy. Nevertheless, it seems that the curve for $\alpha = 0.28$ is growing strongest at $t = 8\Delta^{-1}$ and may be the one that reaches the largest equilibrium value. We would therefore suppose to find the critical $\alpha$ near this value, agreeing with the NRG value $\alpha_c = 0.30$ [97].

The plot for $s = 0.5$ looks similarly and suggests $\alpha_c$ to lie in the range $0.08, ..., 0.10$, again close to $\alpha_{NRG} = 0.106$ (not shown). For $s = 0.25$, we get the problem that the relevant couplings are comparatively small and the dynamics needs rather long to saturate. Both circumstances increase the statistical spreading. However, we can at least get a handle of the second problem by preparing the TLS in a non-diagonal state with $P_x(0) = 0.8$ and $P_z(0) = 0.6$. This is done because $P_x$ saturates much faster than $P_z$.

The results can be seen in Fig. 4.14. After a transient period, the smallest entanglement values occur in the uniquely delocalized ($\alpha = 0.015$) and localized ($\alpha = 0.05$) regime, whereas the values close to $\alpha_{NRG} = 0.022$ accompany a maximum of $S$, suggesting the approximative PIMC value to be in coincidence. Note that soft numerical discrepancies between NRG and PIMC could be a consequence of different cut-off schemes.
Sure, if one did not know about the quantum phase transition in the sub-Ohmic model, our non-saturated data could certainly not serve as a proof of its existence. Still, our findings would be at least a tentative hint.

4.6 Conclusions and outlook

We found quantum mechanical coherences to survive for even arbitrary strong system-bath coupling. To my knowledge, there is no other system that shows such a behavior when brought in contact to a broadband reservoir. However, this effect was first found with our PIMC method, although it is already governed in the NIBA [65]. Later on, other groups could verify this effect qualitatively [113] and find similar patterns for a purely dephasing model [2, 115].

We learned a lot in this chapter and the abundance of details may be a bit annoying. Still, the take-home message can be formulated in simple words: A dissipative bath is not always disturbing. As we have seen, it can be a source of understanding and might even be helpful for real applications.

Concerning the MC simulations, most regions of parameter space are illuminated. One might ask what happens, if the spectral exponent is exactly zero or becomes even negative. Another interesting question could be, how the indirect hints to the phase transition behave for finite temperatures. Here, we are in the quantum critical regime, where no phase transition occurs, but several quantities behave anomalously [97, 102]. The MC could help to check what happens on the transient time scale.

Specifically, our results ought to challenge the colleagues from the experimental side. As outlined in the beginning of this chapter, there are some promising candidates that could realize a SBM with sub-Ohmic coupling for small $s$. Clearly, some features are much easier from the theorist’s point of view. One of them is the question of how these spectra behave in the slow-modes regime. In real life, each system must have a smallest frequency, corresponding to a cut-off in the infra-red range. We have learned that the fast bath-induced oscillations depend very sensitively on exactly this detail. However, an advantage might be that environments with $s \to 0$ are rather inert against thermal fluctuations.
Chapter 5

Band-Gap Reservoirs

Whereas Ohmic and sub-Ohmic baths are a common choice for the spin-boson (SB) dynamics, we now switch to a type of reservoir that is rather untypical, as it originates from other physical fields: We want to study the effect of a gap in the spectral density onto the dynamics, sticking the connection to photonic band-gap materials. Clearly, gaps in electronic densities of states are well-known from semiconductor physics [7]. In contrast, similar spectra in bosonic reservoirs are a rather new field of research for a simple reason. Nature has given us semiconductor crystals, where the periodic potential of atoms produces forbidden regions in energy space. Realizing the analogon for electromagnetic excitations is really hard engineering in the length scales of microns. Nevertheless, the field of photonic crystal gained increased attention, as the idea of replacing semiconductor-based computation by photons is very promising [131]. Communication with speed of light and a negligible heat generation are invaluable advantages against our established information technology.

Due to recent developments in integrating single quantum dots into photonic crystals [132, 133, 134], such gapped electromagnetic spectra are also of interest with regard to their interaction to a single two-level system (TLS). Here, our model comes into play: In this short chapter, we study the effect of a band-gap in an Ohmic spectrum in comparison to the ungapped case.

5.1 Motivation

The field of photonic crystals arose in the 1980s and the idea behind it is to apply concepts known from electronic structure in solid states to the propagation of electromagnetic waves in transparent materials [126]. However, just the way as electrons scatter off atoms in the bulk, thereby causing forbidden zones in electronic k-space that we call gaps, photons can scatter off structures with periodically changing refraction indices. This is done by drilling thousands of small holes into transparent materials, such that the refraction index of glass changes with that of air. A first milestone in this field was the prediction of photon
localization [124]. In 1991, Austrian physicist Eli Yablonovitch was the first to succeed in creating a photonic crystal with a full band-gap, hindering not only photons of one single frequency to propagate, but in fact a full interval in frequency space [125].

Since then, enormous progress in fabricating such structures invigorated the whole field, so that first applications are already commercialized. Some of them may even be able to compete silicon-based information and communication technology and to realize the dream of all-optical computing [131] – or at least evolve to an indispensable compound in a synthesis of both electronic and photonic techniques, which defines the field of opto-electronics. Clearly, photonic band-gap materials are a very hot topic and we could fill books with describing fascinating applications and discussing the tremendous potential for future developments.

Relating to our work, also the coupling of such reservoirs to artificial two-level atoms was studied theoretically [128, 129, 130]. As mentioned above, corresponding experimental devices work with semiconductor quantum dots that are integrated into photonic crystals. By omitting single holes in the crystal structure, one can implement waveguides, thereby allowing for communication and entanglement between the dots [133].

We do not want to go further into details and instead discuss the question that can be answered by our Path Integral Monte Carlo (PIMC) simulations, namely, how does such a gap in the bosonic spectrum influence the dynamics of a TLS? The modeling is simple. We choose an Ohmic spectral density that has no modes in an interval of broadness $b$, which is symmetrically located around a characteristic gap frequency $\omega_0$.

\[
I(\omega) = 2\pi\alpha\omega e^{-\omega/\omega_c} \left\{ \Theta[(\omega_0 - b/2) - \omega] + \Theta[\omega - (\omega_0 + b/2)] \right\}. \tag{5.1}
\]

Trivially, the gap borders are at $\omega_{l/r} = \omega_0 \pm b/2$. The correlation function $Q(t)$ is determined numerically via Eq. (1.17). As the factor $\omega^{-2}$ causes trouble in the Riemann sum, we split the frequency integral into two parts, $\int_0^\infty d\omega \rightarrow \int_0^\epsilon d\omega + \int_\epsilon^\infty d\omega$. In the first one, the trigonometric functions are expanded and the integral is solved exactly. The second integral can be evaluated without problems by making use of a Newton-Cotes formula of order 6 [8].

### 5.2 Effective driven two-level system

The presence of a gap in the spectrum is supposed to influence the spin dynamics significantly, if the bare frequency $\Delta$ is enclosed. We therefore focus on situations where the middle of the gap is located at the bare TLS frequency, $\omega_0 = \Delta$. This way, the spectrum is clearly divided into a low- and a high-frequency part, which leads us to the idea of breaking down the whole model on effective quantities: Eq. (3.3) teaches us that the fast degrees of freedom act to first approximation as a cloud of modes which slows down the oscillation and renormalizes the tunnel coupling, $\Delta \rightarrow \Delta_{\text{eff}}$. In addition, the slow modes are known to cause a bias of size $-\mu \dot{Q}''(t)$ due to Eq. (1.37). We therefore map the dissipative model onto a time-dependent...
5.2. EFFECTIVE DRIVEN TWO-LEVEL SYSTEM

Figure 5.1: A spin-boson model (SBM) with Ohmic spectrum and a gap ranging from $\omega_l = 0.2\Delta$ to $\omega_r = 1.8\Delta$ can qualitatively be described by a bare driven model (renormalized TLS, rTLS) due to Eqs. (5.2), but only if $\alpha$ is rather small. Here, temperature is zero.

TLS with

$$\Delta_{\text{eff}} = \Delta \exp \left[ -\alpha \int_{\omega_l}^{\infty} \frac{d\omega}{\omega^2 + \Delta_{\text{eff}}^2} \exp(-\omega/\omega_c) \right]$$

$$\epsilon_{\text{eff}}(t) = -2\alpha\mu \int_{0}^{\omega_l} d\omega e^{-\omega/\omega_c} \cos(\omega t) \approx -2\alpha\mu\omega_l\text{sinc}(\omega_l t).$$  

(5.2)

with $\exp(-\omega/\omega_c) \approx 1$ in the second equation and $\dot{Q}''$ from Eq. (1.17). Note that the exact analytical time evolution requires a time-ordered product, as the driven TLS Hamiltonian does not commute at different times. To keep things easy, we use multiple short-time propagators with constant $\epsilon$ for very small intervals.

In order to test the quality of this simple effective TLS model, we plot the results in Fig. 5.1 for $T = 0$ and a gap of width $b = 1.6\Delta$. The colored lines refer to the description according to Eqs. (5.2), whereas the symbols show Monte Carlo (MC) data. While the qualitative behavior is similar, quantitative agreement becomes worse for increasing $\alpha$.

Clearly, a breaking down of the modes to a bias and a dressing of the tunnel matrix element cannot be sufficient to describe the whole effect of the bath. Our approximation is expected to break down, when more and more modes with a frequency near $\Delta$ come into play. This can be seen in Fig. 5.2, where we have $b = 0.8\Delta$. Already a rather small coupling ($\alpha = 0.3$) leads to deviations are considerably, whereas even qualitative agreement is absent for $\alpha = 0.5$. However, the black line shows the dynamics for a renormalized TLS without bias and a renormalized tunnel coupling that corresponds to $\alpha = 0.3$, proving that the description with Eqs. (5.2) is at least better than a pure $\Delta$-renormalization.

As this simplification contains no dissipation, it is condemned to disagree for stronger cou-
Figure 5.2: Same as in Fig. 5.1, but with $b = 0.8\Delta$, i.e. $\omega_l = 0.6\Delta$ and $\omega_r = 1.4\Delta$. The mapping fails, but works better than a free model with renormalized $\Delta$ and without bias (black line).

pling or in presence of modes that are rather close to the bare frequency $\Delta$. Still, it reproduces the dynamics in a qualitatively correct way in the opposite limit and we can learn that the modes which lie closest to $\Delta$ are in fact the ones that dissipate energy from the system to the surrounding most efficiently.

### 5.3 Coherent-incoherent transition and imprinted oscillations

Switching to non-zero temperatures, the approximative approach from the previous section fails clearly (not shown). A more important question in this regime might be, whether the broadness of the gap causes a transition to coherent oscillations, if we start with parameters that are related to overdamped decay for an Ohmic reservoir. The answer for $\alpha = 0.4$ and $T = 0.8\Delta$ can be seen in Fig. 5.3.

Clearly, the $P_z$ dynamics becomes underdamped and starts to oscillate, if the gap width grows. However, fixing a transition point obviously fails. Especially the curve for $b = 0.8\Delta$ shows a monotonic decay, but with an imprinted oscillation. Even the curves with smaller $b$ show this feature when the exponentially decaying part is subtracted. Similar structures are visible, when the reservoir is Ohmic with an additional pronounced mode at a distinct frequency instead of a gap [62].

Interestingly, the frequency of the imprinted oscillation is close to $\Delta$. This is clearly visible in Fig. 5.4, where we show the deviation of the $P_z$ dynamics from a fitted exponential
5.3. COHERENT-INCOHERENT TRANSITION & IMPRINTED OSCILLATIONS

Figure 5.3: In a parameter range where the Ohmic model decays monotonically ($T = 0.8\Delta$, $\alpha = 0.4$), the presence of a broad gap forces $P_z(t)$ to oscillate. Still, we cannot define a clear transition point between incoherent and oscillating regime.

decay: The zeros of the shifted sine curve with frequency $\Delta$ lie very close to the zeros of the oscillation. This effect in itself can be understood from the behavior of the auto-correlation $L = \dot{Q}$, which has the same characteristic frequency (see inset). In terms of our MC approach, it is easy to understand, why this transfers from $L'(t)$ to the dynamics: The spin values at $t$ and $t + \Delta$ are correlated during the sampling, as the discretized version of $L'(t)$ directly enters the MC weight.

However, the auto-correlation does not know anything about the free system’s evolution. This suggests that the stamped frequency corresponds to the center of the gap, and not to $\Delta$. In fact, several simulations with $\omega_0 \neq \Delta$ show oscillations with frequency $\approx \omega_0$ after subtraction of the exponential “background”.

All this is just a rough approximation. If we take a closer look at Fig. 5.4, we find that the zeros are not equidistant, neither for $e^{-\lambda t} - P_z(t)$, nor for $L(t)$. When observing an oscillation with slightly changing period, we inevitably think of a beat. Actually, this is what we see in Fig. 5.5, when we plot both the real and the imaginary part of $L(t)$ for the same bath parameters as before, but for longer times.

The black lines match them very good, especially in the long-time limit. They refer to a straightforward analytic approximation: We insert the spectral density (5.1) into the general expression for $L(t)$, Eq. (1.15), and adjust the integration borders according to the gap. The calculation is simple analytics, if we assume the thermal energy to lie somewhere in the gap, $T \approx \Delta$. Then, we can approximate $\coth(\omega\beta/2) \approx 2/\omega\beta$ for the low frequencies and $\coth(\omega\beta/2) \approx 1$ for the high frequencies. Neglecting all terms that decay faster than $t^{-1}$, we
Figure 5.4: We show the discrepancy between the blue curve in Fig. 5.3 to a fitted exponential. Clearly, oscillations are present and the black curve $\propto \sin(\Delta t + \delta)$ suggests that their frequency corresponds to $\Delta$. The inset shows similar features for the bath auto-correlation function $L(t)$.

end up with

$$L(t) = 2\alpha \left[ \int_{0}^{\infty} d\omega + \int_{\omega_r}^{\infty} d\omega \right] \omega e^{-\frac{\omega}{\omega_c}} \left[ \coth \left( \frac{\omega\beta}{2} \right) \cos(\omega t) - i \sin(\omega t) \right]$$

$$\approx \frac{2\alpha}{t} \left[ 2Te^{-\frac{\omega_l}{\omega_c}} \sin(\omega_l t) - \omega_r e^{-\frac{\omega_r}{\omega_c}} \sin(\omega_r t) \right]$$

$$+ i \frac{2\alpha}{t} \left[ \omega_l e^{-\frac{\omega_l}{\omega_c}} \cos(\omega_l t) - \omega_r e^{-\frac{\omega_r}{\omega_c}} \cos(\omega_r t) \right]$$

(5.3)

Still, it is not clear whether this can also be seen in the $P_z$ dynamics. Trying to find this beat with MC simulations, one would require very long times and rather good statistics. At this point, we skip further investigations and propose several ideas in the outlook.

### 5.4 Conclusions and outlook

Our results show that a rather soft incision in the structure of a broadband reservoir makes itself felt. Although we cannot answer the question, whether the beat of the gap border frequencies can be seen in the population dynamics, this is a very interesting feature. However, if we could observe the beat, we would be able to do it the other way round and ask, which frequencies are missing in the spectrum, when $P_z(t)$ for an Ohmic bath with unknown gap is given. This way, the dynamics of the TLS gets a spectroscopic aspect. Clearly, this is just a playing, but in fact a very interesting one.

Apart from the search for the beat in the dynamics, what are the further challenges? Relating
Figure 5.5: The auto-correlation $L(t)$ is plotted for longer times. Astonishingly, the real part is perfectly described by a beat with an amplitude $\propto t^{-1}$ and frequencies $\omega_l$ and $\omega_r$, cf. Eq. (5.3).

to other theoretical works, one might ask, if the Chain Path Integral Monte Carlo is able to describe quenching for reservoirs that do not only change their parameters during time evolution [82], but instead switch the whole bath structure, e.g. from Ohmic to gapped. Another theoretical work presents interesting results for the system-bath entanglement [130]. The authors couple a TLS to Lorentzian spectral densities, but with a pseudo-gap in between, such that the spectral density is zero for one single frequency. A further idea might be to model sub-Ohmic baths with spectral gaps. As their memory kernel decays slower, the beat effect could be more pronounced compared to the Ohmic case. In addition, a view at the coherence dynamics might be very helpful for understanding these phenomena.

To put it in a nutshell, there is still a lot of work to do and in contrast to the Ohmic model, new findings with PIMC simulations seem to be within range.
Chapter 6

Populations and Entanglement for Interacting Spins

In Chaps. 3 to 5, we presented a variety of results for the one-spin dynamics. This final chapter is reserved for a system of two spins, that couple to one and the same environment, described by the interacting spins model (ISM). The most important issues concerning the model and its implementation were discussed in Subsecs. 1.3 and 2.3. In addition, numerical difficulties, especially the problem of an enlarged configuration space, were mentioned.

Although this hinders us to reach comparable system times as for the spin-boson model (SBM), we expect more diverse physics due to the presence of a second spin. Especially effects like decoherence-free subspaces (DFSs) and reservoir-induced spin-spin entanglement are of substantial interest for quantum information purposes [6]. Again, we start with motivating the model and presenting some background information. Then, we study the effects of spin-spin coupling and bath-transferred interaction for the comparatively simple case of Ohmic reservoirs. Motivated by the absence of a quantum-classical transition in the deep sub-Ohmic regime (see Chap. 4), we immediately switch to this regime and check, whether similar features occur also for a two-spin system. Finally, we discuss creation and conservation of entanglement depending on various environmental parameters.

6.1 Motivation

The dynamics of interacting two-level systems (TLSs) is important with regard to different issues. Coherence properties are of interest in the context of energy transfer in biomolecules, where similar models are used to describe the effects of surrounding degrees of freedom onto exciton transfer dynamics [138, 139]. In this field, a boost of activities was caused by the work of Fleming et al. [140], who discovered electronic coherences in the Fenna-Matthew-Olson complex, a pigment-protein structure that appears in green sulfur bacteria. This experiment has been a matter of debate for seven years now, starting a war of opinions about the origin and the role of these oscillations.
As decoherence is the main problem in quantum communication, people are typically interested in devices with minimized system-bath coupling. Unfortunately, this is the limit in which Path Integral Monte Carlo (PIMC) simulations are unfavorable due to the enhanced dynamical sign problem, see Subsec. 2.1.2. However, as entanglement is a fundamental ingredient and on the heart of the field [6], our results may still contribute to a better understanding of interactions between qubits in the presence of a reservoir. In the context of quantum dissipation, the influence of the environment on the creation of entanglement has been studied in different works [155, 156, 157, 158, 159, 160]. In addition, we make contact with DFSs, which are of practical utility in this busy field [145].

Entanglement is a phenomenon that challenges theoretical physicists since the times of Einstein and Schrödinger [136, 137]. However, it was not before the early 1980’s that its experimental evidence succeeded [148, 149]. While the early experiments typically used non-linear crystals and beam splitters to entangle photons via their polarization degree of freedom, nowadays even entangled atomic ensembles can be designed [150, 151].

There are a couple of ideas stemming from the quantum computing community, how to implement such a model in the lab. We only spend some few words on these possible experimental realizations [26]. Porras et al. suggested to couple the internal states of two laser-addressed ions in a Coulomb crystal to the axial modes of the lattice [141]. Ng et al. proposed a way to realize the “two spin-boson model” by a 1D Coulomb crystal [142]. These crystals have been realized by Paul [143] and Penning traps [144] already some years ago and are probably the most promising candidates for quantum computing.

Let us switch to the numerical results. The model Hamiltonian is given by Eq. (1.61). If not stated differently, we use $\Delta_A = \Delta_B = \Delta$ and $\epsilon_A = \epsilon_B = 0$, see Eq. (1.54). If the tunneling matrix elements differ, $\Delta_A$ is chosen to be the time and energy scale. The reservoirs are Ohmic and sub-Ohmic, where the cut-off frequency is $\omega_c = 10\Delta_A$ for all simulations.

### 6.2 Effect of direct and indirect spin-spin coupling on Ohmic baths

The first question that imposes is, how does the possibility of interaction between the spins change the dynamics compared to the SBM? Here, we have to distinguish between direct interaction that is due to a non-zero spin-spin coupling $J$ and indirect interaction that is transmitted by the bath. As the latter is always present, the former cannot be studied independently. So, for $J \neq 0$, we always have cooperative effects of both interaction types.

To keep things easier, we want to restrict ourselves to Ohmic baths in this section. The purpose is to make some qualitative statements in order to get a first feeling for the new physics. We thereby study the dynamics of the observables that were introduced in Sec. 1.3.1, and postpone the discussion of spin-spin entanglement to Subsec. 6.4.
6.2. EFFECT OF SPIN-SPIN COUPLING ON OHMIC BATHS

Figure 6.1: We see $P_1(t)$ for a system with initial state $|1\rangle$ coupled to an Ohmic bath with $\alpha = 0.6$, $\mu = 1$ and $T = 0$. Finite coupling between the two spins makes the dynamics more coherent as long as $J > 0$, whereas decreasing the coupling (especially $J < 0$) suppresses tunneling and pins the system close to its initial state.

### 6.2.1 Influence of spin-spin coupling

The effects of direct interaction are investigated with regard to the coherent-incoherent transition. A single spin coupled to an Ohmic bath changes from oscillating to overdamped motion for $\alpha > \alpha_{CI} \approx 0.5$ at $T = 0$. The analytical result for two coupled spins without a bath, that are initially prepared in the state $|1\rangle = |+\ , +\rangle$, reads

$$P_1(t) = \frac{3 + 2 \cos((2J + \Delta)t) + 2 \cos((2J - \Delta)t) + \cos(2\Delta t)}{8}.$$  

(6.1)

Note that $P_1$ is independent of the sign of $J$ and that the dynamics is not only characterized by one frequency, but also by combinations of $\Delta$ and $J$.

In Fig. 6.1, the two spins couple to a reservoir with parameters $\alpha = 0.6$, $\mu = 1$ and $T = 0$, for which a single spin already shows a monotone decay. First of all, we see that the presence of the bath slows down the decay of the initial state drastically. However, this is an effect that is not related to spin-spin interaction and occurs also for the SBM: Both the $\Delta$ renormalization of the fast modes and the initial bath position are responsible herefore. Concentrating on the curves with non-negative $J$, one can ascertain that increasing coupling makes the dynamics “more coherent”: For large $J$, $P_1$ decays faster and is suspected to swing below its equilibrium value. The interplay of different oscillations for the free system makes things more complex. For this reason and because the sign problem causes an enormous trouble, we skip quantitative statements.

Surprisingly, the symmetry to a change in the sign of $J$ is massively broken: Increasing $|J|$ with $J < 0$ pins the population close to its initial state. This can be understood by the
equilibration properties of the free system. Calculating canonical averages, one sees that the $T = 0$ density matrix switches suddenly at $J = -0.5\Delta$. As the interaction energy between the individual $\sigma_z$ eigenstates of the spins dominates for $J > -0.5\Delta$, the system approaches the pure state $(|1\rangle + |2\rangle + |3\rangle + |4\rangle)/2$ with $\rho_{ij} = 0.25$ for all $i, j \in [1, 4]$. However, when $J < -0.5\Delta$, the interaction that is mediated by $J$ dominates the tunneling amplitudes $\Delta$ and we arrive at a density $\rho_{ij}$ with 0.25 at the diagonal and -0.25 at the counterdiagonal with $i + j = 5$, corresponding to a mixed ensemble with states $(|1\rangle - |4\rangle)/\sqrt{2}$ and $(|2\rangle - |3\rangle)/\sqrt{2}$.

Hence, only coherences caused by direct spin-spin interaction survive, while all the others vanish. As this jump-like behavior is an effect of the equilibration values, it is smeared out in the dynamics. This is why we see a creeping suppression of tunneling when $J$ decreases.

### 6.2.2 Bath-induced interaction

Now, we switch off direct coupling and pose the question, how an indirect interaction via the bath makes itself felt. As a reference, we use results for the SBM. Therefore, spin A is degraded to a background actor and the SBM observables of spin B are governed from the ISM density matrix. While A is always prepared in a $\sigma_z$ eigenstate, both $\sigma_z$ and $\sigma_x$ initial states are studied for spin B: When talking of a $\sigma_\nu$ eigenstate, we mean $P_\nu(0) = 1$ for the SBM and a factorizing spin-spin density with $P^A_\nu(0) = P^B_\nu(0) = 1$ for the ISM.

In Fig. 6.2, results are shown for the coherent range ($T = 0$, $\alpha = 0.3$, and $\mu = 0$). Lines refer to the SBM results, while symbols indicate the ISM dynamics. For the population dynamics
6.2. EFFECT OF SPIN-SPIN COUPLING ON OHMIC BATHS

Figure 6.3: The same as in Fig. 6.2 but with finite temperature, $T = 0.3\Delta$ and $\alpha = 0.8$. The bath adjusts faster compared to the $T = 0$ case.

evolving out of a $\sigma_z$ eigenstate, there is no deviation for $t \lesssim 2\Delta^{-1}$. Afterwards, the ISM curve drifts away and it seems that it is already closer to a monotone decay than the SBM. $P_x$ passes a very small hollow in the two-spin dynamics compared to a monotone increase for a single spin.

If a single spin is prepared in a $\sigma_x$ eigenstate without a bath, we clearly do not see any dynamics at all. Fig. 6.2 shows that this is still true for $P_z$ and a dissipative SBM, as we do not have any preference direction due to $\mu = 0$. However, things change for the ISM. Here, spin A is prepared in the $|+1\rangle$ state and therefore breaks the symmetry between up and down state for spin B. Notice that this is an effect that proves indirect interaction via the bath: If the surrounding was not present, we had $P^B_z \equiv 0$. $P_x$, however, shows again a hollow for both models. The plotted time scale is not large enough to bring both $P_x$ curves together.

This changes for the parameters chosen in Fig. 6.3 ($T = 0.3\Delta$, $\alpha = 0.8$). Here, the bath time scale $\hbar\beta$ is finite and all the $P_z$ curves meet. Note that the hollow that occurs for the ISM makes the $P_x$ curves converge for both initial states, even before they reach their equilibrium value. The observation for $P_z$ is qualitatively the same: The SBM curve makes no move to leave from the symmetric situation ($P_z \equiv 0$), while the ISM drifts towards $|-1\rangle$, before it slowly returns to zero. Compared to the prior parameter set, the distance to the SBM dynamics ($P_z(t) \equiv 0$) is smaller.

Bath-mediated interaction between the spins is therefore evident. Choosing a bath with comparatively short-ranged interaction is sufficient to get a first feeling for the two-spin dynamics. However, we will see right now that the sub-Ohmic bath contains again much more interesting features.
6.3 Oscillations in the deep sub-Ohmic regime

Our results in Chap. 4 reveal that a sub-Ohmic bath gives rise to unexpected quantum effects, if the spectral exponent is small and temperature is not too large. We also know about the sensitive dependence on the initial bath state $\mu$. Consequently, we are advised to see what happens, if we couple such a bath to a system of two spins and vary $\mu$. As we already know what matters, we focus on a very special region of parameter space. Fig. 6.4 shows the dynamics of population $P_1$ depending on $\mu$ for a system initially prepared in state $|1\rangle$. We have a very small spectral exponent ($s = 0.1$) and $\alpha = 0.1$. Further, temperature is zero and the spins are uncoupled.

What we observe is even stranger than for a single spin: Well-known oscillations with frequency $\Omega \approx \Lambda_{cl}$ appear for the polarized bath, $\mu = 1$. However, they suddenly vanish for $\mu = 0.5$, but recur for $\mu = 0$, $P_1$ thereby having a soft tendency to decay. Shifting the bath to the opposite site, $\mu = -1$, makes the oscillations faster, but with smaller amplitude (see inset). A quantitative inspection shows that the effective frequency is as large as $\Omega \approx 3\Lambda_{cl}$.

Fig. 6.5 shows the same for spectral exponent $s = 0.25$. The qualitative behavior is the same and extracted frequencies correspond again to $\Lambda_{cl}$ and $3\Lambda_{cl}$. The main difference is

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1. Although the error bars are of the same size as the amplitude, simulations with shorter $t$ and smaller error bars prove that these oscillations are indeed present (not shown).
6.3. OSCILLATIONS IN THE DEEP SUB-OHMIC REGIME

Figure 6.5: Qualitative dependence of the oscillatory patterns does not change when $s$ is slightly increased to 0.25. The main difference is that the curve for $\mu = 0$ decays faster.

that the population decays faster for $\mu = 0$ compared to the prior case.

However, we can fully understand these effects by taking a closer look at the influence functional (IF) (cf. Eq. (E.1), see also the quantitative discussion in Subsec. 4.4.2). It turns out that both the classical parts $\Lambda_j$ and the terms $X_j$ with $j \geq 1$ are negligibly small compared to $X_0$. Note that the latter is not present in the SBM, where we always have $\zeta_j\eta_j = 0$. Due to combinations of the form $\zeta_j^A\eta_j^B$ and vice versa, this is no longer true for the ISM. $X_0$, however, is of the same magnitude as the (approximatively constant) terms $X_j^{(\mu)}$, but with opposite sign. Both are proportional to $\dot{Q}''$, reading in this limit $\dot{Q}'' \approx 2\alpha\omega_c/s$, as we have $Q(t) \approx i2\alpha\omega_c t/s$. It may seem confusing that $X_0$ is so large compared to $X_j^{(\mu)}$, as all these quantities are an average of $\ddot{\dot{Q}}_{t''}$ over a small area in the $t' - t''$ plane. In fact, this is only true for $X_j^{(\mu)}$. $X_0$, however, additionally contains the full influence of the counter term that causes a static Markovian interaction. This contribution grows with $\Lambda cl$ and diverges for $s \to 0$. Details can be found in App. E.

We can therefore do the following approximation for the IF,

$$
\Phi^{ISM} \approx iX_0 \left[ 0.5(\eta_1^A\zeta_1^B + \zeta_1^A\eta_1^B) + \sum_{j=2}^{q}(\eta_j^A\zeta_j^B + \zeta_j^A\eta_j^B) \right] + i2\mu \sum_{j=1}^{q} X_j^{(\mu)}(\zeta_j^A + \zeta_j^B) \\
\approx i\Lambda cl\tau \left[ 0.5(\eta_1^A\zeta_1^B + \zeta_1^A\eta_1^B) + \sum_{j=2}^{q}(\eta_j^A\zeta_j^B + \zeta_j^A\eta_j^B) - \mu(\zeta_1^A + \zeta_1^B) - 2\mu \sum_{j=2}^{q}(\zeta_j^A + \zeta_j^B) \right] \\
\approx i\Lambda cl\tau \left[ 0.5(\zeta_1^B + \zeta_1^A) + \sum_{j=2}^{q}(\zeta_j^B + \zeta_j^A) - \mu(\zeta_1^A + \zeta_1^B) - 2\mu \sum_{j=2}^{q}(\zeta_j^A + \zeta_j^B) \right], \quad (6.2)
$$

thereby assuming the dynamics to be pinned close to the initial state, i.e. $1 - P_1 \ll 1$ and
\(\eta_j^A, \eta_j^B \approx 1^2\). The IF as a whole does obviously act as a bias of size \((1 - 2\mu)\Lambda_{cl}\) on each spin. The part \(-2\mu\Lambda_{cl}\) stems from the bath initial state, while the bias with constant size of \(\Lambda_{cl}\) is an effect of the counter term. This way, spin A forces the bath to act like a static bias on spin B and vice versa. At this point, we should become aware of the importance of the counter term. Neglecting this contribution would change the pattern of oscillations substantially. We would get a situation similar to the SBM, where \(\mu = 0\) means no bias on the system.

As the sign of the bias of a free TLS with \(P_z(0) = 1\) drops, cf. Eq. (4.8), the whole situation seems to be symmetric around \(\mu = 0.5\): Here, the oscillations vanish, but they reappear with same amplitude for \(\mu = 1\) and \(\mu = 0\), merely showing the slight asymmetry that \(P_1\) softly decays for the latter case. Even this feature can be understood from Eq. (6.2): For \(\mu = 0\), there is no quasi-static bias stemming from the initial bath state. Therefore, the approximation \(\eta_j^A, \eta_j^B \approx 1\) is violated and the spins are not pinned at their initial site. The bath shows its dissipative character and cannot simply be narrowed down to a time-independent bias on a free system. This becomes more and more visible, when \(s\) is increased.

A finite spin-spin coupling of order \(J \lesssim \Delta\) does not change the dynamics significantly, at least not for the bath preparations that go hand in hand with fast oscillations (not shown). As the bias is still the dominant energy scale, this is exactly what we would expect: The influence of spin-spin interaction is comparatively weak, so it is not able to change the dynamics visibly. We also skip a plot that visualizes suppression of coherences by thermal fluctuations. This was already shown for the SBM and transfers to the ISM. Though, the effect of finite temperatures becomes interesting, when we discuss spin-spin entanglement in the deep sub-Ohmic range.

### 6.4 Entanglement and decoherence-free subspaces

We already made contact with entanglement in Secs. 3.3 and 4.5. There, the von Neumann entropy was used as a measure for entanglement between system and reservoir. Now, the situation is different: We are interested in entanglement between the spins, thereby degrading the bath to a spectator – but a spectator that gets involved.

What is entanglement formally? A multipartite system is said to be in an entangled state, if it cannot be written as a product of states of its single entities. In terms of mixed states, a bipartite system is called not entangled or separable, if and only if its density matrix can

\[\sum_{j=2}^q(\eta_j^A + \eta_j^B)(\zeta_j^A + \zeta_j^B)\]

instead of

\[\sum_{j=2}^q(\eta_j^A\zeta_j^B + \zeta_j^A\eta_j^B)\]

Inserting the approximation \(\eta_j^A, \eta_j^B \approx 1\) would then lead to an additional factor 2 in Eq. (6.2). This contradiction is solved by recognizing that, in a strict sense, \(\zeta_j^A, \zeta_j^B = 0\), if we set the \(\eta\)'s to 1. Therefore, this term is either 0 or “2·0”. The approximation must therefore be read such that always few \(\eta\)'s are zero, making the corresponding \(\zeta\)'s non-zero. This way, terms like \(\eta_j^A\zeta_j^B\) give a contribution, whereas \(\eta_j^A\zeta_j^A\) and \(\eta_j^B\zeta_j^B\) are always exactly zero.

\(^2\)Note than one could also write \(\sum_{j=2}^q(\eta_j^A + \eta_j^B)(\zeta_j^A + \zeta_j^B)\) instead of \(\sum_{j=2}^q(\eta_j^A\zeta_j^B + \zeta_j^A\eta_j^B)\). Inserting the approximation \(\eta_j^A, \eta_j^B \approx 1\) would then lead to an additional factor 2 in Eq. (6.2). This contradiction is solved by recognizing that, in a strict sense, \(\zeta_j^A, \zeta_j^B = 0\), if we set the \(\eta\)'s to 1. Therefore, this term is either 0 or “2·0”. The approximation must therefore be read such that always few \(\eta\)'s are zero, making the corresponding \(\zeta\)'s non-zero. This way, terms like \(\eta_j^A\zeta_j^B\) give a contribution, whereas \(\eta_j^A\zeta_j^A\) and \(\eta_j^B\zeta_j^B\) are always exactly zero.
take the form

$$\rho = \sum_{k=1}^{n} p_k \rho_k^A \otimes \rho_k^B$$

(6.3)

with probabilities $p_k$ fulfilling $\sum_k p_k = 1$. The $2 \times 2$ objects $\rho_k^{A/B}$ are spin density matrices of each subsystem with $\text{Tr}(\rho_k^{A/B}) = 1$.

These definitions are evident, but how can one actually quantify the degree of entanglement? There have been proposed a lot of entanglement measures [146, 147, 152]. One popular choice is the so-called \textit{concurrence} $C$, which is a complicated function of the density matrix $\rho$ of a two-qubit system [153]. It is defined as

$$C(\rho) := \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4),$$

(6.4)

where $\lambda_i$ are the eigenvalues of the matrix

$$R := (\rho^{1/2} \tilde{\rho} \rho^{1/2})^{1/2},$$

(6.5)

sorted in descending order. In addition, we have

$$\tilde{\rho} := (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y),$$

(6.6)

where $\rho^*$ means complex conjugation and \emph{not} adjunction. The square root of a Hermitian matrix $A$ is determined by diagonalizing $A$ and reapplying the unitary transformation on the matrix that has the square root of the eigenvalues on its diagonal. Sure, Eq. (6.4) is not at all instructive. We do not care about the question, why the concurrence is a measure of entanglement and instead declare its most important properties: $C$ vanishes for factorizing states and it is always less or equal than one for a proper $4 \times 4$ density.

The missing clearness is a general problem, when one deals with entanglement – for the simple reason that this quantity has in no sense any relation to our everyday life. Everybody knows Albert Einstein’s winged word, who called it a “spooky action at a distance”. The strangeness of the phenomenon entanglement is captured in the violation of a very fundamental relation: This is \textit{Bell’s inequality} [135] that sets a limit for the size of correlations between independent measurements at separated locations. The underlying assumptions are very intriguing, and both the inequality and its violation by quantum mechanics can be easily reconstructed, see e.g. [6]. However, to really \textit{understand} what is going on when entanglement enters the stage and exceeds the limits of Bell’s inequality is more or less impossible.

However, such questions are much too fundamental to be discussed here. Instead, we want to study the occurrence of entanglement in dissipative two-spin systems and approach this phenomenon from two sides: First, we investigate its creation starting from a separable state, before we ask for its evolution out of a maximally entangled preparation. Both cases yield deep insight into the physics of interacting spins. The sign problem forces us to concentrate on the short-time scale.
Figure 6.6: Two uncoupled spins at $T = 0$ and for non-shifted bath preparation become entangled by interaction with the bath, if the spectral exponent is deep in the sub-Ohmic range: We see entanglement for $s = 0.25$ and $s = 0.5$, but not for $s = 0.75$ and $s = 1$. In accordance, directly generated entanglement ($J = 0.5\Delta$) is better conserved for $s = 0.5$ compared to $s = 1$.

6.4.1 Creation of entanglement

First of all, one has to get clear about the fact that there are two possibilities to “produce” entanglement in a bipartite system: First, it can result out of a direct interplay between the entities, i.e. $J \neq 0$. Indeed, we find for two free and unbiased qubits with $\Delta_A = \Delta_B$ that the concurrence behaves as

$$C(\rho(t)) = |\sin(2Jt)|,$$  \quad (6.7)

obviously even reaching states with maximal entanglement at $t = \pi(n + 1/2)/2J$ (see also the black curve in Figs. 6.6 and 6.7). The second way is more interesting and usually not so easy to understand. This is the possibility of bath-induced entanglement. Its appearance is ideally studied for non-interacting spins, for obvious reasons. In the general case, both sources can be present and we get another difficulty, if we want to distinguish between them.

Preliminarily, we focus on the latter. As the parameter space is very large, we restrict to the initial spin state $|1\rangle$ and study the dependence on the bath type by changing the spectral exponent $s$ and by switching off everything that could disturb the process of interest, i.e. $T = 0$, $\mu = 0$, and $J = 0$. Determining error bars is not possible, because the concurrence is a very intricate function of the observables. As the discussion ought to be rather qualitative, this does not matter for our purpose.

Let us take a look at Fig. 6.6. Comparing the curves for $s = 0.25$, $s = 0.5$, $s = 0.75$, and
s = 1, we see that entanglement starts to rise after a short period of time, but only in the deep sub-Ohmic regime, s = 0.25, and distinctly smaller for s = 0.5. In contrast, we see no entanglement for s = 0.75 and an Ohmic bath, s = 1. We also plot the concurrence for s = 0.5 and s = 1, but with J = 0.5. Entanglement is created at the very beginning, but the sub-Ohmic environment conserves it better than the Ohmic. Comparing this to the black line that shows the concurrence evolution for the bare system, we see that the behavior is similar for very short times.

These results justify a limitation to s = 0.25 for all the following investigations. As we know from the previous section that the initial bath state is good enough for surprises in this regime, we want to study, whether the coherence effects detected in Sec. 6.3 transfer to the entanglement dynamics. For this purpose, we take a look at the concurrence as a function of µ for both the uncoupled and the coupled case (J = 0 and J = 0.5Δ), respectively. Again, we have α = 0.05 and T = 0.

View Fig. 6.7 for the interesting results. The concurrence starts to increase after a short transient period, but only for µ = 0 and µ = 0.5. When the population P_{1} is pinned close to 1 (i.e. µ = 1, cf. Fig. 6.5), we see no entanglement at all. Switching on spin-spin coupling, it is still this bath preparation that is not able to pave the way for effective entanglement conservation. In contrast, µ = 0.5 seems to be the optimal value, henceforth.

How can this actually be understood? Resorting to prior arguments, we find that the all this is in complete agreement with the results from Sec. 6.3. Why? As the biasing terms dominate, the preparation with initially polarized environment (µ = 1) behaves like a non-
Fixing $s = 0.25$ and switching off direct coupling, $J = 0$, we see that temperature has the tendency to erase effects from the initial bath position. While the curves for varying $\mu$ differ drastically at $T = 0$, they approach each other for finite $T$, leading to the curiosity of zero entanglement at $T = 0$ and finite entanglement for $T = 2\Delta$ when $\mu = 1$. Increasing $\alpha$ slightly makes the concurrence rise earlier. The total entanglement on the plotted time scale decreases, if the coupling becomes even stronger.

This gives rise to another completely counter-intuitive effect that can be seen in Fig. 6.8. Up to now, we have worked at zero temperature in order to avoid destruction of entanglement by thermal fluctuations. Contrarily, the curves in Fig. 6.8 indicate, that there seems to be the possibility to, in a way, create entanglement thermally, at least for $\mu = 1$: We have $C \equiv 0$ for $T = 0$, but not for $T = 2\Delta$! Although being completely confusing at first sight, we can understand this behavior from our preceding arguments. Finite temperature suppresses non-classical paths and shrinks the relative weight of the bath preparation term in the IF. Therefore, the picture of a bare system which is subject to a bias does no longer apply. On the other hand, thermal fluctuations are not that large that they could destroy entanglement completely. Therefore, the concurrence becomes non-zero for increasing temperature, but vanishes at $T = 0$. This explanation is conserved by the observation that the finite-$T$ curves for different $\mu$ converge.

In addition, we see a curve for $\alpha = 0.2$. Compared to $\alpha = 0.05$, the concurrence starts to arise much earlier. As the bath coupling is the reason for creation of entanglement, larger $\alpha$ is indeed expected to cause the spins to entangle more. Increasing the coupling even more
6.4. ENTANGLEMENT AND DECOHERENCE-FREE SUBSPACES

has again the tendency to destroy entanglement, which is confirmed by the $\alpha = 0.4$ curve.

Now, how does entanglement actually arise? It is suitable to switch to the Bell state basis, Eqs. (1.59), for this discussion. Then, the system is prepared in the state $|1\rangle \equiv (|\Phi^+\rangle + |\Phi^-\rangle)/\sqrt{2}$. In the next section, we show that the population of $|\Psi^-\rangle$ is always zero, if it is orthogonal to the initial state. During the time evolution, the bare system and the bath push the population towards the state $|\Psi^+\rangle$. This is confirmed by the fact that $P_{x,23} > 0$ and $P_{x,23} \gg P_{x,ij}$ for all the cases, in which we see large entanglement.

All our results suggest that what we see are the phenomena of sudden birth and sudden death of entanglement [160], i.e. that entanglement is created or fully destroyed at a certain time instead of reaching a value asymptotically. In addition, we suppose that there exists a kind of effective frequency for entanglement creation, similar to Eq. (6.7), but in the absence of direct spin-spin coupling. Still, it seems rather unlikely that such systems show a steady-state entanglement, i.e. $C > 0$ for $t \to \infty$. However, the accessible time scales are much too short to make definite statements about this. Hence, we can switch to the problem of entanglement conservation for systems that evolve out of a maximally entangled state.

6.4.2 Dynamics of maximally entangled states

Now, we do it the other way round: We prepare the system in a Bell state, cf. Eq. (1.59) and observe, how the concurrence evolves. The goal is not to distinguish between different bath parameters or spin-spin couplings, but to understand the dependence on the particular Bell state, no matter how the bath properties look like.

The result is shown in Fig. 6.9. Here, the environment is Ohmic with $\alpha = 0.5$ and $T = 0.5\Delta$, while both spins are unbiased, have identical tunnel coupling and interact via $J = 0.3\Delta$. We see that entanglement decreases very fast for the $|\Phi\rangle$ states. Contrarily, the other two states $|\Psi^\pm\rangle$ allow themselves plenty of time for reducing their entanglement. Actually, the state $|\Psi^-\rangle$ conserves it completely, except from small fluctuations, that are nothing but statistical noise from the MC sampling. The same state shows a small loss of concurrence, when the spins do not have identical $\Delta$’s.

These differences can be explained by a closer look on the way, how system and bath couple to each other. As the states $|\Psi^\pm\rangle$ are eigenstates of $\sigma^A_z + \sigma^B_z$ with eigenvalue 0, they do not feel the influence of the environment and therefore make no move to show decoherence: They span a DFS, which is not the case for $|\Phi^\pm\rangle$.

But how can one explain the soft decay for $|\Psi^+\rangle$ on the one hand and the full refusal to lose entanglement for $|\Psi^-\rangle$ on the other hand? This is easily explained by calculating the effect of the bare Hamiltonian on these states. Whereas $|\Psi^-\rangle$ is an eigenstate of $H_{2TLS}$ (as long as $\epsilon_A = \epsilon_B$ and $\Delta_A = \Delta_B$), this is different for $|\Psi^+\rangle$. Therefore, the latter is mixed with the states $|\Phi^\pm\rangle$ that feel the bath, but the former stays unperturbed for all times. Further,

\[ Notice that the density matrix for a pure $|\Psi^+\rangle$ state reads $\rho_{22} = \rho_{33} = \rho_{23} = \rho_{32} = 1/2$ and zero for all the other matrix elements.\]
assigning different values to $\Delta_A$ and $\Delta_B$ mixes $|\Psi^-\rangle$ with the other states and makes the system feel dissipation.

For this initial preparation, not only the concurrence, but indeed all observables show no dynamics at all. A series of simulations has proven that this is the case for all types of surroundings and parameters: Ohmic, sub-Ohmic, zero and finite temperatures, standard and shifted bath preparation, and even arbitrary spin-spin coupling strengths! Note that this is one out of few exact proofs of principle for a correct implementation. Its relevance therefore exceeds the pure physical component: As long as this behavior is not visible in the dynamics, there must be something wrong in the code.

The presence of decoherence-free states influences the way, how the system equilibrates [154]. In Fig. 6.10, we show the population dynamics for two spins that are prepared in the factorizing state with $P^A_x(0) = P^B_x(0) = 1$, which is orthogonal to $|\Psi^-\rangle$. We choose $J = 0.5\Delta$ and an Ohmic bath with $\alpha = 0.05$. In order to speed up equilibration and to shrink the error bars, temperature is as large as $20\Delta$.

Clearly, the states $|1\rangle$ and $|4\rangle$ approach to $1/3$, whereas $P_2$ and $P_3$ rush down towards $1/6$. As all their energies are the same, these states should be equally populated in thermal equilibrium. The fact that this is not the case is an indirect hint to a DFS. Starting in a state that is orthogonal to $|\Psi^-\rangle$, neither the free system, nor the bath are able to transfer any population to $|\Psi^-\rangle$. Therefore, this state remains unoccupied and we end up with
Figure 6.10: The population dynamics gives an indirect hint at the existence of a DFS. The spins are prepared in a factorizing state with $P^A_x(0) = P^B_x(0) = 1$ and couple to an Ohmic bath with $\alpha = 0.05$ and $T = 20\Delta$. Further, we have $J = 0.5\Delta$. The observation that two states converge to 1/3, while the others approach 1/6 in equilibrium, is a consequence of the state $|\Psi^-\rangle$ that neither couples to the bath, nor mixes with the other states in the evolution of the bare system.

$P_1 = P_4 = P_{|\Psi^+\rangle} = 1/3$ in equilibrium. As $|\Psi^+\rangle$ is composed of $|2\rangle$ and $|3\rangle$, their populations converge to 1/6.

Obviously, the occurrence of these DFSs is connected to a very special choice of coupling that might be difficult to be perfectly realized in experiment. On the other hand, all the spectral bath properties are irrelevant, if a system has been found that couples to the environment via the operator $\sigma^A_z + \sigma^B_z$. At least in theory, we can conserve coherences and entanglement over a wide range of bath spectra and even for arbitrary temperature.

### 6.5 Conclusions and outlook

Again, it is the deep sub-Ohmic range, where we get the most exciting results. Next to fast coherent oscillations that arise from an interplay of the reservoir’s initial state and the counter term, we find bath-induced entanglement for small spectral exponents. The deep sub-Ohmic environments seem to be most suitable to observe quantum effects.

Now, what about the outlook? Strangely, scientific problems have the ability to reproduce themselves in a very efficient way: With every solved problem, there arises at least one further that awaits a solution. This is found to be perfectly true for this work: After studying the SBM in great detail, we add a second spin to the model and are suddenly confronted with
a plenty of new problems.

For this reason, a couple of issues could not be treated within this work. Not only the scan of parameter space is incomplete, but also a look at observables like the von Neumann entropy might give new insights. One could also study the dependence on the type of spin-spin interaction or implement an approach that adopts the ideas of CH-PIMC. Further, systems of three or even more spins might be interesting, e.g. with regard to entanglement of tripartite systems [130].

This list could be continued even more. As we deal with topics that are of fundamental importance for current basic research, the MC can surely serve well in the next years. A fundamental question will be how to speed up the simulations, e.g. by parallelization.
Summary

In this work, we study the dynamics of spin-1/2 systems in contact with dissipative bosonic reservoirs [1, 2, 20]. Our investigations are motivated by recent progress in designing and controlling atomic and solid state structures of growing complexity [32, 33, 34, 35, 36]. The interplay between the bare system and the environment is of substantial importance for understanding the dynamics of such devices. Spin systems that are embedded in bosonic reservoirs are described by the famous spin-boson model (SBM) and have been studied for several decades [21, 20]. Recent work has shown that two-level systems in contact with sub-Ohmic reservoirs are of fundamental interest in view of both theoretical considerations [97, 99] and their experimental relevance [87, 88, 89]. This is why we focus on the dynamics of systems that couple to a sub-Ohmic environment [65, 67]. Additionally, impressive experimental progress in embedding quantum dots into photonic crystals [125, 132, 133] encouraged us to investigate the dynamics of two-level systems coupled to surroundings with spectral gaps.

During the first part of the work, we study the dynamics of the SBM with different spectral densities. Later on, we extend the SBM towards a model of two spins that interact with the same environment and therefore couple indirectly (interacting spins model, ISM). In addition, the spins are allowed to interact also directly. We are interested in the dynamics of populations and coherences for non-equilibrium initial states, where the system and bath densities factorize. The former can be in an arbitrary initial state, while the latter is in thermodynamical equilibrium with respect to the bath and the interaction Hamiltonian for a fixed spin position $\mu$. Typically, the bath is equilibrated with respect to the initial spin position ($\mu = 1$) or the position between the spin eigenstates ($\mu = 0$).

The density matrix evolves in time according to the Liouville-von Neumann equation. As the surrounding reservoir is modeled as a collection of harmonic oscillators with quasi-continuous spectrum, these degrees of freedom can be integrated exactly via path integrals (PIs) [22, 23]. We end up with an influence functional (IF) in the action containing all effects of the surrounding on the system. The corresponding integral kernels are solely determined by temperature and the spectral density of the environment. This way, the reduced density matrix, which only captures the information of the system of interest, is given by a twofold PI over forward and backward path, respectively.

The double PI is discretized by dividing the system time $t$ into $q$ intervals of equal size. One part of the IF suppresses the large majority of spin paths exponentially. However, both the
action of the free system and the IF have imaginary parts stemming from the unitary time evolution. This way, we sample numbers that spread quite irregularly in the complex plane, leading to extreme interference of single path contributions. As the signal-to-noise ratio decreases exponentially with the system time $t$, this limits the times which are reachable by our simulations. In order to shrink this problem, one performs the sum over half of the coordinates exactly with the cost of a matrix product, thereby remaining with a $q + 1$-fold sum over the other half of the variables [54]. Now, a Metropolis sampling is implemented, that reduces the number of contributing paths enormously [43, 44]. In addition, we present a way to measure both diagonal and off-diagonal observables at all intermediate time steps out of one single simulation.

The dynamics of the reduced density matrix is studied for different non-Ohmic spectra. In general, the spectral density behaves as $\alpha\omega^s\exp(-\omega/\omega_c)$ with dimensionless coupling parameter $\alpha$, spectral exponent $s$, and cut-off frequency $\omega_c$. Ohmic baths are defined by $s = 1$, whereas sub-Ohmic reservoirs with $0 < s < 1$ are connected to very long-ranged bath-mediated interactions.

Nevertheless, we focus on Ohmic reservoirs in the beginning and use them as a test-bed for an approximative method called Chain Path Integral Monte Carlo (CH-PIMC) [66]. The idea behind is to propagate the reduced density up to a time $t_s$, that can easily be reached with a standard Monte Carlo (MC) simulation, and to use the measured values at $t_s$ as initial density for another MC run. Doing this again and again and sticking all the results together, we arrive at a total time $nt_s$. Although the bath memory is cut at every matching point, we can partially recover the reservoir’s state for the subsequent segments by adjusting $\mu$. A modified approach tries to restrict the continuation to the populations, thereby explicitly allowing for jumps in the coherences. These jumps are used as fit parameters, where a simple scheme determines the values for perfect matching.

For Ohmic baths, the CH-PIMC works at all coupling strengths as long as $T \gtrsim \Delta$ (where $\Delta$ is the TLS tunnel matrix element). Within the modified approach, this can be extended to $T \gtrsim 0.5\Delta$, but only when the coupling to the bath is so large that the population dynamics shows a monotone relaxation. In addition, a discussion of coherence and entropy dynamics brings insight into the reliability of the analytic non-interacting blip approximation (NIBA) and confirms a maximum of system-bath entanglement for $0.5 < \alpha < 1$ in the scaling limit $\omega_c \gg \Delta$ at $T = 0$.

For sub-Ohmic baths, we find that the modified CH-PIMC works in the regime of incoherent dynamics as long as $T \gtrsim 0.5\Delta$ and $s \geq 0.5$. This is sufficient for a study of the incoherent decay dynamics over a broad range of temperatures and system-bath couplings at $s = 0.5$. Extracted rates decrease exponentially with $\alpha$ and agree with analytical results from the non-interacting blip approximation (NIBA). In addition, we study the $P_z$ dynamics and find signatures of the $T = 0$ phase transition to a localized phase in the time evolution of the von Neumann entropy.

As we do not underly the restrictions that set the limits for other approaches, our PIMC scheme is able to answer the hitherto unresolved question about the transition from coher-
ent underdamped dynamics to overdamped decay in the deep sub-Ohmic range at $T = 0$ [112, 114]. For spectral exponents $s \geq 0.5$, our findings agree with other approaches that observe a transition to overdamped relaxation, when the system-bath coupling increases. In contrast, the results for $s < 0.5$ run against our intuitive understanding of dissipative quantum systems: For small temperatures, oscillatory structures are visible at very large $\alpha$. In fact, we do not get rid of coherent oscillations for all spectral exponents $s < 0.5$ at $T = 0$ and arbitrary strong system-bath coupling! These coherences persist not although the bath is present, but rather because of the bath. We can clearly identify the slow modes as being responsible herefore, as their initial setting causes a bias that becomes quasi-static for $s \to 0$ and dominates all other energy scales. This is in coincidence with analytical results that we extract out of the NIBA. Studying the dependence of oscillatory patterns on several distortions, we observe a drastic change for very soft IR cut-offs, but not for modifications of the UV cut-off. In addition, the system becomes rather inert against thermal noise, if $s$ approaches zero.

Next, we study the effects of gaps in an Ohmic spectrum onto the population dynamics. This is modeled by simply setting the spectral density in the range $[\omega_0 - b/2; \omega_0 + b/2]$ to zero, where $\omega_0 = \Delta$ is the center of the gap and $b$ its broadness. Reducing the modes to their ability either to cause a time-dependent bias ($\omega < \Delta$) or to renormalize the tunnel matrix element ($\omega > \Delta$) works only at small system-reservoir couplings, broad gaps, and close to $T = 0$. When we study the dynamics of an Ohmic bath in the overdamped regime and compare it to a gapped spectrum with identical $\alpha$ and $T$ and stepwise increasing gap width, one clearly observes oscillations. However, a definite transition border between coherent and incoherent dynamics cannot be determined, because the reservoir stamps the frequency of its gap onto the decay dynamics. Closer inspections suggest that not a single frequency $\omega_0$ is imprinted, but rather a beat with frequencies $\omega_0 \pm b/2$.

Finally, a variety of results is found for the ISM. First of all, we study the two spin system in contact with an Ohmic reservoir from different sides. We find that the dependence on the spin-spin coupling $J$ — especially on its sign — is more complicated than for a bare system and can be understood from a comparison of interaction energies for tunneling $\Delta$ and coupling $J$, respectively. For $J = 0$, bath-induced interaction between the spins causes significant changes in both population and coherence dynamics, compared to the SBM. Another question that imposes is, how the fast bath-induced oscillations that occur for the SBM at $s < 0.5$ transfer to the ISM. We find that the bias caused by the initial bath position gets an opponent that stems from the counter term. The latter is necessary in order to avoid a potential renormalization for the ISM, whereas it is just an irrelevant constant for the SBM. If the bath modes are equilibrated with respect to the position $\mu = 0.5$, both contributions cancel. However, for $\mu \neq 0.5$, always one of them dominates and causes fast oscillations, corresponding to a quasi-static bias of size $(1 - 2\mu)\Lambda_{cl}$ with reorganization energy $\Lambda_{cl} \propto \alpha/s$.

When investigating the concurrence dynamics as a measure of entanglement, we see that a sub-Ohmic bath is better for both creation and conservation of entanglement. Here, the sensitive dependence on the bath displacement is again present. As a system with $\mu = 1$
SUMMARY

corresponds to a first approximation to a non-dissipative arrangement of uncoupled qubits, which are subject to a large bias, there is no bath-induced entanglement at all. By contrast, entanglement arises for $\mu = 0.5$ and $\mu = 0$. Surprisingly, finite temperatures go hand in hand with entanglement for all values of $\mu$. This is because thermal noise suppresses the influence of the initial preparation. Further investigations study entanglement that is induced by spin-spin interaction and its dependence on the system-bath coupling. In addition, we are able to prove the existence of a decoherence-free subspace, meaning that parts of the system Hilbert space are completely decoupled from the bath. Summarizing, the combination of directly interacting spins, that couple indirectly due to the presence of a reservoir, shows physical features that go beyond the effects we see for the SBM.

Several open questions are formulated within the work, ranging from the potential of parallelizing the code towards an extension to systems with more than two spins. Of course, also experimental progress in controlling solid state systems on the nanoscale could help to check our results and to modify theoretical models, thereby leading to synergy effects. In summary, there are still a lot of problems that await a solution and, concerning those that are related to the MC numerics, I am convinced that the method is good enough to tackle most of them. New ideas may ensure that the progress of this work is not limited to these pages, but also serves as a basis for further developments, so that the PIMC will continue helping us to get a deeper understanding of the dynamics of dissipative spin systems.
Appendix A

Path Integral for the Harmonic Oscillator

In this appendix, we want to give a short instruction, how to calculate the path integral (PI) for a driven harmonic oscillator [22],

\[
\int_{x(0)=x_1}^{x(t)=x_f} \mathcal{D}x \exp \left[ i \int_0^t dt' \left( \frac{m}{2} \dot{x}^2(t') - \frac{m\omega^2}{2} x^2(t') + \frac{c}{2} \sigma(t')x(t') \right) \right]. \tag{A.1}
\]

The exponent is nothing but \(iS[x(t')]\) with the action functional \(S\) for a harmonic system that is subject to a driving force \(c\sigma(t')/2\). Notice that \(t\) is a fixed time that is not related to \(\omega\) in any way. The first step is to separate the amount of paths to be summed over into the classical trajectory \(x_{cl}(t')\) fulfilling the boundary conditions \(x(0) = x_1, \ x(t) = x_f\), and the deviations \(\xi(t')\) that vanish at \(t' = 0\) and \(t' = t\):

\[
x(t') = x_{cl}(t') + \xi(t'). \tag{A.2}
\]

As \(x_{cl}(t')\) minimizes the action \(S\), there appear no contributions that are linear in \(\xi\). This is why the PI factorizes,

\[
\int_{x(0)=x_1}^{x(t)=x_f} \mathcal{D}x \exp \left[ iS[x(t')] \right] = A \exp \left[ iS[x_{cl}(t')] \right]. \tag{A.3}
\]

We first want to care about the classical part. The equation of motion reads

\[
m\ddot{x}_{cl}(t') + m\omega^2 x_{cl}(t') = \frac{c}{2} \sigma(t'). \tag{A.4}
\]

Using the Green’s function of the harmonic oscillator, we get the full solution

\[
x_{cl}(t') = A \cos(\omega t') + B \sin(\omega t') + \frac{c}{2m\omega} \int_0^{t'} dt'' \sin[\omega(t' - t'')] \sigma(t'')
\]

\[
= x_1 \frac{\sin[\omega(t-t')]}{\sin(\omega t)} + x_f \frac{\sin(\omega t')}{\sin(\omega t)} - \frac{c}{2m\omega \sin(\omega t)} \int_0^{t'} dt'' \sin[\omega(t-t'')] \sigma(t'')
\]

\[
+ \frac{c}{2m\omega} \int_0^{t'} dt'' \sin[\omega(t'-t'')] \sigma(t''), \tag{A.5}
\]
where we inserted the boundary conditions in the second step. Rearranging the classical action by performing an integration by parts and exploiting the equation of motion, we get

$$S_{cl} = S[x_{cl}(t')] = \int_{0}^{t} dt' \left[ \frac{m}{2} \dot{x}_{cl}^2(t') + \frac{m\omega^2}{2} x_{cl}^2(t') + \frac{c}{2} \sigma(t') x_{cl}(t') \right]$$

$$= \frac{m}{2} [\dot{x}_{cl}(t)x_{cl}(t) - \dot{x}_{cl}(0)x_{cl}(0)] + \frac{c}{4} \int_{0}^{t} dt' \sigma(t') x_{cl}(t').$$  \hspace{1cm} (A.6)

Inserting $x_{cl}(t')$ yields after some steps

$$S_{cl} = -\frac{m \omega x_{1} x_{f}}{\sin(\omega t)} + \frac{m \omega}{2} \cot(\omega t) (x_{1}^{2} + x_{f}^{2}) + \frac{c}{2} \int_{0}^{t} dt' \sigma(t') \frac{x_{f} \sin(\omega t') + x_{1} \sin[\omega(t-t')]}{\sin(\omega t)}$$

$$- \frac{c^{2}}{4m\omega} \int_{0}^{t} dt' \sigma(t') \int_{0}^{t'} dt'' \sigma(t'') \frac{\sin[\omega(t-t')]}{\sin(\omega t)} \frac{\sin(\omega t'')}{\sin(\omega t)}. \hspace{1cm} (A.7)$$

Now we can turn to the factor arising from the deviations $\xi(t')$. As we already know that there is no linear contribution, we only must calculate

$$A_{\xi} = \int_{\xi(0)=0}^{\xi(t)=0} D\xi \exp \left[ i \int_{0}^{t} dt' \frac{m}{2} \left( \dot{\xi}^2(t') - \omega^2 \xi^2(t') \right) \right]. \hspace{1cm} (A.8)$$

The main ingredient is the idea how to scan all the paths that connect the points $\xi(0) = 0$ and $\xi(t) = 0$. It is well-known that every function living on the interval $[0; t]$ can be described by an infinite Fourier series. Due to the boundary conditions, we only have to take into account the sine terms, so that our ansatz reads

$$\xi(t') = \sum_{n=1}^{\infty} \xi_{n} \sin \left( \frac{n\pi t'}{t} \right). \hspace{1cm} (A.9)$$

It is obvious that the PI is just the integral over all Fourier coefficients $\xi_{n}$, modified with normalization factors $N_{n}$, that correspond to the Jacobian of the underlying coordinate transformation. We insert Eq. (A.9) into the PI expression (A.8) and use the orthogonality of sine and cosine functions,

$$A_{\xi} = \prod_{n=1}^{\infty} \int d\xi_{n} N_{n} \exp \left\{ i \frac{m}{2} \sum_{n=1}^{\infty} \xi_{n}^{2} \int_{0}^{t} dt' \left[ \frac{n^{2}\pi^{2}}{t^{2}} \cos^{2} \left( \frac{n\pi t'}{t} \right) - \omega^2 \sin^{2} \left( \frac{n\pi t'}{t} \right) \right] \right\}$$

$$= \prod_{n=1}^{\infty} \int d\xi_{n} N_{n} \exp \left[ i \frac{m}{4t} \sum_{n=1}^{\infty} \xi_{n}^{2} \left( n^{2}\pi^{2} - \omega^{2}t^{2} \right) \right]$$

$$= \prod_{n=1}^{\infty} \int d\xi_{n} N_{n} \exp \left[ i \frac{m}{4t} \xi_{n}^{2} n^{2}\pi^{2} \left( 1 - \frac{\omega^{2}t^{2}}{n^{2}\pi^{2}} \right) \right]. \hspace{1cm} (A.10)$$

Performing the Gaussian integrals, we get

$$A_{\xi} = \left( \prod_{n=1}^{\infty} N_{n} \sqrt{\frac{4t}{im\pi n^{2}}} \right) \left[ \prod_{n=1}^{\infty} \left( 1 - \frac{\omega^{2}t^{2}}{n^{2}\pi^{2}} \right) \right]^{-\frac{1}{2}}. \hspace{1cm} (A.11)$$
In the limit $\omega \to 0$, the oscillator becomes a free particle. Its PI expression is well-known and reads
\[
\int_{x(0)=x_1}^{x(t)=x_f} \mathcal{D}x \: e^{iS_{\text{free}}[x(t)']} = \sqrt{\frac{m}{2\pi i t}} \exp \left[ i \frac{m}{2t} (x_f - x_1)^2 \right]. \tag{A.12}
\]

One can easily convince that the exponential part in Eq. (A.12) stems from the contribution of $x_{\text{cl}}(t')$ and so we can identify $\sqrt{m/2\pi i t}$ with the contribution from $\int \mathcal{D}\xi$. A comparison between (A.11) and (A.12) for $\omega \to 0$ yields
\[
\prod_{n=1}^{\infty} N_n \sqrt{\frac{4t}{i m n^2 \pi^2}} = \sqrt{\frac{m}{2\pi i t}}. \tag{A.13}
\]

With the formula $\prod_{n=1}^{\infty} (1 - \omega^2 t^2/n^2 \pi^2) = \sin(\omega t)/\omega t$, we finally arrive at
\[
A_\xi = \sqrt{\frac{m\omega}{2\pi i \sin(\omega t)}}. \tag{A.14}
\]

The full expression for the PI of the harmonic oscillator is given by $A_\xi e^{iS_{\text{cl}}}$ with the classical action functional in (A.7).
Appendix B

Derivation and Discretization of the Influence Functional

In this chapter, we sketch the most important steps in the derivation of the influence functional [22]. We derive the path integral (PI) expression by inserting complete sets in the time evolution and taking the continuum limit. Later on, we re-discretize the resulting formula in order to make it treatable for the numerics.

For simplicity, the following calculation is restricted to one single environmental mode with position \( x \), momentum \( p \), and parameters \( m, \omega, \) and \( c \). It is easy to see that the effect of \( N \) modes is just the product over the single mode contributions; so the generalization to a broadband reservoir is simple.

First of all, we decompose the time evolution into \( q \) equidistant steps of length \( \tau = t/q \) and insert \( 2q + 2 \) complete sets,

\[
\langle A(t) \rangle = \mathcal{Z}^{-1} \text{Tr} \left[ \rho_0 e^{-\beta H_B} 1_{1'} e^{iH\tau} 1_{2'} \cdots 1_q e^{iH\tau} 1_{(q+1)'} A 1_{q+1} e^{-iH\tau} 1_q \cdots 1_2 e^{-iH\tau} 1_1 \right] \quad (B.1)
\]

with

\[
1_{i'} = \int dx_i^{(\prime)} |x_i^{(\prime)}\rangle \langle x_i^{(\prime)}| \sum_{\sigma_i^{(\prime)} = \pm 1} |\sigma_i^{(\prime)}\rangle \langle \sigma_i^{(\prime)}| \quad \text{for } 1 \leq i^{(\prime)} \leq q + 1. \quad (B.2)
\]

Using an asymmetric Trotter-Suzuki expansion, \( e^{-iH_{SB}\tau} = e^{-i(H_B+H_I)\tau/2} e^{-iH_{TLS}\tau} e^{-i(H_B+H_I)\tau/2} \), with a corresponding discretization error of order \( \tau^3 \), the matrix element for a small evolution in time reads

\[
\langle x_i,\sigma_i|e^{-iH\tau}|x_{i+1},\sigma_{i+1}\rangle = \sqrt{\frac{m}{2\pi i\tau}} K(\sigma_{i+1},\sigma_i) \\
\times \exp \left\{ i\frac{m\tau}{2} \left[ \left( \frac{x_{i+1} - x_i}{\tau} \right)^2 - \omega^2 \frac{x_i^2 + x_{i+1}^2}{2} \right] - i\frac{c\tau}{4} (\sigma_i x_i + \sigma_{i+1} x_{i+1}) \right\} \quad (B.3)
\]

with the bare TLS propagator \( K(\sigma_{i+1},\sigma_i) = \langle \sigma_i|e^{-iH_{TLS}\tau}|\sigma_{i+1}\rangle \). We made use of the \( \sigma_z \)
eigenvalue equation and perform now the trace over system and bath, \( \text{Tr} = \text{Tr}_S \text{Tr}_B, \)

\[
\langle A(t) \rangle = Z^{-1} \sum_{\sigma_1, \ldots, \sigma_-} K^*(\sigma'_1, \sigma'_2, \ldots)K^*(\sigma'_{q+1}) \langle A|\sigma_{q+1}\rangle K(\sigma_{q+1}, \sigma_q) \ldots K(\sigma_2, \sigma_1)
\]

\[
\times \text{Tr}_B \left[ \int dx_2 \ldots dx_{q+1} d\sigma' \int x_{q+1} e^{-\beta H_B} \langle x_{q+1} \rangle \langle x'_{q+1} | e^{i\tau H_s} | x'_{q+1} \rangle \ldots \langle x'_{q+1} | e^{-i\tau H_{s+1}} | x'_{q+1} \rangle \right] 
\]

\[
\times \delta(x_{q+1} - x'_{q+1}) \langle x_{q+1} | e^{-i\tau H_{s+1}} | x_{q+1} \rangle \ldots \langle x_3 | e^{-i\tau H_2} | x_2 \rangle \langle x_2 | e^{-i\tau H_1} | x_1 \rangle 
\]

(B.4)

where \( H_{s+1} = H_B + c(\sigma_i x_i + \sigma_{i+1} x_{i+1})/4. \) We insert (B.3), denote the trace over the bath degree of freedom with \( x_1 \) and name \( x_{q+1} = x'_{q+1} = x_f. \) The expert eye immediately recognizes a double PI in the limit \( \tau \to 0, q \to \infty, q\tau = \text{const}.: \)

\[
\text{Tr}_B[\ldots] = \int dx_1 dx'_1 dx f_1 x_1 e^{-\beta H_B} \langle x'_{q+1} \rangle \int dx \int x'_{q+1} D x' \exp \left\{ i S_{cl}[x(t)] - i S_{cl}[x'(t')] \right\} 
\]

\[
= \int dx_1 dx'_1 dx f_1 x_1 e^{-\beta H_B} \langle x'_{q+1} \rangle 
\]

\[
\times \int_{x(0) = x_1}^{x(t) = x_f} D x \exp \left\{ i \int_0^t dt' \left( \frac{m}{2} \dot{x}^2(t') - \frac{m \omega^2}{2} x^2(t') - \frac{c}{2} \sigma(t') x(t') \right) \right\} 
\]

\[
\times \int_{x'(0) = x'_1}^{x'(t) = x_f} D x' \exp \left\{ -i \int_0^t dt' \left( \frac{m}{2} \dot{x'}^2(t') - \frac{m \omega^2}{2} x'^2(t') - \frac{c}{2} \sigma'(t') x'(t') \right) \right\} \] \quad (B.5)

This is the PI for a driven harmonic oscillator, fulfilling the classical equation of motion \( m \ddot{x}_d(t') + m \omega^2 x_d(t') = c \sigma(t')/2. \) The calculation of the PI is shown in App. A. Inserting the heat kernel

\[
\langle x_1 | e^{-\beta H_B} | x'_1 \rangle = \frac{m \omega}{2 \pi \sinh(\omega \beta)} \exp \left\{ -\frac{m \omega}{2 \sinh(\omega \beta)} [(x_1^2 + x_1'^2) \cosh(\omega \beta) - 2 x_1 x'_1] \right\} \] \quad (B.6)

and the results of the double PI into (B.5), we get

\[
\text{Tr}_B[\ldots] = \sqrt{\frac{m \omega}{2 \pi i \sin(\omega t)}} \sqrt{\frac{m \omega}{2 \pi (-i) \sin(\omega t)}} \sqrt{\frac{m \omega}{2 \pi \sinh(\omega \beta)}} \times \exp \left\{ -i \frac{c^2}{4 m \omega} \int_0^t dt' \int_0^{t'} dt'' \frac{\sin[\omega (t - t')] \sin(\omega t'')}{\sin(\omega t)} [\sigma(t') \sigma(t'') - \sigma'(t') \sigma''(t'')] \right\} 
\]

\[
\times \int dx_1 dx'_1 \exp \left\{ -i \frac{c}{2} \int_0^t dt' \frac{\sin[\omega (t - t')]}{\sin(\omega t)} [x_1 \sigma(t') - x'_1 \sigma'(t')] \right\} 
\]

\[
+ i \frac{m \omega}{2} \cot(\omega t) (x_1^2 - x'_1^2) - \frac{m \omega}{2 \sinh(\omega \beta)} [(x_1^2 + x'_1^2) \cosh(\omega \beta) - 2 x_1 x'_1] \right\} \right\} \right. 
\]

\[
\times \int dx f \exp \left\{ i x f \left[ -\frac{m \omega}{\sin(\omega t)} (x_1 - x'_1) - \frac{c}{2} \int_0^t dt' \frac{\sin(\omega t')}{\sin(\omega t)} [\sigma(t') - \sigma'(t')] \right] \right\} \] \quad (B.7)

The last integral gives a delta distribution so that we can drop the \( x_1 \) integral and remain with a Gaussian integral over \( x'_1. \) To combine the integrals with different borders, the relation
\[
\int_0^t dt' \int_0^t dt'' f(t',t'') = \int_0^t dt' \int_0^t dt''[f(t',t'') + f(t'',t')]
\]
is often useful. We introduce sum- and difference coordinates
\[
\zeta(t) := \frac{\sigma(t) - \sigma'(t)}{2}, \quad \eta(t) := \frac{\sigma(t) + \sigma'(t)}{2}, \tag{B.8}
\]
\(\zeta, \eta \in \{-1,0,1\}\), and arrive at
\[
\text{Tr}_B[\ldots] = \frac{1}{2 \sinh \left( \frac{\omega \beta}{2} \right)} \exp \left[ -i \kappa \int_0^t dt' \int_0^t dt'' \frac{\sin[\omega(t-t')] \sin(\omega t'')}{\sin(\omega t)} \left[ \zeta(t') \eta(t'') + \eta(t') \zeta(t'') \right] + i \kappa \int_0^t dt' \int_0^t dt'' \frac{\sin[\omega(t-t')] \sin(\omega t'')}{\sin(\omega t)} \left[ \zeta(t) \eta(t') + \eta(t) \zeta(t') \right] - \kappa \coth \left( \frac{\omega \beta}{2} \right) \int_0^t dt' \int_0^t dt'' \cos(\omega t') \cos(\omega t'') \zeta(t') \zeta(t'') - i \kappa \int_0^t dt' \int_0^t dt'' \cos(\omega t') \sin(\omega t'') \zeta(t') \zeta(t'') - \frac{\kappa}{2} \tanh \left( \frac{\omega \beta}{2} \right) \int_0^t dt' \int_0^t dt'' \sin(\omega t') \sin(\omega t'') \zeta(t') \zeta(t'') \right] \tag{B.9}
\]
with \(\kappa = c^2/2m\omega\). Here, we made use of \([\cosh(\omega \beta) - 1]/\sinh(\omega \beta) = \tanh(\omega \beta/2)\) and \(\sinh(\omega \beta) \tanh(\omega \beta/2) = 2 \sinh^2(\omega \beta/2)\). By collecting the terms quadratic in \(\zeta\) and independent of \(\beta\), the ones quadratic in \(\zeta\) and \(\beta\)-dependent, and the ones containing \(\zeta\) and \(\eta\), we see that the first vanish and the second and third can be brought into the form
\[
\text{Tr}_B[\ldots] = -\frac{c^2}{2m\omega} \int_0^t dt' \int_0^t dt'' \zeta(t') \left[ \coth \left( \frac{\omega \beta}{2} \right) \cos(\omega t') \zeta(t'') - i \sin(\omega t) \eta(t'') \right], \tag{B.10}
\]
using the identity \(2 \coth(\omega \beta) = \coth(\omega \beta/2) + \tanh(\omega \beta/2)\). The prefactor in (B.9) cancels with the sum of states. We take the product over all environmental modes and finally get the compact expression
\[
e^{-\Phi^{SB}[\zeta,\eta]} = \exp \left\{ - \int_0^t dt' \int_0^t dt'' \zeta(t') \left[ L'(t' - t'') \zeta(t'') + i L''(t' - t'') \eta(t'') \right] \right\}, \tag{B.11}
\]
where \(L'(t)\) and \(L''(t)\) are the real and the imaginary parts of the bath auto-correlation function (1.15) with the spectral density
\[
I(\omega) := \pi \sum_\alpha \frac{\epsilon^2_\alpha}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha). \tag{B.12}
\]
For the numerical implementation, it is important to re-discretize the whole stuff [40]. Therefore, we write the paths as
\[
\eta(t) = \eta_1 \Theta \left( \frac{\tau}{2} - t \right) + \sum_{j=2}^q \eta_j \Theta \left[ \left( j - \frac{1}{2} \right) \tau - t \right] \Theta \left[ t - \left( j - \frac{3}{2} \right) \tau \right] + \eta_{q+1} \Theta \left[ t - \left( q - \frac{1}{2} \right) \tau \right]
\]
\[
\zeta(t) = \zeta_1 \Theta \left( \frac{\tau}{2} - t \right) + \sum_{j=2}^q \zeta_j \Theta \left[ \left( j - \frac{1}{2} \right) \tau - t \right] \Theta \left[ t - \left( j - \frac{3}{2} \right) \tau \right]. \tag{B.13}
\]
and insert them into Eq. (B.11), taking also into account the part that arises from the initial bath preparation, see Eq. (1.37). Calculating the integrals is a simple exercise. We make use of $L(t) = ˙{\dot{Q}}(t)$, $Q(0) = 0$, $\text{Re}[\dot{Q}(0)] = 0$, $\zeta_{q+1} = 0$, and $\zeta_{i\eta_{i}} = 0$. The result is

$$\Phi^{SB} = \sum_{j=2}^{q} \zeta_j \sum_{k=2}^{j} \Lambda_{j-k} \zeta_k + \zeta_1 \sum_{j=1}^{q} \Lambda^{(1)}_j \zeta_j + i \sum_{j=2}^{q} \zeta_j \sum_{k=2}^{j-1} X_{j-k} \eta_k$$

$$+ \text{i} \eta_1 \sum_{j=2}^{q} X^{(1)}_j \zeta_j + i \mu \sum_{j=1}^{q} X^{(\mu)}_j \zeta_j$$  \hspace{1cm} (B.14)

where the appearing terms read

$$\Lambda_0 := \text{Re} \left[ Q(\tau) \right] ,$$
$$\Lambda_{1 \leq j \leq q-2} := \text{Re} \left[ Q[(j+1)\tau] - 2Q(j\tau) + Q[(j-1)\tau] \right] ,$$
$$X_{1 \leq j \leq q-2} := \text{Im} \left[ Q[(j+1)\tau] - 2Q(j\tau) + Q[(j-1)\tau] \right] ,$$

$$\Lambda^{(1)}_1 := \text{Re} \left[ Q(\tau/2) \right] ,$$
$$\Lambda^{(1)}_{2 \leq j \leq q} := \text{Re} \left[ Q[(j-1/2)\tau] - Q[(j-1)\tau] - Q[(j-3/2)\tau] + Q[(j-2)\tau] \right] ,$$
$$X^{(1)}_{2 \leq j \leq q} := \text{Im} \left[ Q[(j-1/2)\tau] - Q[(j-1)\tau] - Q[(j-3/2)\tau] + Q[(j-2)\tau] \right] ,$$

$$X^{(\mu)}_{1} := -\text{Im} \left[ Q(\tau/2) \right] ,$$
$$X^{(\mu)}_{2 \leq j \leq q} := -\text{Im} \left[ Q[(j-1/2)\tau] - Q[(j-3/2)\tau] \right] .$$  \hspace{1cm} (B.15)
Appendix C

Measurement Operators for the Spin Boson Model

The question to be answered in this chapter is, how can we determine all relevant spin-boson observables at all intermediate time steps \( t = (i - 1)\tau \) with \( 2 \leq i \leq q \) out of one single run? This is a rather technical matter, but of fundamental importance for the implementation (see also the supplemental material of Ref. [65]).

Let us first reduce the discussion to the case without dissipation, \( \alpha = 0 \). Then, it is easier to work with the spin coordinates \( \sigma \) and \( \sigma' \) instead of \( \zeta \) and \( \eta \). The expectation value of any observable that is diagonal in the basis of localized eigenstates, say \( P_{z,i} \equiv \langle \sigma_z ((i - 1)\tau) \rangle \), reads in discretized form

\[
P_{z,i} = \sum_{\sigma_1, \ldots, i} \rho_0(\sigma_1, \sigma'_i) \left[ \prod_{j=1}^{i-1} K^*(\sigma'_j, \sigma_{j+1}) K(\sigma_{j+1}, \sigma_j) \right] \delta_{\sigma_i, \sigma_i'}(\delta_{\sigma_i, 1} - \delta_{\sigma_i, -1}). \tag{C.1}
\]

We write \( \delta_{\sigma_i, \sigma_i'}^2 \) instead of \( \delta_{\sigma_i, \sigma_i'} \) for reasons that will become clear later. Eq. (C.1) is easily proved by decomposing \( \langle \sigma_z (t) \rangle = \text{Tr} \left[ e^{iH_{TLS} t} \sigma_z e^{-iH_{TLS} t} \rho_0 \right] \) into infinitesimal steps of length \( \tau \) and inserting \( 1 = \sum_{\sigma = \pm 1} |\sigma \rangle \langle \sigma | \) with \( H_{TLS} \) from Eq. (1.26). The paths that contribute to the expectation value are obviously closed at the end, \( \sigma_i = \sigma'_i \). This is why we can adjoin a “rest path” that starts in a fixed state \( \sigma_i \) and ends in a state \( \sigma_{q+1} = \sigma'_{q+1} \), which corresponds to the discretization of \( \text{Tr} \left( e^{iH_{TLS} t} |\sigma_i \rangle \langle \sigma'_i | e^{-iH_{TLS} t} \right) = \delta_{\sigma_i, \sigma'_i} \),

\[
\delta_{\sigma_i, \sigma'_i} = \sum_{\sigma_{i+1, \ldots, q+1}} \left[ \prod_{j=i}^{q} K^*(\sigma'_j, \sigma_{j+1}) K(\sigma_{j+1}, \sigma_j) \right] \delta_{\sigma_{q+1}, \sigma'_{q+1}}. \tag{C.2}
\]

Accordingly, \( P_{z,i} \) can be read out of the whole path by applying the measurement operator

\[
M_{z,i}^{\alpha = 0} = \delta_{\sigma_i, \sigma'_i}(\delta_{\sigma_i, 1} - \delta_{\sigma_i, -1}) \tag{C.3}
\]
onto the sum over the complete set of diagonal paths, i.e.

\[ P_{z,i} = \sum_{\sigma_1, \ldots, q+1 \atop \sigma'_{1, \ldots, q+1}} \rho_0(\sigma_1, \sigma_1') \left[ \prod_{j=1}^{i-1} K^*(\sigma_j', \sigma_{j+1}') K(\sigma_{j+1}, \sigma_j) \right] M_{z,i}^{\alpha=0} \delta_{\sigma_{q+1}, \sigma_{q+1}'}. \]  

Things become more complicated, when we measure the off-diagonal observables, say \( P_{x,i} \equiv \langle \sigma_x((i-1)\tau) \rangle \): We have to sum over the paths that flip at the end, hence

\[ P_{x,i} = \sum_{\sigma_1, \ldots, i \atop \sigma'_{1, \ldots, i}} \left[ \prod_{j=1}^{i-1} K^*(\sigma_j', \sigma_{j+1}') K(\sigma_{j+1}, \sigma_j) \right] \delta_{\sigma_i, \sigma_i'}. \]

If we want to add a rest path in the same way we did before, we have to “propagate artificially” to a diagonal state at \( i + 1 \). This is done by multiplying (C.5) with

\[ 1 = \frac{1}{2} \sum_{\sigma_{i+1}, \sigma_{i+1}'} K^*(\sigma_{i+1}', \sigma_{i+1}) K(\sigma_{i+1}, \sigma_{i+1}). \]

We replace \( \delta_{\sigma_{i+1}, \sigma_{i+1}'} \) in the same way as before and straightforwardly achieve

\[ P_{x,i} = \sum_{\sigma_1, \ldots, q+1 \atop \sigma'_{1, \ldots, q+1}} \left[ \prod_{j=1}^{i-1} K^*(\sigma_j', \sigma_{j+1}') K(\sigma_{j+1}, \sigma_j) \right] M_{x,i}^{\alpha=0} \delta_{\sigma_{q+1}, \sigma_{q+1}'}; \]

with the measurement operator

\[ M_{x,i}^{\alpha=0} := \frac{\delta_{\sigma_i, \sigma_i'} \delta_{\sigma_{i+1}, \sigma_{i+1}'}}{2K^*(\sigma_{i+1}', \sigma_{i+1}) K(\sigma_{i+1}, \sigma_i)}. \]

Note that the total path is still diagonal in the end, even though we ask for the off-diagonal elements. This is a main condition for extracting both the diagonal and the off-diagonal quantities from one simulation. The other important measurement operators are

\[ M_{P_{\pm 1,i}}^{\alpha=0} := \delta_{\sigma_i, \sigma_i'} \delta_{\sigma_{i+1}, \pm 1}; \]

\[ M_{y,i}^{\alpha=0} := \frac{\delta_{\sigma_i, \sigma_i'} \delta_{\sigma_{i+1}, \sigma_{i+1}'}}{2K^*(\sigma_{i+1}', \sigma_{i+1}) K(\sigma_{i+1}, \sigma_i) i(\delta_{\sigma_i, 1} - \delta_{\sigma_i, -1}).} \]

Notice that \( P_x \) and \( P_y \) are determined by checking the spin coordinates on two sites. Therefore, \( M_{x/y,q+1} \) is not accessible within our approach.

When turning to the case \( \alpha > 0 \), a further difficulty arises. It is connected with the way, how the path is discretized and does only matter for the off-diagonal observables. As \( \sigma_y \) works analogously, we just discuss the case of \( \sigma_x \) and mention in passing, why this problem has no relevance for the populations.

The naive ansatz would be to paste \( \exp[-\Phi_{SB}^I] \) into Eq. (C.4). Unfortunately, this is not the complete truth. Why not? Due to the factor \( \delta_{\sigma_i, \sigma_i'} \), the path is diagonal in the end.
Hence, the contributions containing $\zeta_i = (\sigma_i - \sigma'_i)/2$ vanish. However, this is not true for the off-diagonal operators. As a consequence, we have to include the interactions of $\zeta_i$ with earlier times.

Due to the path discretization (B.13), $\zeta_i$ corresponds to the value of the path $\zeta(t)$ in the interval $(i - 3/2)\tau \leq t \leq (i - 1/2)\tau$. Note that the flips occur at $(i + 1/2)\tau$, whereas the observables are measured at $(i - 1)\tau$. When we want to get $P_x((i - 1)\tau)$, we therefore have to drop half of this interval, i.e. $(i - 1)\tau...((i - 1/2)\tau$ due to causality. This means that we have to multiply the measurement operator with

$$
\exp \left[ \Phi_{i,SB}^{od} \right] = \exp \left\{ \int_0^1 dt' \zeta_i \Theta [t' - (i - 1)\tau] \int_0^{t'} dt'' [L'(t'' - t')\zeta(t'') + iL''(t'' - t')\eta(t'')] \right\},
$$

where “od” stands for off-diagonal. Obviously, this correction vanishes for the diagonal elements. The evaluation is similar to the one in App. B and ends with

$$
\Phi_{i,SB}^{od} = \zeta_i \left[ \sum_{j=2}^i \Lambda_{i-j}^{od} \zeta_j + i \sum_{j=2}^{i-1} X_{i-j}^{od} \eta_j + \Lambda_i^{od,1} \zeta_i + i X_i^{od,1} \eta_i + i \mu X_i^{(\mu),od} \right],
$$

where

$$
\Lambda_0^{od} := \text{Re} \left[ Q(\tau) - Q(\tau/2) \right],
$$
$$
\Lambda_{i-1}^{od} := \text{Re} \left[ Q[j + 1,\tau] - Q[j + 1/2,\tau] - Q(j,\tau) + Q[(j - 1/2,\tau) \right],
$$
$$
X_{i-1}^{od} := \text{Im} \left[ Q[j + 1,\tau] - Q[j + 1/2,\tau] - Q(j,\tau) + Q[(j - 1/2,\tau) \right],
$$
$$
\Lambda_i^{od,1} := \text{Re} \left[ Q[i - 1/2,\tau] - 2Q[i - 1,\tau] + Q[(i - 3/2,\tau) \right],
$$
$$
X_i^{od,1} := \text{Im} \left[ Q[i - 1/2,\tau] - 2Q[i - 1,\tau] + Q[(i - 3/2,\tau) \right].
$$

Using the measurement operators

$$
M_{z/\pm 1,i}^{\alpha=0} \text{ or } M_{x/y,i}^{\alpha=0} \exp \left[ \Phi_{i,SB}^{od} \right],
$$

one can again read the corresponding quantity out one simulation ranging from time slice 2 up to $q + 1$.

Adding the influence functional (B.14) in (C.4) or (C.7) and assuming an arbitrary measurement operator $M_{\nu,i}$, we end up with

$$
P_{\nu,i} = \sum_{\eta_1,...,q+1} \rho_0(\eta_1,\zeta_1) \prod_{j=1}^{q} KK_{\eta_j,\eta_{j+1}}(\zeta_j,\zeta_{j+1}) \exp \left[ -\Phi^{SB} \right] M_{\nu,i},
$$

with $\zeta_{q+1} = 0$. In (C.15), we additionally defined the combined propagators

$$
KK_{\eta_j,\eta_{j+1}}(\zeta_j,\zeta_{j+1}) := K^*{\sigma'_j,\sigma'_{j+1}}K{\sigma_{j+1},\sigma_j}|_{\sigma,\sigma'\rightarrow \eta,\zeta}.
$$
These are \((2 - |\zeta_j|) \times (2 - |\zeta_{j+1}|)\) matrices whose indices depend only on the \(\eta\)'s, while the \(\zeta\)'s are frozen. Accordingly, the \(\zeta_j\)'s run from \(-1\) to \(1\) and the corresponding \(\eta_j\) from \(-1 + |\zeta_j|\) to \(1 - |\zeta_j|\). It will become clear in App. D, why we write parts of the coordinates as matrix indices and the others as function variables.
Appendix D

Elimination of the $\eta$ Coordinates

We now describe the way how to reduce the number of degrees of freedom by performing the sum over the coordinates $\eta_1...\eta_q$ exactly [40, 54]. This is possible because the $\eta$'s occur only linearly in the influence functional (IF), while the $\zeta$'s appear in a bilinear form.

The approach in itself is quite simple. We write down the full expression (2.8) and plug in both the IF and the measurement operator for the more general off-diagonal case. Further, we use the functional equation $\exp(\sum_j a_j) = \prod_j \exp(a_j)$ and rewrite $\sum_{j=2}^q \zeta_j \sum_{k=2}^{j-1} X_{j-k} \eta_k = \sum_{j=2}^q \eta_j \sum_{k=1}^{q-j} \zeta_{j+k} X_k$, yielding

$$P_{\nu,i} = \sum_{\zeta_1,...,q} \exp \left[ -i\mu \sum_{j=1}^q \zeta_j X_j^{(\mu)} + i\zeta_i M_i^{(\mu),od} - \sum_{j=2}^q \sum_{k=2}^j \zeta_j A_{j-k} \zeta_k - \zeta_1 \sum_{j=1}^q \Lambda_j^{(1)} \zeta_j \right]$$

$$\times \exp \left[ \zeta_i \sum_{j=2}^q A_{1-j} \zeta_j + \zeta_i A_i^{od,1} \zeta_i \right] \sum_{\eta_1,...,q+1} \rho_0(\eta_1, \zeta_1) M_{\nu,i}^{0=0} \left[ \prod_{j=1}^q K K_{\eta_j, \eta_{j+1}} (\zeta_j, \zeta_{j+1}) \right]$$

$$\times \exp \left[ i\eta_1 \left( \zeta_i X_i^{od,1} - \sum_{j=2}^q \zeta_j X_j^{(1)} \right) \right] \prod_{j=2}^{i-1} \exp \left( i\eta_j X_j^{od} \right) \prod_{j=2}^q \exp \left( -i\eta_j \sum_{k=1}^{q-j} \zeta_{j+k} X_k \right)$$

$$= \sum_{\zeta_1,...,q,\eta_{q+1}} \exp \left[ -i\mu \varphi(\mu)(\zeta_1,...,q) \right] \exp \left[ -w(\zeta_1,...,q) + w^{od}(\zeta_1,...,i) \right] \sum_{\eta_1} \prod_{j=1}^q K K_j^{(1)} (\zeta_1,...,q) \right]$$

(D.1)

In the last step, have defined the factor $\varphi(\mu)$ and collected the terms that are bilinear in $\zeta$ in $w$:

$$\varphi(\mu)(\zeta_1,...,q) := -i \left( \sum_{j=1}^q \zeta_j X_j^{(\mu)} - \zeta_i X_i^{(\mu),od} \right)$$

$$w(\zeta_1,...,q) := \sum_{j=2}^q \sum_{k=2}^j \zeta_j A_{j-k} \zeta_k + \zeta_1 \sum_{j=1}^q \Lambda_j^{(1)} \zeta_j$$

$$w^{od}(\zeta_1,...,i) := \zeta_i \sum_{j=2}^i \Lambda_i^{od,1} \zeta_j + \zeta_i A_i^{od,1} \zeta_i$$

(D.2)
Notice that Eq. (D.1) contains indeed a matrix product and not a product over matrix entries such as in (2.8). If we wanted to calculate any diagonal quantity instead, we would just have to set all the terms labeled by “od” to zero. In Eq. (D.1), a variety of \( \widetilde{K} K^j \) matrices is defined. These objects are generated by manipulating the row entries of the combined propagators \( K K \) and absorbing the initial preparation \( \rho_0 \) and the measurement operator \( M_{\nu,i}^{\alpha=0} \),

\[
\begin{align*}
\widetilde{K} K^1_{\eta_1,\eta_2}(\zeta_1,...,q) &:= K K_{\eta_1,\eta_2}(\zeta_1,\zeta_2)\rho_0(\eta_1,\zeta_1)\exp\left[ i\eta_1 \left( \zeta_i X_1^{\text{od,1}} - \sum_{k=2}^{q-1} \zeta_k X_k^{(1)} \right) \right] \\
\widetilde{K} K^j_{\eta_j,\eta_{j+1}}(\zeta_j,...,q) &:= K K_{\eta_j,\eta_{j+1}}(\zeta_j,\zeta_{j+1})\exp\left[ i\eta_j \left( \zeta_i X_1^{\text{od}} - \sum_{k=1}^{q-j} \zeta_{j+k} X_k \right) \right] \\
&\quad \text{for } 2 \leq j \leq i - 1, \\
\widetilde{K} K^i_{\eta_i,\eta_{i+1}}(\zeta_i,...,q) &:= K K_{\eta_i,\eta_{i+1}}(\zeta_i,\zeta_{i+1})M_{\nu,i}^{\alpha=0}(\eta_i,\eta_{i+1},\zeta_i,\zeta_{i+1})\exp\left( -i\eta_i \sum_{k=1}^{q-i} \zeta_{i+k} X_k \right) \\
&\quad \text{for } i + 1 \leq j \leq q. 
\end{align*}
\]

\( \text{(D.3)} \)

There is one instance that makes the accumulation of \( \sigma_{x/y} \) harder to handle: The off-diagonal correction in the measurement operator makes all \( \widetilde{K} K \) matrices for \( j \leq i \) depending on the time step on which we want to measure, so they have to be re-calculated for every \( i \). This is why the procedure to be explained right now only works in a restricted way for \( P_x \) and \( P_y \).

Taking a closer look at the product of \( \widetilde{K} K \) matrices, we see that we can define the “matrices” \( M^{\text{left},i} \) and \( M^{\text{right},i} \) (in fact, they are row and column vectors; do not mix them up with the measurement operators!) of dimensions \( 1 \times (2 - |\zeta_i|) \) and \( (2 - |\zeta_{i+1}|) \times 1 \),

\[
\begin{align*}
M^{\text{left},i}_{\eta_i} &= \sum_{\eta_i} \left( \prod_{j=1}^{i-1} \widetilde{K} K^j \right)_{\eta_j,\eta_i} \\
M^{\text{right},i}_{\eta_{i+1}} &= \left( \prod_{j=i+1}^{q} \widetilde{K} K^j \right)_{\eta_{i+1},\eta_{q+1}}. 
\end{align*}
\]

Note that \( \eta_{q+1} \) is frozen in the same way as \( \zeta_1,...,q \). By this, one can express the whole product by \( M^{\text{left},i} \widetilde{K} K^{j<i} M^{\text{right},i} \). This way, the \( M \) matrices can be calculated inductively, which saves a notable amount of CPU time. Due to the \( i \)-dependence of the \( \widetilde{K} K^{j<i} \) matrices, this simplification can only be applied to the \( M^{\text{right}} \) matrices, when \( P_x \) and \( P_y \) are measured.

Eq. (D.1) is the final result that has to be implemented. It is shown in Sec. 2.2.1 how the Metropolis sampling for the coordinates \( \zeta_1,...,\zeta_q \) and \( \eta_{q+1} \) works.
Appendix E

Details for the Interacting Spins Model

In this section, we want to give a brief overview about the corresponding expressions of the previous appendix chapters for the interacting spins model (ISM), thereby refraining from any derivations. First of all, we have to sketch the discretized influence functional (IF) for a system of two interacting spins, that is governed from Eq. (1.62) by inserting paths of the form (B.13) for spins $A$ and $B$, yielding

$$\Phi^{ISM} = \sum_{j=2}^{q} (\zeta_j^A + \zeta_j^B) \sum_{k=2}^{j} \Lambda_{j-k}(\zeta_k^A + \zeta_k^B) + (\zeta_1^A + \zeta_1^B) \sum_{j=1}^{q} \Lambda_j^{(1)}(\zeta_j^A + \zeta_j^B)$$

$$+ i \sum_{j=2}^{q} (\zeta_j^A + \zeta_j^B) \sum_{k=2}^{j} X_{j-k}(\eta_k^A + \eta_k^B) + i(\eta_1^A + \eta_1^B) \sum_{j=1}^{q} (\zeta_j^A + \zeta_j^B) X_j^{(1)}$$

$$+ i2\mu \sum_{j=1}^{q} (\zeta_j^A + \zeta_j^B) X_j^{(\mu)}. \quad (E.1)$$

Note that this expression is not just a modification of Eq. (B.14) by replacing $\zeta \rightarrow \zeta^A + \zeta^B$ and $\eta \rightarrow \eta^A + \eta^B$. Whereas the terms $\zeta_j \eta_j$ vanish in case of the spin-boson model, their ISM counterparts do not so. As a consequence, we have to change the summation borders slightly, thereby including the terms

$$X_0 := \text{Im}[Q(\tau)], \quad X_1^{(1)} := \text{Im}[Q(\tau/2)]. \quad (E.2)$$

For the same reason, the IF without counter term contains a further contribution, that does not appear in the SBM. It reads

$$- i\Lambda_{cl}\tau \left[ \frac{1}{2}(\zeta_1^A \eta_1^B + \eta_1^A \zeta_1^B) + \sum_{j=2}^{q} (\zeta_j^A \eta_j^B + \eta_j^A \zeta_j^B) \right] \quad (E.3)$$

and cancels exactly with the counter term contribution in Eq. (1.62). Therefore, the full counter term is included in $X_0$. If we simply dropped it, we would get $X_0 = \text{Im}[Q(\tau)] - \Lambda_{cl}\tau$. 

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While the latter expression is of order $\tau^2$, Eq. (E.2) grows linearly with $\tau$. This is of fundamental importance when the reorganization energy is the dominating scale.

Now, we should have a look at the measurement operators. The division into four categories of observables, that was already mentioned in Sec. 1.3, comes again into play. The simplest observables are the ones where both spins remain in a diagonal state: These are the populations $P_\nu$ with $\nu \in \{1; 2; 3; 4\}$. One easily derives that the measurement operators for both the free and the dissipative case at time step $i \doteq (i-1)\tau$ read

$$M^{\alpha=0}_{\nu,i} := \delta_{\eta^A \nu,0} \delta_{x_{i,0}^A,0} \delta_{y_{i,0}^B,0} = \delta_{\eta^A_{i,\pm1},0} \delta_{x_{i,\pm1}^A,0} \delta_{y_{i,0}^B,0}$$

with the collective coordinate $\eta^{AB}$ that is explained below.

All the remaining observables are off-diagonal in the total Hilbert space, but eight of them are diagonal in the subspaces of spins $A$ or $B$. We have already seen in Sec. (1.3), how these twelve observables are categorized. The free system allows to apply measurement operators similar to those of the SBM. For the observation of $P_{x/y12}$ (connected to the matrices $\sigma_{x/y12}$; see Eq. (1.60)), we get

$$M^{\alpha=0}_{x12,i} := \frac{\delta_{\eta^A_{i,1},0} \delta_{x_{i,0}^A,0} \delta_{y_{i,0}^B,0}}{4KK_{SM}(\zeta_{i,0}^{AB}, \zeta_{i+1}^{AB})_{\eta^A_{i,0}, \eta^B_{i,0}}}$$

$$M^{\alpha=0}_{y12,i} := \frac{\delta_{\eta^A_{i,1},0} \delta_{x_{i,0}^A,0} \delta_{y_{i,0}^B,0}}{4KK_{SM}(\zeta_{i,0}^{AB}, \zeta_{i+1}^{AB})_{\eta^A_{i,0}, \eta^B_{i,0}}}$$

which is already expressed in terms of the combined propagator

$$KK_{SM}(\eta^A_{i,0}, \eta^B_{i+1})_{\zeta^A_{i,0}, \zeta^B_{i+1}} := K^* (\sigma_j^{A/B}, \sigma_j^{A/B}) K(\sigma_j^{A/B}, \sigma_j^{A/B})$$

Again, the $\zeta$ path is kept fixed during accumulation. Then, the combined propagator $KK_{SM}(\zeta_{i}, \zeta_{i+1})$ is a $(2 - |\zeta_{i}|) \cdot (2 - |\zeta_{i+1}|)$ matrix, so there are one, two or four rows and columns possible. Further, we introduced the "working indices" $\eta^A_{j} \text{ and } \zeta^A_{j} \text{ and } \eta^B_{j} \text{ and } \zeta^B_{j}$ that are collective coordinates for both spins and important for book-keeping in the implementation. For $\zeta^{AB}_j$, we have

$$\zeta^{AB}_j := 3\zeta^A_j + \zeta^B_j \in [-4; 4].$$

It is easily checked that the corresponding values for $\zeta^A_j \text{ and } \zeta^B_j$ can be uniquely recast by

$$\zeta^A_j := \lfloor(\zeta^{AB}_j + 4)/3\rfloor - 1, \quad \zeta^B_j = \text{mod}(\zeta^{AB}_j + 4, 3) - 1$$

where $\lfloor x \rfloor$ means the next integer less or equal than $x$. The $\eta^A_{j}$es are mainly used as vector and matrix indices and are just numbers between 1 and $(2 - |\zeta^A_j| \cdot (2 - |\zeta^B_j|))$. Their connection to the values $\eta^A_{j}$ is rather complicated and can only be implemented by a sequence of if-statements. When $\zeta^{A/B} = 0$, $\eta^{AB}$ is nothing but the value of the ISM state according to Eq. (1.55).
After this short excursion, we turn back to the off-diagonal measurement operators. Again, we have to paste a cancellation factor that repairs the IF correctly. For the ISM, it reads
\( \exp[\Phi_{\text{od,ISM}}] \) with
\[
\Phi_{\text{od,ISM}}^i = (\zeta_i^A + \zeta_i^B) \left\{ \sum_{j=2}^i \left[ \Lambda_{i-j}^{\text{od}} (\zeta_j^A + \zeta_j^B) + i X_{i-j}^{\text{od}} (\eta_j^A + \eta_j^B) \right] \right. \\
+ \Lambda_{i-1}^{\text{od,1}} (\zeta_i^A + \zeta_i^B) + i X_i^{\text{od,1}} (\eta_i^A + \eta_i^B) + i 2 \mu \hat{X}^{(\mu,\text{od})}_i \right\},
\tag{E.9}
\]

cf. Eq. (C.13). In the meantime, it is annoying to mention, but the way how the measurement operator enters is just the same as for the SBM: The entries of \( \hat{K}_K \) are modified with the operators \( M_{\nu,i}^{\alpha=0} \exp[\Phi_{\text{od,ISM}}] \). We have additional contributions due to the fact that the time-local part of the blip-sojourn interaction is non-zero. It is captured in the term containing \((\zeta_i^A + \zeta_i^B) \cdot (\eta_i^A + \eta_i^B)\), so we define
\[
X_0^{\text{od}} := \text{Im} \left[ Q(\tau) - Q(\tau/2) \right].
\tag{E.10}
\]

Now, what is the full expression that we have to implement? In principle, it is exactly the same as in Eq. (2.11), but with different definitions for the \( \hat{K}K \) matrices,
\[
\hat{K}_K^{\text{ISM,1}}_{\eta_i^A, \eta_i^B, \eta_j^A, \eta_j^B} (\zeta_{i,...,q}) := K K_{\eta_i^A, \eta_j^A}^{\text{ISM}} (\zeta_i^A, \zeta_j^A) \rho_0 (\eta_i^A, \eta_j^A) \\
\times \exp \left[ i (\eta_i^A + \eta_j^B) \left( (\zeta_i^A + \zeta_j^B) X_{i,j}^{\text{od,1}} - \sum_{k=1}^q (\zeta_k^A + \zeta_k^B) X_k^{(1)} \right) \right]
\]
\[
\hat{K}_K^{\text{ISM,j}}_{\eta_j^A, \eta_j^B, \eta_j+1} (\zeta_{j,...,q}) := K K_{\eta_j^A, \eta_{j+1}}^{\text{ISM}} (\zeta_j^A, \zeta_{j+1}) \\
\times \exp \left[ i (\eta_j^A + \eta_j^B) \left( (\zeta_j^A + \zeta_j^B) X_{j,j}^{\text{od,1}} - \sum_{k=0}^{j-1} (\zeta_{j+k}^A + \zeta_{j+k}^B) X_k \right) \right]
\]
\[
\text{for } 2 \leq j \leq i - 1,
\]
\[
\hat{K}_K^{\text{ISM,i}}_{\eta_i^A, \eta_i^B, \eta_i+1} (\zeta_{i,...,q}) := K K_{\eta_i^A, \eta_i+1}^{\text{ISM}} (\zeta_i^A, \zeta_{i+1}) M_{\nu,i}^{\alpha=0} (\eta_i^A, \eta_{i+1}, \zeta_i^A, \zeta_{i+1}) \\
\times \exp \left( i (\eta_i^A + \eta_i^B) (\zeta_i^A + \zeta_i^B) X_i^{\text{od}} - i (\eta_i^A + \eta_i^B) \sum_{k=0}^{q-i} (\zeta_{i+k}^A + \zeta_{i+k}^B) X_k \right)
\]
\[
\hat{K}_K^{\text{ISM,j}}_{\eta_j^A, \eta_j^B, \eta_j+1} (\zeta_{j,...,q}) := K K_{\eta_j^A, \eta_j+1}^{\text{ISM}} (\zeta_j^A, \zeta_{j+1}) \exp \left( -i (\eta_j^A + \eta_j^B) \sum_{k=0}^{q-j} (\zeta_{j+k}^A + \zeta_{j+k}^B) X_k \right)
\]
\[
\text{for } i + 1 \leq j \leq q.
\tag{E.11}
\]
and the functions $w$, $w^{\text{od}}$, and $\varphi^{(\mu)}$,

\[
\varphi^{\text{ISM},(\mu)}(\zeta_{A,B}^{1,...,q}) := -i \left( \sum_{k=1}^{q} (\zeta_k^A + \zeta_k^B) \hat{X}_k^{(\mu)} - (\zeta_i^A + \zeta_i^B) X_i^{(\mu),\text{od}} \right)
\]

\[
w^{\text{ISM}}(\zeta_{A,B}^{1,...,q}) := \sum_{j=2}^{q} \sum_{k=2}^{j} (\zeta_j^A + \zeta_j^B) \Lambda_{j-k}(\zeta_k^A + \zeta_k^B) + (\zeta_i^A + \zeta_i^B) \sum_{j=1}^{q} \Lambda_j^{(1)}(\zeta_j^A + \zeta_j^B)
\]

\[
w^{\text{ISM},\text{od}}(\zeta_{A,B}^{1,...,i}) := (\zeta_i^A + \zeta_i^B) \sum_{j=2}^{i} \Lambda_{i-j}^{\text{od}}(\zeta_j^A + \zeta_j^B) + (\zeta_i^A + \zeta_i^B) \Lambda_i^{\text{od},1}(\zeta_i^A + \zeta_i^B).
\]

(E.12)

The implementation is tedious, but in principle not difficult.
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Hiermit erkläre ich, daß ich die vorliegende Arbeit selbständig angefertigt, keine anderen als die angegebenen Quellen und Hilfsmitteln benutzt, sowie wörtlich oder inhaltlich übernommene Stellen als solche kenntlich gemacht und die Satzung der Universität Ulm zur Sicherung guter wissenschaftlicher Praxis in der aktuell gültigen Fassung vom 16.10.2009 beachtet habe.

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