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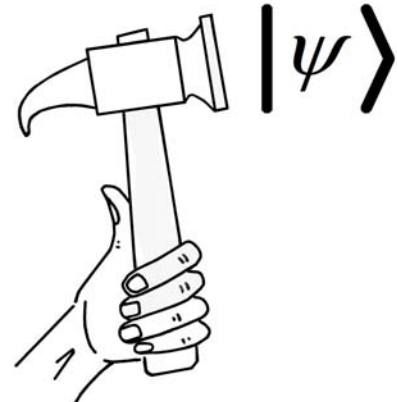

Bahar Mehmani

Classical Manipulation of a Quantum System

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to Sanli
My most beloved companion in life

Paranimfen: Telli Faez en Shanna Haaker

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Contents

CHAPTER 1

Introduction

One of the main goals of modern technology is to design and control the microscopic world. Quantum information, quantum chemistry and quantum thermodynamics are some aspects of this general trend. Manipulating quantum systems is an important issue in these fields. Simple quantum mechanical systems are the main objects in quantum information. Since in many situations only two states of a system are important in this subject, two state systems are the best candidates. Some examples are the ground state and first excited state of an electron in an atom; the mutually exclusive polarization states of a photon (horizontal and vertical if it is linearly polarized, or left and right if it is circularly polarized), the respectively up and down states (when only the spin degree of freedom is considered) of a spin-$\frac{1}{2}$ particle possessing a magnetic moment which can be influenced by some external magnetic field. The Hilbert space of all these examples can be spanned by two basis states and all operators in the Hilbert space can be combined from the 2×2 Pauli matrices. From the mathematical point of view any two-level system with non-degenerate energy levels can be described by the same 2×2 matrices and thus is analogous to a spin-$\frac{1}{2}$ system. The determination of the unknown state of a spin-$\frac{1}{2}$ system is one of the most

important issues in the field of quantum information. In doing so, one needs to measure the spin components in three different directions. As currently described in many textbooks, the z-component of the spin of of a spin-$\frac{1}{2}$ system, can statistically be determined by means of a repeated Stern-Gerlach experiment. In this process, the x and y component of the spin are destroyed as a consequence of the non-commutation property of the spin operator in the transversal directions. Likewise, the state of any two-level system can be determined only through measurement of three linearly independent observables which do not commute and cannot be simultaneously measured. In chapter 2 we address this issue and show that it is possible to identify the state of a two-level system by simultaneous measurements. In particular, we show that the unknown state of such a system can be determined indirectly by means of a set of measurements performed simultaneously on the system itself and an auxiliary system which is called assistant. We let the system which is initially in an unknown state interact with the assistant with initially a known state. After some elapsed time we perform simultaneous measurements of an observable of the system of interest and an observable of the assistant. We show that this process enables us to recover the initial state of the system. In chapter 2 we study two cases: both employing another two-level system, for solid state applications, and a single mode of electromagnetic field as an assistant, for quantum optics applications.

In manipulating quantum systems, controlling their interaction with the surrounding environment is an important issue. This is best addressed in the subject of open quantum systems. An open system is nothing more than one which has interactions with some environment. The dynamics of a closed system is described by a unitary transformation. A natural way to describe the dynamics of an open system is to regard it as arising from an interaction between the system of interest and an environment, which together form a closed system. This is a recurrent theme in modern physics. Depending on the type of environment, there are different conditions under which this procedure is possible. A group of methods, which goes under the name of system-bath interaction, amounts to isolating a quantum system with a few degrees of freedom in contact with an equilibrium environment (thermal bath) which usually is considered to have many degrees of freedom. One of the main consequences of this approach is the appearance of a Langevin equation, which supplements the Newton equation of motion for the quantum system by two additional forces: a random conservative force and a non-conservative (i.e., non-Lagrangian), velocity-dependent friction force.

In chapter 3 we focus on the spin-boson model which describes the dynamics of a two-level system coupled to a thermal bath modeled by a set of harmonic oscillators. Employing this model we study the dynamics of a pulsed spin-$\frac{1}{2}$ system in the presence of another spin-$\frac{1}{2}$ system located at some distance from it. We show that although the spins are considered non-interacting, the presence of the bath yields the polarization transfer among them. More precisely, the back reaction of spins on the bath induces the polarization transfer. Here the presence of the bath is crucial since it is the only interactive component between the spins. This is in contrast with the usual school of thought in spin-boson model were the bath is considered to be a hindrance.

The quantum back reaction force plays an important role in another area in physics, namely, quantum-classical approximations. It provides a straightforward derivation route, in which one starts with a fully quantum treatment and takes the classical limit for some degrees of freedom. This provides a powerful scheme that facilitates understanding and manipulating the microscopic world. Quantum-classical approximations are particularly useful when one can easily identify quantum and classical subsystems by mass, energy, time scale. This is another set-up that allows studying the dynamics of an open system. In chapters 4 and 5 we consider a quantum system coupled to a classical system and identify the two systems by a time scale separation. Chapter 4 is devoted to the evolution of the fast quantum subsystem. In this chapter we employ the adiabatic perturbation theory based on time scale separation and derive higher order corrections to the adiabatic wave function in terms of a small parameter ϵ. We define ϵ as the small ratio of the characteristic times of the quantum over the classical system, respectively. According to the adiabatic theorem a quantum system under the influence of its surrounding environment remains in its instantaneous eigenstate if the environment which is acting on it evolves slowly enough and if there is a gap between the initial eigenvalue and the rest of the energy spectrum.
Our ultimate goal is to understand the nature of the back reaction force exerted by the quantum system on its classical environment. This is the subject of chapter 5. In this chapter we study the dynamics of the slow classical system by adiabatically excluding the fast quantum system. We try to understand to which extent the ensuing dynamics of the slow classical system can be described by autonomous Lagrangian-generated equations for the classical coordinates. For the quantum-classical dynamics it is well known that in the leading order the influence of the quantum system on the classical one can be described by the Born-Oppenheimer potential energy term [1]. It was

shown by Berry and Robbins that in the first order of ϵ one gets an effective magnetic field, which manifests itself as the velocity-dependent term in the classical Lagrangian [2]. Recently, Goldhaber has shown that in the second order ϵ^2 one gets in the Lagrangian an additional kinetic energy term, i.e., a quadratic form in slow velocities [3].
What happens in the next orders? In particular, how far we can continue the expansion over ϵ, still keeping the classical system Lagrangian? Most importantly, are there new physical effects essentially related to post-adiabatic corrections?

Here we answer these questions. It appears that at every order over ϵ one can derive Lagrange equations for the dynamics of the classical system. However, there is an important difference between the orders ϵ and ϵ^2 and all successive orders. At the order ϵ^3 the classical dynamics is Lagrangian, but the Lagrangian starts to depend on the higher-order time-derivatives of the classical coordinates: While the classical Lagrangians normally depend on the coordinates and their first-order time-derivatives (velocities), at the order ϵ^3 we get a Lagrangian that is a functional of the classical coordinates, velocities, and accelerations. Moreover, in the third order of ϵ, the Lagrangian depends linearly on the classical accelerations.
This fact is of conceptual relevance. Classical physics is essentially based on the Newton's second law that equates acceleration to the force, which depends only on coordinates and velocities. As a consequence, the trajectory of the classical motion is fixed via initial coordinates and initial velocities. In its turn, the Newton's second law is generated by a Lagrangian, which depends on coordinates and velocities. Dependence on higher-order derivatives in the Lagrangian implies a number of essential changes in the kinematics of the classical system: the momentum of the classical system depends on the acceleration, while the full angular momentum tensor is a sum of the usual orbital part and a term that can be interpreted as the spin of the classical system. In the simplest non-trivial case this spin is proportional to the squared velocity of the classical particle. We show that this implies the existence of the zitterbewegung effect, where the momentum of the classical particle (system) is governed by the projected time-derivative of the spin. So far the zitterbewegung effect was known only in the physics of relativistic Dirac electron, while we show the same effect appears in a purely non-relativistic slowly evolved classical system due to its coupling to a fast quantum system. It appears now that this effect is a part of the physics generated by higher-order post-adiabatic corrections. Similar dependence on higher-order

derivatives is expected at higher orders ϵ^n with $n \geq 4$, though in this thesis we restrict ourselves to deriving the effective classical Lagrangian up to the order ϵ^4.

CHAPTER 2

Quantum State Tomography

In this chapter the question of determining the unknown state of a quantum system is addressed. First, some of the interpretations of the notion of the quantum state is mentioned. Then quantum state tomography is introduced as a procedure of reconstructing the quantum state from measurements of observables of the system. This method aims to determine the unknown state of a quantum system from a linear transformation of a set of experimental data. Then the quantum state tomography of a two-level system or a "qubit" in the terminology of quantum information by simultaneous measurement of two commuting observables is studied. This can be done by letting the qubit interact with another qubit which is in a known initial state, or with a single mode of a quantized electromagnetic field. In the latter case, the interaction is studied within the Jaynes-Cummings Model. It is shown that it is possible to determine the unknown initial state of the qubit from two sets of measurements of commuting observables each belonging to one of the systems. In order to make sure that the reconstructed density matrix is a Hermitian, semipositive matrix with a unit trace, the maximum likelihood reconstruction method is applied. In this approach the density matrix that is most likely to have produced the measured data set is characterized by numerical optimization.

2.1 Introduction

The ability to determine and characterize the state of a quantum system is one of the most important areas in nowadays physical research specifically in quantum computation, quantum cryptography, and quantum communication. Given the state of a quantum system, one can calculate the expectation value of any observable of the system [4]. However, the inverse problem of determining the state by performing different measurements is not a trivial task. This problem was first discussed by Pauli in 1933 [5]. He raised the question of how to reconstruct the unknown wave function of an ensemble of identical spinless particles via the corresponding position and momentum probability densities. The interest in the state determination problem grew considerably since then, and is now a well-recognized subject [6–12].
In general, the process of reconstructing the quantum state (density matrix) of a system by means of performing measurements on different observables of the system is called quantum state tomography. In various experimental setups it is reasonably straightforward to reconstruct the state of a quantum system employing a linear tomographic technique. This way the elements of the density matrix can be linearly related to a set of measured quantities. But since different observables of a quantum system may not commute with each other, one often has to perform series of successive measurements of observables which cannot be done simultaneously. Simultaneous measurement of observables costs less time and energy and is more beneficial. However, there is one drawback in this method. The recovered state might not correspond to a physical state due to the experimental noise. For example, density matrices for any quantum system must be semipositive, Hermitian matrices with unit trace. The matrices resulting from a tomographic measurement may fail to be positive semidefinite. To avoid this issue the "maximum likelihood" method is adopted.

In section 2.2 we discuss some of the interpretations of quantum state and quantum measurement. Then we outline the strategy of quantum state tomography with simultaneous measurement of observables. Sections 2.3-2.4 are devoted to describe specific models we employ to this end. In section 2.7 we introduce the maximum likelihood method. This method is used to reconstruct the most proper density matrix based on a measured data set by numerical optimization. The numerical results are demonstrated in appendices A and B.

2.2 The state of a quantum system

In classical physics, the state of a system is characterized by specifying the values of all physical quantities, for instance the positions and the velocities of the particles that constitute the system. In quantum mechanics the situation is complicated by the fact that the physical quantities are mathematically represented by specific type of operators called observables, which in general are elements of a *non-commutative algebra*. Hence their values cannot be simultaneously specified, as emphasized in the Heisenberg's uncertainty principle. Instead, the measurement results of each observable is characterized by a probability distribution, which involves statistical fluctuations. The "state of the system" is then represented by a mathematical notion that allows us to express the probability distribution of all the observables for an ensemble of identically prepared systems.

Various interpretations have been given to the concept of state in quantum mechanics. Here we list three of them [13–15]:

- According to the Schrödinger interpretation, a state is represented by a wave function or by a ket vector in the Hilbert space on which the observables of the considered system act. In this interpretation, the wavefunction is regarded as an intrinsic property of the system and it directly describes its physical properties. The probability distribution of the position of a particle, for instance, is obtained from the modulus square of its wave function. The distribution of the momentum is given by the modulus square of the Fourier transform of the wave function.

- In "information interpretation", on the opposite point of view, the state does not pertain to the system itself, but only gathers the information we have on it [15]. The problem in this concept is that the wave function of a physical system would depend on the observer in analogy with classical probability [13]: If two observers have different information on the same physical system, they should use two different wave functions for describing it.

- In the statistical interpretation of quantum mechanics [14], to which we adhere, the state of a system is a mathematical object from which we can derive any probabilistic prediction about the physical quantities attached to this system. One typically imagines some experimental apparatus and procedure which "prepares" this quantum state; the

mathematical object then reflects the setup of the apparatus. This way, the quantum state accounts for the full information available about the preparation of the system, from which we wish to derive consequences for future experiments. Since this knowledge is probabilistic it does not refer to a single system or single event. What we call a state, which is most of the time a mixed state, characterizes a statistical ensemble of systems of the same type, which are all prepared under identical physical considerations. The physical state is thus a mathematical representation of the result of a certain state preparation procedure; it accounts for our information about this preparation and upon knowing it we can elaborate consistent probabilistic predictions. It is thus a concept which merges objective and subjective aspects [16].

A standard tool to implement the statistical definition of state is the density matrix, which generalizes the pure state represented by a wave function. Indeed, there is no conceptual difference between wave function and density matrix which are both mathematical means for evaluating expectation values of the observables of the system or probabilities.

In the frame work of the statistical interpretation, the laws of quantum mechanics can be summarized as follows:

- An observable $\hat{\mathcal{O}}$ is represented by a self-adjoint linear operator acting on the Hilbert space pertaining to the system. It has a spectral representation, $\hat{\mathcal{O}} = \sum_i o_i \hat{P}_i$ where o_i are the eigenvalues of $\hat{\mathcal{O}}$ and $\hat{P}_i$ are the orthogonal projection operators related to the orthonormal eigenvectors of $\hat{\mathcal{O}}$, i.e., $\hat{P}_i = \sum_m |m, o_i\rangle\langle m, o_i|$. The parameter m labels the degenerate eigenvectors of $\hat{\mathcal{O}}$.

- The state of a system at a given time is represented by its density matrix, $\hat{\rho}$, which is a self-adjoint operator in Hilbert space with a unit trace. The density matrix should also be semipositive to ensure that any variance of the observables of the system is non-negative. Pure states correspond to the special case

$$\hat{\rho}^2 = \hat{\rho}. \tag{2.1}$$

- The dynamics of the system can be obtained by

$$\hat{\rho}(t) = \hat{U}(t, t_0)\, \hat{\rho}(t_0)\, \hat{U}^\dagger(t, t_0), \tag{2.2}$$

  where $\hat{U}(t, t_0)$ is the unitary time evolution operator.

- Given the density matrix $\hat{\rho}$ of a system, one can find the expectation value of any observable $\hat{\mathcal{O}}$ of the system in the considered situation as

$$\langle\hat{\mathcal{O}}\rangle = \mathrm{tr}[\hat{\rho}\,\hat{\mathcal{O}}], \tag{2.3}$$

  where $\mathrm{tr}[\cdots]$ stands for the trace of a matrix.

Let us emphasize that through out this thesis the operators are always distinguished by a ˆ sign.
As it was mentioned earlier, we wish to reconstruct the density matrix of a quantum system. Consider we are given an ensemble of systems S which we don't know its initial state. In other words, the probability to observe some result or another in the measurement of an observable is unknown. The following question then is of our interest. How can one determine the density matrix by identification of a set of observables, the measurement of which permits the precise determination of $\hat{\rho}$? In other words, how can one determine the quantum statistical operator that describes the preparation of the system?

Procedures of reconstructing the quantum state from measurements are known as *quantum state tomography*. Recently, they have found some applications in quantum information processing [17]. For example, in quantum cryptography one needs a complete specification of the qubit state both as it is emitted from the source and as it is received after transmission [18].

In the simplest example of a spin-$\frac{1}{2}$ system or equivalently any two-level quantum system the state is described by a 2×2 matrix. In the two-dimensional Hilbert space, any observable is a linear combination of the Pauli operators, which satisfy

$$\begin{aligned} &\hat{\sigma}_\alpha^2 = \hat{1}, \quad \alpha = x, y, z, \\ &\hat{\sigma}_x\hat{\sigma}_y = i\hat{\sigma}_z, \end{aligned} \tag{2.4}$$

and are represented by the Pauli matrices

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.5}$$

A state is characterized by three real numbers: one for the diagonal elements of the 2×2 density matrix $\hat{\rho}$, and two for its off-diagonal elements. Equivalently, we can introduce the polarization vector, $\vec{r}$, the components of which are the expectation values of the Pauli matrices.

$$r_\alpha = \mathrm{tr}\left(\hat{\rho}\,\hat{\sigma}_\alpha\right), \qquad \alpha = x, y, z. \tag{2.6}$$

Once we know the value of these parameters, we are able to determine the value of the density matrix, making use of the identity

$$\hat{\rho} = \frac{1}{2}\left(\mathbf{1} + \vec{r}\cdot\vec{\hat{\sigma}}\right). \tag{2.7}$$

Thus, according to the above argument, one has to perform three incompatible measurements for the unknown state determination, e.g., measuring the spin components along the x-, y- and z- axes via a Stern-Gerlach setup. However, during the measurement procedure of each component one loses the information about the two other components, since the spin operators in different directions do not commute. Thus, to determine the state of a spin-$\frac{1}{2}$ system, one needs to use three sets of Stern–Gerlach measurements performed along orthogonal directions. In this approach, the state of any two-level system, represented by a 2×2 density matrix $\hat{\rho}$, can be fully determined only through measurement of three linearly independent observables which do not commute and cannot be simultaneously measured.

In what follows we show that the unknown density matrix of such a system S, in particular the full polarization vector of a spin-$\frac{1}{2}$ system, can be determined indirectly. This can be done by means of a single set of measurements performed simultaneously on both the system S and another auxiliary system (assistant or ancilla) A, where A starts its evolution from a known state [12, 19–22]. The suggested strategy is the following: initially S is in an unknown state that we wish to determine, while the state of the assistant A is known. During some time lapse S and A interact in a known fashion. As a result their joint state is modified: it involves correlations and keeps memory of the initial state of S. Two commuting observables of the combined system S+A are then simultaneously measured. Repeating this process provides then the necessary statistical data: the expectation values of the observables and also their correlation. We will show that one can infer the three components of the initial polarization vector of S, and hence the state of the system from these three sets of data. This way, performing one simultaneous measurement on observables of S+A plays the same role as performing successive measurements on three non-commuting observables of S. This type of information transfer is remarkable. Initially, an unknown information was embedded in the matrix elements of $\hat{\rho}$, or equivalently in the components of the polarization vector of S. It had a *quantum nature*, and could not be represented by an ordinary probability distribution, due to the non-commutation of the three components of the spin operator. After the interaction between

S and A this unknown initial information about S, together with the known information about A, is redistributed among the matrix elements of the joint density matrix of the overall system, S+A. However, the resulting *classical* joint probability distribution for the observables of the system S and the assistant A can keep full memory of the initial quantum information about S. The process on which we rely amounts to a transformation of quantum information into classical information, which can be gained by a classical type of measurement involving commuting observables only. This measurement modifies the state of S+A, but it can recover all the matrix elements of $\hat{\rho}$.

The idea of transforming quantum into classical information by using an assistant system A was first proposed by D' Ariano [19] who showed the possibility of mapping the density matrix of S onto a single observable of S+A. It was explicitly implemented in a dynamical form by Allahverdyan *et al.* [12] of which the present work is a continuation. In particular, they showed that one can determine the unknown state of a spin-$\frac{1}{2}$ system with a single apparatus by using another spin-$\frac{1}{2}$ system as an assistant. This idea was recently implemented by Peng et al. [21] who used pulses to induce the proper dynamics of the interaction between the spin-$\frac{1}{2}$ system and its assistant. They verified the initial state of the system obtained from this procedure with the result of the direct measurement of the three components of the spin vector of the system. Later it was shown that one can employ a single mode of coherent light as an assistant in order to reconstruct the initial state of a two-level system [20].

In the next section 2.3 we briefly review the proposed procedure by Allahverdyan *et al* [12] about determination of the state of a spin-$\frac{1}{2}$ system employing another spin-$\frac{1}{2}$ system as an assistant.
Then we specifically show that the unknown density matrix of an ensemble of two-level systems (atom or spin) can be determined via interaction with a single mode of the electromagnetic field. The atom-field interaction is studied within the Jaynes-Cummings model (JCM) [23] . The unknown state of a two-level system is characterized by repeated measurement of two commuting observables: the population difference of the system $\hat{\sigma}_z$, and the photon number of the field $\hat{a}^\dagger\hat{a}$. This measurement supplies three averages: $\langle\hat{\sigma}_z\rangle$, $\langle\hat{a}^\dagger\hat{a}\rangle$, and $\langle\hat{\sigma}_z\,\hat{a}^\dagger\hat{a}\rangle$, which will be linearly related to the elements of the initial density matrix of the ensemble of the two-level systems. Note that since $\hat{\sigma}_z$ and $\hat{a}^\dagger\hat{a}$ commute, $\langle\hat{\sigma}_z\,\hat{a}^\dagger\hat{a}\rangle$ is recovered from the gathered data of $\hat{\sigma}_z$ and $\hat{a}^\dagger\hat{a}$ by counting the number of coincidences.

2.3 Spin-$\frac{1}{2}$ assistant

Consider a two-level system, S, the state of which we wish to determine. The aim is to find an indirect procedure involving only measurements of commuting observables, which therefore can be performed by means of a single apparatus. To this end, we let the system S be coupled to an auxiliary two-level system A. A is in a known state.
Let us recall the general form of an unknown state of S from (2.7)

$$\hat{\rho} = \frac{1}{2}\left(1 + \vec{r}\cdot\vec{\hat{\sigma}}\right), \tag{2.8}$$

where the polarization vector $\vec{r}$ is defined as

$$\vec{r} = \mathrm{tr}\left[\hat{\rho}\,\hat{\sigma}_\alpha\right], \qquad \alpha = x, y, z. \tag{2.9}$$

The state is called pure if $|\vec{r}| = 1$. $|\vec{r}| < 1$ represents a mixed state, and $|\vec{r}| > 1$ is physically excluded.

We choose the state of the assistant, represented by $\hat{R}$ as

$$\hat{R} = \frac{1}{2}\left(1 + \lambda\hat{s}_z\right), \qquad 0 \le \lambda \le 1 \tag{2.10}$$

where $\hat{s}_x$, $\hat{s}_y$, and $\hat{s}_z$ are the Pauli matrices in the Hilbert space belonging to the assistant A.
Initially there is no interaction between S and A. Therefore the initial state of the overall system, $\hat{\Omega}_0$, can be written as

$$\hat{\Omega}_0 = \hat{R}\otimes\hat{\rho} = \frac{1}{4}\begin{pmatrix}(1+\lambda)\left(1+\vec{r}\cdot\vec{\hat{\sigma}}\right) & 0\\ 0 & (1-\lambda)\left(1+\vec{r}\cdot\vec{\hat{\sigma}}\right)\end{pmatrix}. \tag{2.11}$$

Now we let the two systems interact for some time. The interaction can be described with the help of a 4×4 unitary matrix $\hat{U} = e^{-i\hat{H}}$, where we set $t = 1$. Here, we don't specify our Hamiltonian and consider a general unitary matrix and we parametrize it such that it generates a proper time-evolved overall density matrix at later time $t = 1$, given by $\hat{\Omega}_f$ such that the initial state of S can be read off easily. The observables of which the measurements yields the determination of the initial state of S are the final polarization of each spin of the overall system S+A [12]. They can be measured simultaneously and the correlation of the two can be derived from the gathered data. We

show that it is possible to read off the initially unknown state of the system S from the three above mentioned sets of data. Let us decompose $\hat{U}$ into the following 2×2 block matrix,

$$\hat{U} = \begin{pmatrix} \hat{A} & \hat{C} \\ \hat{B} & \hat{D} \end{pmatrix}, \tag{2.12}$$

and express the unitarity of $\hat{U}$ in terms of the 2×2 matrices $\hat{A}$, $\hat{B}$, $\hat{C}$, $\hat{D}$ in the Hilbert space of S. The polar decomposition of $\hat{A}$ and $\hat{B}$ yields

$$\hat{A} = \hat{v}\hat{k}, \qquad \hat{B} = \hat{w}\hat{k}', \tag{2.13}$$

where $\hat{v}$, and $\hat{w}$ are unitary matrices while $\hat{k}$ and $\hat{k}'$ are semi-positive Hermitian matrices. Since $\hat{v}$, and $\hat{w}$ are unitary, it is easy to see that $\hat{k}$ and $\hat{k}'$ are the non-negative square roots of $\hat{A}^\dagger\hat{A}$ and $\hat{B}^\dagger\hat{B}$, respectively. If $\hat{k}$ and $\hat{k}'$ have a vanishing eigenvalue, these representations of $\hat{A}$ and $\hat{B}$ still hold but are no longer unique. We shall restrict ourselves to the case where $\hat{k}$ and $\hat{k}'$ are strictly positive.
The condition $\hat{U}\hat{U}^\dagger = 1$ implies

$$\hat{C}\hat{C}^\dagger = 1 - \hat{A}\hat{A}^\dagger, \qquad \hat{D}\hat{D}^\dagger = 1 - \hat{B}\hat{B}^\dagger, \tag{2.14}$$

$$\hat{A}\hat{B}^\dagger + \hat{C}\hat{D}^\dagger = 0, \tag{2.15}$$

while $\hat{U}^\dagger\hat{U} = 1$ implies

$$\hat{A}^\dagger\hat{A} + \hat{B}^\dagger\hat{B} = 1, \qquad \hat{C}^\dagger\hat{C} + \hat{D}^\dagger\hat{D} = 1, \tag{2.16}$$

$$\hat{A}^\dagger\hat{C} + \hat{B}^\dagger\hat{D} = 0. \tag{2.17}$$

Implementing (2.16) on the polar decomposition of $\hat{A}$ and $\hat{B}$ given by (2.13) yields

$$\hat{k}' = \sqrt{1 - \hat{k}^2}. \tag{2.18}$$

Thus $\hat{C}\hat{C}^\dagger$ and $\hat{D}\hat{D}^\dagger$ can be simplified as

$$\hat{C}\hat{C}^\dagger = \hat{v}\hat{k}'^2\hat{v}^\dagger, \qquad \hat{D}\hat{D}^\dagger = \hat{w}\hat{k}^2\hat{w}^\dagger. \tag{2.19}$$

Since $\hat{k}$ and $\hat{k}'$ are strictly positive and $\hat{u}$ and $\hat{w}$ are unitary matrices, we can define unitary matrices $\hat{x}$ and $\hat{y}$ such that $\hat{C}$ and $\hat{D}$ have the form

$$\hat{C} = \hat{v}\hat{k}'\hat{x}, \qquad \hat{D} = \hat{w}\hat{k}\hat{y}. \tag{2.20}$$

The remaining unitary condition $\hat{A}^\dagger\hat{C} + \hat{B}^\dagger\hat{D} = 0$ reads $\hat{k}\hat{k}'(\hat{x} + \hat{y}) = 0$. Again, since $\hat{k}$ and $\hat{k}'$ are strictly positive this implies $\hat{y} = -\hat{x}$, which fixes $\hat{y}$ in a unique way.
The unitary matrix $\hat{U}$ then becomes:

$$\hat{U} = \begin{pmatrix} \hat{v} & 0 \\ 0 & \hat{w} \end{pmatrix} \begin{pmatrix} \hat{k} & \hat{k}' \\ \hat{k}' & -\hat{k} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \hat{x} \end{pmatrix}. \tag{2.21}$$

In order to get a more symmetric form for $\hat{U}$, we introduce a unitary matrix $\hat{X}$ such that $(\hat{X}^\dagger)^2 = \hat{x}$ and define the matrices $\hat{V} = \hat{v}\hat{X}^\dagger$ and $\hat{W} = \hat{w}\hat{X}^\dagger$, $\hat{K} = \hat{X}\hat{k}\hat{X}^\dagger$, $\hat{K}' = \hat{X}\hat{k}'\hat{X}^\dagger$. We can then write the 4×4 unitary transformation operator $\hat{U}$ as

$$\hat{U} = \begin{pmatrix} \hat{V} & 0 \\ 0 & \hat{W} \end{pmatrix} \begin{pmatrix} \hat{K} & \hat{K}' \\ \hat{K}' & -\hat{K} \end{pmatrix} \begin{pmatrix} \hat{X} & 0 \\ 0 & \hat{X}^\dagger \end{pmatrix}, \tag{2.22}$$

in terms of the three unitary matrices $\hat{V}$, $\hat{W}$, $\hat{X}$ and the non-negative hermitian matrices $\hat{K}$ and $\hat{K}' = \sqrt{1 - \hat{K}^2}$. Since $\hat{K}$ and $\hat{K}'$ are strictly positive, this decomposition is unique, provided we fix the signs of the eigenvalues of $\hat{X} = \sqrt{\hat{x}^\dagger}$ by some convention, for instance, $(\hat{X} + \hat{X}^\dagger) \geq 0$.
Having the unitary matrix given by (2.22) we can calculate the state of the overall system at later time as

$$\hat{\Omega}_f = \hat{U}\hat{\Omega}_0\hat{U}^\dagger, \tag{2.23}$$

where $\hat{\Omega}_0$ is given by (2.11). The observables that can be simultaneously measured by means of the same apparatus on the state $\hat{\Omega}_f$ are the z-components of the spin of each system. In case S and A are generally two-level systems, the z component of quasi-spin is related to the level occupation and thus the energy of the system. This corresponds to the following averages

$$\begin{aligned} \langle \hat{s}_z \rangle &= \mathrm{tr}\left[\hat{\Omega}_f\, \hat{s}_z\right], \\ \langle \hat{\sigma}_z \rangle &= \mathrm{tr}\left[\hat{\Omega}_f\, \hat{\sigma}_z\right], \\ \langle \hat{s}_z\, \hat{\sigma}_z \rangle &= \mathrm{tr}\left[\hat{\Omega}_f\, (\hat{s}_z\, \hat{\sigma}_z)\right]. \end{aligned} \tag{2.24}$$

We notice that the correlation $\langle \Omega_f\, (\hat{s}_z\, \hat{\sigma}_z) \rangle$ can be recovered form the gathered data of $\hat{\sigma}_z$ and $\hat{s}_z$ via the number of coincidences.
Inserting the unitary time-evolution operator in the expectation values (2.24)

we get a linear relation between the gathered data of measurements of $\hat{s}_z$, $\hat{\sigma}_z$ and their correlation on one hand and the the elements of the initial density matrix of S given by r_x, r_y and r_z on the other hand. But before calculating the above mentioned expectation values, let us first parametrize the unitary time evolution operator $\hat{U}$.
Since $\hat{K}$ is a Hermitian matrix with $0 \leq \hat{K} \leq 1$, we can parametrize it as

$$\hat{K} = \cos\theta\cos\phi + \sin\theta\sin\phi\,(\vec{\chi}\cdot\vec{\hat{\sigma}}), \tag{2.25}$$

where $\vec{\chi}$ is a unit vector and $0 < \phi \leq \theta \leq \frac{\pi}{2} - \phi$. It is straightforward to see that $\hat{K}'$ is given by

$$\hat{K}' = \sin\theta\cos\phi - \cos\theta\sin\phi\,(\vec{\chi}\cdot\vec{\hat{\sigma}}). \tag{2.26}$$

Since the initial overall density matrix $\hat{\Omega}_0$ is block diagonal, multiplication of the unitary matrix $\hat{X}$ by a phase factor does not affect $\hat{U}\hat{\Omega}_0\hat{U}^\dagger$ although it modifies $\hat{U}$. Therefore, we can parametrize $\hat{X}$ as

$$\hat{X} = e^{i\psi(\vec{\xi}\cdot\vec{\hat{\sigma}})} = \cos\psi + i(\vec{\xi}\cdot\vec{\hat{\sigma}})\sin\psi, \tag{2.27}$$

where $\vec{\xi}$ is a unit vector which we assume to be perpendicular to $\vec{\chi}$ for simplicity, and $0 \leq \psi \leq \pi$.
Parametrization of $\hat{V}$ and $\hat{W}$ can be done due to the fact that we are not interested in the off-diagonal block elements of $\hat{\Omega}_f$. In other words, the three expectation values (2.24) do not require the determination of the off-diagonal elements of the overall density matrix and it would be sufficient to determine the action of $\hat{V}$ and $\hat{W}$ on the $\hat{\sigma}_z$:

$$\hat{V}^\dagger\hat{\sigma}_z\hat{V} = \vec{\eta}\cdot\vec{\hat{\sigma}}, \qquad \hat{W}^\dagger\hat{\sigma}_z\hat{W} = \vec{\zeta}\cdot\vec{\hat{\sigma}}, \tag{2.28}$$

where η and ζ are three dimensional unit vectors.
Inserting the expression for $\hat{\Omega}_f$ from (2.23) into (2.24) using the parametrization introduced by (2.25)-(2.28) yields

$$\begin{aligned}\langle\hat{s}_z\rangle &= \lambda\cos 2\theta\cos 2\phi + \lambda\,(\vec{\chi}\cdot\vec{r})\sin 2\theta\sin 2\phi\cos 2\psi \\ &+ \left[(\vec{\xi}\times\vec{\chi})\cdot\vec{r}\right]\sin 2\theta\sin 2\phi\sin 2\psi,\end{aligned} \tag{2.29}$$

and

$$\begin{aligned}
&\langle\hat{\sigma}_z\rangle + \langle\hat{s}_z\,\hat{\sigma}_z\rangle = \lambda(\vec{\chi}\cdot\vec{\eta})\sin 2\theta\sin 2\phi \\
&+(\vec{\chi}\cdot\vec{\eta})\,(\vec{\chi}\cdot\vec{r})\,(1-\lambda\cos 2\theta)(1-\cos 2\phi)\cos 2\psi \\
&+(\vec{\chi}\cdot\vec{\eta})\left[(\vec{\xi}\times\vec{\chi})\cdot\vec{r}\right](\lambda-\cos 2\theta)(1-\cos 2\phi)\sin 2\psi \\
&+(\vec{\xi}\cdot\vec{\eta})\left(\vec{\xi}\cdot\vec{r}\right)(\cos 2\phi+\lambda\cos 2\theta)(1-\cos 2\psi) \\
&+(\vec{\eta}\cdot\vec{r})\,(\cos 2\phi+\lambda\cos 2\theta)\cos 2\psi \\
&+\left[(\vec{\xi}\times\vec{\eta})\cdot\vec{r}\right](\lambda\cos 2\phi+\cos 2\theta)\sin 2\psi. \qquad (2.30)
\end{aligned}$$

Finally, $\langle\hat{\sigma}_z\rangle - \langle\hat{s}_z\,\hat{\sigma}_z\rangle$ can be obtained by transforming 2θ to $2\theta+\pi$ and replacing $\vec{\eta}$ with $\vec{\zeta}$ in (2.30).

For the sake of simplicity, we assume that $\vec{\xi}$ is the unit vector in the $x-$direction and that the unit vector $\vec{\chi}$ lies in the $y-$direction:

$$\vec{\xi}=(1,0,0), \qquad \vec{\chi}=(0,1,0), \qquad \vec{\xi}\times\vec{\chi}=(0,0,1). \qquad (2.31)$$

Therefore the components of the two vectors $\vec{\eta}$ and $\vec{\zeta}$ on $\vec{\xi}$ and $\vec{\chi}$ can be defined as

$$\begin{aligned}
&\eta_x \overset{def}{=} \vec{\xi}\cdot\vec{\eta}, \qquad \eta_y \overset{def}{=} \vec{\chi}\cdot\vec{\eta}, \qquad \eta_z=[\vec{\xi}\times\vec{\chi}]\cdot\vec{\eta} \\
&\zeta_x \overset{def}{=} \vec{\xi}\cdot\vec{\zeta}, \qquad \zeta_y \overset{def}{=} \vec{\chi}\cdot\vec{\zeta}, \qquad \zeta_z=[\vec{\xi}\times\vec{\chi}]\cdot\vec{\zeta}. \qquad (2.32)
\end{aligned}$$

The important issue in this part of parametrization is to consider the vectors $\vec{\chi}$ and $\vec{\xi}$ are perpendicular to each other which substantially simplifies the calculation of the expectation values. Within the above choice of the unit vectors we can relate the measured values of the population difference of the two energy-levels of A and S to the initial state of the system S as

$$\begin{pmatrix}\langle\hat{s}_z\rangle\\ \langle\hat{\sigma}_z\rangle\\ \langle\hat{s}_z\,\hat{\sigma}_z\rangle\end{pmatrix} = \mathcal{C}\begin{pmatrix}r_x\\ r_y\\ r_z\end{pmatrix}+\mathcal{F}, \qquad (2.33)$$

where $\mathcal{C}$ is a 3×3 matrix of the coefficients whose elements are given by

$$\begin{aligned}
c_{11} &= 0, \\
c_{12} &= \lambda \sin 2\theta \sin 2\phi \cos 2\psi, \\
c_{13} &= \sin 2\theta \sin 2\phi \sin 2\psi, \\
c_{21} &= (\eta_x + \zeta_x) \cos 2\phi + \lambda(\eta_x - \zeta_x) \cos 2\theta, \\
c_{22} &= (\eta_y + \zeta_y) \cos 2\psi + \lambda(\eta_y - \zeta_y) \cos 2\theta \cos 2\phi \cos 2\psi \\
&- \sin 2\psi \left[\lambda(\eta_z + \zeta_z) \cos 2\phi + (\eta_z - \zeta_z) \cos 2\theta\right], \\
c_{23} &= \lambda(\eta_y + \zeta_y) \sin 2\psi + (\eta_y - \zeta_y) \cos 2\theta \cos 2\phi \sin 2\psi \\
&+ \cos 2\psi \left[(\eta_z + \zeta_z) \cos 2\phi + \lambda(\eta_z - \zeta_z) \cos 2\theta\right], \\
c_{31} &= (\eta_x - \zeta_x) \cos 2\phi + \lambda(\eta_x + \zeta_x) \cos 2\theta, \\
c_{32} &= (\eta_y - \zeta_y) \cos 2\psi + \lambda(\eta_y + \zeta_y) \cos 2\theta \cos 2\phi \cos 2\psi \\
&- \sin 2\psi \left[\lambda(\eta_z - \zeta_z) \cos 2\phi + (\eta_z + \zeta_z) \cos 2\theta\right], \\
c_{33} &= \lambda(\eta_y - \zeta_y) \sin 2\psi + (\eta_y + \zeta_y) \cos 2\theta \cos 2\phi \sin 2\psi \\
&+ \cos 2\psi \left[(\eta_z - \zeta_z) \cos 2\phi + \lambda(\eta_z + \zeta_z) \cos 2\theta\right],
\end{aligned} \tag{2.34, 2.35}$$

and $\mathcal{F}$ is the vector of constants given by:

$$\mathcal{F} = \lambda \begin{pmatrix} \cos 2\theta \cos 2\phi \\ (\eta_y - \zeta_y) \sin 2\theta \sin 2\phi \\ (\eta_y + \zeta_y) \sin 2\theta \sin 2\phi \end{pmatrix}. \tag{2.36}$$

The elements of the initially unknown density matrix of S which are encoded by $\vec{r}$ are related to these expectation values, so they can be recovered if and only if the determinant of the coefficient matrix $\mathcal{C}$ is non-zero. With some algebra we can calculate the determinant of the coefficient matrix, represented by D, as

$$\begin{aligned}
\frac{8D}{\sin 2\theta \sin 2\phi} &= \frac{(1-\lambda^2) \sin 4\psi}{2} [(\cos 2\phi + \lambda \cos 2\theta)\, \eta_x \zeta_y \\
&- (\cos 2\phi - \lambda \cos 2\theta)\, \eta_y \zeta_x] \\
&+ \eta_z \zeta_x (\cos 2\phi - \lambda \cos 2\theta)[\lambda \cos 2\phi \\
&+ \cos 2\theta(\lambda^2 \cos^2 2\psi + \sin^2 2\psi)] \\
&- \eta_x \zeta_z (\cos 2\phi + \lambda \cos 2\theta)[\lambda \cos 2\phi \\
&- \cos 2\theta(\lambda^2 \cos^2 2\psi + \sin^2 2\psi)].
\end{aligned} \tag{2.37}$$

Thus the initial state of the system S can be determined from $\langle \hat{s}_z \rangle$, $\langle \hat{\sigma}_z \rangle$ and $\langle \hat{s}_z \, \hat{\sigma}_z \rangle$ provided that the determinant D is non-zero.
In what follows we consider two limiting cases: *i*) when the assistant is initially in a completely disordered state ($\lambda = 0$), and *ii*) when it starts its evolution from a pure state, i.e. $\lambda = 1$. Then we maximize the value of D over the parameters of $\hat{U}$ and reconstruct the initial state of S.

2.3.1 Assistant with completely disordered initial state

Inserting $\lambda = 0$ in the expression for the determinant given by (2.37) yields

$$\begin{aligned} D &= \frac{1}{16} \sin 2\theta \sin 4\phi \sin 2\psi [\cos 2\psi (\eta_x \zeta_y - \eta_y \zeta_x) \\ &+ \cos 2\theta \sin 2\psi (\eta_z \zeta_x + \eta_x \zeta_z)]. \end{aligned} \tag{2.38}$$

It is clear that this determinant is maximized over the parameter ϕ if $\phi = \pm \frac{\pi}{8}$. Furthermore, the maximum of $D = \frac{1}{16} \sin 2\theta \sin 2\psi [\cos 2\psi (\eta_x \zeta_y - \eta_y \zeta_x) + \cos 2\theta \sin 2\psi (\eta_z \zeta_x + \eta_x \zeta_z)]$ over $\vec{\eta}$ and $\vec{\zeta}$ is reached when

$$\vec{\eta} = \vec{\zeta} = (\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}). \tag{2.39}$$

Thus we have

$$D = \frac{1}{16} \sin 2\theta \sin 2\psi \sqrt{1 - \sin^2 2\theta \sin^2 2\psi}. \tag{2.40}$$

The determinant (2.40) reaches its maximum value $1/32$ for $\theta = \pi/8$ and $\psi = \pi/4$. Such non-zero determinant guarantees the procedure of inversion and characterizing the initial state of the system. Inserting the above values of the parameters in the expressions for the expectation values of the z-component of spins, (2.29), (2.30) we can reconstruct the initial density matrix of S:

$$\begin{aligned} r_x &= 2\langle \hat{\sigma}_z \rangle, \\ r_y &= -2\langle \hat{s}_z \, \hat{\sigma}_z \rangle, \\ r_z &= 2\langle \hat{s}_z \rangle. \end{aligned} \tag{2.41}$$

We see that for a suitable choice of the evolution operator $\hat{U}$ it is possible to determine the initial state of a spin-1/2 system implying an assistant which is initially in completely disordered state.

2.3.2 Assistant with a pure initial state

Considering the assistant starts its evolution from a pure state is equivalent to set $\lambda = 1$ in the general expression for the determinant given by (2.37), which yields

$$D = \frac{1}{8}\sin 2\theta \sin 2\phi(\cos^2\phi - \cos^2\theta)(\eta_z\zeta_x - \eta_x\zeta_z). \tag{2.42}$$

The maximum value of the determinant, $|D| = 1/12\sqrt{3}$, in this case is reached when $\vec{\eta}$ and $\vec{\zeta}$ are perpendicular to each other

$$\vec{\eta} = (\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}), \qquad \vec{\zeta} = (\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}), \tag{2.43}$$

$\phi = \pm\frac{\pi}{4}$, and $\sin^2(2\theta) = 1/3$ while ψ which determines a phase in the unitary operator remains an arbitrary parameter.
Thus the initial state of S can be determined as

$$\begin{aligned} r_x &= \sqrt{3}\langle\hat{s}_z\,\hat{\sigma}_z\rangle, \\ r_y &= \sqrt{3}\left(\cos 2\psi\langle\hat{s}_z\rangle - \sin 2\psi\langle\hat{\sigma}_z\rangle\right), \\ r_z &= \sqrt{3}\left(\sin 2\psi\langle\hat{s}_z\rangle + \cos 2\psi\langle\hat{\sigma}_z\rangle\right). \end{aligned} \tag{2.44}$$

If we choose the phase $\psi = \pi/4$, we get

$$\begin{aligned} r_x &= \sqrt{3}\langle\hat{s}_z\,\hat{\sigma}_z\rangle, \\ r_y &= -\sqrt{3}\langle\hat{\sigma}_z\rangle, \\ r_z &= \sqrt{3}\langle\hat{s}_z\rangle. \end{aligned} \tag{2.45}$$

We conclude this section by mentioning that one can fully determine the unknown state of a spin-$\frac{1}{2}$ system by simultaneous measurements of the population difference of the system and the assistant provided that the determinant D is non-zero. Very small determinant means the errors made in the measurement procedures are substantial and one cannot infer the initial state from the gathered data. Comparing the maximum values of D when the assistant is in pure state and when it is in completely random state, shows that there is not much gain in using an assistant in a pure state. In other words, it is possible to characterize the initial state of S by coupling it to an assistant being in completely disordered state. Such assistants are much easier to produce from a technical point of view.

2.4 The Jaynes-Cummings model

In previous section we did not restrict ourselves to a specific Hamiltonian in order to describe the interaction between S and A. The next section will be devoted to the case where a single coherent mode of electromagnetic field plays the role of the assistant. In this case the interaction Hamiltonian is known as the Jaynes-Cummings model. We will first introduce the model and then implement it for characterizing the initial state of a two-level atom by simultaneous measurements.

The Jaynes-Cummings model (JCM) [23] plays an important role in quantum optics and atomic physics [24–26]. This model describes the interaction of a two-level atom with a single mode of electromagnetic field, and it was employed by Jaynes and Cummings for studying the quantum features of spontaneous emission. Later on, the model generated several non-trivial theoretical predictions such as collapse and revivals of the atomic population that are related to the discretness of the photon [27, 28]. These predictions were successfully tested in experiments [29]. In particular, the model explains experimental results on one-atom masers [29], and on the passage of (Rydberg) atoms through cavities [30–33]. JCM is also used for describing quantum correlation and formation of macroscopic quantum states. It was recently employed in quantum information theory [34, 35]. More recently, the JCM has found applications in semiconductors [36], and in Josephson junctions [37–39]. JCM has denoted a family of models, since the original model of Jaynes and Cummings. It has been generalized several times for more adequate description of the atom-field interaction (e.g., multi-mode fields, multi-level atoms, damping) [40–42]. We shall however study the simplest original realization of JCM that involves a two-level atom interacting with a single mode of electromagnetic field. In particular, we neglect the effects of noise and dissipation. This situation has direct experimental realizations [29, 43, 44] . For instance with superconducting microcavities one can achieve ~ 0.1s for the average lifetime of the cavity photon. This is much larger than the typical field-atom interaction time $\sim 100 - 500\mu s$ [30, 33].

2.4.1 Atom-field interaction Hamiltonian

The Jaynes-Cummings Hamiltonian is an specific type of a general atom-field interaction Hamiltonian. In this section we cast the JC Hamiltonian from this interaction Hamiltonian.

The interaction of a radiation field $\hat{\vec{E}}$ with an atom within the dipole approximation can be written as

$$\hat{H} = \hat{H}_A + \hat{H}_F - e\hat{\vec{\varrho}} \cdot \hat{\vec{E}}. \tag{2.46}$$

Here $\hat{H}_A$ and $\hat{H}_F$ represent the Hamiltonian of the atom and field, respectively, in the absence of interaction. $\vec{\varrho}$ is the position of the electron and $\hat{\vec{E}}$ represents the electric field.

In the dipole approximation the atom size is considered to be much smaller than the wavelength of the radiation field. Hence, the field is assumed to be uniform over the whole atom.

The energy of the free field is given in terms of the bosonic creation $\hat{a}_k^\dagger$ and annihilation $\hat{a}_k$ operators, where k is the number of modes. Neglecting the zero-point energy we have

$$\hat{H}_F = \sum_\lambda \sum_k \hbar \nu_{k\lambda} \hat{a}_{k\lambda}^\dagger \hat{a}_{k\lambda}, \tag{2.47}$$

where ν_k is the frequency of the $k-$th mode, and λ is the polarization index.

$\hat{H}_A$ and $e\hat{\vec{r}}$ can be expressed by the atom transition operator

$$\hat{\sigma}_{ij} = |i\rangle\langle j|, \tag{2.48}$$

where $\{|i\rangle\}$ represents a complete set of atomic energy eigenstates, i.e.,

$$\sum_i |i\rangle\langle i| = 1. \tag{2.49}$$

It then follows

$$\hat{H}_A = \sum_i E_i |i\rangle\langle i| = \sum_i E_i \hat{\sigma}_{ii}, \tag{2.50}$$

also

$$e\vec{\varrho} = \sum_{i,j} e|i\rangle\langle i|\hat{\vec{\varrho}}|j\rangle\langle j| = \sum_{i,j} \vec{\mathcal{D}}_{ij} \hat{\sigma}_{ij}. \tag{2.51}$$

The coefficient $\vec{\mathcal{D}}_{ij} = e\langle i|\hat{\vec{\varrho}}|j\rangle$ is the electric-dipole transition matrix element.

In the dipole approximation, the electric field operator is evaluated at the position of the point atom. For the atom being at the origin it the follows

$$\hat{\vec{E}} = \sum_{k,\lambda} \vec{\varepsilon}_{k\lambda} \mathcal{E}_{k\lambda} (\hat{a}_{k\lambda} + \hat{a}_{k\lambda}^\dagger), \tag{2.52}$$

where $\mathcal{E}_{k\lambda} = (\hbar\nu_{k\lambda}/2\epsilon_0 V)^{1/2}$. Here V represents the volume. $\vec{\varepsilon}_{k\lambda}$ are the real unit vectors of the linear polarization basis.

Inserting $\hat{H}_A, \hat{H}_F, e\hat{\vec{r}}$, and $\hat{\vec{E}}$ from Eqs. (2.47), (2.50), (2.51), and (2.52) into the total Hamiltonian given by (2.46) for a polarized field we get

$$\hat{H} = \sum_k \hbar\nu_k \hat{a}_k^\dagger \hat{a}_k + \sum_i E_i \hat{\sigma}_{ii} + \hbar \sum_{i,j} \sum_k g_k^{ij} \hat{\sigma}_{ij} (\hat{a}_k + \hat{a}_k^\dagger), \tag{2.53}$$

where

$$g_k^{ij} = -\frac{\vec{\mathcal{D}}_{ij} \cdot \vec{\varepsilon}_k \mathcal{E}_k}{\hbar}. \tag{2.54}$$

We now proceed to the case of a two-level atom and single mode radiation field.

We denote the eigenstates of the two-level atom by $|+\rangle$, and $|-\rangle$ with the eigenenergies E_+, and E_-, respectively.

We notice that in this case g_k^{ij} reduces to a single scalar parameter, known as the atom-field coupling constant:

$$g_k^{ij} = g. \tag{2.55}$$

The energy of the two-level system reads as

$$\hat{H}_A = E_+ |+\rangle\langle+| + E_- |-\rangle\langle-|. \tag{2.56}$$

Defining $\hat{\sigma}_z$ as

$$\hat{\sigma}_z = \frac{1}{2} \left(|+\rangle\langle+| - |-\rangle\langle-| \right), \tag{2.57}$$

the Hamilton of the atom up to an irrelevant constant energy reads

$$\hat{H}_A = \hbar\omega\hat{\sigma}_z, \tag{2.58}$$

where $\omega = (E_+ - E_-)/\hbar$ is the atom frequency and a shift $(E_+ + E_-)/2$ has been omitted.

Therefore, the Hamiltonian for the interaction of a two-level system with a single mode field reads

$$\hat{H} = \hbar\omega\hat{\sigma}_z + \hbar\nu\hat{a}^\dagger\hat{a} + \hbar g(\hat{a}^\dagger + \hat{a})\hat{\sigma}_x \tag{2.59}$$

In quantum optical realizations of JCM the coupling constant g is normally much smaller than ω and ν, e.g., it is typical to have $\nu \sim \omega \sim g \times 10^5$ ($\omega \sim \nu$ =10GHz, $g \sim \Delta$ =10–100KHz). Therefore the subsequent reasoning based on the interaction representation is legitimate. We note that in the interaction representation the coupling term reads:

$$\hbar g(\hat{a}^\dagger\, e^{-i\nu t} + \hat{a}\, e^{i\nu t})(\hat{\sigma}_-\, e^{-i\omega t} + \hat{\sigma}_+ e^{i\omega t}), \tag{2.60}$$

where we introduced the raising and lowering spin operators

$$\hat{\sigma}_+ = \hat{\sigma}_x + i\hat{\sigma}_y, \qquad \hat{\sigma}_- = \hat{\sigma}_x - i\hat{\sigma}_y,$$

with the following commutation rules:

$$[\hat{\sigma}_\pm, \hat{\sigma}_z] = \mp\hat{\sigma}_\pm, \;\; [\hat{\sigma}_+, \hat{\sigma}_-] = 2\hat{\sigma}_z, \;\; \hat{\sigma}_+\hat{\sigma}_- + \hat{\sigma}_-\hat{\sigma}_+ = 1.$$

We now apply the rotating wave approximation to (2.59): the atom and field frequencies are assumed to be close to each other, therefore the factors proportional to $e^{\pm it(\nu+\omega)}$ in (2.59) oscillate in time much stronger than those proportional to$e^{\pm it(\nu-\omega)}$. Thus the rapidly oscillating terms can be neglected within this approximation and we arrive at

$$\hat{H} = \hbar\omega\hat{\sigma}_z + \hbar\nu\hat{a}^\dagger\hat{a} + \hbar g(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^\dagger), \tag{2.61}$$

which is called the JC Hamiltonian We shall denote

$$\Delta \stackrel{def}{=} \omega - \nu,$$

for the detuning parameter. For our future purposes we note that Δ is a tunable parameter. Within the atom-cavity realizations of the JCM, the detuning Δ can be controlled by changing the shape of the cavity and this changes the mode frequency ν. Alternatively, Δ can be changed via the atom frequency ω by applying an electric field across the cavity [45]. Then ω is modified due to the Stark effect.

The above standard derivation of (2.61) is based on small detuning Δ and weak atom-mode coupling g:

$$\Delta \ll \min(\omega, \nu), \qquad g \ll \min(\omega, \nu).$$

Both these conditions are normally satisfied for quantum optical realizations of JCM.

There are however situations—especially for the solid state physics applications of the Hamiltonian (2.59)—where the atom-field interaction constant g is not small. It is useful to know that sometimes the counter-rotating terms $\propto e^{\pm it(\nu+\omega)}$ vanish due to specific selection rules, and then JCM applies in the strong-coupling situation as well. This can be achieved by proper choice of circular polarization basis for the electromagnetic field [46].

In the next section we use the fact that the Hamiltonian (2.61) is exactly solvable and derive the corresponding unitary time evolution operator. Having that at hand, we would be able to calculate the expectation value of the observables of the overall system at any time t.

2.4.2 The unitary time evolution operator

In this section, we show that the time evolution operator of the Jaynes-Cummings (JC) Hamiltonian can be calculated exactly.
We begin with rewriting the JC Hamiltonian as the sum of two commuting terms:

$$\hat{H} = \hat{H}_1 + \hat{H}_2,$$

where

$$\hat{H}_1 = \hbar\nu\hat{\sigma}_z + \hbar\nu\hat{a}^\dagger\hat{a}, \tag{2.62}$$

$$\hat{H}_2 = \hbar\Delta\hat{\sigma}_z + \hbar g\left(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^\dagger\right). \tag{2.63}$$

Since the two parts of the JC Hamiltonian commute with each other, the unitary time evolution operator can be factorized:

$$\hat{U}(t,0) = e^{-i\hat{H}t/\hbar} = e^{-i\hat{H}_1 t/\hbar}e^{-i\hat{H}_2 t/\hbar}. \tag{2.64}$$

The first factor in the expression (2.64) is diagonal:

$$\hat{U}_1(t) = e^{-i\hat{H}_1 t/\hbar} = e^{-i\nu t\hat{a}^\dagger\hat{a}}\begin{pmatrix} e^{-i\nu t/2} & 0 \\ 0 & e^{i\nu t/2}\end{pmatrix}. \tag{2.65}$$

In order to calculate $\hat{U}_2$, we expand the expression $e^{-i\hat{H}_2 t/\hbar}$:

$$\begin{aligned}\hat{U}_2(t) = e^{-i\hat{H}_2 t/\hbar} &= \sum_{n=0}^{\infty}\frac{(-it/\hbar)^n}{n!}(\hat{H}_2)^n \\ &= \sum_{n=0}^{\infty}(-i)^n\frac{t^n}{n!}\begin{pmatrix}\frac{\Delta}{2} & g\hat{a} \\ g\hat{a}^\dagger & -\frac{\Delta}{2}\end{pmatrix}^n,\end{aligned} \tag{2.66}$$

where we have inserted the expression (2.63) for $\hat{H}_2$.

Decomposing the matrix power series into even and odd powers, it is straight forward to see that for any integer number l, the even powers read

$$\begin{pmatrix} \frac{\Delta}{2} & g\hat{a} \\ g\hat{a}^\dagger & -\frac{\Delta}{2} \end{pmatrix}^{2l} = \begin{pmatrix} (\hat{\varphi}+g^2)^l & 0 \\ 0 & \hat{\varphi}^l, \end{pmatrix} \tag{2.67}$$

where

$$\hat{\varphi} = g^2\hat{a}^\dagger\hat{a} + \frac{\Delta^2}{4}. \tag{2.68}$$

Note that $\hat{\varphi}$ is not commuting with $\hat{a}$ and $\hat{a}^\dagger$. We notice that

$$\hat{a}\hat{\varphi} = (\hat{\varphi}+g^2)\hat{a}. \tag{2.69}$$

It then follows that for the odd powers we get

$$\begin{pmatrix} \frac{\Delta}{2} & g\hat{a} \\ g\hat{a}^\dagger & -\frac{\Delta}{2} \end{pmatrix}^{2l+1} = \begin{pmatrix} \frac{\Delta}{2}(\hat{\varphi}+g^2)^l & g(\hat{\varphi}+g^2)^l\hat{a} \\ g\hat{\varphi}^l\hat{a}^\dagger & -\frac{\Delta}{2}\hat{\varphi}^l \end{pmatrix}, \tag{2.70}$$

which then yields

$$\hat{U}_2(t) = \begin{pmatrix} \cos[t\sqrt{\hat{\varphi}+g^2}] - i\frac{\Delta}{2}\frac{\sin[t\sqrt{\hat{\varphi}+g^2}]}{\sqrt{\hat{\varphi}+g^2}} & -ig\frac{\sin[t\sqrt{\hat{\varphi}+g^2}]}{\sqrt{\hat{\varphi}+g^2}}\hat{a} \\ -ig\frac{\sin[t\sqrt{\hat{\varphi}}]}{\sqrt{\hat{\varphi}}}\hat{a}^\dagger & \cos[t\sqrt{\hat{\varphi}}] + i\frac{\Delta}{2}\frac{\sin[t\sqrt{\hat{\varphi}}]}{\sqrt{\hat{\varphi}}} \end{pmatrix}. \tag{2.71}$$

Equations (2.65) and (2.71) determine time evolution operator $\hat{U} = \hat{U}_1\hat{U}_2$. In the eigenbasis of the two-level system $\hat{U}$ reads:

$$\begin{aligned} \hat{U}(t) = {} & e^{-i\nu t(\hat{a}^\dagger\hat{a}+\frac{1}{2})}\left(\cos[t\sqrt{\hat{\varphi}+g^2}] - i\frac{\Delta}{2}\frac{\sin[t\sqrt{\hat{\varphi}+g^2}]}{\sqrt{\hat{\varphi}+g^2}}\right)|+\rangle\langle+| \\ & -ige^{-i\nu t(\hat{a}^\dagger\hat{a}+\frac{1}{2})}\frac{\sin[t\sqrt{\hat{\varphi}+g^2}]}{\sqrt{\hat{\varphi}+g^2}}\,\hat{a}|+\rangle\langle-| \\ & -ige^{-i\nu t(\hat{a}^\dagger\hat{a}-\frac{1}{2})}\frac{\sin t\sqrt{\hat{\varphi}}}{\sqrt{\hat{\varphi}}}\,\hat{a}^\dagger|-\rangle\langle+| \\ & +e^{-i\nu t(\hat{a}^\dagger\hat{a}-\frac{1}{2})}\left(\cos t\sqrt{\hat{\varphi}} + i\frac{\Delta}{2}\frac{\sin t\sqrt{\hat{\varphi}}}{\sqrt{\hat{\varphi}}}\right)|-\rangle\langle-|, \end{aligned} \tag{2.72}$$

where $|\pm\rangle$ are the eigenstates of $\hat{\sigma}_z$ with eigneenergies $E_\pm$.

The unitarity of $\hat{U}(t)$ is satisfied because of the identities

$$\begin{aligned} \frac{\sin\left[t\sqrt{\hat{\varphi}+g^2}\right]}{\sqrt{\hat{\varphi}+g^2}}\ \hat{a} &= \hat{a}\ \frac{\sin\left[t\sqrt{\hat{\varphi}}\right]}{\sqrt{\hat{\varphi}}}, \\ \cos\left[t\sqrt{\hat{\varphi}+g^2}\right]\ \hat{a} &= \hat{a}\ \cos\left[t\sqrt{\hat{\varphi}}\right]. \end{aligned} \tag{2.73}$$

Having $\hat{U}$ at hand, we can calculate any property of $S+A$ we wish.

2.5 Initial states

We consider the most general form of the initial state for the atom. This is described by some general mixed density matrix $\hat{\rho}_S$:

$$\begin{aligned} \hat{\rho}_S = &\left(\frac{1}{2}+r_z\right)|+\rangle\langle+| + (r_x - ir_y)\,|+\rangle\langle-| \\ &+ (r_x + ir_y)\,|-\rangle\langle+| + \left(\frac{1}{2}-r_z\right)|-\rangle\langle-|, \end{aligned} \tag{2.74}$$

where we have written the initial state of S in the eigen-basis of $\hat{\sigma}_z$, and where $\vec{r}$ defines unknown elements of the initial state of S.

For the assistant, we shall assume that the single cavity mode starts its evolution from a coherent state with a known parameter α:

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\,|n\rangle, \tag{2.75}$$

where $|\alpha\rangle$ is the eigenvector of the annihilation operator $\hat{a}$,

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle,$$

and where $|n\rangle$ is the eigenvector of the photon number operator $\hat{a}^\dagger\hat{a}$,

$$\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle.$$

The assumption (2.75) on the initial state of the field is natural since these are the kinds of fields produced by classical currents [47], and also, to a good approximation, by sufficiently intense laser fields.

We assume the system and the assistant are initially separated and do not interact with each other. As a result, the overall initial density matrix is factorized,

$$\hat{\rho}(0) = \hat{\rho}_S \otimes |\alpha\rangle\langle\alpha|. \tag{2.76}$$

The initial state of the field is given by

$$|\alpha\rangle\langle\alpha| = e^{-|\alpha|^2} \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{\alpha^n \alpha^{*m}}{\sqrt{n!}\sqrt{m!}} |n\rangle\langle m|. \tag{2.77}$$

The state of $S + A$ at a later time t can be calculated with the help of the unitary operator (2.72) calculated in section 2.4.2:

$$\hat{\rho}(t) = \hat{U}(t)\,\hat{\rho}(0)\,\hat{U}^{\dagger}(t). \tag{2.78}$$

Then the expectation value of any observable $\hat{\mathcal{O}}$ of the overall system at time t is

$$\langle\hat{\mathcal{O}}\rangle = \mathrm{tr}\left[\hat{\rho}(t)\hat{\mathcal{O}}\right]. \tag{2.79}$$

2.6 Commuting observables

The siplest set of two commuting observables of $S + A$ with which we can build up the initial state of the atom are the energies of each system, which are described by the atom population difference $\hat{\sigma}_z$ and $\hat{a}^{\dagger}\hat{a}$. Using (2.72), (2.74), (2.77), and (2.78), the atom population difference at later time t, denoted by $\langle\hat{\sigma}_z\rangle_t$ reads

$$\begin{aligned}
\langle\hat{\sigma}_z\rangle_t = {} & \frac{g^2}{2}\sum_{n=0}^{\infty}(n+1)(c_{n+1}-c_n)\frac{\sin^2(\Omega_n t/2)}{(\Omega_n t/2)^2} \\
& +4g\,r_x\sum_{n=0}^{\infty} c_n \frac{\sin(\Omega_n t/2)}{\Omega_n}\Im\{\chi_n(t)\} \\
& +4g\,r_y\sum_{n=0}^{\infty} c_n \frac{\sin(\Omega_n t/2)}{\Omega_n}\Re\{\chi_n(t)\} \\
& +r_z\left\{1 - g^2\sum_{n=0}^{\infty}(n+1)(c_{n+1}+c_n)\frac{\sin^2(\Omega_n t/2)}{(\Omega_n/2)^2}\right\},
\end{aligned} \tag{2.80}$$

where r_x, r_y, and r_z, are the unknown elements of the initial atom density matrix, which we want to find out. $\Re$ and $\Im$ stand for the real and the imaginary parts, respectively. The parameters $\chi_n(t)$, c_n are defined as

$$\chi_n(t) \stackrel{def}{=} \alpha \left[\cos\left(\frac{\Omega_n\, t}{2}\right) + i\Delta\, \frac{\sin\left(\Omega_n t/2\right)}{\Omega_n}\right], \tag{2.81}$$

and

$$c_n \stackrel{def}{=} e^{-|\alpha|^2}\, \frac{\alpha^{2n}}{n!}, \tag{2.82}$$

where the corresponding Rabi frequency, Ω_n, is defined as

$$\Omega_n \stackrel{def}{=} \sqrt{4(n+1)g^2 + \Delta^2}. \tag{2.83}$$

The average number of photons in the cavity, $\langle \hat{a}^\dagger \hat{a} \rangle_t$, can be calculated in a similar way

$$\begin{aligned}
\langle \hat{a}^\dagger \hat{a} \rangle_t = & \sum_{n=0}^{\infty} n c_n - \frac{g^2}{2} \sum_{n=0}^{\infty} (n+1)(c_{n+1} - c_n) \frac{\sin^2(\Omega_n t/2)}{(\Omega_n/2)^2} \\
& -4g\, r_x \sum_{n=0}^{\infty} c_n \frac{\sin\left(\Omega_n t/2\right)}{\Omega_n} \Im\{\chi_n(t)\} \\
& -4g\, r_y \sum_{n=0}^{\infty} c_n \frac{\sin\left(\Omega_n t/2\right)}{\Omega_n} \Re\{\chi_n(t)\} \\
& +g^2\, r_z \sum_{n=0}^{\infty} (n+1)(c_{n+1} + c_n) \frac{\sin^2(\Omega_n t/2)}{(\Omega_n/2)^2}.
\end{aligned} \tag{2.84}$$

The correlation of the two observables, $\langle \hat{\sigma}_z\, \hat{a}^\dagger \hat{a} \rangle_t$, which amounts to the number of coincidences, reads

$$\begin{aligned}
\langle \hat{\sigma}_z\, \hat{a}^\dagger \hat{a} \rangle_t = & \frac{g^2}{4} \sum_{n=0}^{\infty} (n+1) \left[(2n+3)c_{n+1} - (2n+1)c_n\right] \frac{\sin^2(\Omega_n t/2)}{(\Omega_n/2)^2} \\
& +2g\, r_x \sum_{n=0}^{\infty} c_n (2n+1) \frac{\sin\left(\Omega_n t/2\right)}{\Omega_n} \Im\{\chi_n(t)\} \\
& +2g\, r_y \sum_{n=0}^{\infty} c_n (2n+1) \frac{\sin\left(\Omega_n t/2\right)}{\Omega_n} \Re\{\chi_n(t)\} \\
& +r_z \left\{ \sum_{n=0}^{\infty} n c_n - \frac{(n+1)g^2}{2} \left[(2n+3)c_{n+1} + (2n+1)c_n\right] \frac{\sin^2(\Omega_n t/2)}{(\Omega_n/2)^2} \right\}.
\end{aligned} \tag{2.85}$$

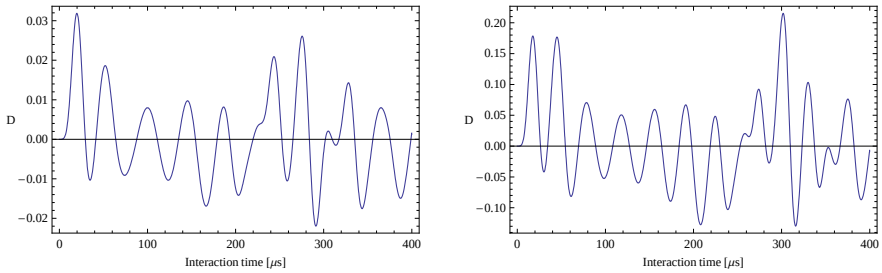
Expectedly, these three quantities, i.e., the atom population difference $\langle\hat{\sigma}_z\rangle_t$, the average number of photons $\langle\hat{a}^\dagger\hat{a}\rangle_t$, and the correlation of these two observables $\langle\hat{\sigma}_z\,\hat{a}^\dagger\hat{a}\rangle_t$ are linearly related to the three unknown parameters r_x, $\langle r_y$, r_z of the initial atom density matrix:

$$\begin{pmatrix} \langle\hat{\sigma}_z\rangle_t \\ \langle\hat{a}^\dagger\hat{a}\rangle_t \\ \langle\hat{\sigma}_z\,\hat{a}^\dagger\hat{a}\rangle_t \end{pmatrix} = \mathcal{M}\begin{pmatrix} r_x \\ r_y \\ r_z \end{pmatrix} + \mathcal{B}, \qquad \mathcal{B} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}. \tag{2.86}$$

The elements of the 3×3 matrix $\mathcal{M}$ and the vector $\mathcal{B}$ are read off from Eqs. (2.80) – (2.85). They depend on the parameter α of the initial assistant state, on the detuning parameters Δ, coupling g of the JC Hamiltonian, and on the interaction time t. Thus, if the matrix $\mathcal{M}$ is non-singular, i.e., the determinant of $\mathcal{M}$ is not zero, one can invert $\mathcal{M}$ and express the unknown parameters of the initial atom density matrix via known quantities. Although the elements of $\mathcal{M}$ are complicated, the determinant itself is much simpler. It takes the explicit form

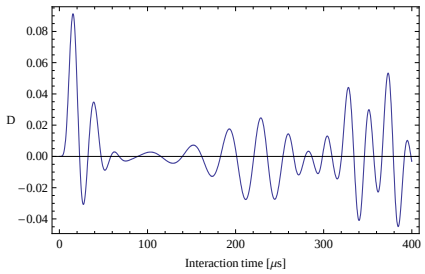
$$D(t) \stackrel{def}{=} \det[\mathcal{M}] = 4\Delta\, g^2 e^{-2|\alpha|^2} \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{|\alpha|^{2(n+m+1)}}{n!m!}(n-m) \times$$
$$\left[\frac{\sin^2(\Omega_n t/2)\ \sin\Omega_m t}{\Omega_n^2\Omega_m} - \frac{\sin^2(\Omega_m t/2)\ \sin\Omega_n t}{\Omega_m^2\Omega_n}\right]. \tag{2.87}$$

We note that the determinant $D(t)$ is real. At the initial time $t = 0$, $D(0)$ is naturally zero, since the initial state of the overall system is factorized. According to the expression (2.87) a non-zero detuning Δ is essential for a non vanishing determinant. Thus some non-zero detuning is crucial for the present scheme of the state determination. Although in the resonant case, i.e., when the frequency of the two-level system is equal to the cavity mode frequency, it is not possible to determine the initial state of a two-level system by measuring the the energies of the system and the assistant, however, this scheme is still applicable for spin-$\frac{1}{2}$ systems because in order to recover the initial state of the spin-$\frac{1}{2}$ system one can measure the transversal component of spin (x or y component) instead of the z component [48]. But in general, for two-level systems other than spins, it is rather difficult to measure the transversal component since it cannot be defined well. While the z component of quasi-spin is related to the level occupation and thus the energy of the two-level system. The crucial point in this case is that

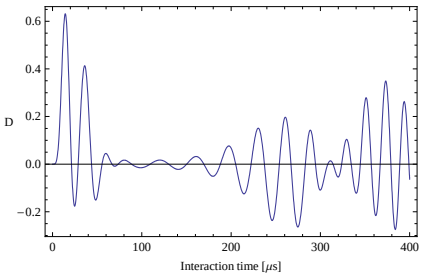


(a) $\bar{n} = 2, \Delta = 10$ KHz.

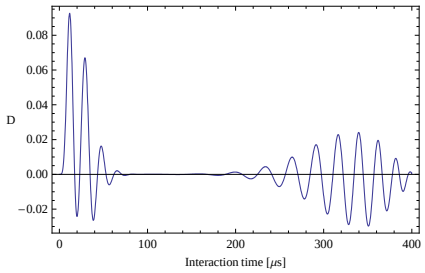
(b) $\bar{n} = 2, \Delta = 100$ KHz.



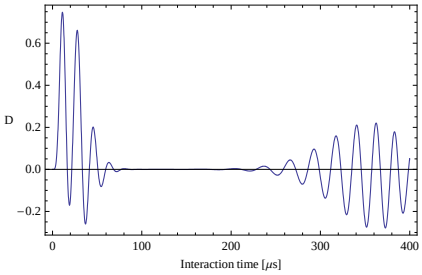
(c) $\bar{n} = 5, \Delta = 10$ KHz.



(d) $\bar{n} = 5, \Delta = 100$ KHz.



(e) $\bar{n} = 10, \Delta = 10$ KHz.



(f) $\bar{n} = 10, \Delta = 100$ kHz.

Figure 2.1: The dynamics of the determinant of the matrix $\mathcal{M}$ in the Jaynes-Cummings model for different values of the mean photon number in the cavity $\bar{n} = 2, 5, 10$ with two detuning parameters: $\Delta = 10$ KHz and $\Delta = 100$ KHz The coupling constan $g = 50$ KHz in all different cases.

there should be a detuning between the frequency of the field and that of the system of interest in order to invert the relevant relations between simultaneously measured observables in one hand and the elements of the initial density matrix of the two-level system on the other hand [20].
It is seen in Figs. 2.1(a)–2.1(f) that for a non-zero detuning, the determinant $D(t)$ is non-zero for a certain initial period $t > 0$. On the other hand, large

$D(t)$ implies that the state of the atom and the field are entangled [49]. Comparing figures Fig. 2.1(a) and Fig. 2.1(c) we see that although higher initial photon numbers $\bar{n}$ lead to bigger values for the determinant, they cause rapid oscillations in the value of the determinant. This makes the measurement process more difficult. (Note in this context that the determinant depends on the absolute value of α and $\bar{n} = |\alpha|^2$ is the average number of photons.)

If the average number of photons $\bar{n} = |\alpha|^2$ in the initial state of the field is sufficiently large, the determinant is nearly zero for intermediate times; see Figs. 2.1(e) and 2.1(f). This collapse can be understood by looking at (2.87). It has the same origin as the collapse of the atomic population difference well known for the JCM [26]. Each term in the right hand side of (2.87) oscillates with a different frequency. With time these oscillations get out of phase and $D(t)$ vanishes (collapses). However, since the number of significant oscillations in $D(t)$ is finite, they partially get in phase for later times producing the revival of $D(t)$, as seen in the Figs. 2.1(e) and 2.1(f).

It is seen that D does not depend on separate frequencies ω and ν of the two-level system and the field, only their difference $\Delta = \omega - \nu$ is relevant. This is due to the choice of the measurement basis—see the left hand side of (2.86)—that involves quantities which are constants of motion for $g \to 0$. The value of $D(t)$ changes by varying the detuning parameter Δ. Comparing the figures Fig. 2.1(a) with Fig. 2.1(b), Fig. 2.1(c) with Fig. 2.1(d), and Fig. 2.1(e) with Fig. 2.1(f) one observes that the value of the highest peak of $D(t)$ increases by an order of magnitude when the detuning parameter changes from 10kHz to 100kHz. Note that in Eq. (2.87) for the determinant $D(t)$ the contribution from the diagonal $n = m$ matrix elements of the assistant initial state $|\alpha\rangle\langle\alpha|$ cancels out. Thus, it is important to have an initial state of the assistant with non-zero diagonal elements in the $\{|n\rangle\}$ basis. In other words, if we consider an initial Gibbsian state for the electromagnetic field, i.e., a thermal bath at equilibrium with temperature T, the determinant vanishes and we cannot deduce the initial state of the atom by performing simultaneous measurements of the bath's photon number and the population difference of the atom beam.

The principal message of this section is that the determinant $D(t)$ is not zero for a realistic range of the parameters. This means that the initial unknown state of the two level system can be determined by specifying the average atom population difference $\langle\hat{\sigma}_z\rangle_t$, the average number of photons $\langle\hat{a}^\dagger\hat{a}\rangle_t$, and their correlation $\langle\hat{\sigma}_z\,\hat{a}^\dagger\hat{a}\rangle_t$. These quantities are obtained from

measuring two commuting observables: the atom population difference $\hat{\sigma}_z$ and the photon number $\hat{a}^\dagger\hat{a}$. Having at hand the proper measurement data for these two observables, one can calculate $\langle\hat{\sigma}_z\rangle_t$, $\langle\hat{a}^\dagger\hat{a}\rangle_t$, and find $\langle\hat{\sigma}_z\,\hat{a}^\dagger\hat{a}\rangle_t$ via the number of coincidences.

2.6.1 Random interaction time

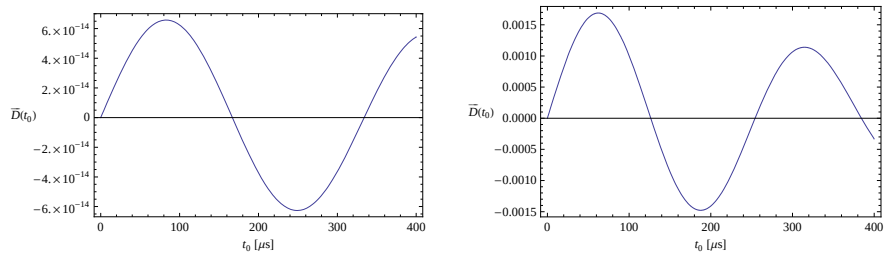
We saw in the previous sections that the success of the presented scheme is to a large extent determined by the ability to select properly the interaction time t, since this ultimately should ensure a non-zero (and sufficiently large) determinant $D(t)$ (It is clear that a small determinant will amplify numerical errors. This is illustrated in appendix B.

To quantify the robustness of the presented scheme it is reasonable to assume that there is no perfect control in choosing the interaction time. To this end let us assume that the interaction time t is a random, Gaussian distributed quantity centered at t_0 with a dispersion σ and that an ensemble of measurements is performed to map out this spread. The corresponding probability distribution $P(t)$ of thus reads

$$P(t) = \frac{1}{2\pi\sigma}\, e^{-(t-t_0)^2/(2\sigma)}. \tag{2.88}$$

We notice that the expectation value of each observable as it is described in section 2.2, is calculated by making an its ensemble average. Now we have to take into account that the repeated measurement of counting the number of the photon in the cavity and the population difference of atoms are performed at a random t in each set of measurement, which obeys the Gaussian distribution. Thus we have to perform a time-average in the relevant time window as well. Since we just want to get a rough estimation about the consequence of such way of measurement on the value of the determinant, we avoid the tedious time-averaging calculation of $\langle\hat{a}^\dagger\rangle$, $\langle\hat{\sigma}_z\rangle$, and their correlation by making a shortcut and perform the time-averaging of the determinant itself.
Averaging the determinant $D(t)$ over this distribution yields

$$\begin{aligned}\overline{D}(t_0) = 4\Delta\, g^2 e^{-2|\alpha|^2} \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{|\alpha|^{2(n+m+1)}}{n!m!} \times \\ \times(n-m)\left[w(\Omega_n,\Omega_m;t_0) - w(\Omega_m,\Omega_n;t_0)\right],\end{aligned} \tag{2.89}$$



(a) $\Delta = 10$ KHz, $\sigma = 0.1\mu$s (b) $\Delta = 100$ KHz, $\sigma = 0.01\mu$s

Figure 2.2: The time averaged determinant $\bar{D}$ in the Jaynes-Cummings model as a function of t_0 when the mean photon number in the cavity is $\bar{n} = 2$, and $g = 50$ KHz for different values of Δ and σ; see Eqs. (2.88)–(2.90).

where

$$\begin{aligned} w(\Omega_n, \Omega_m; t_0) &= \frac{1}{4\Omega_n^2 \Omega_m} \Big\{ 2e^{-\frac{\sigma}{2}{\Omega_m}^2} \sin[t_0 \Omega_m] \\ &- e^{-\frac{\sigma}{2}(\Omega_m+\Omega_n)^2} \sin[t_0(\Omega_m + \Omega_n)] \\ &- e^{-\frac{\sigma}{2}(\Omega_m-\Omega_n)^2} \sin[(\Omega_m - \Omega_n)t_0] \Big\}. \end{aligned} \tag{2.90}$$

It is seen that the oscillations of $D(t)$ turn after averaging into exponential factors $e^{-\frac{\sigma^2}{2}(\Omega_m \pm \Omega_n)^2}$ and $e^{-\frac{\sigma^2}{2}\Omega_m^2}$ in (2.89, 2.90), due to which the averaged determinant $\overline{D}(t_0)$ gets suppressed for a sufficiently large "indeterminacy" σ. This suppression is illustrated in Fig. 2.2(a) and Fig. 2.2(b). By comparing Fig. 2.2(a) and Fig. 2.2(b) we realize that when the dispersion σ grows by one order of magnitude, the value of the averaged determinant drops dramatically.

2.7 Maximum likelihood method

In section 2.5 we have shown how one determines the initial spin density matrix of a spin-$\frac{1}{2}$ system given the three averages $\langle \hat{\sigma}_z \rangle_t$, $\langle \hat{a}^\dagger \hat{a} \rangle_t$, and $\langle \hat{\sigma}_z \, \hat{a}^\dagger \hat{a} \rangle_t$. However, there is one important issue about this method: the recovered state from the above mentioned three averages might not correspond to a physical state because of experimental noise. By a physical state we mean a density matrix which is Hermitian, semipositive matrix with unit trace. In order to

avoid this problem, we employ the method of "maximum likelihood" reconstruction [50,51] in the following section. In this approach the density matrix that is "mostly likely" to have produced the above mentioned measured data set is determined by numerical optimization.

Our scheme operates by measuring only the commuting variables. As a result, for the approximate state reconstruction we do not need anything beyond the most standard (classical) Maximum Likelihood (ML) method. Since one measures the number of photons and the spin direction along the z-axes (these quantities are represented by the operators $\hat{a}^\dagger\hat{a}$ and $\hat{\sigma}_z$, respectively), the incomplete data in our case means that we are given frequencies $\nu_a(m)$ of events, where one registered m photons ($m = 0, 1, \ldots$), and where, simultaneously, the spin component assumed values $a = \pm 1$. In the ML method the probabilities $p_a(m)$ (given the frequencies $\nu_a(m)$) are obtained by maximizing the likelihood function over $p_a(m)$ [1]

$$L[p_a(m)] = \sum_{a=\pm 1} \sum_{m=0}^{\infty} \nu_a(m) \ln [p_a(m)] \,. \tag{2.91}$$

This maximization over $p_a(m)$ is to be carried out in the presence of relevant constraints. For our case the initial spin density matrix $\hat{\rho}_S$ must be a positive-definite, normalized matrix. Thus we get a single constraint

$$r_x^2 + r_y^2 + r_z^2 \leq 1. \tag{2.92}$$

Working out (2.86) we write this constraint as a function of the probabilities $p_a(m)$:

$$(u - \mathcal{B})^T \mathcal{C} (u - \mathcal{B}) \leq 1, \tag{2.93}$$

where ^{T} means the transpose of a matrix.

$$\mathcal{C} \stackrel{def}{=} (\mathcal{M}\mathcal{M}^T)^{-1}. \tag{2.94}$$

The matrix $\mathcal{M}$ and the vector $\mathcal{B}$ are defined in (2.86), and where finally

$$u = \begin{pmatrix} \sum_{a=\pm 1} \sum_{m=0}^{\infty} a \, p_a(m) \\ \sum_{a=\pm 1} \sum_{m=0}^{\infty} m \, p_a(m) \\ \sum_{a=\pm 1} \sum_{m=0}^{\infty} a \, m \, p_a(m) \end{pmatrix}. \tag{2.95}$$

[1] Equivalently, one can minimize over $p_a(m)$ the relative entropy $\sum_{a=\pm 1} \sum_{m=0}^{\infty} \nu_a(m) \ln \frac{\nu_a(m)}{p_a(m)}$. This measure of distinguishability between $p_a(m)$ and $\nu_a(m)$ is equal to zero if and only if $p_a(m) = \nu_a(m)$.

If the constraint (2.93) is satisfied automatically, the maximization of $\mathcal{L}[p_a(m)]$ in (2.91) produces

$$p_a(m) = \nu_a(m), \tag{2.96}$$

i.e., that the sought probabilities are equal to the frequencies, as one would expect intuitively [52]. However, in general this constraint is not satisfied automatically and has to be included explicitly in the maximization of $\mathcal{L}[p_a(m)]$ over $p_a(m)$. Indeed, looking at (2.91) and (2.93) we may deduce qualitatively that the constraint (2.93) will be satisfied automatically by (2.96), if the frequencies are not very far from the actual probabilities (the ones that would be obtained in the perfect experiment) and, simultaneously, the determinant $\det[\mathcal{M}]$ is not very close to zero.

2.8 Conclusion

In this chapter we described a method for quantum state tomography. The usual way of solving this inverse problem of quantum mechanics is to make measurements of non-commuting quantities. Single apparatus tomography proceeds differently employing controlled interaction and measuring commuting observables. This is done via coupling the system of interest to an auxiliary system (assistant) that starts its evolution from a known state. The essence of the method is that the proper coupling is able to transfer the information on the initial state of the system to a commuting basis of observables for the composite system (system + assistant).

It is important to implement the single-apparatus tomography for a situation with a physically transparent measurement base and with a realistic system-assistant interaction. Here we carried out this program for a two-level atom (system) interacting with a single mode of electromagnetic field (assistant). The atom-field interaction is given by the Jaynes-Cummings Hamiltonian, which has direct experimental realizations in quantum optics [25,29–33], superconductivity [37–39], semiconductor physics [36], etc. As the measurement base we have taken the simplest set of observables related to the energies of the atom and field: population difference of the atoms $\hat{\sigma}_z$ and the number of photons $\hat{a}^\dagger\hat{a}$ in the field. We have shown that one can determine the unknown initial state of the atom via post-interaction values of 1) the average atomic population difference $\langle\hat{\sigma}_z\rangle$, 2) the average number of photons

$\langle \hat{a}^\dagger \hat{a} \rangle$ and 3) the correlation of these quantities $\langle \hat{\sigma}_z \, \hat{a}^\dagger \hat{a} \rangle$. The third quantity does not need a separate measurement, since it can be recovered from the simultaneous measurement of the two basic observables $\hat{\sigma}_z$ and $\hat{a}^\dagger \hat{a}$.

Since our scheme is based on measuring commuting observables, we can apply the classical Maximum Likelihood setup for an approximate reconstruction of the unknown density matrix given the incomplete (noisy) measurement data.

CHAPTER 3

Spin Cooling and Polarization Transfer

In this chapter the spin polarization transfer among two non-interacting spatially separated spins coupled to a common heat bath is studied. The bath is modeled by an ensemble of harmonic oscillators. Under certain considerations the model is exactly solvable making it possible to derive the exact time-evolution of the spin components. It is shown that by introducing external forces in the form of short and strong pulses acting on one spin one can purify its state, i.e. can make relatively pure states from initially mixed ones in the presence of the other spin.

3.1 Introduction

It was shown in the previous chapter that it is possible to recover the initial state of a system by letting it interact with another quantum system. In this chapter two non-interacting quantum systems surrounded by a common environment are studied.
Quantum mechanics usually deals with the dynamics of isolated systems, but in the real world there are no perfectly closed systems. Quantum systems always interact with their surrounding environment, which are typically

modeled by thermal baths.
The interaction between a quantum system with one or a few degrees of freedom and a thermal bath with many degrees of freedom is the central concept in the theory of open quantum systems and quantum information [47,53,54]. Common approaches to study open quantum systems are based on system-plus-bath models so that the overall closed system can be described by a Hamiltonian of the general form

$$\hat{H} = \hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{I}}, \tag{3.1}$$

where $\hat{H}_{\mathrm{S}}$ corresponds to the Hamiltonian of the system, $\hat{H}_{\mathrm{B}}$ represents the Hamiltonian of the bath, and $\hat{H}_{\mathrm{I}}$ stands for the interaction Hamiltonian between the system and the bath. It is worth noting that the Hilbert space belonging to $\hat{H}$ is composed of the tensor product of the Hilbert space of the system S and the bath B: $S \otimes B$.
Thus the state of S changes as a consequence of its internal dynamics as well as its interaction with the surrounding environment. Hence, in order to study the dynamics of an open quantum system, one has to consider the dynamics of its surroundings as well. In fact, the dynamics of the environment can imply substantial changes in the dynamics of the quantum system. For instance, the action of many variables of the bath on the system modifies the time-evolution of observables of the system by inclusion of random terms [55]. In order to describe only the dynamics of the system one usually traces out the environment degrees of freedom. This results in an effective description of the dynamics of the subsystem, the so-called *reduced* dynamics.
As for the quantum system one usually considers a two-level system. These are the simplest quantum systems to work with and the only physical systems whose Hilbert space corresponds exactly to that of a qubit in quantum information theory. Two-level systems describe many physical and chemical systems with discrete degrees of freedom such as spin-$\frac{1}{2}$ particles, the polarization of a photon or a many level system where the two lowest levels are the only accessible ones. Systems having continuous degree of freedom subject to a potential energy function with two separated minima can also be modeled by two-level systems. Examples of such situations could be some type of chemical reaction involving electron transfer processes or the motion of defects in some crystalline solid [54]. Since two-level systems mathematically can be described by Pauli matrices for spin-$\frac{1}{2}$ systems and, the bath is usually considered as an ensemble of bosons, the global model system has

been dubbed the *spin-boson model*.
The Hamiltonian of a two-level system may be expressed by

$$\hat{H}_{\mathrm{S}} = -\frac{\delta}{2}\hat{\sigma}_x + \frac{\varepsilon}{2}\hat{\sigma}_z, \tag{3.2}$$

where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the x and z components of the Pauli matrices. In the continuous degree of freedom example δ corresponds to the transition probability between wells of the potential and ε stands for their energy difference. In the case of spin-$\frac{1}{2}$ systems, δ and ε correspond to a static magnetic field acting on the z and x direction, respectively.

The bosonic bath is modeled by a set of harmonic oscillators, thus bosons. Harmonic oscillators can represent a bath of phonons to describe the electron spin resonance(ESR) [53]. The set of harmonic oscillators is also used in quantum optics when one wants to describe a two-level atom interacting with a photonic bath [56].
The most important properties of a bosonic bath are:

- The bath is a macroscopic entity in a stable equilibrium state with temperature T.

- The interaction between the system and the bath weakly perturbs the equilibrium state of the bath. Thus the system is influenced by the excitations, which can be considered as harmonic oscillator excitations. Hence the Hamiltonian of the bath is taken as

$$\hat{H}_{\mathrm{B}} = \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k, \qquad [\hat{a}_k, \hat{a}_l^\dagger] = \delta_{kl}, \tag{3.3}$$

  where $\hat{a}_k^\dagger$ and $\hat{a}_k$ are bosonic creation and annihilation operators of the bath mode of wave vector k with frequency ω_k.

- The coupling of the system to the bath operator is linear in the bath harmonic oscillator operators. This corresponds to energy transfer to and from the bath by the absorption or emission of a bath quanta. This is due to the assumption of set of harmonic oscillators for the bath and the weak perturbation of the bath's state by the system. As a result, a linear interaction is sufficient to bring the system in equilibrium state with the bath at temperature T [57, 58]. Thus the

interaction Hamiltonian in the spin-boson model may be written as

$$\hat{H}_{\mathrm{I}} = \frac{\hbar}{2} \sum_{\alpha=x,y,z} \sum_{k} \hat{\sigma}_{\alpha} \left(g_k^{\alpha} \hat{a}_k^{\dagger} + g_k^{\alpha *} \hat{a}_k \right), \tag{3.4}$$

where g_k^{α} is the coupling of the α component of the system to the bath mode of wave vector k and $g_k^{\alpha *}$ is its complex conjugate. This interaction couples the bath to all spin components. It is usually simplified by considering the bath is only coupled to $\hat{\sigma}_z$.

- The spectrum of oscillator frequencies is smooth and dense. Thus the effect of the interaction between the bath and the system can be described by a single *spectral function* $J(\omega)$. This is the case when the thermodynamic limit is taken for the bath. As a result, all quantities involving the interaction with the bath will be composed of integrals of the spectral density.

- The coupling constant of the system to operators of the bath is a smooth function of the frequency of the oscillators. In the thermodynamic limit, it is not important to consider the coupling to each of the harmonic oscillators and a global description for the spin-bath interaction suffices to obtain all the interesting physics.
  The couplings g_k are parameterized via the spectral density function $J(\omega)$ as
  $$J(\omega) = \sum_{k} |g_k|^2 \, \delta(\omega - \omega_k). \tag{3.5}$$

Within the above mentioned properties of the spin-boson model the problem is completely defined by the parameters ε and δ and the function $J(\omega)$. However, it cannot be solved analytically. Here we study a simplification of this model that enables us to calculate the dynamics of the spin-$\frac{1}{2}$ system in a specific range of parameters. More precisely, we study the possibility of the polarization transfer between two spatially separated non-interacting spin-$\frac{1}{2}$ systems coupled to a common heat bath by means of an external perturbation of one of them. We show that if the initial polarization of both spins, i.e., the occupation of their ground states, is low, by applying short and strong pulses on one of them we can improve its final polarization (cool it down). Cooling spins, i.e., generating pure states from initially mixed ones is important in fields such as NMR spectroscopy and quantum information.

In NMR experiments the result depends strongly on the initial polarization of spins. Enhancing the polarization, enhances the output signal in the experiment. It is also important to have pure states in quantum information so that one can address them properly within a quantum algorithm.
The origin of cooling effect in the present model is in shifting the spins frequency by factors arising from the enhanced back reaction of the spin(via the pulses) on the collective coordinate of the bath. In the presence of another spin, this effect gets shared between the two spins.
On the other hand, the presence of the other spin yields the polarization transfer. If its initial polarization is considerable, it can be incompletely transferred to the initially unpolarized spin by applying external pulses on the latter. The existence of a thermal bath is crucial in our consideration and this process can take place due to the presence of the common thermal bath. Clearly, the effect could not survive the independent-bath approximation.

The content of this chapter is the following: In sections 3.2 we consider two independent spins at a distance r from each other both immersed in a common heat bath. We show that under specific considerations the spin-boson model describing the situation is exactly solvable. Sections 3.3-3.5 are devoted to the study of the dynamics of spins observables as well as the dynamics of the bath. Then we introduce an external field in the form of sharp pulses acting on one spin in section 3.6. In section 3.7 we show how one can achieve the cooling and spin transfer via external perturbations of one spin. We also show that the results could not be achieved without the presence of the bath. This is in contrast to the usual belief that the bath is a serious hindrance one can not get rid of.

3.2 The model

Our model consists of two spatially separated non-interacting spin-$\frac{1}{2}$ systems (qubits) coupled to a common heat bath [59]. spins S_1 and S_2 are subjected to static magnetic fields in the $z-$direction with the Zeeman Hamiltonian

$$\hat{H}_{\mathrm{S}_i} = \frac{\hbar\Omega_i}{2}\hat{\sigma}_z^{(i)}, \qquad i = 1, 2 \tag{3.6}$$

where $\hat{\sigma}_x^{(i)}$, $\hat{\sigma}_y^{(i)}$, $\hat{\sigma}_z^{(i)}$ are Pauli matrices describing two spins.
The energy levels of each spin are then $\pm\frac{1}{2}\varepsilon_i$:

$$\varepsilon_i = \hbar\Omega_i, \qquad i = 1, 2, \tag{3.7}$$

and where Ω_i is the frequency of the $i-$th spin. We consider S_1 and S_2 to be separated by a distance r along the $z-$axis and be surrounded by a common bosonic bath with the Hamiltonian

$$\hat{H}_{\mathrm{B}} = \sum_k \hbar\omega_k \, \hat{a}_k^\dagger \hat{a}_k. \tag{3.8}$$

As for the interaction between the bath and spins we notice that the main role of a thermal bath is to derive spins initially in non-stationary state toward a stationary state. In this respect, for two-level systems (spin-$\frac{1}{2}$ systems) we distinguish two types of relaxation processes and the corresponding time-scales [60]:

- The $\mathcal{T}_2$-time scale related to the relaxation of the average transverse components $\langle\hat{\sigma}_x^{(i)}\rangle$, and $\langle\hat{\sigma}_y^{(i)}\rangle$ of the $i-$th spin (decoherence), where $i = 1, 2$.
- The $\mathcal{T}_1$-time scale related to the relaxation[1]of $\langle\hat{\sigma}_z^{(i)}\rangle$, $i = 1, 2$

It is customary to have situations where

$$\mathcal{T}_2 \ll \mathcal{T}_1. \tag{3.9}$$

The physical reason of this assumption is that the transversal components (in the sense of Zeeman Hamiltonian for the spins) are not directly related to the energies of the spins.
It is worth mentioning that there are experimentally realized examples of two-level systems with sufficiently long $\mathcal{T}_2$ time scale properties with $\mathcal{T}_1$ being several orders of magnitude larger than $\mathcal{T}_2$. For example, for atoms in optical traps $\mathcal{T}_2 \sim 1$ s, while the response time of the bath is 10^{-8}s [61]. For an electric spin injected or optically excited in a semiconductor $\mathcal{T}_2 \sim 1\mu$s [62] and for an exciton created in a quantum dot $\mathcal{T}_2 \sim 10^{-9}$s [63], where in both situations the response time of the bath is of order $10^{-9} - 10^{-13}$ s. Typical femtosecond (10^{-15}s) laser pulses then are suitable for the pulsed dynamics that our model is based on. In NMR physics $\mathcal{T}_2$ ranges between $10^{-6} - 10^3$ s, with bath's response time of the order of one micro second and the duration of the pulses can vary between 1 ps and 1μs [64].In all these examples the

[1] There is also a third relaxation time which has a different origin. It appears due to different energies or de-phasing of the non-interacting spins. In our model we assume that ϵ_1 and ϵ_2 are close to each other such that this time scale is large enough

response time of the bath is much shorter than the internal time of spins. We restrict ourselves to times much less than the relaxation time $\mathcal{T}_1$ of the longitudinal components $\langle\hat{\sigma}_z^{(i)}\rangle$ of the two spins. We choose the spin-bath interaction Hamiltonian such that the bath induces only transversal relaxation [65, 66].

$$\hat{H}_{\rm int} \;=\; \sum_{i=1,2} \frac{\hbar}{2} \hat{X}^{(i)}\, \hat{\sigma}_z^{(i)}, \qquad i = 1, 2 \tag{3.10}$$

where $\hat{X}^{(1)}$ and $\hat{X}^{(2)}$ are collective coordinates of the bath seen by each spin and are defined as

$$\hat{X}^{(1)} \stackrel{def}{=} \sum_k \left(g_k^1\, \hat{a}_k^\dagger + g_k^{1*}\, \hat{a}_k \right), \tag{3.11}$$

$$\hat{X}^{(2)} \stackrel{def}{=} \sum_k \left(g_k^2\, \hat{a}_k^\dagger + g_k^{2*}\, \hat{a}_k \right), \tag{3.12}$$

In general the couplings are complex and out of phase with each other. We choose different couplings to the bath labeled by g_k^1 and g_k^2 since S_1 and S_2 have an explicit spatial separation. To make this evident, we assume two spins are separated by distance r in the $z-$direction such that the local interaction of each spin with the bath can be represented by

$$g_k^1 \;=\; g_k\, e^{(i/2)\, kr\cos\theta_k} \tag{3.13}$$

$$g_k^2 \;=\; g_k\, e^{-(i/2)\, kr\cos\theta_k} \tag{3.14}$$

where θ is the polar angle measured against the $z-$axis in $k-$space, and

$$|g_k^1| = |g_k^2| = g_k. \tag{3.15}$$

This form of coupling is capable of preserving the translational invariance of the system in the absence of an external potential. Couplings of the form (3.14-3.14) appear in the interaction of a particle with a fermionic bath [67] or in the polaron problem [54].
The bath spectral density function $J(\omega)$ is parameterized as

$$J(\omega) = \sum_k |g_k|^2\, \delta(\omega - \omega_k). \tag{3.16}$$

We notice that due to (3.15) it is the same for both spins. The thermodynamic limit of the bath will be taken later in section 3.5.

The overall system can be studied within the spin-boson model [57, 65, 66, 68–73] with the the Hamiltonian

$$\hat{H} = \hat{H}_{\mathrm{S}_1} + \hat{H}_{\mathrm{S}_2} + \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{int}}, \tag{3.17}$$

$$\hat{H} = \sum_{i=1}^{2} \frac{\hbar\Omega_i}{2}\hat{\sigma}_z^{(i)} + \sum_k \hbar\omega_k\, \hat{a}_k^\dagger \hat{a}_k + \frac{\hbar}{2}\sum_{i=1}^{2} \hat{X}^{(i)}\hat{\sigma}_z^{(i)}. \tag{3.18}$$

It is seen that the $z-$components of both spins commute with $\hat{H}$ and hence they are conserved, so the energy of the spins are constant of motion[2]. This is due to restricting the model to times much less than the relaxation time $\mathcal{T}_1$ and omitting the related terms form (3.18). On the other hand $\langle\hat{\sigma}_x^{(i)}\rangle$, and $\langle\hat{\sigma}_y^{(i)}\rangle$ do undergo an evolution. In other words, this model describes a purely decohering mechanism, where no energy exchange between the spins and the bath is present. In fact, energy exchange processes typically involve time scales much longer than the decoherence mechanisms.
In all the above mentioned examples the response time of the bath is much shorter than the internal time $1/\Omega_1$ of the spin. Although this model now has a restricted validity, it is exactly solvable under the above imposed constraints. The last ingredient of this model is to introduce external fields acting on one of the spins. This will be discussed in section 3.6 where we formulate the external field as short pulses in order to keep the model analytically solvable.

3.3 Time evolution of the bath and spin operators

In this section we calculate the time evolution of the components of the spin of two systems as well as the time evolution of the bath collective coordinate using the Heisenberg equation:

$$\dot{\hat{A}} = \frac{i}{\hbar}[\hat{H}, \hat{A}], \tag{3.19}$$

[2]We notice that if the two spins were identical, i.e. $\Omega_1 = \Omega_2$ and they were sitting on top of each other, e.g. at $r = 0$, besides the quantities $\hat{\sigma}_z^{(1)}$, $\hat{\sigma}_z^{(2)}$, and $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}$, the quantities $\hat{\sigma}_+^{(1)} \otimes \hat{\sigma}_-^{(2)}$ and $\hat{\sigma}_+^{(2)} \otimes \hat{\sigma}_-^{(1)}$ would be conserved as well. This means, any initial density matrix of the two spins that can be presented as a linear combination of these operators will remain unchanged in the course of time under the evolution given by (3.18).

where $\hat{A}$ stands for any observable of the overall system and $\dot{\hat{A}}$ represents the time derivative of $\hat{A}$.

3.3.1 Time evolution of the bath operators

The dynamics of the bath annihilation operator is given by

$$\dot{\hat{a}}_k = -i\omega_k \hat{a}_k - \frac{i}{2}\,\hat{\sigma}_z^{(1)}\, g_k\, e^{(i/2)kr\cos\theta_k} - \frac{i}{2}\,\hat{\sigma}_z^{(2)}\, g_k\, e^{-(i/2)kr\cos\theta_k}. \quad (3.20)$$

This differential equation can be solved by a Laplace transformation and one gets

$$\begin{aligned} \hat{a}_k(t) &= e^{-i\omega_k t}\hat{a}_k(0) + \frac{g_k}{2\omega_k}\,\hat{\sigma}_z^{(1)}\, e^{(i/2)kr\cos\theta_k}\left(e^{-i\omega_k t} - 1\right) \\ &+ \frac{g_k}{2\omega_k}\,\hat{\sigma}_z^{(2)}\, e^{-(i/2)kr\cos\theta_k}\left(e^{-i\omega_k t} - 1\right). \end{aligned} \quad (3.21)$$

The complex conjugate of (3.21) gives the dynamics of the creation operator. Thus for $\hat{X}^{(1)}(t)$ and $\hat{X}^{(2)}(t)$ given by (3.11, 3.12) we have [see appendix C]

$$\hat{X}^{(1)}(t) = \hat{\eta}_r(t) - \hat{\sigma}_z^{(1)} G(t) - \hat{\sigma}_z^{(2)} G_r(t), \quad (3.22)$$

$$\hat{X}^{(2)}(t) = \hat{\eta}_{-r}(t) - \hat{\sigma}_z^{(1)} G_{-r}(t) - \hat{\sigma}_z^{(2)} G(t). \quad (3.23)$$

The functions $G(t)$ and $G_{\pm r}(t)$ are the response functions quantifying the *back reaction* of S_1 and S_2 on the collective coordinate operator of the bath.

$$G_{\pm r}(t) = \sum_k \frac{g_k^2}{\omega_k}\left[\cos\left(kr\cos\theta_k\right) - \cos\left(\omega_k t \pm kr\cos\theta_k\right)\right]. \quad (3.24)$$

While $G(t)$ is defined as $G_{r=0}(t)$

$$G(t) = \sum_k \frac{|g_k|^2}{\omega_k}\left(1 - \cos\omega_k t\right). \quad (3.25)$$

We define the time integral of $G_{\pm r}(t)$ by $F_{\pm r}(t)$, as the back reaction factor of spin at distance $\pm r$

$$F_{\pm r}(t) \stackrel{def}{=} \int_0^t ds\, G_{\pm r}(s) = \quad (3.26)$$

$$\sum_k \frac{|g_k|^2}{\omega_k^2}\left[\omega_k t\cos\left(kr\cos\theta_k\right) - \sin\left(\omega_k t \pm kr\cos\theta_k\right)\right].$$

while $F(t)$, the back reaction factor of the very same spin under the study, is defined as

$$F(t) = \sum_k \frac{|g_k|^2}{\omega_k^2} \left[\omega_k t - \sin(\omega_k t)\right]. \tag{3.27}$$

In a similar fashion, when both spins are sitting on top of each other, $F_{r=0}(t) = F(t)$.

In the following sections we will see that the back reaction factor plays an important role in the cooling and polarization transfer process and the presence of the bath is essential in this scheme.
The operator $\hat{\eta}_r(t)$ in (3.22), and (3.23) is defined as

$$\hat{\eta}_r(t) \stackrel{def}{=} \sum_k g_k \left[\hat{a}_k^\dagger(0) e^{i\left(\frac{kr}{2}\cos\theta_k + \omega_k t\right)} + \hat{a}_k(0) e^{-i\left(\frac{kr}{2}\cos\theta_k + \omega_k t\right)}\right]. \tag{3.28}$$

Setting $r = 0$ yields

$$\hat{\eta}(t) = \sum_k g_k \left[\hat{a}_k^\dagger(0) e^{i\omega_k t} + \hat{a}_k(0) e^{-i\omega_k t}\right]. \tag{3.29}$$

$\hat{\eta}_r(t)$ is named quantum noise operator which acts as a random force on spins separated by distance r. We notice that $\hat{\eta}_r(t)$ is determined directly in terms of bath operators at the initial time $t = 0$. Therefore the nature of the initial state of the bath plays a significant role. It is also remarkable that the commutator of the noise operator is a $c-$numbered function of time [55] and it is independent of r [see appendix D]

$$[\hat{\eta}_r(t), \hat{\eta}_r(t')] = -2\,i\,\mathrm{sign}(t-t') \sum_k |g_k|^2 \sin[\omega_k(t-t')], \tag{3.30}$$

where $\mathrm{sign}(t-t')$ represents the sign function. This commutator can be written in terms of the back reaction factor $F(t)$ as

$$[\hat{\eta}_r(t), \hat{\eta}_r(t')] \;=\; -2i\ddot{F}(t-t'). \tag{3.31}$$

This is a straightforward consequence of the definition (3.28) and the creation and annihilation operator commutation relations.

3.3.2 Time evolution of spin operators

We are interested in spin subsystems properties, in particular, in expectation values of the spin operators S_1 and S_2 at later times after coupling to the bath.

Choosing the Heisenberg representation we can exactly solve the Heisenberg equations of motion of the spin operators and then calculate their ensemble averages.
Let us first recall the following standard relations between the spin operators

$$\hat{\sigma}_{\pm}^{(i)} = \hat{\sigma}_{x}^{(i)} \pm \hat{\sigma}_{y}^{(i)}, \qquad i = 1, 2, \tag{3.32}$$

$$\left[\hat{\sigma}_{z}^{(i)}, \hat{\sigma}_{\pm}^{(i)}\right] = \pm 2\hat{\sigma}_{\pm}^{(i)}, \tag{3.33}$$

$$\hat{\sigma}_{z}^{(i)}\hat{\sigma}_{\pm}^{(i)} = \pm\hat{\sigma}_{\pm}^{(i)}. \tag{3.34}$$

Since the overall Hamiltonian (3.18) commutes with $\hat{\sigma}_{z}^{(i)}$, for $i = 1, 2$, the Heisenberg equation for $\hat{\sigma}_{z}^{(i)}$ reads

$$\dot{\hat{\sigma}}_{z}^{(i)} = 0, \qquad \hat{\sigma}_{z}^{(i)}(t) = \hat{\sigma}_{z}^{(i)}(0). \tag{3.35}$$

It is easier to calculate the time evolution of the raising and lowering operators $\hat{\sigma}_{\pm}^{(i)}$, which act on the energy eigenstates of spins rather than working out transversal components $\hat{\sigma}_{x}^{(i)}$ and $\hat{\sigma}_{y}^{(i)}$,

$$\dot{\hat{\sigma}}_{\pm}^{(i)} = \frac{i}{\hbar}\left[\hat{H}, \hat{\sigma}_{\pm}^{(i)}\right]. \tag{3.36}$$

Inserting $\hat{H}$ from (3.18) and implying (3.33), for the spin S_1 we have

$$\dot{\hat{\sigma}}_{\pm}^{(1)} = \pm i\Omega_1\hat{\sigma}_{\pm}^{(1)} \pm i\hat{X}^{(1)}\,\hat{\sigma}_{\pm}^{(1)}. \tag{3.37}$$

Inserting $\hat{X}^{(1)}(t)$ given by (3.22) into (3.37) and using (3.34) relations yields

$$\dot{\hat{\sigma}}_{\pm}^{(1)} = i\left[\pm\Omega_1 \pm \hat{\eta}_r(t) - G(t) \mp G_r(t)\hat{\sigma}_{z}^{(2)}\right]\hat{\sigma}_{\pm}^{(1)}. \tag{3.38}$$

The equation (3.38) is a quantum Langevin-type equation with quantum noise $\hat{\eta}_r(t)$, and back reactions $G(t)$ and $G_r(t)$.
Solving the differential equation (3.38) yields

$$\hat{\sigma}_{\pm}^{(1)}(t) = \exp\left[\pm i\Omega_1 t - iF(t)\right]\,\hat{\Pi}_{r}^{\pm}(0,t)\,\hat{\sigma}_{\pm}^{(1)}(0)\exp\left[\mp iF_r(t)\,\hat{\sigma}_{z}^{(2)}\right], \tag{3.39}$$

where $\hat{\Pi}_{r}^{\pm}(t_0, t_1)$ is defined as

$$\hat{\Pi}_{r}^{\pm}(t_0, t_1) \stackrel{def}{=} \mathcal{T}\exp\left[\pm i\int_{t_0}^{t_1} ds\,\hat{\eta}_r(s)\right], \tag{3.40}$$

and where $\mathcal{T}$ stands for the time-ordering operator. The explicit expression for $\hat{\Pi}_r^{\pm}(t_0, t_1)$ will be given later.

The dynamics of S_2 located at distance r from S_1 can be straightforwardly derived using the same analogy

$$\hat{\sigma}_{\pm}^{(2)}(t) = \exp\left[\pm i\Omega_2 t - iF(t)\right] \hat{\Pi}_{-r}^{\pm}(0,t) \exp\left[\mp iF_{-r}(t)\hat{\sigma}_z^{(1)}\right] \hat{\sigma}_{\pm}^{(2)}(0), \quad (3.41)$$

where $\hat{\Pi}_{-r}^{\pm}(t_0, t_1)$ is defined as

$$\hat{\Pi}_{-r}^{\pm}(t_0, t_1) \stackrel{def}{=} \mathcal{T} \exp\left[\pm i \int_{t_0}^{t_1} ds\, \hat{\eta}_{-r}(s)\right]. \quad (3.42)$$

It is seen from (3.39) and (3.41) that there are three effects generated by the spin-bath interaction:

- random influences of the common bath on each spin due to the quantum noise operator; this is understandable since two non-interacting spins are open (not isolated) systems, their dynamics are not deterministic but rather contain stochastic elements due to the interaction with the thermal bath.
- A deterministic influence generated by the back reaction term of the spin under study,
- the influence generated by the back reaction term of the other spin at distance r which initially assumed not to be directly interacting with the other one.

For later considerations, it is useful to calculate the time evolution of $\hat{\Pi}_{\pm r}^{\pm}(t_0, t_1)$.
Defining $\mathcal{E}_t\hat{A}$ as the Heisenberg time evolution of an operator $\hat{A}$ over a period t,

$$\mathcal{E}_t\hat{A} \equiv e^{it\hat{H}/\hbar}\, \hat{A}\, e^{-it\hat{H}/\hbar}, \quad (3.43)$$

the Heisenberg dynamics of the quantum noise operator reads

$$\begin{aligned} &\mathcal{E}_t\hat{\eta}_r(s) = \\ &\hat{\eta}_r(t+s) + \hat{\sigma}_z^{(1)} \sum_k \frac{|g_k|^2}{\omega_k} \left\{\cos\left[\omega_k(t+s)\right] - \cos\left(\omega_k s\right)\right\} \quad (3.44) \\ &+\hat{\sigma}_z^{(2)} \sum_k \frac{|g_k|^2}{\omega_k} \left\{\cos\left[\omega_k(t+s) + kr\cos\theta_k\right] - \cos\left(\omega_k s + kr\cos\theta_k\right)\right\}. \end{aligned}$$

Inserting the expressions for the back reaction given by (3.24) in the expression for $\mathcal{E}_t\hat{\eta}_{r,\theta}(s)$ [see appendix D] we get

$$\begin{aligned}\mathcal{E}_t\hat{\eta}_r(s) &= \hat{\eta}_r(t+s) + [G(s) - G(t+s)]\ \hat{\sigma}_z^{(1)} \\ &+ [G_r(s) - G_r(t+s)]\ \hat{\sigma}_z^{(2)}. \end{aligned} \tag{3.45}$$

By analogy,

$$\begin{aligned}\mathcal{E}_t\hat{\eta}_{-r}(s) &= \hat{\eta}_{-r}(t+s) + [G_{-r}(s) - G_{-r}(t+s)]\ \hat{\sigma}_z^{(1)} \\ &+ [G(s) - G(t+s)]\ \hat{\sigma}_z^{(2)}. \end{aligned} \tag{3.46}$$

Thus, the of the operator $\hat{\Pi}^{\pm}_{\pm r}(0,t_1)$ reads

$$\begin{aligned}&\mathcal{E}_t\hat{\Pi}^{\pm}_{r}(0,t_1) = \\ &\hat{\Pi}^{\pm}_{r}(t,t+t_1)\ \exp\left[\pm i\chi(0,t_1,t)\hat{\sigma}_z^{(1)}\right]\ \exp\left[\pm i\chi_r(0,t_1,t)\hat{\sigma}_z^{(2)}\right],\end{aligned} \tag{3.47}$$

$$\begin{aligned}&\mathcal{E}_t\hat{\Pi}^{\pm}_{-r}(0,t_1) = \\ &\hat{\Pi}^{\pm}_{-r}(t,t+t_1)\exp\left[\pm i\chi_{-r}(0,t_1,t)\hat{\sigma}_z^{(1)}\right]\ \exp\left[i\chi(0,t_1,t)\hat{\sigma}_z^{(2)}\right].\end{aligned} \tag{3.48}$$

where $\chi_r(0,t_1,t)$ is defined as

$$\chi_{\pm r}(0,t_1,t) \stackrel{def}{=} \int_0^t ds[G_{\pm r}(s) - G_{\pm r}(t_1+s)], \tag{3.49}$$

$$= F_{\pm r}(t_1) + F_{\pm r}(t) - F_{\pm r}(t_1+t), \tag{3.50}$$

When deriving (3.50), we used the definition $F_{\pm r}(t_1) \equiv \int_0^{t_1} ds\, G_{\pm r}(s)$.

3.4 Factorized initial state

We assume that the spins are prepared independently from each other and the bath an then brought in contact with the bath at time $t = 0$. Thus at initial time $t = 0$ the common density matrix of the bath and spins, represented by $\hat{\rho}(0)$ is factorized:

$$\hat{\rho}(0) = \hat{\rho}_{\rm B}(0) \otimes \hat{\rho}_{\rm S_1}(0) \otimes \hat{\rho}_{\rm S_2}(0), \tag{3.51}$$

where $\hat{\rho}_{\rm S_1}(0)$ and $\hat{\rho}_{\rm S_2}(0)$ are the initial density matrices of each spin. $\hat{\rho}_{\rm B}$ stands for the Gibbs state of the bath, which is initially in equilibrium at inverse temperature β,

$$\hat{\rho}_{\rm B} = \frac{e^{-\beta\hat{H}_B}}{\mathrm{tr}\left[e^{-\beta\hat{H}_B}\right]}. \tag{3.52}$$

Since the spins and the bath are initially independent, $\hat{\rho}(0)$ can be written as

$$\hat{\rho}(0) = \frac{e^{-\beta \hat{H}_0}}{\mathrm{tr}\left[e^{-\beta \hat{H}_0}\right]}, \tag{3.53}$$

where $\hat{H}_0$ is the Zeeman Hamiltonian of each spin added to the bath Hamiltonian and is described by

$$\hat{H}_0 = \frac{1}{2}\sum_{i=1,2} \hbar \Omega_i \hat{\sigma}_z^{(i)} + \sum_k \hbar \omega_k \hat{a}_k^\dagger \hat{a}_k. \tag{3.54}$$

The factorized initial state (3.53) implies

$$\langle \hat{\sigma}_\pm^{(i)}(0) \rangle = 0 \qquad i = 1, 2, \tag{3.55}$$

$$\langle \hat{\sigma}_z^{(i)}(0) \rangle = -\tanh\left(\frac{\beta \hbar \Omega_i}{2}\right). \tag{3.56}$$

We note that depending on the response of spins to an external static magnetic field, the initial polarization $|\langle \hat{\sigma}_z^{(i)} \rangle|$ varies. This is best characterized by frequency/field ratio, which is for example 42 MHz/T for a proton. For an electron this ratio is 10^3 times larger due to the difference between atomic and nuclear Bohr magnetons. Thus at temperature $T = 1$ K and magnetic field $B = 1$ T, the equilibrium polarization of proton is only

$$|\langle \hat{\sigma}_z \rangle| = \tanh\left(\frac{\hbar \mu B}{2K_B T}\right) = 10^{-3}, \tag{3.57}$$

while for an electron it is 1000 times larger, $|\langle \hat{\sigma}_z \rangle| \sim 1$.

Since the bath is initially in a Gibbs state, employing (3.51) we have

$$\langle \hat{a}_k(0) \rangle = \langle \hat{a}_k^\dagger(0) \rangle = 0, \tag{3.58}$$

$$\langle \hat{a}_k(0) \hat{a}_{k'}^\dagger(0) \rangle = (\langle n_k \rangle + 1)\delta_{kk'}, \tag{3.59}$$

$$\langle \hat{a}_k^\dagger(0) \hat{a}_{k'}(0) \rangle = \delta_{kk'} \langle n_k \rangle, \tag{3.60}$$

$$\langle \hat{a}_k^\dagger(0) \hat{a}_k(0) + \hat{a}_k(0) \hat{a}_k^\dagger(0) \rangle = \coth\left(\frac{\beta \hbar \omega_k}{2}\right), \tag{3.61}$$

where $\langle n_k \rangle = \left[e^{\beta \hbar \omega_k} - 1\right]^{-1}$ is the thermal occupation of mode k.
The relation (3.58) implies that the quantum noise has the property of

$$\langle \hat{\eta}_r(t) \rangle = 0. \tag{3.62}$$

We recall that $\hat{\eta}_r(t)$ is determined via $\hat{a}_k(0)$ and $\hat{a}_k^\dagger(0)$.
Taking the average of the commutator of the noise given by (3.31) over the initial state of the bath yields

$$\langle[\hat{\eta}_r(t), \hat{\eta}_r(t')]\rangle = -2\,i\,\dot{G}(t-t') = -2\,i\,\ddot{F}(t-t'), \tag{3.63}$$

where the back reaction factor $F(t)$ is given by (C.22).
We notice that thermal state of the bath and the anticommutation rules between the creation and annihilation operators of the bath implies (3.63) which is independent of the distance r between two spins.
Implying (3.61) we can also calculate the average of the anticommutator of the noise operator [see the appendix D] as

$$\langle\{\hat{\eta}_r(t), \hat{\eta}_r(t')\}\rangle = 2\sum_k |g_k|^2 \coth\left(\frac{\beta\hbar\omega_k}{2}\right)\cos\left[\omega_k(t-t')\right], \tag{3.64}$$

which is independent of the separation distance r between two spins due to the initial thermal state of the bath and the anti-commutation relations betwee the bath creation and annihilation operators.
From (3.64) the symmetrized correlation function of quantum noise operator $K(t-t')$ reads

$$K(t-t') = \frac{1}{2}\,\langle\{\hat{\eta}_r(t), \hat{\eta}_r(t')\}\rangle\,. \tag{3.65}$$

Then, the time-order correlation function of the noise operator defined by

$$K_{\mathcal{T}}(t-t') \stackrel{def}{=} \left\langle \mathcal{T}\big(\hat{\eta}_r(t)\,\hat{\eta}_r(t')\big)\right\rangle \tag{3.66}$$

can be described in terms of the symmetrized correlation function given by (3.64) and the back reaction forces as

$$\begin{aligned} K_{\mathcal{T}}(t-t') &= K(t-t') - i\dot{G}(t-t'), \\ &= K(t-t') - i\ddot{F}(t-t'). \end{aligned} \tag{3.67}$$

Since $\langle\hat{\eta}_r(t)\rangle = 0$, we can use Wick's theorem for decomposing higher-order products of the noise operator [74]. This is important since our ultimate goal is to calculate the ensemble average of the time-evolved spin operators. Wick's theorem is related to the fact that the commutator of the quantum noise operator is a $c-$number. According to this theorem if $\langle\hat{\eta}_r(t)\rangle = 0$, any correlation of an odd number of $\hat{\eta}_r(t)$ vanishes. A correlation of an

even number of $\hat{\eta}_r(t)$ is equal to the sum of products of pair correlations, the sum being taken over all pairings. Thus the Wick's decomposition of $\langle \mathcal{T}\big(\hat{\eta}_r(t_1)\cdots\hat{\eta}_r(t_{2k})\big)\rangle$ will be a sum of $(2k-1)!! = (2k-1)(2k-3)\cdots 3$ terms. These are the characteristic properties of a classical stationary Gaussian stochastic process [75]. Therefore, the operators $\hat{\eta}_r(t)$ are called Gaussian operators [76].
We employ this property in order to calculate the time-ordered exponential of the time integral of the quantum noise which appears in (3.48) and (3.40) [66]:

$$\begin{aligned}\langle\hat{\Pi}_r^{\pm}(t_0,t_1)\rangle &= \sum_{k=0}^{\infty}\frac{(-1)^k}{(2k)!}\int_{t_0}^{t_1}\cdots\int_{t_0}^{t_1} ds_1\cdots ds_{2k}\langle\mathcal{T}\big(\hat{\eta}_r(s_1)\cdots\hat{\eta}_r(s_{2k})\big)\rangle \\ &= \exp\left[-\frac{1}{2}\int_{t_0}^{t_1}\int_{t_0}^{t_1} ds_1 ds_2 K_{\mathcal{T}}(s_1-s_2)\right] \\ &= \exp\left[-\xi(t_1-t_0)+i\,F(t_1-t_0)\right]. \end{aligned} \tag{3.68}$$

The function $\xi(t_1-t_0)$ is defined in terms of the symmetrized correlation function of the quantum noise as

$$\xi(t_1-t_0)=\frac{1}{2}\int_{t_0}^{t_1}\int_{t_0}^{t_1} ds_1 ds_2 K(s_1-s_2). \tag{3.69}$$

Since the commutator and the anticommutator of the noise operator is independent of r, in the same fashion

$$\langle\hat{\Pi}_{-r}^{\pm}(t_0,t_1)\rangle = \exp\left[-\xi(t_1-t_0)+i\,F(t_1-t_0)\right]. \tag{3.70}$$

having the expressions for the time-evolved transversal components of the spins given by (3.39), (3.41), we can calculate their ensemble averages as following:

$$\langle\hat{\sigma}_{\pm}^{(1)}(t)\rangle = e^{\pm i\Omega_1 t - iF(t)}\langle\Pi_r^{\pm}(0,t)\rangle\,\langle\sigma_{\pm}^{(1)}(0)\rangle\,\langle e^{\mp iF_r(t)\hat{\sigma}_z^{(2)}}\rangle, \tag{3.71}$$

$$\langle\hat{\sigma}_{\pm}^{(2)}(t)\rangle = e^{\pm i\Omega_2 t - iF(t)}\langle\Pi_{-r}^{\pm}(0,t)\rangle\,\langle e^{\mp iF_{-r}(t)\hat{\sigma}_z^{(1)}}\rangle\,\langle\sigma_{\pm}^{(2)}(0)\rangle. \tag{3.72}$$

Inserting the averaged time-ordered operator from (3.68), we see that the back reaction forces $F(t)$ cancel out. As a result the transversal components of spins decay due to the interaction with the bath as

$$\langle\hat{\sigma}_{\pm}^{(1)}(t)\rangle = e^{\pm i\Omega_1 t - \xi(t)}\,\langle\sigma_{\pm}^{(1)}(0)\rangle\,\langle e^{\mp iF_r(t)\hat{\sigma}_z^{(2)}}\rangle, \tag{3.73}$$

$$\langle\hat{\sigma}_{\pm}^{(2)}(t)\rangle = e^{\pm i\Omega_2 t - \xi(t)}\,\langle e^{\mp iF_{-r}(t)\hat{\sigma}_z^{(1)}}\rangle\,\langle\sigma_{\pm}^{(2)}(0)\rangle. \tag{3.74}$$

Thus the factor $e^{-\xi(t)}$ with $\xi(t)$ defined by (3.69) leads to decoherence for a general factorized initial state.
In section 3.6 we show that $F(t)$ which disappears from(3.74) plays an important role when S_1 undergoes a perturbation by implying short pulses.

3.5 Ohmic spectrum of the bath

For the spin-bath interaction, we shall consider the ohmic regime [57]. The most studied ohmic case corresponds to an environment which induces a dissipative force linear in the velocity of a Brownian particle moving in it. In the ohmic regime the spectral density function reads

$$J(\omega) = \gamma\,\omega\,e^{-\omega/\Gamma}, \tag{3.75}$$

where γ is a dimensionless coupling constant, and where Γ (usually much larger than Ω_1 and Ω_2) is the maximal characteristic frequency of the bath's response.
For the inverse dispersion relation we take the most natural one

$$k = \frac{\omega_k}{c}, \tag{3.76}$$

where c is the phonon velocity in the bath.

The symmetrized correlation function of the quantum noise operator in ohmic case is given by

$$\begin{aligned} K(t) &= \int_0^\infty d\omega\, J(\omega)\, \coth\left(\frac{\beta\hbar\omega}{2}\right)\cos(\omega t) \\ &= \gamma\int_0^\infty d\omega\, e^{-\omega/\Gamma}\,\omega\coth\left(\frac{\beta\hbar\omega}{2}\right)\cos(\omega t), \end{aligned} \tag{3.77}$$

where we have inserted (3.16) and (3.75) into the expression for the quantum noise correlator given by (3.64).
We notice that the decay factor $\xi(t)$ is related to $K(t)$ via Eq. (3.69). Thus we can get an exact expression for $\xi(t)$ [66]

$$\xi(t) = \gamma\ln\left[\frac{\mathbf{\Gamma}^2\,(1+\Theta)\,\sqrt{1+\Gamma^2t^2}}{\mathbf{\Gamma}\,(1+\Theta-i\Theta\,\Gamma\,t)\;\mathbf{\Gamma}\,(1+\Theta+i\Theta\,\Gamma\,t)}\right], \tag{3.78}$$

where $\mathbf{\Gamma}$ is Euler's gamma function, and Θ is defined as

$$\Theta \stackrel{def}{=} \frac{1}{\beta\hbar\Gamma}, \tag{3.79}$$

which is called a dimensionless temperature [65]. This implies that in low temperatures the decay behaves as the following power-law expression

$$\Theta \ll 1: \qquad e^{-\xi(t)} = \left(1+\Gamma^2 t^2\right)^{-\gamma/2}. \tag{3.80}$$

For $\Theta \gtrsim 1$ $e^{-\xi(t)}$ starts as a Gaussian, but continues as $e^{-t/\mathcal{T}_2}$ with $\mathcal{T}_2 = \hbar/2\beta\gamma$ [66, 69, 70, 72].

In order to calculate the time derivative of the back reaction factor $G_r(t)$ in the ohmic regime, we first average $G_r(t)$ given by (3.24) over all θ_k and denote it by $\bar{G}_r(t)$

$$\begin{aligned} \bar{G}_r(t) &= \frac{1}{2}\int_0^\pi d\theta_k \, \sin\theta_k \, G_r(t) \qquad (3.81)\\ &= \sum_k \frac{g_k^2}{2\omega_k}\frac{1}{kr}\left[2\sin(kr) - \sin\left(\omega_k t + kr\right) + \sin\left(\omega_k t - kr\right)\right]. \end{aligned}$$

We notice that

$$\bar{G}_r(t) = \bar{G}_{-r}(t). \tag{3.82}$$

Implying $k = \omega_k/c$ and inserting the bath spectral density in (3.81) we get

$$\bar{G}_r(t) = \int_0^\infty d\omega \, \frac{J(\omega)}{2\omega^2\tilde{t}}\left\{2\sin\omega\tilde{t} - \sin\left[\omega(t+\tilde{t})\right]\sin\left[\omega(t-\tilde{t})\right]\right\}, \tag{3.83}$$

where we define $\tilde{t}$ as the time spent by phonons to travel between S_1 and S_2

$$\tilde{t} \stackrel{def}{=} \frac{r}{c}. \tag{3.84}$$

Considering the ohmic regime and inserting (3.75) into (3.87) we get

$$\bar{G}_r(t) = \frac{\gamma}{2\tilde{t}}\int_0^\infty \frac{d\omega}{\omega}\, e^{-\omega/\Gamma}\left\{2\sin\omega\tilde{t} - \sin\left[\omega(t+\tilde{t})\right]\sin\left[\omega(t-\tilde{t})\right]\right\}, \tag{3.85}$$

which can be worked out [see appendix C] as

$$\begin{aligned} &\bar{G}_r(t) = \qquad (3.86)\\ &\frac{\gamma}{2\tilde{t}}\left\{2\arctan(\Gamma\tilde{t}) - \arctan\left[\Gamma(t+\tilde{t})\right] + \arctan\left[\Gamma(t-\tilde{t})\right]\right\}. \end{aligned}$$

Let us recall $G(t)$ given by (3.25)

$$G(t) = \int_0^\infty d\omega \, \frac{J(\omega)}{\omega} \left(1 - \cos \omega t\right). \tag{3.87}$$

In the ohmic regime this function reads

$$\begin{aligned} G(t) &= \gamma \int_0^\infty d\omega \, e^{-\omega/\Gamma} \left(1 - \cos \omega t\right) \\ &= \gamma\Gamma \left(1 - \frac{1}{1+\Gamma^2 t^2}\right). \end{aligned} \tag{3.88}$$

We notice that in the limit where r approaches zero, $\bar{G}_r(t)$ corresponds to $G(t)$.
Calculation of the back reaction factor $F_r(t)$ in the ohmic regime yields [see appendix C]

$$\begin{aligned} \bar{F}_r(t) &= \frac{\gamma}{2\tilde{t}} \Bigg\{ \frac{1}{2\Gamma} \ln \left(\frac{1 + \left[\Gamma(t+\tilde{t})\right]^2}{1 + \left[\Gamma(t-\tilde{t})\right]^2} \right) + 2t \arctan\left(\Gamma\tilde{t}\right) \\ &- (t+\tilde{t}) \arctan\left[\Gamma(t+\tilde{t})\right] + (t-\tilde{t}) \arctan\left[\Gamma(t-\tilde{t})\right] \Bigg\}. \end{aligned} \tag{3.89}$$

We notice that setting $r = 0$ in (3.86) reproduces the result for a single spin coupled to a heat bath in the ohmic regime [66]. Moreover, for fixed r, at the characteristic time $1/\Gamma$, $\bar{G}_r(t)$ and $\bar{F}_r(t)$ become constant. It is remarkable that the time-scale of the back reaction factor $\bar{F}_r(t)$ is temperature-independent while the decoherence time does depend on T.

3.6 Pulsed dynamics

In this section we study the case where one of the spins, say S_1, is acted on by two successive pulses. The aim is to see how this would result to a higher polarized spin state for S_1. The reason for applying two pulses and not just one lies in the no-cooling principle [77]. According to the no-cooling principle which is related to the second law of thermodynamics, an equilibrium system cannot be cooled by means of a cyclic external field. One cannot achieve cooling by implying a single pulse since it sees the initial local equilibrium state of the spin, and then according to the no-cooling principle

it can only heat the spins state up. Thus we have to employ at least two pulses [65].

The external field acting on S_1 is described by a time-dependent Hamiltonian as

$$\hat{H}_{\mathrm{P}} = \frac{1}{2} \sum_{\alpha=x,y,z} h_\alpha(t) \hat{\sigma}_\alpha^{(1)}, \tag{3.90}$$

with magnitudes $h_\alpha(t)$. We consider H_{P} to be a pulse. A pulse of duration δ is defined by sudden switching on the external field at some time $t > 0$, and then suddenly switching off at time $t + \delta$.
Adding $\hat{H}_{\mathrm{P}}$ to the Hamiltonian $\hat{H}$ of the overall system given by (3.18) makes the total Hamiltonian time-dependent

$$\hat{H}(t) = \hat{H} + \hat{H}_{\mathrm{P}}(t). \tag{3.91}$$

In the pulsed regime [68] $\vec{h}(t)$ differs from zero only for a very short time interval δ being there very large, $\vec{h}(t)\delta \sim 1$, to achieve a finite effect. This kind of interaction was used to describe spin-echo phenomena [78], which deals with the refocusing of the precessing of nuclear spin magnetization. It is also implied in the processes of switching off undesired interactions, such as those causing decoherence [73].
It is well known that during a sudden switching on and and switching off, the density matrix of the system does not change [79] while the Hamiltonian gets a finite change. For the moment, we keep an arbitrary form of the external field Hamiltonian in the time interval $(t, t + \delta)$. The operator for the Hamiltonian $\hat{H}(t)$ given by (3.91) in the time interval $(0, t + \tau)$, where $\tau > \delta$ reads

$$\begin{aligned} &\mathcal{T} \exp\left[-\frac{i}{\hbar} \int_0^{t+\tau} ds \hat{H}(s)\right] = \\ &e^{-i[t+\tau-(t+\delta)]\hat{H}/\hbar} \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_t^{t+\delta} ds \hat{H}(s)\right] e^{-i\hat{H}t/\hbar}, \end{aligned} \tag{3.92}$$

where $\mathcal{T}$ represents the time-ordering operator. In (3.92) we have separated out the time intervals $(0, t)$ and $(t + \delta, t + \tau)$, at which the system evolves freely and the actual time-dependence of the Hamiltonian appears only in $(t, t + \delta)$.
We denote the pulse evolution operator $\hat{U}_p(t)$ as

$$\hat{U}_{\mathrm{P}}(t) \stackrel{def}{=} e^{i\delta\hat{H}/\hbar} \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_t^{t+\delta} ds \hat{H}(s)\right], \tag{3.93}$$

and want to show that it can be represented by a rotation operator acting on the spin of S_1.
We notice that the expression (3.93) satisfies the same first-order differential equation in δ with the same boundary condition $\delta = 0$ as the following expression:

$$\mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^{\delta} ds\, e^{is\hat{H}/\hbar}\, \hat{H}_{\mathrm{P}}(s+t)\, e^{-is\hat{H}/\hbar}\right]. \tag{3.94}$$

This can be shown by calculating the derivative of (3.93) and (3.94) with respect to δ. For the derivative of (3.93) with respect to δ we have

$$\begin{aligned}
&\frac{\partial}{\partial\delta} e^{i\delta\hat{H}/\hbar}\mathcal{T} \exp\left[-\frac{i}{\hbar}\int_t^{t+\delta} ds\hat{H}(s)\right] = \\
&= \frac{i}{\hbar}\left[\hat{H} - e^{i\delta\hat{H}/\hbar}\hat{H}(t+\delta)e^{-i\delta\hat{H}/\hbar}\right] e^{i\delta\hat{H}/\hbar}\mathcal{T} \exp\left[-\frac{i}{\hbar}\int_t^{t+\delta} ds\hat{H}(s)\right] \\
&= -\frac{i}{\hbar} e^{i\delta\hat{H}/\hbar}\hat{H}_{\mathrm{P}}(t+\delta)e^{-i\delta\hat{H}/\hbar}\, e^{i\delta\hat{H}/\hbar}\mathcal{T} \exp\left[-\frac{i}{\hbar}\int_t^{t+\delta} ds\hat{H}(s)\right], \qquad (3.95)
\end{aligned}$$

where we have used $\hat{H}(t) = \hat{H} + \hat{H}_{\mathrm{P}}(t)$.
On the other hand the derivative of (3.94) with respect to δ reads

$$\begin{aligned}
&\frac{\partial}{\partial\delta}\mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^{\delta} ds\, e^{is\hat{H}/\hbar}\, \hat{H}_{\mathrm{P}}(s+t)\, e^{-is\hat{H}/\hbar}\right] = \qquad (3.96) \\
&-\frac{i}{\hbar} e^{i\delta\hat{H}/\hbar}\, \hat{H}_{\mathrm{P}}(t+\delta)\, e^{-i\delta\hat{H}/\hbar}\, \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^{\delta} ds\, e^{is\hat{H}/\hbar}\, \hat{H}_{\mathrm{P}}(s+t)\, e^{-is\hat{H}/\hbar}\right].
\end{aligned}$$

Thus $\hat{U}_{\mathrm{P}}(t)$ can be written as

$$\begin{aligned}
\hat{U}_{\mathrm{P}}(t) &= e^{i\delta\hat{H}/\hbar}\mathcal{T} \exp\left[-\frac{i}{\hbar}\int_t^{t+\delta} ds\hat{H}(s)\right] \\
&= \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_t^{t+\delta} ds\, e^{i(s-t)\hat{H}/\hbar}\, \hat{H}_{\mathrm{P}}(s)\, e^{i(t-s)\hat{H}/\hbar}\right] \\
&= \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^{\delta} ds\, e^{is\hat{H}/\hbar}\, \hat{H}_{\mathrm{P}}(s+t)\, e^{-is\hat{H}/\hbar}\right]. \qquad (3.97)
\end{aligned}$$

Now we show that by considering very short pulses, we can mathematically represent them with unitary operators. When the pulses acting on S_1 are

very short so that during the time interval $(t, t+\delta)$ the terms containing $\hat{\sigma}_z^{(1)}$ in the Hamiltonian can be neglected, we can take the first term in the Taylor expansion

$$\begin{aligned} e^{is\hat{H}/\hbar}\,\hat{H}_{\rm P}(s+t)\,e^{-is\hat{H}/\hbar} &= \hat{H}_{\rm P}(s+t) + \frac{is}{\hbar}\left[\hat{H}, \hat{H}_{\rm P}(s+t)\right] + \cdots \\ &\approx \hat{H}_{\rm P}(s+t). \end{aligned} \tag{3.98}$$

Thus for the pulse evolution operator we get

$$\hat{U}_{\rm P}(t) = \mathcal{T}\exp\left[-\frac{i}{\hbar}\int_0^{\delta} ds \hat{H}_{\rm P}(s+t)\right]. \tag{3.99}$$

Thus a very short pulse can be represented by a unitary operator in the Hilbert space of the spin it is acting on. This means that a pulse rotates the Bloch vector $\langle\vec{\hat{\sigma}}^{(1)}\rangle$. We parameterize pulses by coefficients $c_{n,ab}$ as

$$\mathcal{P}_\alpha\hat{\sigma}_a^{(1)} \stackrel{def}{=} \hat{U}_{\rm P}^\dagger(t)\hat{\sigma}_a^{(1)}\hat{U}_{\rm P}(t) = \sum_{b=\pm,z} c_{n,ab}\hat{\sigma}_b^{(1)}, \qquad a=\pm,z,\;\; n=1,2, \tag{3.100}$$

where $n=1,2$ counts the number of pulses.
We notice that there is no need to neglect the bath and S_2 Hamiltonian during application of pulses, since external fields are acting on S_1 only and the influence of the bath and S_2 Hamiltonian disappear automatically. For a more detailed application, we will need the explicit form of $\hat{U}_{\rm P}^\dagger(t)$ given by (3.99). We parameterize the pulse by a 2×2 unitary matrix as

$$\hat{U}_{\rm P}^\dagger(t) = \begin{pmatrix} e^{-i\varphi}\cos\vartheta & -e^{-i\psi}\sin\vartheta \\ e^{i\psi}\sin\vartheta & e^{i\varphi}\cos\vartheta \end{pmatrix}, \tag{3.101}$$

where

$$\varphi \geq 0, \qquad \psi \leq 2\pi \qquad 0 \leq \vartheta \leq \frac{\pi}{2}. \tag{3.102}$$

Such parameterizations are common in experiments where the spin is rotated in certain degrees over a well-defined axis [78]. For this specific form of parametrization of the pulse, the coefficients $c_{k,ab}$ read

$$\begin{aligned} c_{n,+z} &= -e^{i(\psi_n-\varphi_n)}\sin 2\vartheta_n, & c_{n,++} &= e^{-2i\varphi_n}\cos^2\vartheta_n, \\ c_{n,+-} &= -e^{2i\psi_n}\sin^2\vartheta_n, & c_{n,zz} &= \cos 2\vartheta_n, \\ c_{n,z+} &= \frac{1}{2}e^{-i(\psi_n+\varphi_n)}\sin 2\vartheta_n, & c_{n,z-} &= \frac{1}{2}e^{i(\psi_n+\varphi_n)}\sin 2\vartheta_n, \end{aligned} \tag{3.103}$$

where $n=1,2$ stands for the index of the pulses.

3.7 Cooling and polarization transfer

The problem we address in this section is set up as follows. Two non-interacting spins S_1, and S_2 separated at distance r in the $z-$direction are coupled to a common thermal bath. Suddenly at time t, which we set to be much larger than the response time of the thermal bath, S_1 undergoes two successive pulses one at time t and the other at time $t+\tau$. As a result S_1 cools down. Since the spins are coupled to the same bath, we observe polarization transfer between two spins. In order to study spin cooling and polarization transfer, we calculate the final polarization of both spins as well as the final averaged transversal components of spins.

The final expressions for $\sigma_z^{(1)}$ after applying two pulses $\mathcal{P}_1$ at time t and $\mathcal{P}_2$ at time $t+\tau$ reads

$$\sigma_z^{(1)}(t+\tau) \;=\; \mathcal{E}_t\,\mathcal{P}_1\,\mathcal{E}_\tau\,\mathcal{P}_2\,\hat{\sigma}_z^{(1)}. \tag{3.104}$$

Implying (3.100) for $\mathcal{P}_2\,\hat{\sigma}_z^{(1)}$ we get

$$\sigma_z^{(1)}(t+\tau) \;=\; \mathcal{E}_t\,\mathcal{P}_1\,\mathcal{E}_\tau\,\left[c_{2,zz}\hat{\sigma}_z^{(1)} + 2\Re\{c_{2,z+}\hat{\sigma}_+^{(1)}\}\right]. \tag{3.105}$$

The operator $\mathcal{E}_\tau$ acting on $\hat{\sigma}_z^{(1)}$ does not change it while for $\hat{\sigma}_+^{(1)}(\tau)$ we can insert the expression (3.39) into (3.105) and get

$$\begin{aligned}\sigma_z^{(1)}(t+\tau) = \mathcal{E}_t\,\mathcal{P}_1 \quad &\Big[\quad c_{2,zz}\hat{\sigma}_z^{(1)} \\ &+ \quad 2\Re\left\{c_{2,z+}e^{i[\Omega_1\tau - F(\tau)]}\hat{\Pi}_r^+(0,\tau)\,\hat{\sigma}_+^{(1)}\,e^{-i\bar{F}_r(\tau)\hat{\sigma}_z^{(2)}}\right\}\Big],\end{aligned} \tag{3.106}$$

where, for brevity, we drop the initial time $t=0$ argument of $\hat{\sigma}_\pm^{(i)}$ and $\hat{\sigma}_z^{(i)}$. Operation of the pulse $\mathcal{P}_1$ on S_1 results in

$$\begin{aligned}&\sigma_z^{(1)}(t+\tau) = c_{2,zz}\,\mathcal{E}_t\,\left[c_{1,zz}\hat{\sigma}_z^{(1)} + 2\Re\{c_{1,z+}\hat{\sigma}_+^{(1)}\}\right] \\ &+2\mathcal{E}_t\Re\Big\{c_{2,z+}\,e^{i[\Omega_1\tau - F(\tau)]}\hat{\Pi}_r^+(0,\tau)\,\times \\ &\times\left[c_{1,z+}\hat{\sigma}_z^{(1)} + c_{1,++}\hat{\sigma}_+^{(1)} + c_{1,+-}\hat{\sigma}_-^{(1)}\right]e^{-i\bar{F}_r(\tau)\hat{\sigma}_z^{(2)}}\Big\}.\end{aligned} \tag{3.107}$$

Applying the time evolution operator $\mathcal{E}_t$ on the spin components using (3.39), (3.49), (3.69), and (3.49) finally yields

$$\begin{aligned}
&\sigma_z^{(1)}(t+\tau) = c_{2,zz}c_{1,zz}\sigma_z^{(1)} \qquad (3.108)\\
&+2\,c_{2,zz}\Re\Big\{c_{1,z+}e^{i[\Omega_1 t-F(t)]}\,\hat{\Pi}_r^+(0,t)\,\hat{\sigma}_+^{(1)}\,e^{-i\bar{F}_r(t)\hat{\sigma}_z^{(2)}}\Big\}\\
&+2\Re\Big\{c_{2,z+}c_{1,+z}e^{i[\Omega_1\tau-F(\tau)]}\hat{\Pi}_r^+(t,t+\tau)\,\hat{\sigma}_z^{(1)}\,e^{i\chi(\tau,t)\hat{\sigma}_z^{(1)}}\,e^{i\left[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)\right]\hat{\sigma}_z^{(2)}}\Big\}\\
&+2\Re\Big\{c_{2,z+}\,c_{1,++}e^{i[\Omega_1(t+\tau)-F(t+\tau)]}\,\hat{\Pi}_r^+(t,t+\tau)\hat{\Pi}_r^+(0,t)\,\hat{\sigma}_+^{(1)}\,e^{-i\bar{F}_r(t+\tau)\hat{\sigma}_z^{(2)}}\Big\}\\
&+2\Re\Big\{c_{2,z+}\,c_{1,+-}e^{i[\Omega_1(\tau-t)-\chi(\tau,t)-F(t)-F(\tau)]}\,\hat{\Pi}_r^+(t,t+\tau)\hat{\Pi}_r^-(0,t)\,\hat{\sigma}_-^{(1)}\,\times\\
&\times\,e^{i\hat{\sigma}_z^{(2)}\left[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)+\bar{F}_r(t)\right]}\Big\},
\end{aligned}$$

where we have used the definition of $\bar{\chi}_r(\tau,t)$ as the averaged value of $\chi_r(\tau,t)$ over θ_k, which is given by

$$\bar{\chi}_r(\tau,t) = \bar{F}_r(t) + \bar{F}_r(\tau) - \bar{F}_r(t+\tau), \qquad (3.109)$$

where $\bar{F}_r(t)$ is given by (3.90). We notice that the back reaction factor $F(t)$ shifts the frequency Ω_1 of S_1. In other words, applying pulses amounts to enhancement of the back reaction force of the spin on the collective coordinates of the bath.
Averaging (3.108) over the bath and both spin states results the final polarization of S_1 as

$$\begin{aligned}
&\langle\hat{\sigma}_z^{(1)}(t+\tau)\rangle = c_{1,zz}\,c_{2,zz}\langle\hat{\sigma}_z^{(1)}\rangle \qquad (3.110)\\
&+2e^{-\xi(\tau)}\Re\left\{c_{2,z+}\,c_{1,+z}\,e^{i\Omega_1\tau}\,\langle e^{i\chi(\tau,t)\hat{\sigma}_z^{(1)}}\,\hat{\sigma}_z^{(1)}\rangle\,\langle e^{i\left[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)\right]\hat{\sigma}_z^{(2)}}\right\},
\end{aligned}$$

where implied the initial condition (3.56) and set $\langle\hat{\sigma}_\pm^{(1)}\rangle = 0$ in deriving (3.110).
We notice that there are two factors that come from the bath:

- $e^{-\xi(\tau)}$ which amounts to the decoherence of the transversal spin components, of the system located at the origin, in the time period τ between the two pulses. Note that the transversal terms are generated by the first pulse.

- $\chi(\tau,t)$, and $\chi_r(\tau,t)$, defined by (3.50), representing back reaction factors of both spins on the collective coordinate operator of the bath. As we saw in section 3.4, Eqs. (3.74–3.74), this effect is not relevant for decoherence, but it is crucial in this context.

We now work out the second term of the expression (3.110) for the final polarization of the pulsed spin after two successive pulses.

$$\begin{aligned} & 2e^{-\xi(\tau)}\Re\left\{c_{2,z+}\,c_{1,+z}\,e^{i\Omega_1\tau}\,\langle e^{i\chi(\tau,t)\hat{\sigma}_z^{(1)}}\hat{\sigma}_z^{(1)}\rangle\,\langle e^{i\left[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)\right]\hat{\sigma}_z^{(2)}}\rangle\right\} \\ & = 2e^{-\xi(\tau)}\Re\left\{c_{2,z+}\,c_{1,+z}\,e^{i\Omega_1\tau}\,P_r\right\}, \end{aligned} \tag{3.111}$$

where

$$\begin{aligned} P_r \;\stackrel{def}{=}\; & i\sin\left[\chi(\tau,t)\right]\cos\left[\chi_r(\tau,t)-F_r(\tau)\right] \\ + \;& i\langle\hat{\sigma}_z^{(1)}\rangle\,\langle\hat{\sigma}_z^{(2)}\rangle\cos\left[\chi(\tau,t)\right]\sin\left[\chi_r(\tau,t)-F_r(\tau)\right] \\ + \;& \langle\sigma_z^{(1)}\rangle\cos\left[\chi(\tau,t)\right]\cos\left[\chi_r(\tau,t)-F_r(\tau)\right] \\ - \;& \langle\sigma_z^{(2)}\rangle\sin\left[\chi(\tau,t)\right]\sin\left[\chi_r(\tau,t)-F_r(\tau)\right]. \end{aligned} \tag{3.112}$$

For the following results we set $\Gamma t \gg 1$ which means we wait long enough so the systems and the bath reach the equilibrium. Then we apply two successive pulses on the spin S_1. This guaranties the independency of the outcome result on the details of the initial state preparation. In this limit $\chi(\tau,t)$ and $\chi_r(\tau,t)-F_r(\tau)$ read [see appendix C]

$$\chi_r(\tau,t)-F_r(\tau) \;=\; -\frac{\gamma\tau c}{r}\arctan\left(\frac{\Gamma r}{c}\right), \tag{3.113}$$

$$\chi(\tau,t) \;=\; -\gamma\,\arctan(\Gamma\tau). \tag{3.114}$$

Inserting (3.113) into the expression of P_r given by (3.112) yields

$$\begin{aligned} P_r \;=\; & -i\sin\left[\gamma\,\arctan(\Gamma\tau)\right]\cos\left[\frac{\gamma\tau c}{r}\arctan\left(\frac{\Gamma r}{c}\right)\right] \\ - \;& i\langle\hat{\sigma}_z^{(1)}\rangle\,\langle\hat{\sigma}_z^{(2)}\rangle\cos\left[\gamma\,\arctan(\Gamma\tau)\right]\sin\left[\frac{\gamma\tau c}{r}\arctan\left(\frac{\Gamma r}{c}\right)\right] \\ + \;& \langle\sigma_z^{(1)}\rangle\cos\left[\gamma\,\arctan(\Gamma\tau)\right]\cos\left[\frac{\gamma\tau c}{r}\arctan\left(\frac{\Gamma r}{c}\right)\right] \\ - \;& \langle\sigma_z^{(2)}\rangle\sin\left[\gamma\,\arctan(\Gamma\tau)\right]\sin\left[\frac{\gamma\tau c}{r}\arctan\left(\frac{\Gamma r}{c}\right)\right]. \end{aligned} \tag{3.115}$$

Inserting (3.112) and the parameters describing the pulses from (3.103) into (3.110), the final polarization of the pulsed spin reads

$$\begin{aligned}\langle\sigma_z^{(1)}(t+\tau)\rangle &= \cos 2\vartheta_1 \cos 2\vartheta_2 \langle\sigma_z^{(1)}\rangle \\ &- \sin 2\vartheta_1 \sin 2\vartheta_2\, e^{-\xi(\tau)} \Re\left\{e^{i\Omega_1\tau}\, e^{i\varsigma}\, P_r\right\},\end{aligned} \tag{3.116}$$

where P_r is defined by (3.115) and

$$\varsigma \stackrel{def}{=} \psi_1 - \psi_2 - \varphi_1 - \varphi_2. \tag{3.117}$$

This expression is one of our main results. We notice that due the presence of the first term in the expression for P_r given by (3.115) the final polarization of the pulsed spin can be non-zero even if both spins are initially completely unpolarized, i.e. in the case where $\langle\hat{\sigma}_z^{(1)}\rangle = 0 = \langle\hat{\sigma}_z^{(2)}\rangle$. In this case the expression for P_r given by (3.115) reads

$$P_r = -i \sin\left[\gamma \arctan(\Gamma\tau)\right] \cos\left[\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right)\right]. \tag{3.118}$$

Thus the final polarization of S_1 will be

$$\begin{aligned}&\langle\sigma_z^{(1)}(t+\tau)\rangle = -e^{-\xi(\tau)} \sin 2\vartheta_1 \sin 2\vartheta_2 \times \\ &\times \sin\left[\gamma \arctan(\Gamma\tau)\right] \cos\left[\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right)\right] \Im\{e^{i\Omega_1\tau}\, e^{i\varsigma}\}.\end{aligned} \tag{3.119}$$

Since Ω_1 is negligible due to the initial conditions,

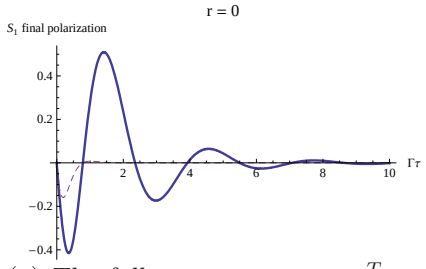
$$\begin{aligned}&\langle\sigma_z^{(1)}(t+\tau)\rangle = -e^{-\xi(\tau)} \sin 2\vartheta_1 \sin 2\vartheta_2 \times \\ &\times \sin\left[\gamma \arctan(\Gamma\tau)\right] \cos\left[\gamma\Gamma\tau\cos(kr\cos\theta)\right] \Im\{e^{i\varsigma}\}.\end{aligned} \tag{3.120}$$

This expression can be maximized over the pulse parameters by choosing

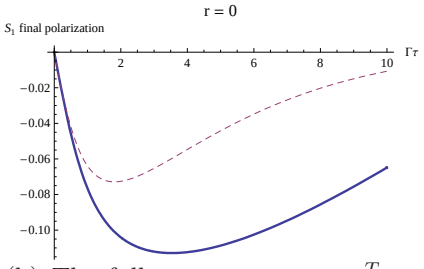
$$\vartheta_1 = \vartheta_2 = \frac{\pi}{4}, \qquad \varsigma = \frac{\pi}{2}. \tag{3.121}$$

In terms of pulses this means to apply a $\frac{\pi}{2}$ pulse along the $x-$axis at time t followed by another $-\frac{\pi}{2}$ pulse along the $y-$direction at time $t+\tau$.
We represent a $\frac{\pi}{2}$ pulse along the $x-$axis as [66]

$$\mathcal{P}_1\left(x, \frac{\pi}{2}\right), \tag{3.122}$$



(a) The full curve represents $\frac{T}{\hbar\Gamma} = 0.1$ while the dashed curve $\frac{T}{\hbar\Gamma} = 1$. The bath coupling constant $\gamma = 2$.



(b) The full curve represents $\frac{T}{\hbar\Gamma} = 0.1$ while the dashed curve $\frac{T}{\hbar\Gamma} = 1$. The bath coupling constant $\gamma = 0.1$.

Figure 3.1: The final polarization of S_1 after two successive pulses in terms of $\Gamma\tau$ for different temperatures when the dimensionless bath coupling constant $\gamma = 2$ and $\gamma = 0.1$. We compare these two cases when both spins are initially unpolarized and are located at the same place, $r = 0$.

where

$$\mathcal{P}_1\left(x, \frac{\pi}{2}\right)\hat{\sigma}_z \equiv e^{i\hat{\sigma}_x\pi/4}\,\hat{\sigma}_z\,e^{-i\hat{\sigma}_x\pi/4}. \tag{3.123}$$

The first $\frac{\pi}{2}$ pulse in the $x-$direction applied on $\hat{\sigma}_z^{(1)}$ can be described by

$$\mathcal{P}_1\left(x, \frac{\pi}{2}\right)\hat{\sigma}_z^{(1)} = \frac{1}{2i}\hat{\sigma}_+^{(1)} - \frac{1}{2i}\hat{\sigma}_-^{(1)}, \tag{3.124}$$

which in terms of the pulse coefficients $c_{n,ab}$ means

$$c_{1,zz} = 0, \qquad c_{1,z+} = \frac{1}{2i}. \tag{3.125}$$

Therefore

$$\psi_1 + \varphi_1 = \frac{\pi}{2}. \tag{3.126}$$

Applying $-\frac{\pi}{2}$ pulse in the $y-$direction on $\hat{\sigma}_z^{(1)}$ gives

$$\mathcal{P}_2\left(y, -\frac{\pi}{2}\right)\hat{\sigma}_z^{(1)} = e^{-i\hat{\sigma}_y^{(1)}\pi/4}\,\hat{\sigma}_z^{(1)}\,e^{i\hat{\sigma}_y^{(1)}\pi/4}, \tag{3.127}$$

which yields

$$\mathcal{P}_2\left(y, -\frac{\pi}{2}\right)\hat{\sigma}_z^{(1)} = \frac{1}{2}\hat{\sigma}_+^{(1)} + \frac{1}{2}\hat{\sigma}_-^{(1)}. \tag{3.128}$$

Therefore the pulse coefficients read

$$c_{2,zz} = 0, \qquad c_{2,z+} = \frac{1}{2}. \tag{3.129}$$

$c_{2,z+} = \frac{1}{2}$ implies

$$\psi_2 + \varphi_2 = 0. \tag{3.130}$$

As a result the final polarization of S_1 is

$$\begin{aligned} &\langle \sigma_z^{(1)}(t+\tau)\rangle = \\ &-e^{-\xi(\tau)} \sin\left[\gamma \arctan(\Gamma\tau)\right] \cos\left[\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right)\right]. \end{aligned} \tag{3.131}$$

The physical reason of getting non-zero final polarization is the back reaction of both spins which is now shared between them. The generation of coherence by the first $\frac{\pi}{2}$ pulse couples S_1 to the bath and S_2. The polarization of S_1 changes under the shifted frequency. We notice that the final polarization of S_1 depends on the distance between the two spins and the time τ between two pulses. The final polarization decays with the factor $e^{-\xi(\tau)}$, which describes the decoherence of the transversal terms produced by the first pulse in the time interval between the two pulses. Thus the time interval between two pulses should be such that it does not let the decoherence overcome the influence of the first pulse. The factor $e^{-\xi(\tau)}$ implies that the final value of the polarization of S_1 decreases with γ (weaker back reaction) and $1/T$ (larger decoherence).

When we set $r \to \infty$ which means we consider two separates spins each with its own bath, $\cos\left[\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right)\right] = 1$ and we get the same result as in the single qubit case [65]:

$$\langle \sigma_z^{(1)}(t+\tau)\rangle = -e^{-\xi(\tau)} \sin\left[\gamma \arctan(\Gamma\tau)\right]. \tag{3.132}$$

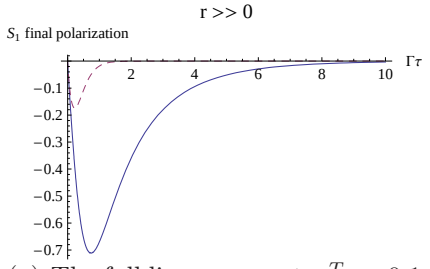
While considering both spins sitting on top of each other, $r = 0$ yields

$$\langle \sigma_z^{(1)}(t+\tau)\rangle = -e^{-\xi(\tau)} \sin\left[\gamma \arctan(\Gamma\tau)\right] \cos\left(\gamma\Gamma\tau\right). \tag{3.133}$$

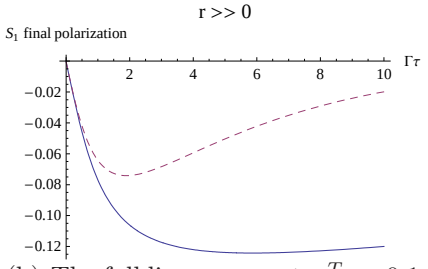
Another interesting phenomenon is the case of spin transfer, which takes place if the initial polarization of S_2 is larger than the initial polarization of S_1. This can be seen from the last term in the expression (3.116) for P_r given by

$$-\langle \sigma_z^{(2)}\rangle \sin\left[\gamma \arctan(\Gamma\tau)\right] \sin\left[\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right)\right]. \tag{3.134}$$

Thus when S_2 is initially highly polarized while S_1 is unpolarized, P_r given



(a) The full line represents $\frac{T}{\hbar\Gamma} = 0.1$ while the for the dashed curve $\frac{T}{\hbar\Gamma} = 1$. The bath coupling constant $\gamma = 2$.



(b) The full line represents $\frac{T}{\hbar\Gamma} = 0.1$ while the for the dashed curve $\frac{T}{\hbar\Gamma} = 1$. The bath coupling constant $\gamma = 0.1$.

Figure 3.2: The final polarization of S_1 after two successive pulses in terms of $\Gamma\tau$ for different temperatures when the dimensionless bath coupling constant $\gamma = 2$ and $\gamma = 0.1$. We compare these two cases when both spins are initially unpolarized and are located at the same place, $r \gg 0$.

by (3.115) reads

$$\begin{aligned} P_r &= -i \sin\left[\gamma \arctan(\Gamma\tau)\right] \cos\left[\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right)\right] \\ &\quad -\langle\hat{\sigma}_z^{(2)}\rangle \sin\left[\gamma \arctan(\Gamma\tau)\right] \sin\left[\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right)\right], \end{aligned} \tag{3.135}$$

and the final polarization of an initially unpolarized spin reads

$$\langle\sigma_z^{(1)}(t+\tau)\rangle = -e^{-\xi(\tau)} \sin 2\vartheta_1 \sin 2\vartheta_2 \, \Re\left\{e^{i\varsigma} P_r\right\}, \tag{3.136}$$

where P_r is given by (3.135).
The polarization transfer from S_2 to S_1 takes place when we consider to following pulse parameters

$$\vartheta_1 = \vartheta_2 = \frac{\pi}{4}, \qquad \varsigma = 0. \tag{3.137}$$

The above condition can be fulfilled by applying a $-\frac{\pi}{2}$ pulse in the $x-$direction followed by a $-\frac{\pi}{2}$ pulse in the $y-$direction after a time period of τ. A $-\frac{\pi}{2}$ pulse in the $x-$direction means

$$\mathcal{P}_1\left(x, -\frac{\pi}{2}\right) \hat{\sigma}_z^{(1)} = e^{-i\hat{\sigma}_x^{(1)}\pi/4} \, \hat{\sigma}_z^{(1)} \, e^{i\hat{\sigma}_x^{(1)}}, \tag{3.138}$$

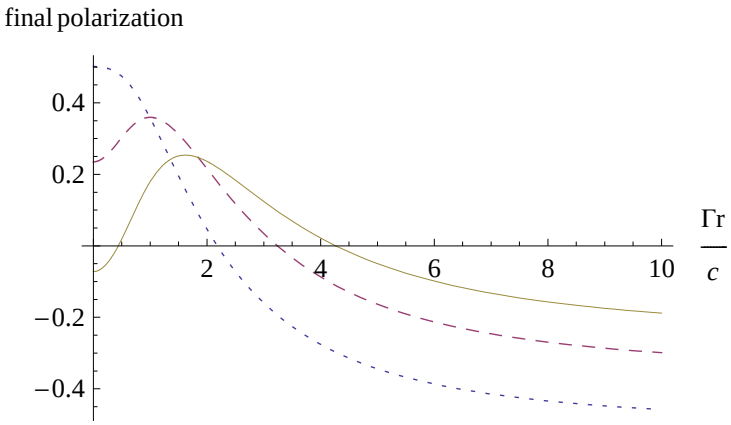


Figure 3.3: The final polarization of S_1 after two successive pulses in terms of the dimensionless distance$\Gamma r/c$ for different pulse durations $\Gamma\tau$. The dimensionless bath coupling constant $\gamma = 2$, and $\frac{T}{\hbar\Gamma} = 0.1$. Both spins are initially unpolarized. The dotted curve: $\Gamma\tau = 1.5$, the dashed curve: $\Gamma\tau = 2$, and the solid curve: $\Gamma\tau = 2.5$.

which yields to

$$\mathcal{P}_1\left(x, -\frac{\pi}{2}\right)\hat{\sigma}_z^{(1)} = -\frac{1}{2i}\hat{\sigma}_+^{(1)} + \frac{1}{2i}\hat{\sigma}_-^{(1)}. \tag{3.139}$$

Therefore

$$\psi_1 + \varphi_1 = \frac{3\pi}{4}. \tag{3.140}$$

Thus the final polarization of S_1 in this case reads

$$\begin{aligned}&\langle\sigma_z^{(1)}(t+\tau)\rangle = \\ &e^{-\xi(\tau)}\,\langle\hat{\sigma}_z^{(2)}\rangle \sin\left[\gamma\,\arctan(\Gamma\tau)\right]\sin\left[\frac{\gamma\tau c}{r}\arctan\left(\frac{\Gamma r}{c}\right)\right].\end{aligned} \tag{3.141}$$

Thus we see the initial polarization of S_2 is partially transferred to S_1 without modifying the initial polarization of S_2. This is not in contradiction with the no-cloning theorem, which states that no well-defined state can be attributed to a subsystem of an entangled state. Since in our case the quantum states are represented by commuting density matrices, they can be cloned (copied) exactly.
Thus the existence of S_2 improves the cooling effect via polarization transfer provided it is initially sufficiently polarized.

Now we calculate $\langle\hat{\sigma}_{\pm}^{(1)}(t+\tau)\rangle$ to see how the transversal components of S_1 which initially are zero evolve after applying two successive pulses on S_1. Following the same analogy as we employed in deriving the final polarization of S_1 we have

$$\hat{\sigma}_{\pm}^{(1)}(t+\tau) = \mathcal{E}_t\mathcal{P}_1\mathcal{E}_\tau\mathcal{P}_2\hat{\sigma}_{\pm}^{(1)}, \tag{3.142}$$

which then yields

$$\begin{aligned}
&\hat{\sigma}_{\pm}^{(1)}(t+\tau) = c_{2,\pm z}\, c_{1,zz}\hat{\sigma}_z^{(1)} \\
&+2\, c_{2,\pm z}\Re\left\{c_{1,z\pm}e^{i[\Omega_1 t - F(t)]}\,\hat{\Pi}_r^{+}(0,t)\,\hat{\sigma}_{+}^{(1)}e^{-i\bar{F}_r(t)\hat{\sigma}_z^{(2)}}\right\} \\
&+c_{2,\pm+}\, c_{1,+z}\, e^{i[\Omega_1\tau - F(\tau)]}\,\hat{\Pi}_r^{+}(t,t+\tau)\, e^{i\chi(\tau,t)\hat{\sigma}_z^{(1)}}\,\hat{\sigma}_z^{(1)}\, e^{i\left[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)\right]\hat{\sigma}_z^{(2)}} \\
&+c_{2,\pm-}\, c_{1,-z}\, e^{-i[\Omega_1\tau + F(\tau)]}\,\hat{\Pi}_r^{-}(t,t+\tau)\, e^{-i\chi(\tau,t)\hat{\sigma}_z^{(1)}}\,\hat{\sigma}_z^{(1)}\, e^{-i\left[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)\right]\hat{\sigma}_z^{(2)}} \\
&+c_{2,\pm+}\, c_{1,++}\, e^{i[\Omega_1(t+\tau) - F(t+\tau)]}\,\hat{\Pi}_r^{+}(t,t+\tau)\Pi_r^{+}(0,t)\,\hat{\sigma}_{+}^{(1)}e^{-i\bar{F}_r(t+\tau)\hat{\sigma}_z^{(2)}} \\
&+c_{2,\pm-}\, c_{1,--}\, e^{-i[\Omega_1(\tau+t) + F(\tau+t)]}\,\Pi_r^{-}(t,t+\tau)\,\hat{\Pi}_r^{-}(0,t)\,\hat{\sigma}_{-}^{(1)}\, e^{i\bar{F}_r(t+\tau)\hat{\sigma}_z^{(2)}} \\
&+c_{2,\pm+}\, c_{1,-+}\, e^{-i[\Omega_1(\tau-t) - F(t+\tau) + 2F(\tau) + 2F(t)]}\,\hat{\Pi}_r^{-}(t,t+\tau)\hat{\Pi}_r^{+}(0,t)\,\times \\
&\times\hat{\sigma}_{+}^{(1)}\, e^{i\left[\bar{F}_r(t+\tau) - 2\bar{F}_r(t)\right]\hat{\sigma}_z^{(2)}} \\
&+c_{2,\pm+}\, c_{1,+-}\, e^{i[\Omega_1(\tau-t) + F(t+\tau) - 2F(\tau) - 2F(t)]}\,\hat{\Pi}_r^{+}(t,t+\tau)\hat{\Pi}_r^{-}(0,t)\,\times \\
&\times\hat{\sigma}_{-}^{(1)}\, e^{-i\left[\bar{F}_r(t+\tau) - 2\bar{F}_r(t)\right]\hat{\sigma}_z^{(2)}}.
\end{aligned} \tag{3.143}$$

Taking the ensemble averages and implying the initial condition

$$\langle\hat{\sigma}_{\pm}^{(1)}\rangle = 0, \tag{3.144}$$

yields

$$\begin{aligned}
&\langle\hat{\sigma}_{\pm}^{(1)}(t+\tau)\rangle = c_{2,\pm z}\, c_{1,zz}\,\langle\hat{\sigma}_z^{(1)}\rangle + \\
&+c_{2,\pm+}\, c_{1,+z}\, e^{i\Omega_1\tau - \xi(\tau)}\,\langle e^{i\chi(\tau,t)\hat{\sigma}_z^{(1)}}\hat{\sigma}_z^{(1)}\rangle\,\langle e^{i[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)]\hat{\sigma}_z^{(2)}}\rangle \\
&+c_{2,\pm-}\, c_{1,-z}\, e^{-i\Omega_1\tau - \xi(\tau)}\,\langle e^{-i\chi(\tau,t)\hat{\sigma}_z^{(1)}}\hat{\sigma}_z^{(1)}\rangle\,\langle e^{-i[\bar{\chi}_r(\tau,t)-\bar{F}_r(\tau)]\hat{\sigma}_z^{(2)}}\rangle,
\end{aligned} \tag{3.145}$$

Inserting the pulse coefficients from (3.103) and employing the definition of P_r from (3.115) for $\langle\hat{\sigma}_{+}^{(1)}(t+\tau)\rangle$ we get

$$\begin{aligned}
&\langle\hat{\sigma}_{+}^{(1)}(t+\tau)\rangle = \\
&-e^{-i(\psi_2-\varphi_2)}\sin 2\vartheta_2\cos 2\vartheta_1\langle\hat{\sigma}_z^{(1)}\rangle - \sin 2\vartheta_1\, e^{-\xi(\tau)}\,\times \\
&\times\Big\{\cos^2\vartheta_2\, e^{i(\psi_1-\varphi_1-2\varphi_2)}e^{i\Omega_1\tau}\,P_r - \sin^2\vartheta_2\, e^{-i(\psi_1-\varphi_1-2\psi_2)}e^{-i\Omega_1\tau}\,P_r^{*}\Big\},
\end{aligned} \tag{3.146}$$

where P_r^* is the complex conjugate of P_r.
Let us now consider the case where both spins are initially unpolarized; $\langle\hat{\sigma}_z^{(1)}\rangle = 0 = \langle\hat{\sigma}_z^{(1)}\rangle$. Applying a $\frac{\pi}{2}$ pulse along the $x-$direction followed by a $-\frac{\pi}{2}$ pulse along the $y-$direction on S_1 with the pulse parameter

$$\vartheta_1 = \vartheta_2 = \frac{\pi}{4}, \qquad \varsigma = \frac{\pi}{2}, \tag{3.147}$$

results in

$$\mathcal{P}_1\left(\frac{\pi}{2}, x\right)\hat{\sigma}_+^{(1)} = \frac{1}{2}\hat{\sigma}_+^{(1)} + \frac{1}{2}\hat{\sigma}_-^{(1)} - i\hat{\sigma}_z^{(1)} \tag{3.148}$$

$$\mathcal{P}_2\left(-\frac{\pi}{2}\right)\hat{\sigma}_+^{(1)} = \frac{1}{2}\hat{\sigma}_+^{(1)} - \frac{1}{2}\hat{\sigma}_-^{(1)} - \hat{\sigma}_z^{(1)}. \tag{3.149}$$

Thus inserting $\vartheta_1 = \vartheta_2 = \frac{\pi}{4}$ in the expressions for $c_{1,+z}$, $c_{1,++}$, and $c_{2,+z}$ given by (3.103) we get

$$\begin{aligned} &\psi_1 = 0, \qquad \varphi_1 = \frac{\pi}{2} \\ &\psi_2 = \varphi_2 = 0. \end{aligned} \tag{3.150}$$

Now the expression for $\langle\hat{\sigma}_+^{(1)}(t+\tau)\rangle$ reads

$$\langle\hat{\sigma}_+^{(1)}(t+\tau)\rangle = -ie^{-\xi(\tau)}\Re\{P_r\}, \tag{3.151}$$

where we take into account that $\Omega_1\tau$ is negligible. We notice that P_r given by the expression (3.118) is a purely imaginary expression and thus

$$\langle\hat{\sigma}_x^{(1)}(t+\tau)\rangle = 0 = \langle\hat{\sigma}_y^{(1)}(t+\tau)\rangle. \tag{3.152}$$

Thus while the polarization of initially unpolarized S_1 increases by applying a $\frac{\pi}{2}$ pulse in the x-direction and a $-\frac{\pi}{2}$ in the $y-$direction, its transversal components will remain the same when S_2 is also initially unpolarized.
On the other hand, when S_2 is initially highly polarized, $|\langle\hat{\sigma}_z^{(2)}\rangle| \sim 1$, following the same lines of calculation we get a non-zero final transversal component in the y-direction by applying two successive $-\frac{\pi}{2}$ pulses in the x and y direction. In this case we have

$$\psi_1 = \varphi_1 = \frac{3\pi}{4}, \qquad \psi_2 = \varphi_2 = 0. \tag{3.153}$$

Therefore

$$\langle \hat{\sigma}_+^{(1)}(t+\tau)\rangle = -ie^{-\xi(\tau)}\Im\{P_r\}, \tag{3.154}$$

where P_r is given by (3.135). Thus for the final transversal components of the S_1 spin we have

$$\begin{aligned} &\langle \hat{\sigma}_x^{(1)}(t+\tau)\rangle = 0, \\ &\langle \hat{\sigma}_y^{(1)}(t+\tau)\rangle = e^{-\xi(\tau)}\sin\left[\gamma \arctan\left(\Gamma\tau\right)\right]\cos\left[\frac{\gamma\tau c}{r}\arctan\left(\frac{\Gamma r}{c}\right)\right]. \end{aligned} \tag{3.155}$$

We recall that since there are no external forces applying on S_2, the process does not affect its state.

3.8 Conclusion

Spin-$\frac{1}{2}$ systems are quantum systems for which the Hilbert space is two-dimensional and thus can be considered as qubits. Recently, nuclear spins as examples of spin-$\frac{1}{2}$ systems have been suggested as good candidates for realizing quantum information processing [80–82]. Before any quantum algorithm can be executed, the qubits themselves must be initialized into a well-defined state which in most cases should be pure. Unfortunately, the nuclear spin systems are surrounded by the environment. That is to say, they are usually found in a highly mixed state and thus unpolarized. However, there are several techniques for increasing the polarization of nuclear spin. The most common ones are optical pumping [83] in which light is used to enhance the polarization and dynamic nuclear polarization [84], which is based on transferring the spin polarization of electrons to nuclei in a coupled two-spin system with the help of radio frequency pulses applied on both spins. Here we describe another polarization enhancement method based on the back reaction of the environment. In this scheme we consider two spatially non-interacting qubits coupled to a common bath. By applying two successive pulses on one of spins, we can increase its polarization (cool it down) even if the initial polarization of both spins is negligible. When one spin is initially highly polarized, applying two successive pulses on the initially unpolarized spin results in polarization transfer, hence enhancement of polarization of an initially unpolarized spin. We studied this situation within the spin-boson model. We showed that under certain considerations the model can be exactly solvable. For the spectral density of the bath we considered the ohmic

regime. We showed that the origin of polarization enhancement mechanism lies in the shared back reaction of spins to the common bath. Thus the presence of the bath is necessary. In fact, it is the only interactive component between the spins which intermediates the polarization transformation. By applying strong pulses on two non-interacting spins coupled to a common bath, it is possible to reach final non-zero polarization even when both spins are initially unpolarized. In case the pulsed spin is initially unpolarized while the other spin has high initial polarization we obtain rather good polarization transfer.

CHAPTER 4

Adiabatic Perturbation Theory

This chapter is devoted to the adiabatic perturbation theory. It is presented in a different way from the standard presentations by a careful accounting of higher-order terms. The idea is based on the time-scale separation which is usually the case when a massive slow system interacts with a light fast system. In the previous section the spin-boson model was employed to study the evolution of an open quantum system. In this chapter we consider another category of open systems in which the quantum system evolves much faster than its slow classical surrounding environment. The Hamiltonian of the fast system then can be considered as a function of the slowly varying parameters of the slow system. The wavefunction of the fast quantum system is separated into fast and slow components and the slow component is expanded in terms of a small parameter. This parameter is defined as the ratio of the characteristic time scales of the two systems. Within this time scale separation it is possible to determine the state of the open quantum system.

4.1 Introduction

A recurrent theme in modern physics is to study the dynamics of an open system, i.e., a system that interacts with its environment [54]. Depending on the type of environment, there are different conditions under which this procedure is possible. A group of methods, which goes under the name of system-bath interaction, amounts to isolating a relatively small system in contact to an equilibrium environment (thermal bath) [54]. This was the subject of chapter 3. One of the main consequences of this approach is the Langevin equation, which supplements the Newton equation of motion for the small system by two additional forces: random conservative force and non-conservative (i.e., non-Lagrangian), velocity-dependent friction force [54].

There is another set-up that allows studying the dynamics of an open system. Here the essential condition is that the target system is much faster than its environment [2, 3, 85, 86]. Separation of scales plays a fundamental role in understanding the dynamical behavior of the hybrid (slow + fast) systems. It is often possible to drive simple laws for certain slow variables from the underlying fast dynamics whenever the scales are well separated. As an example consider the spinning top. While the top rotates very fast, the rotation axis is usually precessing much slower. The earth is an example of a top where these time scales are well separated. It turns once a day, but the frequency of precession is about 26000 years.
The prototype example in quantum mechanics is a molecule, i.e. a system consisting of two types of particles with very different masses. Electrons are lighter than nuclei by a factor at least 2000, depending on the type of nucleusand and are moving much faster than the nuclei. In this case the fast scale is also the quantum mechanical time scale described by Planck's constant $\hbar$ and the relevant energies. The slow scale is "slow" with respect to the fast quantum scale. For the sake of clarity in the time-scale separation, we define a dimensionless small parameter, ϵ, as the ratio of the characteristic time scales of the two systems. By "the characteristic time" of the fast system we mean the time over which the dynamical quantities associated to the fast system change considerably, while the dynamical quantities associated with the slow system experience a small change. In the adiabatic regime this parameter, ϵ, approaches zero. By adiabatic we mean the regime, where the slow system evolves infinitely slowly in time. This situation is best described by the adiabatic theorem which implies that a system prepared in the instantaneous eigenstate of a time-dependent Hamiltonian will remain close to the

instantaneous eigenstate of the Hamiltonian provided that the Hamiltonian changes sufficiently slowly [87–89]. The adiabatic theorem in quantum mechanics was developed in its early days and it is a useful and a powerful tool for studying the dynamics of a quantum system where the Hamiltonian of the system evolves very slowly (adiabatically) in time. The theory has lots of applications, in the name of adiabatic approximation, in quantum physics (Berry phase) [90], quantum control [91] and adiabatic quantum computation [92].
In the adiabatic regime, the effective dynamics for the slow degrees of freedom, *e.g.* for the nuclei, is known as Born-Oppenheimer approximation and it is important for understanding the molecular dynamics. In this regime the dynamics of the nucleus can be described by considering an effective potential generated by one energy level of the electrons, while the state of the electrons instantaneously adjusts to an eigenstate corresponding to the momentary configuration of the nuclei.
The phenomenon that fast degrees of freedom become slaved by slow degrees of freedom which in turn evolve autonomously is called adiabatic decoupling. In the following two chapters we show that if the slow system, doesn't evolve infinitely slowly, i. e., ϵ is small but not zero, the effective dynamics of the slow system can be described by additional forces exerted on it from the fast quantum system. In doing so, we discuss the adiabatic perturbation theory in section 4.3. Section 4.4 is devoted to the precision of this method. The dynamics of the slow classical system is the subject of the next chapter.

4.2 Slowly evolving systems

Usually the Hamiltonian discussed in the quantum mechanical text books does not depend on time. But in reality it does depend on time due to the presence of the external or environmental factors. Therefore, it is important to study time-dependent Hamiltonians in modeling the real quantum systems. One of the most interesting aspects of time-dependent Hamiltonians is the occurrence of the geometric phase, which had been ignored in quantum physics for half a century. It had not been forgotten but was thought to be unimportant. In 1928, Fock showed that such a phase could be set to unity by redefinition of the phase of the initial wave function . Although Fock's proof was limited to non-cyclic evolutions only, his conclusion was generally accepted until around 1980 when Mead and Truhlar [93] and Berry [90] re-

considered cyclic evolutions.
In the quantum mechanical description of a physical system, one has a finite or infinite dimensional Hilbert space of state vectors and a set of observables described by linear operators acting on these state vectors. If a quantum system is not isolated from its environment, the observables can be described by operators that depend on a set of parameters, $q = (q_1, q_2, \ldots, q_K)$, where K is the number of degrees of freedom of the environment. Each value of q characterizes a particular configuration of the environment. In particular, a changing environment is described by time-dependent parameters, $q = q(t)$. For a quantum system in a classical environment, the parameters q label the points of a smooth manifold $\mathcal{M}$. Every change of the environment is then described by a curve $\mathbf{C} : [0, T] \to \mathcal{M}$, with points $q(t) \in \mathbf{C}$. The manifold $\mathcal{M}$ is called the parameter space of the quantum system. The geometric properties of the parameter space depend of the specifications of the system. In general, the Hamiltonian is a smooth and single valued function of $q \in \mathcal{M}$. By the smoothness of the Hamiltonian we mean that the eigenvalues and the eigenvectors are smooth functions of q.
The evolution of the states of the quantum system in the external environment is described by the time-dependent Schrödinger equation

$$i\partial_t|\Psi\rangle = \hat{H}\left(q(t)\right)|\Psi\rangle, \tag{4.1}$$

where $\partial_t = \frac{\partial}{\partial t}$, and we set $\hbar = 1$.
Here $|\Psi\rangle$ denotes the state vector which belongs to the Hilbert space $\mathcal{H}$ and represents a pure state of the system. The general mixed state is described by a density matrix $\hat{\rho}$ whose evolution is given by the Liouville-von Neumann equation

$$i\partial_t\hat{\rho} = \left[\hat{H}\left(q(t)\right), \hat{\rho}\right]. \tag{4.2}$$

For the sake of simplicity, we shall assume the pure state case.
The adiabatic energy levels $\{E_k\left(q(t)\right)\}_{k=1}^{d}$ and the corresponding eigen-vectors $\{|k; q(t)\rangle\}_{k=1}^{d}$ are defined via the eigen-resolution of the Hamiltonian $\hat{H}\left(q(t)\right)$ at fixed values of $q = (q_1, \ldots, q_K)$:

$$\hat{H}\left(q\right)|k; q\rangle = E_k(q)|k; q\rangle, \qquad \langle k; q|l; q\rangle = \delta_{kl}, \quad k = 1, \ldots, d, \tag{4.3}$$

where d is the total number of energy levels. By $|k; q(t)\rangle$ we mean the eigen state $|k\rangle$ which depend on the time-varying set of parameters $q(t)$.
We shall assume that the adiabatic energy levels are not degenerate.

Given an environmental process along with a time parametrization $q(t)$, one obtains a time-dependent Hamiltonian

$$\hat{H}\left(q(t)\right) = \sum_{k=1}^{d} E_k\left(q(t)\right) \hat{P}_k\left(q(t)\right), \tag{4.4}$$

where

$$\hat{P}_k\left(q(t)\right) = |k; q(t)\rangle\langle k; q(t)|, \tag{4.5}$$

are the time-dependent projectors corresponding to the eigenstates of $\hat{H}\left(q(t)\right)$. We note that the adiabatic representation (4.3) has a gauge freedom:

$$|k; q(t)\rangle \to e^{i\alpha_k(q(t))}|k; q(t)\rangle, \tag{4.6}$$

where $\alpha_k\left(q(t)\right)$ is an arbitrary single-values function of $q = (q_1, \ldots, q_K)$. Hence all physical observables have to be gauge-invariant.

The qualitative *sufficient* condition for the time-scale separation is that the characteristic time of the classical motion is much larger than $\frac{\hbar}{\Delta}$, where Δ is the minimal adiabatic energy gap: $\Delta \equiv \min_{k\neq l}(|E_k - E_l|)$. [1]

To reflect mathematically the fact of time-scale separation we shall write the dependence of the quantum Hamiltonian on the classical coordinates as

$$H\left(q_1(\epsilon t), q_2(\epsilon t), \ldots\right), \tag{4.7}$$

where ϵ is defined as a small dimensionless parameter representing the ratio of the two time-scales.

$$\epsilon \ll 1. \tag{4.8}$$

The time-scale separation, i.e., condition (4.7), can be generated, *e.g.*, by a large mass M of the classical particle. Then the classical particle moves slowly—provided that its initial velocity is small—and $\epsilon \sim 1/\sqrt{M}$. This scenario of time-scale separation is normally met in chemical physics (heavy classical nuclei versus light quantum electrons) [94] and semi-quantum gravity [95].

In the Schrödinger equation (4.1) we shall assume that the initial state $|\Psi(0)\rangle$ is an eigenstate:

$$|\Psi(0)\rangle = |n; q(0)\rangle. \tag{4.9}$$

[1] This condition is sufficient, but not necessary for the validity of the time-scale separation and the consequent adiabatic approach, e.g., the latter can still hold if certain level-crossings are allowed. We shall not consider this more general situation.

Within the adiabatic approach the choice (4.9) does not imply any serious loss of generality. We note that it is sufficient to take a single initial wave vector and not a superposition of them, since any superposition will bring in the adiabatic limit strong oscillations for non-diagonal elements of the resulting density matrix. This will reduce the superposition to the mixture of adiabatic eigen-vectors, which amounts to studying the consequences of (4.9), and then taking the average over the index n with certain time-independent weights.

In the following section we present adiabatic perturbation theory [96,97]. It is a method to solve the time-dependent Schrödinger equation (4.1) under the time-scale separation (4.7) and the adiabatic assumption (4.8).

4.3 Adiabatic perturbation theory

The adiabatic theorem mentioned in section 4.1 yields an approximate solution and it seems natural to ask what will be the non-adiabatic corrections to the solution provided by this approximation especially if the characteristic time scale of the process is not too large.

In this section we study the higher order corrections to the adiabatic wave-function up to any order for non-degenerate adiabatic wave-function. The method we motivate here despite other methods is based on a careful separation of the slow and fast components of the wave-function of the fast quantum system which is under the influence of the slowly varying parameters of its environment. To this end, we define the slow time-variable as

$$s \stackrel{def}{=} \epsilon t.$$

As in any theory that is based on time-scale separation, we should start with dividing the sought solution to the time-dependent Schrödinger equation with the Hamiltonian (4.7) into fast and slow components:

$$|\Psi\rangle = |\psi_n(\epsilon, q(s)\rangle \, e^{i\alpha_n(t)}, \tag{4.10}$$

where

$$\alpha_n(t) \equiv -\int_0^t d\tau \, E_n \left(q(\epsilon\tau)\right),$$

is the dynamical phase.
$e^{i\alpha_n(t)}$ is the fast component of the sought solution since it changes fast, *i.e.*,

as $\sim e^{is/\epsilon}$. Inserting (4.10) into (4.1) we get

$$i\epsilon|\dot{\psi}_n\left(\epsilon, q(s)\right)\rangle = \left[\hat{H}\left(q(s)\right) - E_n\left(q(s)\right)\right]|\psi_n\left(\epsilon, q(s)\right)\rangle, \tag{4.11}$$

where dot is defined as differentiation with respect to the slow time s.
Now we expand the slow wave-function, $\psi_n\left(\epsilon, q(s)\right)$, in the powers of small parameter ϵ:

$$|\psi_n\left(\epsilon, q(s)\right)\rangle = e^{i\gamma_n(q(s))}\left[\,|n; q(s)\rangle + \epsilon|n_1; q(s)\rangle + \epsilon^2|n_2; q(s)\rangle + \ldots\right], \tag{4.12}$$

where

$$\gamma_n\left(q(s)\right) = i\int_0^s du\,\langle n; q(u)|\dot{n}; q(u)\rangle, \tag{4.13}$$

is the Berry phase factor. We separated the Berry phase, $\gamma_n\left(q(s)\right)$ out to facilitate further calculations and ensure the proper gauge-covariance. We notice that $\langle n; q(u)|\dot{n}; q(u)\rangle$ is purely imaginary (due to the fact $\langle n; q(u)|n; q(u)\rangle = 1$).

Substituting power series expansion (4.12) into (4.11) and comparing terms of equal order of ϵ, we get a set of recursive equations

$$0 = \left(\hat{H}\left(q(s)\right) - E_n\left(q(s)\right)\right)|n; q(s)\rangle, \tag{4.14}$$

$$i|\dot{n}; q(s)\rangle - i\langle n; q(s)|\dot{n}; q(s)\rangle\,|n; q(s)\rangle = \left(\hat{H}\left(q(s)\right) - E_n\left(q(s)\right)\right)|n_1; q(s)\rangle, \tag{4.15}$$

$$i|\dot{n}_1(s)\rangle - i\langle n; q(s)|\dot{n}; q(s)\rangle\,|n_1; q(s)\rangle = \left(\hat{H}\left(q(s)\right) - E_n\left(q(s)\right)\right)|n_2; q(s)\rangle, \tag{4.16}$$

$$\vdots,$$

or in general

$$i|\dot{n}_{m-1}; q(s)\rangle - i\langle n; q(s)|\dot{n}; q(s)\rangle|n_{m-1}; q(s)\rangle = \left(\hat{H}\left(q(s)\right) - E_n\left(q(s)\right)\right)|n_m; q(s)\rangle. \tag{4.17}$$

Eq. (4.14) holds automatically for the adiabatic regime, i.e., $\mathcal{O}(\epsilon^0)$.

To solve the higher order equations we introduce the projection operator $\hat{P}\left(q(s)\right)$ and its orthogonal complement $\hat{Q}\left(q(s)\right)$:

$$\hat{P}\left(q(s)\right)(s) = |n; q(s)\rangle\langle n; q(s)|, \qquad \hat{Q}\left(q(s)\right) = \sum\nolimits_k{}'|k; q(s)\rangle\langle k; q(s)|,$$
$$\hat{P} + \hat{Q} = \hat{1}, \qquad \hat{P}\hat{Q} = \hat{Q}\hat{P} = 0. \tag{4.18}$$

where $\sum_k'$ means the term $k = n$ is excluded from the summation $\sum_{k=1}^{d}$.

4.3.1 Post-adiabatic corrections

We start with deriving the first order correction to the adiabatic wavefunction. Then an analogous argument straightforwardly yields all higher order correction as well.
In order to solve the first order equation (4.15), we operate the orthogonal complement projector $\hat{Q}(q(s))$ from left to the both sides of (4.15). Since

$$\begin{aligned} &\hat{Q}(q(s))\,|n;q(s)\rangle = 0, \\ &\hat{Q}(q(s))\,\hat{H}(q(s)) = \sum_k{}' E_k(q(s))\,|k;q(s)\rangle\langle k;q(s)|, \end{aligned} \tag{4.19}$$

we get

$$\begin{aligned} &i\sum_k{}'|k;q(s)\rangle\langle k;q(s)|\dot{n};q(s)\rangle = \\ &\sum_k{}'\Delta_{kn}(q(s))\,|k;q(s)\rangle\langle k;q(s)|n_1;q(s)\rangle, \end{aligned} \tag{4.20}$$

where we have defined

$$\Delta_{kn}(q(s)) \overset{def}{=} E_k(q(s)) - E_n(q(s)). \tag{4.21}$$

Since $\Delta_{k\neq n}(q(s))$ is non-zero, due to the non-degenerate adiabatic energy level assumption, we get

$$\langle k;q(s)|n_1;q(s)\rangle \overset{def}{=} c^{[1]}_{k\neq n}(q(s)) = -i\frac{\langle k;q(s)|\dot{n};q(s)\rangle}{\Delta_{nk}(q(s))}. \tag{4.22}$$

Thus the projection of the first order correction to the adiabatic energy level on $\hat{Q}$, denoted by $|n_1^{\perp};q(s)\rangle$, is defined as

$$|n_1^{\perp};q(s)\rangle \overset{def}{=} \sum_k{}' c^{[1]}_{kn}(q(s))\,|k;q(s)\rangle. \tag{4.23}$$

where $c^{[1]}_{k\neq n}(q(s))$ is defined by (4.22).
The above expression means that the state makes transitions between its energy levels during its evolution in contrast to the adiabatic regime. But

this is not the whole story, in order to define $|n_1; q(s)\rangle$ completely we have to derive its projection on $\hat{P}\left(q(s)\right)$ as well. In doing so, we operate the projection operator $\hat{P}\left(q(s)\right)$ from the left on both sides of the second-order equation (4.16). Keeping in mind that

$$\hat{P}\left(q(s)\right)\left(\hat{H}\left(q(s)\right) - E_n\left(q(s)\right)\right) = 0, \tag{4.24}$$

we get

$$\langle n; q(s)|\dot{n}_1(s)\rangle - \langle n; q(s)|\dot{n}(s)\rangle\langle n; q(s)|n_1; q(s)\rangle = 0. \tag{4.25}$$

Therefore, calculating $\langle n; q(s)|n_1; q(s)\rangle$ requires the calculation of $\langle n; q(s)|\dot{n}_1; q(s)\rangle$. This can be done by differentiating with respect to the slow time, s, both sides of the following identity:

$$|n_1; q(s)\rangle = \hat{P}(s)|n_1; q(s)\rangle + |n_1^{\perp}(s)\rangle, \tag{4.26}$$

and then multiplying both sides from left by $\langle n; q(s)|$ from left:

$$\begin{aligned}
&\langle n; q(s)|\dot{n}_1; q(s)\rangle = \\
&\frac{d}{ds}\left[\langle n; q(s)|n_1; q(s)\rangle\right] + \langle n; q(s)|\dot{n}; q(s)\rangle\langle n; q(s)|n_1; q(s)\rangle \\
&+{\sum_k}' c_{kn}^{[1]} q(s)\langle n; q(s)|\dot{k}(s)\rangle,
\end{aligned} \tag{4.27}$$

where we have used the definition $\langle k; q(s)|n_1; q(s)\rangle = c_{kn}^{[1]}\left(q(s)\right)$. Inserting (4.27) into (4.25) yields

$$\dot{c}_{nn}^{[1]}\left(q(s)\right) = -{\sum_k}'\langle n; q(s)|\dot{k}(s)\rangle c_{kn}^{[1]}\left(q(s)\right), \tag{4.28}$$

where we define

$$c_{nn}^{[1]}\left(q(s)\right) \stackrel{def}{=} \langle n; q(s)|n_1; q(s)\rangle. \tag{4.29}$$

Inserting the definition of $c_{k\neq n}^{[1]}\left(q(s)\right)$ in the above expression we get

$$\begin{aligned}
c_{nn}^{[1]}\left(q(s)\right) &= -{\sum_k}' \int_0^s du\langle n; q(u)|\dot{k}; q(u)\rangle c_{kn}^{[1]}\left(q(u)\right) = \\
&- i{\sum_k}' \int_0^s du \frac{|\langle k; q(u)|\dot{n}; q(u)\rangle|^2}{\Delta_{nk}\left(q(u)\right)}.
\end{aligned} \tag{4.30}$$

It is seen that $c_{nn}^{[1]}(q(s))$ is purely imaginary.
Summarizing the above calculations, we can write the first-order correction to the adiabatic wave-function as

$$|n_1; q(s)\rangle = c_{nn}^{[1]}(q(s))\,|n; q(s)\rangle + |n_1^{\perp}; q(s)\rangle, \tag{4.31}$$

where $|n_1^{\perp}; q(s)\rangle$ is defined by (4.23) and $c_{nn}^{[1]}(q(s))$ is given by (4.30).
It is remarkable that for the first-order adiabatic correction equation (4.22), which describes the transition to the other eigen energy levels in the post-adiabatic regime, is well-known [2, 3]. It is certainly less known that the consistent adiabatic perturbation theory generates another $\mathcal{O}(\epsilon)$ term, i.e., $c_{nn}^{[1]}(q(s))$ [97, 98]. This term is purely imaginary and represents a memory effect of the transitions to other energy levels during the evolution of the quantum system. This term drops out from post-adiabatic corrections to the averaged force.
Following an analogous argument, the higher order post-adiabatic corrections to the wave-function, represented by $|n_m; q(s)\rangle$, with $m > 1$, read

$$|n_m; q(s)\rangle = c_{nn}^{[m]}(q(s))\,|n; q(s)\rangle + |n_m^{\perp}; q(s)\rangle, \tag{4.32}$$

$$|n_m^{\perp}; q(s)\rangle = {\sum_k}' c_{kn}^{[m]}(q(s))\ |k; q(s)\rangle, \tag{4.33}$$

where $c_{k\neq n}^{[m]}(q(s))$ is derived from the following recursive expression

$$c_{k\neq n}^{[m]}(q(s)) = \frac{i\langle n; q(s)|\dot{n}; q(s)\rangle\, c_{k\neq n}^{[m-1]}(q(s)) - i\langle k; q(s)|\dot{n}_{m-1}; q(s)\rangle}{\Delta_{nk}(q(s))}, \tag{4.34}$$

and the scalar function $c_{nn}^{[m]}(q(s))$ is given by

$$\dot{c}_{nn}^{[m]}(q(s)) = -\langle n; q(s)|\dot{n}_m^{\perp}; q(s)\rangle, \tag{4.35}$$

$$c_{nn}^{[m]}(q(s)) = -{\sum_k}' \int_0^s du\, c_{kn}^{[m]}(q(u))\ \langle n; q(u)|\dot{k}; q(u)\rangle. \tag{4.36}$$

Altogether $|\psi_n(\epsilon, (q(s)))\rangle$ in (4.12) can be written as

$$|\psi_n(\epsilon, (q(s)))\rangle = e^{i\gamma_n(q(s))} \sum_k c_{kn}(q(s))\,|k; q(s)\rangle, \tag{4.37}$$

where $c_{kn}(q(s))$ is given by the following expansion over the small parameter ϵ

$$c_{kn}(q(s)) = \delta_{kn} + \epsilon c_{kn}^{[1]}(q(s)) + \epsilon^2 c_{kn}^{[2]}(q(s)) + \cdots. \tag{4.38}$$

The normalization condition of the wave-function implies relations between the coefficients $c_{kn}\left(q(s)\right)$:

$$\sum_{k} \left| c_{kn}\left(q(s)\right) \right|^2 = 1, \tag{4.39}$$

which should be satisfied at each order of ϵ. By separating the term regarding to $k = n$ in the above expression (4.39) for the first few orders we have

$$\begin{aligned}
&\left| c_{nn}\left(q(s)\right) \right|^2 = \qquad (4.40)\\
&1 + \epsilon \left[2\Re\{ c^{[1]}_{nn}\left(q(s)\right) \} \right] + \epsilon^2 \left[2\Re\{ c^{[2]}_{nn}\left(q(s)\right) \} + \left| c^{[1]}_{nn}\left(q(s)\right) \right|^2 \right] \\
&+\epsilon^3 \left[2\Re\{ c^{[3]}_{nn}\left(q(s)\right) + c^{[1]}_{nn}\left(q(s)\right) c^{*[2]}_{nn}\left(q(s)\right) \} \right] \\
&+\epsilon^4 \left[2\Re\{ c^{[4]}_{nn}\left(q(s)\right) + c^{[1]}_{nn}\left(q(s)\right) c^{*[3]}_{nn}\left(q(s)\right) \} + \left| c^{[2]}_{nn}\left(q(s)\right) \right|^2 \right] + \cdots , \\
&\sum_{k}{}' \left| c_{kn}\left(q(s)\right) \right|^2 = \qquad (4.41)\\
&\epsilon^2 \left[\left| c^{[1]}_{kn}\left(q(s)\right) \right|^2 \right] + \epsilon^3 \left[2 \sum_{k}{}' \Re\{ c^{[1]}_{kn}\left(q(s)\right) c^{*[2]}_{kn}\left(q(s)\right) \} \right] \\
&+\epsilon^4 \left[\left| c^{[2]}_{kn}\left(q(s)\right) \right|^2 + 2 \sum_{k}{}' \Re\{ c^{[1]}_{kn}\left(q(s)\right) c^{*[3]}_{kn}\left(q(s)\right) \} \right] + \cdots .
\end{aligned}$$

Inserting the expressions (4.41) and (4.42) into the normalization condition (4.39) brings the following relations at the orders ϵ and ϵ^2, ϵ^3, and ϵ^4 respectively,

$$\begin{aligned}
&\Re\{ c^{[1]}_{nn}\left(q(s)\right) \} = 0, \qquad (4.42)\\
&2\Re\{ c^{[2]}_{nn}\left(q(s)\right) \} + \langle n_1; q(s) | n_1; q(s) \rangle = 0, \qquad (4.43)\\
&\Re\{ c^{[3]}_{nn}\left(q(s)\right) + \langle n_1; q(s) | n_2; q(s) \rangle \} = 0, \qquad (4.44)\\
&2\Re\{ c^{[4]}_{nn}\left(q(s)\right) + \langle n_1; q(s) | n_3; q(s) \rangle \} + \langle n_2; q(s) | n_2; q(s) \rangle = 0, \qquad (4.45)\\
&\vdots
\end{aligned}$$

where we have used the expression of $|n_1; q(s)\rangle$ given by (4.31) in (4.42), and the expression for $|n_m; q(s)\rangle$ for $m = 2$ and $m = 3$ given by (4.32) in (4.44) and (4.45).

4.4 Precision of the adiabatic approximation

The precision of the adiabatic approximation is studied in details by G. A. Hagedorn and A. Joye [97]. They rigorously proved that the adiabatic perturbation theory is correct up to exponentially small errors for time-dependent Hamiltonians. They employed the standard Cauchy estimates in order to estimate the error resulting from the truncation of the asymptotic expansion of the wavefunction and proved that when the expansion is truncated after an optimal number of terms, the resulting approximation , i.e., the difference between the exact and the approximated solution, is exponentially accurate as it is described in the following.
According to (4.12) let us define

$$|{\psi_n}^N(\epsilon, q(s))\rangle = e^{i\gamma_n(q(s))} \sum_{m=0}^{N} \epsilon^m |n_m; q(s)\rangle. \tag{4.46}$$

Let $\{a\}$ define the integer part of a real number a, and let we are given a positive number g. Then it is shown that [97]:

$$\Big|\ |\psi^{\{g/\epsilon\}}(\epsilon, s)\rangle - |\psi_{\text{exact}}(\epsilon, s)\rangle\ \Big| \leq C(g)e^{-\Gamma(g)/\epsilon}, \tag{4.47}$$

where $|\psi_{\text{exact}}(\epsilon, s)\rangle$ is the exact solution of the time-dependent Schrödinger equation (4.11) and at the initial time

$$|\psi^{\{g/\epsilon\}}(\epsilon, 0)\rangle = |\psi_{\text{exact}}(\epsilon, 0)\rangle, \tag{4.48}$$

and where $C(g)$ and $\Gamma(g)$ are bounded positive functions of g. This result implies that the precision of the adiabatic approximation is exponential over ϵ.

4.5 Summary

In this chapter we considered a fast quantum system which is under the influence of a slowly evolving classical system. To describe the situation, we represented the Hamiltonian governing the motion of the fast quantum system as a function of slowly varying parameters of the classical system. We defined a small dimensionless parameter ϵ as the ration of the time scales of the two system and divided the sought solution of the time-dependent

Schrödinger equation into fast and slow components. Within the adiabatic perturbation theory we expanded the slow component over the small parameter ϵ and derived the higher order corrections. The results of this chapter will be employed in the next chapter where we study the dynamics of the slow classical system.

CHAPTER 5

Post Adiabatic Forces

The post-adiabatic corrections to the adiabatic wave function of a fast quantum system coupled to a slow classical system was calculated in the previous chapter. In this chapter some dynamical properties of a slow classical system coupled to a fast quantum system is considered. In particular, the result of the previous chapter is employed in order to calculate the postadiabatic forces exerted by the quantum system on the classical one. Up to higher orders in the small parameter ϵ, which represents the ratio of the time-scales of the two systems, the exerted force can be derived from a Lagrangian. However, at orders higher than two the Lagrangian is not just a functional of the coordinate and velocity of the classical system but it also depends on the acceleration and higher time-derivatives of the slowly varying coordinates. This brings new physical concepts such as spin and zitterbewegung effect in the purely classical regime.

5.1 Introduction

In this chapter we employ the results of the previous chapter and study the dynamics of the classical slow part of the quantum-classical (also called

mean-field or hybrid) dynamics, which describes coupled quantum and classical systems in the adiabatic regime where the characteristic time scale of the system of interest is much slower than that of its fast counterpart. [2,3]. We focus on the slow classical system adiabatically exclude the quantum system and construct an autonomous dynamics for the classical particle in successive orders of the small ratio ϵ of the characteristic times.
One of the well-established results in this direction known from 1922 is the Darwin Lagrangian [85, 99] for a system of slowly moving charges. We know that in electrodynamics the propagation velocity is finite and the fields must be considered as independent systems with their own degrees of freedom. As a result, if we want to build up a Lagrangian for a system of interacting charges in a rigorous way, we have to encounter the quantities related to the internal degrees of freedom of the fields as well as the velocity and the coordinates of the particles in the Lagrangian. However, if the velocities of all the particles in the system are small compared to the velocity of light, the system can be described by a certain approximate Lagrangian called Darwin Lagrangian, named after Charles Galton Darwin a grandson of the great naturalist and has important applications in plasma physics and astrophysics [85]. It turns out to be possible to derive the equation of motion for the particles through a Lagrangian up to $(v/c)^2$ order. This can be done since the radiation of electromagnetic waves by moving charges occurs only in third order of (v/c).
Here, we assume the classical system is slow —a condition that is normally fulfilled in practice. We introduce a small parameter ϵ defined as the ratio of the characteristic times for the quantum over the classical system, respectively. Then we exclude the fast quantum system and study to which extent the ensuing dynamics of the slow classical system can be described by an autonomous Lagrangian-generated equations for the classical coordinates. In the leading order and order of ϵ^1 this includes respectively the Born-Oppenheimer potential and an effective magnetic field related to the Berry phase. Within the order ϵ^2 the motion of the classical particle is described by a Lagrangian that depends on its coordinate and momenta. We show that in the order ϵ^3 the motion of the classical particle is still described by a Lagrangian, but the latter linearly depends on the particle's acceleration [98]. This implies the existence of a spin tensor [non-orbital angular momentum] for the particle. This spin tensor is related to the momentum via an analogue of the zitterbewegung effect. The Hamiltonian structure of the classical system is non-trivial and is defined via non-linear Poisson brackets.

The linear dependence of the effective classical Lagrangian on higher-order derivatives is seen as well in the higher orders ϵ^n [98].
This chapter is organized as the following. In section 5.2 we introduce the quantum-classical dynamics. Section 5.3 is devoted to derivation of the higher order corrections to the post-adiabatic force. In section 5.4 we review the derivation of the classical Lagrangian in the orders ϵ. In particular, we reproduce in a systematic way the results obtained by Berry and Robbins [2]. It is well known that at the zero order of ϵ the influence of the quantum system on the classical one can be described by the Born-Oppenheimer potential energy term [2, 3, 94, 95, 100, 101].

It was shown by Berry and Robbins that in the first order of ϵ one gets an effective magnetic field, which manifests itself as the velocity-dependent term in the classical Lagrangian [2].

Section 5.5 describes the second-order post-adiabatic force using the adiabatic perturbation theory outlined in the previous chapter. In this chapter we reproduce the results recently shown by Goldhaber [3]. Namely, in the second order ϵ^2 one gets in the Lagrangian of the classical system an additional kinetic energy term, i.e., a quadratic form in slow velocities [3]. A very similar result on the order ϵ^2 was obtained earlier by Weigert and Littlejohn for two coupled (fast and slow) quantum systems [100]. Moreover, we show that at the order ϵ^2 the classical Lagrangian corresponds to a classical particle moving along the geodesics of a curved manifold. We calculate the curvature for the simplest non-trivial case and work out its implications for the stability of the effective classical motion at the order ϵ^2. Here we also point out at an unusual scenario related to the metric of the manifold changing its signature [i.e., changing from a Riemannian to a pseudo-Riemannian manifold]. It appears that the slow classical motion within this order can be reduced to a free motion ("geodesic motion") on a Riemannian space with a signature-indefinite metric tensor. This offers the possibility of interchanging time-like and space-like coordinates. Recall in this context that within non-relativistic classical mechanics the geodesic motion on a curved surface proceeds according to a positively-defined metric tensor, while the geodesic motion in the general theory of relativity has a metric tensor with signature $(1, -1, -1, -1)$ [99]. In both cases the signature is fixed.

We are also interested in knowing what happens in the next orders. In particular, we want to understand how far we can continue the expansion over ϵ, still keeping the classical system Lagrangian. Most importantly, we are interested to know whether there are new physical effects essentially related

to post-adiabatic corrections.These questions are answered in sections 5.6 and 5.7. It appears that at every order over ϵ one can derive Lagrange equations for the dynamics of the classical system. However, there is an important difference between the orders ϵ and ϵ^2 and all successive orders. At the order ϵ^3 the classical dynamics is Lagrangian, but the Lagrangian starts to depend on the higher-order time-derivatives of the classical coordinates. It is important to note that the classical Lagrangians normally depend on the coordinates and their first-order time-derivatives (velocities). In section 5.6 we show that at the order ϵ^3 we get a Lagrangian that is linear over the second order time-derivatives, i. e., classical accelerations. This fact is of conceptual relevance. The classical physics is essentially based on the Newton's second law that equates acceleration to the force, which depends only on coordinates and velocities. As a consequence, the trajectory of the classical motion is fixed via initial coordinates and initial velocities. In its turn, the Newton's second law is generated by a Lagrangian, which depends on coordinates and velocities. A Lagrangian depending on higher-order derivatives enlarges the amount of the initial data needed to fix the classical trajectory and produces equations of motion that go beyond the Newton's law. Our result seems to be the first example where a higher-derivative Lagrangian emerges for an open classical system due to time-scale separation. Dependence on higher-order derivatives in the Lagrangian implies a number of essential changes in the kinematics of the classical system: the momentum of the classical system depends on the acceleration, while the full angular momentum tensor is a sum of the usual orbital part and a term that can be interpreted as the spin of the classical system. In the simplest non-trivial case this spin is proportional to the velocity square of the classical particle. We show that this implies the existence of the zitterbewegung effect, where the momentum of the classical particle (system) is governed by the projected time-derivative of the spin. So far the zitterbewegung effect was known only in the physics of relativistic Dirac electron, while we show the same effect appears in a purely non-relativistic slowly evolved classical system due to its coupling to a fast quantum system. It appears now that this effect is a part of the physics generated by higher-order post-adiabatic corrections. We conjecture that similar dependence on higher-order derivatives is expected at higher orders ϵ^n with $n \geq 4$, though we restrict ourselves with deriving the effective classical Lagrangian up to the order ϵ^4. In section 5.7 we deduce the classical Lagrangian at the order ϵ^4 and show that it also depends linearly on higher-order derivatives of the classical coordinates.

5.2 Quantum-classical dynamics

In this section we derive the equation of motion for a classical system coupled to a quantum system. In doing so, we consider the mean-field classical dynamics. In this approach the classical variables are treated as parameters in the Hamiltonian of the quantum system. The dynamics of the quantum system, is described by the Schrödinger equation while the dynamics of the classical system is given by the Newton equation of motion supplemented by the average force acting from the quantum part. As a result, the classical particle experiences an *averaged* force exerted by the quantum system.
It is important to note that in general this force is not generated by an averaged potential. This would only be the case in the adiabatic regime and the first order adiabatic perturbation theory.

As a model we consider a K-degree of freedom classical system with coordinates $q = (q_1, \ldots, q_K)$ and with Lagrangian

$$\mathcal{L}_0 = \frac{M}{2} \sum_{\alpha=1}^{K} \left(\frac{dq_\alpha}{dt} \right)^2 - V(q), \tag{5.1}$$

where M is the mass, and $V(q) = V(q_1, \ldots, q_K)$ is the potential energy of the classical system.

Now this classical system (or particle) couples to a quantum system with Hamiltonian operator $\hat{H}\left(q(t)\right)$, which parametrically depends on the classical coordinates. The quantum system evolves in time according to the Schrödinger equation (for simplicity we put $\hbar = 1$)

$$i\partial_t |\Psi\rangle = \hat{H}\left(q(t)\right) |\Psi\rangle, \tag{5.2}$$

where $|\Psi\rangle$ is the wave-function, and where $\partial_t = \frac{\partial}{\partial t}$.

We can calculate the force exerted by the quantum system on the classical one as

$$F_\mu = \langle \Psi | \partial_\mu \hat{H}\left(q(t)\right) |\Psi\rangle, \tag{5.3}$$

where we defined [1]:

$$\partial_\mu = \frac{\partial}{\partial q_\mu(t)}. \tag{5.4}$$

For the simplicity of notation we absorb the minus sign in the force.

[1] Note that $\partial_\mu = \partial_{q_\mu(t)}$ acts only on the coordinates, but not on the velocities, e.g., $\partial_\mu \dot{q}_\alpha = 0$. In particular, ∂_μ commutes with the total time-derivative $\frac{d}{ds}$.

The classical part of the dynamics is written as [94, 95, 101]

$$M\frac{d^2q_\mu}{dt^2} + \partial_\mu V + \langle\Psi|\partial_\mu \hat{H}\left(q(t)\right)|\Psi\rangle = 0, \qquad \mu = 1, \ldots, K. \tag{5.5}$$

Eq. (5.5) is the Newton equation of motion, where besides the classical force $-\partial_\mu V$, the classical particle experiences an *average* force $-\langle\Psi(t)|\partial_\mu H\left(q(t)\right)|\Psi(t)\rangle$ exerted by the quantum systems. In this sense the classical coordinates play a role of a mean-field [101]. The main purpose of the present chapter is to understand to which extent this force can be generated by a Lagrangian which depends on the classical coordinates $q_\alpha(t)$ and their time-derivatives. It should be clear from (5.2) and (5.5) that the total average energy is conserved in time:

$$\frac{d}{dt}\left(\frac{M}{2}\sum_{\alpha=1}^{K}\left(\frac{dq_\alpha}{dt}\right)^2 + V(q) + \langle\Psi|\hat{H}\left(q(t)\right)|\Psi\rangle\right) = 0. \tag{5.6}$$

We note that the quantum-classical equations of motion (5.2, 5.5) can be derived from a Lagrangian

$$\begin{aligned}\widetilde{\mathcal{L}} &= \frac{1}{2i}\langle\partial_t\Psi|\Psi\rangle - \frac{1}{2i}\langle\Psi|\partial_t\Psi\rangle - \langle\Psi|\hat{H}\left(q(t)\right)|\Psi(t)\rangle \\ &+ \frac{M}{2}\sum_{\alpha=1}^{K}\left(\frac{dq_\alpha}{dt}\right)^2 - V(q),\end{aligned} \tag{5.7}$$

where as a set of independently varying parameters one should take $|\Psi\rangle$ and $q(t)$ (or alternatively $\langle\Psi|$ and $q(t)$)[2]. It is seen that $\widetilde{\mathcal{L}}$ is simply a sum of the corresponding quantum and classical Lagrangians, which points out that combination of classical and quantum degrees of freedom does not violate the Lagrangian formalism. However, In section 5.2.1 we briefly discuss the possibility of derivation of the quantum-classical dynamics from a full quantum-quantum dynamics.

5.2.1 Derivation

The quantum-classical dynamics can be derived from a full quantum-quantum dynamics in the following fashion [94, 101–105].

[2] As usual, when varying (5.7) we put aside the total time-derivatives, e.g., $\frac{d}{dt}\langle\delta\Psi|\Psi\rangle$.

We first consider both coupled systems are on equal footing. Therefore, we assume we are given a two-degree of freedom quantum system with the following Hamiltonian

$$\hat{H}_{tot} = \frac{\hat{p}^2}{2M} + \hat{V}(q) + \hat{H}(q,x) + \frac{\hat{\pi}^2}{2M},$$

where (q,p) and (x,π) are two degrees of freedom.
For simplicity we shall assume that the initial state is factorized for these two degrees of freedom.

The Heisenberg equation generated by this Hamiltonian reads:

$$\frac{d\hat{q}}{dt} = \frac{\hat{p}}{M}, \tag{5.8}$$

$$\frac{d\hat{p}}{dt} = -\partial_q \hat{V}(q) - \partial_q \hat{H}(q,x), \tag{5.9}$$

$$\frac{d\hat{x}}{dt} = \frac{\hat{\pi}}{M}, \tag{5.10}$$

$$\frac{d\hat{\pi}}{dt} = -\partial_x \hat{H}(q,x). \tag{5.11}$$

We separate the motion of $(\hat{q},\hat{p})$ degrees of freedom into two parts:

$$\hat{p}(t) = \overline{\hat{p}}(t) + \hat{p}_f, \qquad \hat{q}(t) = \overline{\hat{q}}(t) + \hat{q}_f, \tag{5.12}$$

where $\overline{\hat{p}}(t)$ and $\overline{\hat{q}}(t)$ are the averages over the initial state, and where $\hat{p}_f$ and $\hat{q}_f$ are the fluctuations. Then we make two assumptions:

- The $(\hat{q},\hat{p})$ degrees of freedom are Gaussian which means they satisfy

$$\overline{\hat{p}}_f = \overline{\hat{q}}_f = 0. \tag{5.13}$$

- The fluctuations of $(\hat{q},\hat{p})$ degrees of freedom are small.

Keeping these assumptions in mind, we substitute (5.12) into (5.8, 5.9, 5.11) and expand (5.8) and (5.11) over small $\hat{q}_f$:

$$\frac{d\overline{\hat{q}}}{dt} + \frac{d\hat{q}_f}{dt} = \frac{\overline{\hat{p}}}{M} + \frac{\hat{p}_f}{M}, \tag{5.14}$$

$$\begin{aligned} \frac{d\overline{\hat{p}}}{dt} + \frac{d\hat{p}_f}{dt} &= -\partial_q \hat{V}(\overline{q}) - \partial_q \hat{H}(\overline{q},x) \\ &- \partial_q^2 \hat{V}(\overline{q}) q_f - \partial_q^2 \hat{H}_{qq}(\overline{q},x) q_f + \mathcal{O}(\hat{q}_f^2), \end{aligned} \tag{5.15}$$

$$\frac{d\pi}{dt} = -\partial_x \hat{H}(\overline{q},x) - \partial_{xq}^2 \hat{H}(\overline{q},x)\, q_f + \mathcal{O}(\hat{q}_f^2). \tag{5.16}$$

Averaging (5.14)-(5.16) over the initial states we obtain

$$\frac{d\overline{\hat{q}}}{dt} = \frac{\overline{\hat{p}}}{M}, \tag{5.17}$$

$$\frac{d\overline{\hat{p}}}{dt} = -\overline{\partial_q \hat{V}(\overline{q})} - \overline{\partial_q \hat{H}(\overline{q}, x)} - \overline{\partial_q^2 \hat{H}(\overline{q}, x) q_f} + \overline{\mathcal{O}(\hat{q}_f^2)}, \tag{5.18}$$

$$\overline{\frac{d\pi}{dt}} = -\overline{\partial_x \hat{H}(\overline{q}, x)} - \overline{\partial_{xq}^2 \hat{H}(\overline{q}, x)\, q_f} + \overline{\mathcal{O}(\hat{q}_f^2)}. \tag{5.19}$$

Based on our second assumption, if in (5.18, 5.19) the terms proportional to $\mathcal{O}(q_f)$ are neglected we get into a quantum-classical equations, where $(\overline{\hat{p}}, \overline{\hat{q}})$ is considered as the classical degree of freedom. Thus, from (5.18) we arrive at the Newton equation of motion for the classical part of the system:

$$M\frac{d^2q}{dt^2} + \partial_q V + \langle \Psi | \partial_q \hat{H}\left(q(t)\right) | \Psi \rangle = 0.$$

We conclude this section by emphasizing that the main assumption involved in the quantum-classical dynamics derivation is that the quantum fluctuation of the classical coordinate(s) are small. The validity of the (mean-field) quantum-classical dynamics is not related to the classical sub-system being slow. The derivations of the quantum-classical dynamics need not neglect fluctuations of all pertinent variables, i.e., it need not impose the full quantum trajectories. It will be sufficient that the to-be classical sector of the dynamics is approximated via suitable Gaussian density matrices [106]. Then, the parameters of this matrices satisfy the equations of motion for some effective classical systems [106].

5.3 Post-adiabatic force

In this section we concentrate on the adiabatic limit of the quantum-classical system, where the classical system is slow and the quantum system is fast, and derive an autonomous equations of motion for the classical part. To this end, we shall solve the time-dependent Schrödinger equation for the fast quantum system under the adiabatic assumption and determine via its solution, the structure of the averaged force.

We employ the adiabatic perturbation theory described in the previous chapter. For the sake of brevity, instead of $|n; q(s)\rangle$ we simply writhe $|n\rangle$ but

we keep in mind that $|n\rangle$ parametrically depnds on the slow time s trough the classical parameters $q(s)$. This notation holds for higher order corrections as well. We will also wrtie $\hat{H}(s)$, and $E_n(s)$ instead of $\hat{H}\left(q(s)\right)$ and $E_n\left(q(s)\right)$. Assuming the quantum system initially starts its evolution from an eigenstate of the Hamiltonina $\hat{H}(s)$, the slow component of the wave-function can be expanded over the small dimensionless parameter ϵ. Let us recall

$$|\psi_n\rangle = e^{\int_0^s du\, \langle \dot{n}|n\rangle}|\phi_n\rangle, \tag{5.20}$$

$$|\phi_n\rangle = |n\rangle + \epsilon|n_1\rangle + \epsilon^2|n_2\rangle + \epsilon^3|n_3\rangle + \ldots, \tag{5.21}$$

The zero order term $|\phi_n\rangle = |n\rangle$ in the expansion (5.21) is the statement of the adiabatic theorem. In (5.20), $e^{\int_0^s du\, \langle \dot{n}|n\rangle}$ is the Berry phase factor; it was separated out for ensuring the proper gauge-covariance [96]; see also below. Note that $\langle \dot{n}|n\rangle$ is purely imaginary (due to $\langle n|n\rangle = 1$). An alternative representation of $|\phi_n\rangle$ is

$$|\phi_n\rangle = \sum_{k=1}^{d} c_{kn}|k\rangle, \qquad c_{kn}(0) = \delta_{kn}, \tag{5.22}$$

$$c_{kn} = \delta_{kn} + \epsilon c_{kn}^{[1]} + \epsilon^2 c_{kn}^{[2]} + \epsilon^3 c_{kn}^{[3]} + \ldots, \tag{5.23}$$

where d is the number of the non-degenerate eigenstates of the Hamiltonian. $c_{k\neq n}^{[m]}$ and $c_{nn}^{[m]}$ are given by

$$c_{k\neq n}^{[m]} = \frac{i\langle n|\dot{n}\rangle\, c_{k\neq n}^{[m-1]} - i\langle k|\dot{n}_{m-1}\rangle}{\Delta_{nk}}, \tag{5.24}$$

$$c_{nn}^{[m]} = -{\sum_{k}}' \int_0^s du\, c_{kn}^{[m]}\, \langle n|\dot{k}\rangle, \tag{5.25}$$

where

$$\Delta_{kn}(s) = E_k(s) - E_n(s).$$

The expression for the exerted force from the fast quantum system to the slow classical system reads

$$F_\mu = \langle\psi_n|\partial_\mu \hat{H}(s)|\psi_n\rangle, \qquad \mu = 1, \ldots, K, \tag{5.26}$$

where K is the number of degrees of freedom of the classical system. Inserting the expression for $|\psi_n\rangle$ from (5.20) into (5.26) we get

$$F_\mu = \partial_\mu \langle\phi_n|\hat{H}(s)|\phi_n\rangle - 2\Re\langle\partial_\mu\phi_n|\hat{H}(s)|\phi_n\rangle. \tag{5.27}$$

We add and subtract $\partial_\mu E_n(s)$ from (5.27). Employing the time-dependent Schrödinger equation for $\hat{H}(s)|\phi_n\rangle$ we get

$$\hat{H}(s)|\phi_n\rangle = i\epsilon\langle\dot{n}|n\rangle|\phi_n\rangle + i\epsilon|\dot{\phi}_n\rangle + E_n(s)|\phi_n\rangle. \tag{5.28}$$

Multiplying both sides of (5.28) from left by $\langle\partial_\mu\phi_n|$, and taking into account that $\langle\phi_n|\partial_\mu\phi_n\rangle$ is purely imaginary since $\langle\phi_n|\phi_n\rangle = 1$, the general expression for the force F_μ acting on the classical system reads

$$F_\mu(s) = \partial_\mu E_n(s) + 2\epsilon\Im\langle\partial_\mu\phi_n|\dot{\phi}_n\rangle + \partial_\mu[\langle\phi_n|\hat{H}(s)|\phi_n\rangle - E_n(s)]. \tag{5.29}$$

We note from (5.22) and (5.23) that the last term of (5.29) is of second order in ϵ and higher:

$$\langle\phi_n|\hat{H}(s)|\phi_n\rangle - E_n(s) = \sum\nolimits_k{}' \Delta_{kn}|c_{kn}|^2 = O(\epsilon^2). \tag{5.30}$$

The factor $\partial_\mu E_n$ is the force generated by the adiabatic (Born-Oppenheimer) potential $E_n(s)$. Thus the last two terms in (5.29) represent the non-adiabatic force. We denote

$$F_\mu = F_\mu^{[0]} + \epsilon F_\mu^{[1]} + \epsilon^2 F_\mu^{[2]} + \epsilon^3 F_\mu^{[3]} + \ldots, \tag{5.31}$$

where $F_\mu^{[0]}(s) = \partial_\mu E_n(s)$.

In the following sections we derive expressions for higher-order post-adiabatic forces and show that they can be generated by a Lagrangian.

5.4 First order post-adiabatic force

The first order post-adiabatic force can be calculated through the only first order term in the general expression for the force, (5.29), given by

$$2\epsilon\Im\langle\partial_\mu\phi_n|\dot{\phi}_n\rangle,$$

where according to (5.21)

$$|\phi_n\rangle = |n\rangle + O(\epsilon). \tag{5.32}$$

Therefore the first order post-adiabatic force reads

$$F_\mu^{[1]} = 2\Im\langle\partial_\mu n|\dot{n}\rangle. \tag{5.33}$$

From now on, for the sake of simplicity, we drop the argument s.
The expression for the first order post-adiabatic force given by (5.33) can be simplified more. Taking into account that

$$|\dot{n}\rangle = \dot{q}_\alpha |\partial_\alpha n\rangle, \tag{5.34}$$

and assuming implicit summation from 1 to K over the repeated Greek indices. the first order post-adiabatic force, $F_\mu^{[1]}$, reads

$$F_\mu^{[1]} = 2\dot{q}_\alpha \Im\langle \partial_\mu n | \partial_\alpha n\rangle. \tag{5.35}$$

We notice $\Im\langle \partial_\mu n | \partial_\alpha n\rangle = -\Im\langle \partial_\alpha n | \partial_\mu n\rangle$, therefore the first order force is antisymmetric. Moreover, the presence of $\dot{q}_\alpha$ which represents the slow velocity of the classical system, suggests that $F^{[1]}$ is effective Lorentz [or gyroscopic] type force [2]. This force emerges from a vector potential whose elements are

$$A_\alpha = \Im\langle \partial_\alpha n | n\rangle. \tag{5.36}$$

Therefore, we see that the first order averaged force can be generated by the following Lagrangian

$$\mathcal{L}^{[1]}(\dot{q}, q) = \epsilon A_\alpha(q)\dot{q}_\alpha. \tag{5.37}$$

Now the complete classical Lagrangian to the first order represented by $\mathcal{L}_1$ is obtained by adding $\mathcal{L}^{[1]}(\dot{q}, q)$ and the Born-Oppenheimer potential $E_n(q)$ to the initial (bare) classical Lagrangian $\mathcal{L}_0$, given by (5.1):

$$\mathcal{L}_1 = \frac{M}{2}\sum_{\alpha=1}^{K}\left(\frac{dq_\alpha}{dt}\right)^2 - V(q) - E_n(q) + \epsilon A_\alpha(q)\dot{q}_\alpha. \tag{5.38}$$

If we rescale the kinetic energy to the slow time, we will get

$$\mathcal{L}_1 = \epsilon^2\frac{M}{2}\sum_{\alpha=1}^{K}(\dot{q}_\alpha)^2 + \epsilon A_\alpha(q)\dot{q}_\alpha - V(q) - E_n(q). \tag{5.39}$$

The generalized momenta then reads

$$p_\alpha = \frac{\partial \mathcal{L}_1}{\partial \dot{q}_\alpha} = \epsilon^2 M\dot{q}_\alpha + \epsilon A_\alpha(q). \tag{5.40}$$

The effective Hamiltonian governing the slow classical system up to the first order, denoted by $\mathcal{H}_1$, can be calculated using the Legendre transformation of the Lagrangian (5.39):

$$\mathcal{H}_1 = \frac{1}{2M\epsilon^2}\sum_{\alpha=1}^{K}\left[p_\alpha - \epsilon A_\alpha(q)\right]^2 + E_n(q) + V(q), \tag{5.41}$$

which has the similar structure of the Hamiltonian of a moving electric charge in an electromagnetic field.

5.5 Second order post-adiabatic force

In this section we calculate the second-order post-adiabatic force and prove that this force can be produced by a kinetic term in the second-order post-adiabatic Lagrangian —and not a potential term— which has a coordinate-dependent mass tensor.
Inserting (5.22) in the third term in the general expression of post-adiabatic force given by (5.29) and considering the second order terms we obtain:

$$\epsilon\Im\langle\partial_\mu\phi_n|\dot{\phi}_n\rangle = \epsilon^2\frac{d}{ds}\Im\langle\partial_\mu n|n_1\rangle + \epsilon^2\partial_\mu\Im\langle n_1|\dot{n}\rangle + \mathcal{O}(\epsilon^3). \tag{5.42}$$

The second term in (5.29) leads to

$$\partial_\mu\left[\langle\phi_n|\hat{H}(s)|\phi_n\rangle - E_n\right] = \epsilon^2{\sum_k}'\Delta_{kn}|c_{kn}^{[1]}|^2 + \mathcal{O}(\epsilon^3). \tag{5.43}$$

Therefore, the second order post-adiabatic force can be written as

$$\begin{aligned} F_\mu^{[2]} &= \partial_\mu{\sum_k}'\Delta_{kn}|c_{kn}^{[1]}|^2 + 2\Im\left\{\langle\partial_\mu n_1|\dot{n}\rangle + \langle\partial_\mu n|\dot{n}_1\rangle\right\} && (5.44)\\ &= \partial_\mu{\sum_k}'\frac{\langle k|\dot{n}\rangle\langle\dot{n}|k\rangle}{\Delta_{kn}} + 2\Im\left\{\frac{d}{ds}\langle\partial_\mu n|n_1\rangle + \partial_\mu\langle n_1|\dot{n}\rangle\right\}. && (5.45)\end{aligned}$$

Let us recall the expression for $|n_1\rangle$ from the previous chapter:

$$\begin{aligned} |n_1\rangle &= c_{nn}^{[1]}|n\rangle + |n_1^\perp\rangle, && (5.46)\\ |n_1^\perp\rangle &= {\sum_k}'c_{kn}^{[1]}|k\rangle, && (5.47)\end{aligned}$$

where

$$c_{k\neq n}^{[1]} = \frac{\langle k|\dot{n}\rangle}{i\Delta_{nk}}. \tag{5.48}$$

Inserting (5.46) into the second expression of (5.45) yields

$$\frac{d}{ds}\langle\partial_\mu n|n_1\rangle = \frac{d}{ds}\Im\langle\partial_\mu n|n_1^\perp\rangle = \frac{d}{ds}\sum\nolimits_k{}' \Im\left\{c_{kn}^{[1]}\langle\partial_\mu n|k\rangle\right\}, \quad (5.49)$$

$$\partial_\mu\langle n_1|\dot{n}\rangle = \partial_\mu\langle n_1^\perp|\dot{n}\rangle = \partial_\mu\sum\nolimits_k{}' \Im\left\{c_{kn}^{[1]*}\langle k|\dot{n}\rangle\right\}, \quad (5.50)$$

where we have inserted the expression (5.47) for $|n_1^\perp\rangle$.
We notice that the non-local (time-integral) contribution $c_{nn}^{[1]}$ drops out from (5.49), and (5.50) since $c_{nn}^{[1]}$ and $\langle n|\partial_\mu n\rangle$ are both purely imaginary. This means that the second order post-adiabatic mean-field force can be interpreted as a local force acting on the classical (slow) system.

Given the expression for $c_{kn}^{[1]}$ by (5.48) and employing the fact that

$$|\dot{k}\rangle = \dot{q}_\alpha|\partial_\alpha k\rangle, \quad (5.51)$$

the second order post-adiabatic force can be written as

$$\begin{aligned} F_\mu^{[2]} &= -2\ddot{q}_\alpha\Re\left\{\sum\nolimits_k{}' \frac{\langle n|\partial_\mu k\rangle\langle\partial_\alpha k|n\rangle}{\Delta_{nk}}\right\} + \dot{q}_\alpha\dot{q}_\beta\partial_\mu\Re\left\{\sum\nolimits_k{}' \frac{\langle n|\partial_\alpha k\rangle\langle\partial_\beta k|n\rangle}{\Delta_{nk}}\right\} \\ &- 2\dot{q}_\alpha\frac{d}{ds}\Re\left\{\sum\nolimits_k{}' \frac{\langle n|\partial_\mu k\rangle\langle\partial_\alpha k|n\rangle}{\Delta_{nk}}\right\}. \end{aligned} \quad (5.52)$$

We recognize in (5.52) the acceleration contribution. Defining

$$G_{\mu\alpha}(q) \stackrel{def}{=} -2\sum\nolimits_k{}' \frac{1}{\Delta_{nk}(q)}\Re\left\{\langle n(q)|\partial_\mu k(q)\rangle\langle\partial_\alpha k(q)|n(q)\rangle\right\}, \quad (5.53)$$

where $G_{\mu\alpha}(q)$ plays the role of a coordinate dependent mass tensor, the second order force reads

$$F_\mu^{[2]} = G_{\mu\alpha}\ddot{q}_\alpha + \dot{q}_\alpha\dot{q}_\beta\left(\frac{1}{2}\partial_\beta G_{\alpha\mu} + \frac{1}{2}\partial_\alpha G_{\beta\mu} - \frac{1}{2}\partial_\mu G_{\alpha\beta}\right). \quad (5.54)$$

We notice from (5.53) that $G_{\alpha\beta}$ is a symmetric matrix: $G_{\alpha\beta} = G_{\beta\alpha}$. It is also a positive matrix, i.e., $G_{\alpha\beta}\phi_\alpha\phi_\beta \geq 0$, for any vector ϕ_α, provided that the the quantum system starts its evolution from the ground state: $\Delta_{kn} \geq 0$. But $G_{\alpha\beta}$ cannot be a positive matrix for all initial states of the quantum system, since, e.g., when the quantum system is a two-level system with $d = 2$, one has $G_{\alpha\beta}[\text{excited state}] = -G_{\alpha\beta}[\text{ground state}]$. This case will be explicitly studied in the next section.

It is clear that the force given by (5.54) is generated by the following Lagrangian

$$\mathcal{L}^{[2]}(\dot{q},q)=\frac{1}{2}G_{\alpha\beta}(q)\dot{q}_{\alpha}\dot{q}_{\beta}. \tag{5.55}$$

Therefore, the dynamics of the slowly evolving classical system under the influence of a fast quantum system up to the second order is described by

$$\mathcal{L}_2=\frac{M}{2}\sum\nolimits_{\alpha=1}^{K}\left(\frac{dq_{\alpha}}{dt}\right)^2-V(q)-E_n(q)+\epsilon\mathcal{L}^{[1]}(\dot{q},q)+\epsilon^2\mathcal{L}^{[2]}(\dot{q},q), \tag{5.56}$$

where $\mathcal{L}^{[1]}(\dot{q},q)$ is given by (5.37).

Note that when the time-scale separation is enforced by a large [bare] mass M of the classical particle, the post-adiabatic Lagrangian $\mathcal{L}^{[1]}(\dot{q},q)$, and $\mathcal{L}^{[2]}(\dot{q},q)$ are small as compared to the large kinetic energy $M\sum_{\alpha=1}^{K}\left(\frac{dq_{\alpha}}{dt}\right)^2$; to make this fact explicit, we rescale this kinetic energy to the slow time via $\epsilon\sim 1/\sqrt{M}$:

$$\mathcal{L}_2=\frac{\epsilon^2}{2}\left[M\delta_{\alpha\beta}+G_{\alpha\beta}(q)\right]\dot{q}_{\alpha}\dot{q}_{\beta}+\epsilon A_{\alpha}(q)\dot{q}_{\alpha}-V(q)-E_n(q). \tag{5.57}$$

5.5.1 Metric tensor and curvature

The kinetic part $\frac{\epsilon^2}{2}[M\delta_{\alpha\beta}+G_{\alpha\beta}(q)]\dot{q}_{\alpha}\dot{q}_{\beta}$ of the second-order Lagrangian (5.57) corresponds to a free particle moving on a Riemannian manifold with metric tensor [99]:

$$g_{\alpha\beta}(q)\equiv\epsilon^2[M\delta_{\alpha\beta}+G_{\alpha\beta}(q)]. \tag{5.58}$$

There is an important particular case, where the complete Lagrangian (5.57) just reduces to this kinetic energy. This happens when

- the eigenvectors $|n\rangle$ can be chosen real, which then nullify the vector potential $A_{\alpha}(q)$,
- the bare potential $V(q)$ and the Born-Oppenheimer potential $E_n(q)$ compensate each other, $V(q)+E_n(q)=0$, or $V(q)$ is zero from the outset, while $E_n(q)$ turns to zero, since the eigenvalues of the quantum Hamiltonian $\hat{H}[q]$ do not depend on the coordinates q (though the eigen-vectors do).

Thus we focus on the purely kinetic Lagrangian

$$\frac{1}{2}g_{\alpha\beta}(q)\dot{q}^{\alpha}\dot{q}^{\beta}. \tag{5.59}$$

Once we are going to exercise on the Riemannian geometry, we recover for the velocities the explicitly contravariant notations [99] dq^{α}. The metric tensor $g_{\alpha\beta}$ is then naturally covariant. The Lagrangian (5.57) yields the following equations of motion

$$\ddot{q}^{\alpha} + \Gamma^{\alpha}_{\mu\nu}\dot{q}^{\mu}\dot{q}^{\nu} = 0. \tag{5.60}$$

This is the geodesic equation $\frac{D\dot{q}^{\alpha}}{ds^2} = 0$, where the covariant differential of any vector C^{α} is defined as

$$DC^{\alpha} = dC^{\alpha} + \Gamma^{\alpha}_{\nu\mu}C^{\nu}dq^{\mu}, \tag{5.61}$$

and where the connections $\Gamma^{\alpha}_{\mu\nu}$ are related to the metric tensor via [99]:

$$\Gamma^{\alpha}_{\mu\nu} = \frac{1}{2}g^{\alpha\sigma}\left(\partial_{\mu}g_{\sigma\nu} + \partial_{\nu}g_{\sigma\mu} - \partial_{\sigma}g_{\mu\nu}\right). \tag{5.62}$$

Here $g^{\alpha\sigma}$ is the inverse of the metric tensor: $g^{\alpha\sigma}g_{\sigma\beta} = \delta^{\alpha}_{\beta}$, and where δ^{α}_{β} is the Kronecker delta-symbol.
The first important question is whether the resulting Riemannian manifold is curved or not. In the case of a flat manifold it is possible to bring $g_{\alpha\beta}$ to a diagonal and coordinate independent form by going to some new coordinates q'. The criterion of this is the Riemannian curvature tensor $R^{\mu}_{\nu\alpha\beta}$ [99]. The explicit formula for the covariant curvature tensor is [99]

$$\begin{aligned} R_{\alpha\,\beta\,\gamma\,\delta} &= \frac{1}{2}\left[\partial^2_{\beta\gamma}g_{\alpha\delta} + \partial^2_{\alpha\delta}g_{\beta\gamma} - \partial^2_{\beta\delta}g_{\alpha\gamma} - \partial^2_{\alpha\gamma}g_{\beta\delta}\right] \\ &+ g^{\mu\nu}\left[\Gamma_{\nu\,\beta\gamma}\Gamma_{\mu\,\alpha\delta} - \Gamma_{\nu\,\beta\delta}\Gamma_{\mu\,\alpha\gamma}\right], \end{aligned} \tag{5.63}$$

where $\Gamma_{\mu\beta\gamma} = g_{\mu\alpha}\Gamma^{\alpha}_{\beta\gamma}$. Eq. (5.63) implies the following symmetry relations:

$$R_{\alpha\,\beta\,\gamma\,\delta} = -R_{\beta\,\alpha\,\gamma\,\delta} = -R_{\alpha\,\beta\,\delta\,\gamma} = R_{\gamma\,\delta\,\alpha\,\beta}. \tag{5.64}$$

The manifold is not curved, if and only if

$$R^{\mu}_{\nu\alpha\beta} = 0. \tag{5.65}$$

For any vector C^α, the curvature tensor determines the non-commutativity degree of the covariant derivatives [99]:

$$C^\alpha_{;\beta\,;\,\gamma} - C^\alpha_{;\gamma\,;\,\beta} = -C^\sigma R^\alpha_{\sigma\beta\gamma}, \qquad C^\alpha_{;\beta} \equiv \frac{DC^\alpha}{\partial q^\beta}. \tag{5.66}$$

It is known that the curvature tensor determines the local behavior of geodesics with respect to perturbing their initial conditions [99]. Let $x^\alpha(s,\phi)$ be a family of geodesics, where s is the time, and ϕ is a scalar continuous parameter which distinguishes the members of the family. Thus by the definition of the geodesic:

$$\frac{Du^\alpha}{ds} = 0, \qquad u^\alpha \equiv \frac{\partial x^\alpha}{\partial s}. \tag{5.67}$$

Let us introduce a vector $v^\alpha \equiv \frac{\partial x^\alpha}{\partial \phi}$, which determines the deviation of two geodesics with slightly perturbed initial conditions. This vector satisfies the following Jacobi-Levi-Civita equation [99] [3]:

$$\frac{D^2 v^\alpha}{ds^2} = R^\alpha_{\beta\gamma\delta} u^\beta u^\gamma v^\delta. \tag{5.68}$$

The vector v^α can be separated into two components $v^\alpha = v^\alpha_{[1]} + v^\alpha_{[2]}$: one orthogonal to u^α ($u_\alpha v^\alpha_{[1]} = 0$) and another one parallel to u^α. One can check with help of (5.64, 5.67) that the orthogonal component $v^\alpha_{[1]}$ satisfies the same equation (5.68), while the parallel component $v^\alpha_{[2]}$ satisfies the geodesic equation (5.67).

Below we calculate the curvature for the simplest example of two classical coordinates q^1 and q^2. The fact of having only two coordinates simplifies the formulas for the curvature. Eqs. (5.64) imply that there is only one independent component of the [covariant] curvature tensor, which can be chosen to be R_{1212}. All other components are either zero or equal to $\pm R_{1212}$. Now $R_{\alpha\,\beta\,\gamma\,\delta}$ is expressed as

$$R_{\alpha\,\beta\,\gamma\,\delta} = \frac{R}{2}[g_{\alpha\,\gamma} g_{\beta\,\delta} - g_{\alpha\,\delta} g_{\beta\,\gamma}], \tag{5.69}$$

$$R = g^{\alpha\gamma} g^{\beta\delta} R_{\alpha\,\beta\,\gamma\,\delta} = \frac{2R_{1212}}{g_{11}g_{22} - g_{12}^2}, \tag{5.70}$$

[3] To derive Eq. (5.68) note that the very definitions of u^α and v^α imply $v^\beta\,\partial_\beta u^\alpha = u^\beta\,\partial_\beta v^\alpha$, which amounts to $u^\alpha_{;\beta}\,v^\beta = v^\alpha_{;\beta}\,u^\beta$. Now calculate directly $\frac{D^2 v^\alpha}{ds^2}$ recalling (5.66) and noting that $u^\alpha_{;\beta} u^\beta = 0$ due to (5.67).

where R is the scalar curvature.
The latter thus determines the whole curvature tensor for the present two-dimensional situation. Substituting (5.69) into (5.68) and recalling that one can take $u_\alpha v^\alpha = 0$ in this equation, we get

$$\frac{D^2 v^\alpha}{ds^2} = -\frac{R}{2} v^\alpha \, (u_\beta u^\beta). \tag{5.71}$$

Note that $u_\beta u^\beta$ does not depend on s; see (5.67).

We now set to calculate the curvature tensor $R^\mu_{\nu\alpha\beta}$ for the simplest possible example, where there are only two classical coordinates q^1, q^2 and the quantum system is a two-level system. For further simplicity we assume that the quantum Hamiltonian is real. This means that the Hamiltonian is a linear combination of the first and third Pauli matrices:

$$\hat{H}[q] = \begin{pmatrix} q^2 & q^1 \\ q^1 & -q^2 \end{pmatrix}. \tag{5.72}$$

The eigenvalues and eigenvectors of $\hat{H}$ read respectively

$$E_+ = \sqrt{(q^1)^2 + (q^2)^2} \equiv \rho, \quad (\rho > 0) \tag{5.73}$$

$$E_- = -\sqrt{(q^1)^2 + (q^2)^2} \equiv -\rho, \tag{5.74}$$

$$|+\rangle = \frac{1}{\sqrt{2\rho}} \begin{bmatrix} \frac{q^1}{\sqrt{\rho - q^2}} \\ \sqrt{\rho - q^2} \end{bmatrix}, \tag{5.75}$$

$$|-\rangle = \frac{1}{\sqrt{2\rho}} \begin{bmatrix} \frac{q^1}{\sqrt{\rho + q^2}} \\ -\sqrt{\rho + q^2} \end{bmatrix}. \tag{5.76}$$

It is seen that the adiabatic energies E_+ and E_- cross at $\rho = 0$.

We shall study in separate the case when the quantum system starts at $t = 0$ from its ground state $|-\rangle$, and from the excited state $|+\rangle$.

Ground state

The metric reads form (5.58) and (5.73–5.76):

$$g_{11} = \epsilon^2 \left[M + \frac{(q^2)^2}{4\rho^5} \right], \qquad g_{22} = \epsilon^2 \left[M + \frac{(q^1)^2}{4\rho^5} \right],$$
$$g_{12} = g_{21} = -\epsilon^2 \left(\frac{q^1 q^2}{4\rho^5} \right). \tag{5.77}$$

The determinant and trace of the metric read

$$\det[g] = \epsilon^4 M \left(M + \frac{1}{4\rho^3} \right), \qquad \mathrm{tr}[g] = \epsilon^2 \left(M + \frac{1}{4\rho^3} \right). \tag{5.78}$$

It is seen from (5.77–5.78) that both the determinant and the trace of $g_{\alpha\beta}$ are positive; thus the eigenvalues are positive as well. This situation refers to a usual classical mechanical particle, which is enforced to move on a two-dimensional surface. For the scalar curvature we get from (5.62, 5.63, 5.70) and (5.77–5.78)

$$R = -\frac{3(1 + 16M\rho^3)}{2\epsilon^2 M\rho^2 \left(1 + 4M\rho^3\right)^2}. \tag{5.79}$$

Thus R is strictly negative. Returning to (5.71) we see that since the metric is positively defined [see (5.77–5.78)] $u^\alpha u_\alpha$ is always non-negative. Then the negativity of R in (5.79) implies that the geodesics are unstable with respect to small perturbation of initial conditions, because (5.71) corresponds to a harmonic oscillator with an inverted (though space-dependent) frequency[4]. We see that R is singular at $\rho = 0$, where the adiabatic energy levels cross.

Excited state

Now we assume that the two-level quantum system starts its evolution from the excited state $|+\rangle$. This case leads to more interesting possibilities, since now the metric reads:

$$\begin{aligned} g_{11} &= \epsilon^2 \left[M - \frac{(q^2)^2}{4\rho^5} \right] \qquad g_{22} = \epsilon^2 \left[M - \frac{(q^1)^2}{4\rho^5} \right], \\ g_{12} &= g_{21} = \epsilon^2 \frac{q^1 q^2}{4\rho^5}, \end{aligned} \tag{5.80}$$

Hence the determinate and trace of g read, respectively,

$$\det[g] = \epsilon^4 M \left[M - \frac{1}{4\rho^3} \right], \qquad \mathrm{tr}[g] = \epsilon^2 \left[M - \frac{1}{4\rho^3} \right]. \tag{5.81}$$

[4]Such a local instability leads to chaos, if the (q^1, q^2)-manifold is compact. This is not the case for the considered situation, though it is presumably not very difficult to compactify the manifold, keeping the conclusion on the local instability of geodesics.

Since the metric (5.80) relates to (5.77) with transformation $M \to -M$ and $\epsilon \to i\epsilon$ ($i^2 = -1$), we get for the scalar curvature directly from (5.79)

$$R = \frac{3(16M\rho^3 - 1)}{2\epsilon^2 M\rho^2 \left(1 - 4M\rho^3\right)^2}. \tag{5.82}$$

When the particle moves sufficiently far from the origin $q^1 = q^2 = 0$ (i.e., when $4M\rho^3 > 1$), the metric is positively defined and the curvature is positive. According to (5.71) this means that the geodesics are not sensitive to perturbations in initial conditions. At $4M\rho^3 = 1$ the metric tensor changes its signature, so that for $4M\rho^3 < 1$ it has one positive and one negative eigenvalue. At $4M\rho^3 = 1$ the scalar curvature is singular. We expect that the adiabatic assumption will become problematic in the vicinity of the singularity, but it seems that it is possible for the particle to "tunnel" between subspaces of different signature.

Since the metric tensor is not positively defined for $4M\rho^3 < 1$, (5.71, 5.82) show that for $\frac{1}{4} < 4M\rho^3 < 1$ the geodesics with initial condition $u_\alpha u^\alpha < 0$ can become unstable[5].

For even smaller values of ρ with $16M\rho^3 < 1$ the curvature becomes negative. Now the unstable geodesics have $u_\alpha u^\alpha > 0$, while those with $u_\alpha u^\alpha < 0$ are (at least locally) stable.
It is thus seen that the initial ground versus the excited state of the quantum system produces rather different dynamic behavior for the classical system.

5.6 Third order post-adiabatic force

We now turn to study the post-adiabatic force at the order ϵ^3. The calculations here are more involved, though their general pattern—employing the adiabatic perturbation theory and then reconstructing the effective Lagrangian—remains the same.
In order to calculate the third-order post-adiabatic force given by (5.29), we have to calculate two terms of (5.29) namely, $\langle\phi_n|H|\phi_n\rangle - E_n = \sum_k{}' \Delta_{kn}|c_{kn}|^2$ and $\epsilon\Im\langle\partial_\mu\phi_n|\dot{\phi}_n\rangle$ up to the third order in ϵ.

[5]In the General Theory of Relativity $u_\alpha u^\alpha < 0$ is prohibited by causality; for massive particles $u_\alpha u^\alpha > 0$ and can be normalized to $u_\alpha u^\alpha = 1$, while for photons $u_u^\alpha = 0$ [99]. However, for the present classical theory with a well-defined global time s nothing prohibits us to consider the class of geodesics with $u_\alpha u^\alpha < 0$.

Employing (5.23) we see that $|c_{kn}|^2$ in the third order of ϵ reads

$$|c_{kn}|^2 = 2\epsilon^3 \Re\{c_{kn}^{[2]}\, c_{kn}^{[1]*}\}. \tag{5.83}$$

Inserting (5.83) into the last expression of the post-adiabatic force (5.29) for the third-order correction we get

$$\partial_\mu[\langle\phi_n|\hat{H}(s)|\phi_n\rangle - E_n] = \partial_\mu {\sum_k}' \Delta_{kn}|c_{kn}|^2 = 2\epsilon^3 \partial_\mu {\sum_k}' \Delta_{kn} \Re\{c_{kn}^{[2]}\, c_{kn}^{[1]*}\}. \tag{5.84}$$

Now let us calculate the other part of the general expression of the third-order post-adiabatic force given by $\epsilon\Im\langle\partial_\mu\phi_n|\dot{\phi}_n\rangle$ for the third-order correction:

$$2\epsilon\Im\langle\partial_\mu\phi_n|\dot{\phi}_n\rangle = 2\frac{d}{ds}\Im\left\{\langle\partial_\mu n|n_2\rangle\right\} + 2\partial_\mu\Im\left\{\langle n_2|\dot{n}\rangle\right\} + 2\Im\left\{\langle\partial_\mu n_1|\dot{n}_1\right\}. \tag{5.85}$$

Then the expression for the third-order force reads

$$\frac{F_\mu^{[3]}}{2} = \partial_\mu {\sum_k}' \Delta_{kn} \Re\{c_{kn}^{[2]}\, c_{kn}^{[1]*}\} + \frac{d}{ds}\Im\langle\partial_\mu n|n_2\rangle + \partial_\mu\Im\langle n_2|\dot{n}\rangle + \Im\langle\partial_\mu n_1|\dot{n}_1\rangle. \tag{5.86}$$

Inserting

$$|n_2\rangle = c_{nn}^{[2]}|n\rangle + {\sum_k}' c_{kn}^{[2]}|k\rangle, \tag{5.87}$$

For the expression $\Im\langle n_2|\dot{n}\rangle$ we get

$$\Im\langle n_2|\dot{n}\rangle = \Im\left\{c_{nn}^{[2]*}\langle n|\dot{n}\rangle\right\} + {\sum_k}' \Delta_{nk} \Re\left\{c_{kn}^{[2]} c_{kn}^{[1]*}\right\}, \tag{5.88}$$

where we used

$$c_{k\neq n}^{[1]*} = i\frac{\langle\dot{n}|k\rangle}{\Delta_{nk}} \tag{5.89}$$

in obtaining (5.88).
Therefore the third term of (5.86) reads

$$\partial_\mu\Im\langle n_2|\dot{n}\rangle = \partial_\mu\Im\left\{c_{nn}^{[2]*}\langle n|\dot{n}\rangle\right\} - \partial_\mu {\sum_k}' \Delta_{kn} \Re\left\{c_{kn}^{[2]} c_{kn}^{[1]*}\right\}, \tag{5.90}$$

where we used $\Delta_{nk} = -\Delta_{kn}$.
Then the third order post-adiabatic force reads

$$\frac{F_\mu^{[3]}}{2} = \frac{d}{ds}\Im\langle\partial_\mu n|n_2\rangle + \partial_\mu\Im\{c_{nn}^{[2]*}\langle n|\dot{n}\rangle\} + \Im\langle\partial_\mu n_1|\dot{n}_1\rangle. \tag{5.91}$$

Now we work out $\Im\langle\partial_\mu n|n_2\rangle$. This can be done by inserting the expression for $|n_2\rangle$, given by 5.87, in the first term of the above expression for the third-order force. Having (5.87) in mind the first term of (5.91) can be written as

$$\begin{aligned}\frac{d}{ds}\Im\langle\partial_\mu n|n_2\rangle &= \Im\left\{c_{nn}^{[2]}\langle\partial_\mu\dot{n}|n\rangle\right\} + \Im\left\{c_{nn}^{[2]}\langle\partial_\mu n|\dot{n}\rangle\right\} \\ &+\Im\left\{\left(\frac{d}{ds}c_{nn}^{[2]}\right)\langle\partial_\mu n|n\rangle\right\} + \frac{d}{ds}\Im\left\{\sum_k{}' c_{kn}^{[2]}\langle\partial_\mu n|k\rangle\right\}.\end{aligned} \tag{5.92}$$

Since $\langle\partial_\mu n|n\rangle$ is purely imaginary, we get

$$\begin{aligned}\frac{d}{ds}\Im\langle\partial_\mu n|n_2\rangle &= \Im\left\{c_{nn}^{[2]}\langle\partial_\mu\dot{n}|n\rangle\right\} + \Im\left\{c_{nn}^{[2]}\langle\partial_\mu n|\dot{n}\rangle\right\} \\ &+\Im\langle\partial_\mu n|n\rangle\Re\left\{\frac{d}{ds}c_{nn}^{[2]}\right\} + \frac{d}{ds}\Im\left\{\sum_k{}' c_{kn}^{[2]}\langle\partial_\mu n|k\rangle\right\}.\end{aligned} \tag{5.93}$$

The second term of (5.87) reads

$$\begin{aligned}&\partial_\mu\Im\left\{c_{nn}^{[2]*}\langle n|\dot{n}\rangle\right\} = -\partial_\mu\Im\left\{c_{nn}^{[2]}\langle\dot{n}|n\rangle\right\} \\ &= -\Im\left\{\left(\partial_\mu c_{nn}^{[2]}\right)\langle\dot{n}|n\rangle\right\} - \Im\left\{c_{nn}^{[2]}\langle\partial_\mu\dot{n}|n\rangle\right\} - \Im\left\{c_{nn}^{[2]}\langle\dot{n}|\partial_\mu n\rangle\right\}.\end{aligned} \tag{5.94}$$

Adding (5.92) and (5.94) together yields

$$\begin{aligned}&\frac{d}{ds}\Im\langle\partial_\mu n|n_2\rangle + \partial_\mu\Im\left\{c_{nn}^{[2]*}\langle n|\dot{n}\rangle\right\} = 2\Im\langle\partial_\mu n|\dot{n}\rangle\Re\left\{c_{nn}^{[2]}\right\} \\ &+\Im\langle\partial_\mu n|n\rangle\frac{d}{ds}\Re\left\{c_{nn}^{[2]}\right\} - \Im\langle\dot{n}|n\rangle\partial_\mu\Re\left\{c_{nn}^{[2]}\right\} + \frac{d}{ds}\Im\left\{\sum_k{}' c_{kn}^{[2]}\langle\partial_\mu n|k\rangle\right\},\end{aligned} \tag{5.95}$$

where we noticed $\langle\dot{n}|n\rangle$ is purely imaginary. Thus

$$\Im\left\{(\partial_\mu c_{nn}^{[2]})\langle\dot{n}|n\rangle\right\} = \Im\langle\dot{n}|n\rangle\partial_\mu\Re\left\{c_{nn}^{[2]}\right\}. \tag{5.96}$$

We also used the fact that

$$\Im\left\{c_{nn}^{[2]}\langle\partial_\mu n|\dot{n}\rangle\right\}-\Im\left\{c_{nn}^{[2]}\langle\dot{n}|\partial_\mu n\rangle\right\}=2\Im\langle\partial_\mu n|\dot{n}\rangle\Re\left\{c_{nn}^{[2]}\right\}. \tag{5.97}$$

Let us recall the normalization condition in the second order of ϵ:

$$\Re\left\{c_{nn}^{[2]}\right\}=-\frac{1}{2}\langle n_1|n_1\rangle. \tag{5.98}$$

Thus, the third-order post-adiabatic force reads

$$\begin{aligned}\frac{F^{[3]}}{2} &= -\Im\left\{\langle\partial_\mu n|\dot{n}\rangle\right\}\,\langle n_1|n_1\rangle-\frac{1}{2}\Im\left[\langle\partial_\mu n|n\rangle\right]\,\frac{d}{ds}\langle n_1|n_1\rangle \\ &- \frac{1}{2}\Im\left[\langle n|\dot{n}\rangle\right]\,\partial_\mu\langle n_1|n_1\rangle+\Im\langle\partial_\mu n_1|\dot{n}_1\rangle \\ &+ \frac{d}{ds}\Im\left\{\sum\nolimits_k{}' c_{kn}^{[2]}\langle\,\partial_\mu n|k\rangle\right\}.\end{aligned} \tag{5.99}$$

In order to simplify (5.99) we first work out the terms containing $|n_1\rangle$. Let us recall the expression for $|n_1\rangle$ and $c_{k\neq n}^{[2]}$ from the previous chapter:

$$|n_1\rangle=c_{nn}^{[1]}|n\rangle+|n_1^\perp\rangle, \tag{5.100}$$

$$c_{k\neq n}^{[2]}=c_{nn}^{[1]}c_{k\neq n}^{[1]}+\tilde{c}_{k\neq n}^{[2]}, \tag{5.101}$$

where $|n_1^\perp\rangle$ and $\tilde{c}_{k\neq n}^{[2]}$ are given by

$$|n_1^\perp\rangle=\sum_k{}' c_{kn}^{[1]}|k\rangle,\qquad c_{kn}^{[1]}=-i\frac{\langle k|\dot{n}\rangle}{\Delta_{nk}}, \tag{5.102}$$

and

$$\begin{aligned}&\tilde{c}_{k\neq n}^{[2]}= \\ &\frac{i}{\Delta_{nk}}\left[c_{kn}^{[1]}\left(\langle n|\dot{n}\rangle-\langle k|\dot{k}\rangle\right)-\frac{d}{ds}\left(c_{k\neq n}^{[1]}\right)+\sum\nolimits_{l(\neq k)}{}' c_{ln}^{[1]}\langle\dot{k}|l\rangle\right].\end{aligned} \tag{5.103}$$

We also notice that

$$\langle n_1|n_1\rangle=|c_{nn}^{[1]}|^2+\langle n_1^\perp|n_1^\perp\rangle, \tag{5.104}$$

$$|\dot{n}_1\rangle=\left(\frac{d}{ds}c_{nn}^{[1]}\right)|n\rangle+c_{nn}^{[1]}|\dot{n}\rangle+\frac{d}{ds}|n_1^\perp\rangle, \tag{5.105}$$

$$\langle\partial_\mu n_1|=\left(\partial_\mu c_{nn}^{[1]*}\right)\langle n|+c_{nn}^{[1]*}\langle\partial_\mu n|+\langle\partial_\mu n_1^\perp|. \tag{5.106}$$

Inserting (5.101), and (5.104)-(5.106) into (5.99) we notice that all the non-local terms consisting $c_{nn}^{[1]}$ are canceled out and we are left with

$$\begin{aligned}\frac{F_\mu^{[3]}}{2} &= -\langle n_1^\perp|n_1^\perp\rangle\Im\langle\partial_\mu n|\dot{n}\rangle - \frac{1}{2}\frac{d}{ds}\left(\langle n_1^\perp|n_1^\perp\rangle\right)\Im\langle\partial_\mu n|n\rangle \\ &- \frac{1}{2}\partial_\mu\left(\langle n_1^\perp|n_1^\perp\rangle\right)\Im\langle n|\dot{n}\rangle \\ &+ \Im\langle\partial_\mu n_1^\perp|\frac{d}{ds}n_1^\perp\rangle + \frac{d}{ds}\Im\left[\sum_k{}' \tilde{c}_{kn}^{[2]}\langle\partial_\mu n|k\rangle\right], \end{aligned} \tag{5.107}$$

where $\tilde{c}_{kn}^{[2]}$ is given by (5.104).

The first three terms of (5.107) can be written in terms of the derivatives of each of the expressions. Therefore the third-order post-adiabatic force reads:

$$\begin{aligned}\frac{F^{[3]}}{2} &= -\frac{1}{2}\frac{d}{ds}\left[\langle n_1^\perp|n_1^\perp\rangle\,\Im\langle\partial_\mu n|n\rangle\right] - \frac{1}{2}\partial_\mu\left[\langle n_1^\perp|n_1^\perp\rangle\Im\langle n|\dot{n}\rangle\right] \\ &+\frac{d}{ds}\left[\Re\left(\sum_k{}'\frac{\langle\partial_\mu n|k\rangle\langle k|\dot{n}\rangle}{\Delta_{nk}^2}\right)\Im\langle n|\dot{n}\rangle\right] + \Im\langle\partial_\mu n_1^\perp|\dot{n}_1^\perp\rangle \\ &+\frac{d}{ds}\Im\left\{\sum_k{}'\left(-\frac{i}{\Delta_{nk}}\frac{d}{ds}\left[c_{kn}^{[1]}\right] + \frac{i}{\Delta_{nk}}\sum_l{}' c_{ln}^{[1]}\langle\dot{k}|l\rangle\right)\langle\,\partial_\mu n|k\rangle\right\}, \end{aligned} \tag{5.108}$$

where we have used $\frac{i}{\Delta_{nk}}c_{k\neq n}^{[1]} = \frac{1}{\Delta_{nk}^2}\langle k|\dot{n}\rangle$ in simplifying the last term of (5.107) such that the term $-\langle k|\dot{k}\rangle c_{k\neq n}^{[1]}$ in the expression (5.104) is absorbed in the summation over the index l and the condition $l \neq k$ is removed.

Defining

$$|n_1^\perp\rangle = -i\dot{q}_\alpha|N_\alpha\rangle \qquad |N_\alpha\rangle \stackrel{def}{=} \sum_k{}'\frac{\langle k|\partial_\mu n\rangle}{\Delta_{nk}}|k\rangle, \tag{5.109}$$

and inserting this expression for $|n_1\rangle$ into the first three terms of the expression (5.108), after some algebra it is straight forward to see that those terms

can be generated by a Lagrangian

$$
\begin{aligned}
&-\frac{1}{2}\frac{d}{ds}\left[\langle n_1^{\perp}|n_1^{\perp}\rangle\,\Im\langle\partial_\mu n|n\rangle\right]-\frac{1}{2}\partial_\mu\left[\langle n_1^{\perp}|n_1^{\perp}\rangle\Im\langle n|\dot{n}\rangle\right]\\
&+\frac{d}{ds}\left[\Re\left(\sum_k{}'\frac{\langle\partial_\mu n|k\rangle\langle k|\dot{n}\rangle}{\Delta_{nk}^2}\right)\Im\langle n|\dot{n}\rangle\right]=\\
&\left(\frac{d}{ds}\frac{\partial}{\partial\dot{q}_\mu}-\frac{\partial}{\partial q_\mu}\right)\frac{1}{3}h_{\alpha\beta\gamma}\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma,
\end{aligned}
\tag{5.110}
$$

where

$$
\begin{aligned}
h_{\alpha\beta\gamma} &= \frac{1}{2}\Im\langle n|\partial_\gamma n\rangle\,\Re\langle N_\alpha|N_\beta\rangle \\
&+ \frac{1}{2}\Im\langle n|\partial_\alpha n\rangle\,\Re\langle N_\gamma|N_\beta\rangle+\frac{1}{2}\Im\langle n|\partial_\beta n\rangle\,\langle N_\alpha|N_\gamma\rangle.
\end{aligned}
\tag{5.111}
$$

$h_{\alpha\beta\gamma}$ is symmetric with respect to any permutation of indices α, β and γ, so that

$$
\frac{1}{3}h_{\alpha\beta\gamma}\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma=\frac{1}{2}\Im\langle n|\partial_\gamma n\rangle\,\Re\langle N_\alpha|N_\beta\rangle\,\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma. \tag{5.112}
$$

Working out the term $\Im\langle\partial_\mu n_1^{\perp}|\dot{n}_1^{\perp}\rangle$ in the expression (5.108) for the third order post-adiabatic force yields

$$
\Im\langle\partial_\mu n_1^{\perp}|\dot{n}_1^{\perp}\rangle=\Im\langle\partial_\mu N_\beta|N_\alpha\rangle\ddot{q}_\alpha\dot{q}_\beta+\Im\langle\partial_\mu N_\beta|\partial_\gamma N_\alpha\rangle\,\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma. \tag{5.113}
$$

It is straight forward to show that the last term of (5.108) can be written as

$$
\begin{aligned}
&\frac{d}{ds}\Im\left\{\sum_k{}'\left(-\frac{i}{\Delta_{nk}}\frac{d}{ds}\left[c_{kn}^{[1]}\right]+\frac{i}{\Delta_{nk}}\sum_l{}'\,c_{ln}^{[1]}\,\langle\dot{k}|l\rangle\right)\,\langle\,\partial_\mu n|k\rangle\right\}\\
&=\frac{d}{ds}\Im\left\{-i\langle N_\mu|\dot{n}_1^{\perp}\rangle\right\}=-\frac{d}{ds}\left[\Im\langle N_\mu|N_\alpha\rangle\,\ddot{q}_\alpha+\Im\langle N_\mu|\partial_\beta N_\alpha\rangle\,\dot{q}_\alpha\dot{q}_\beta\right]\\
&=\frac{d^3q_\alpha}{ds^3}\Im\langle N_\alpha|N_\mu\rangle+\ddot{q}_\alpha\dot{q}_\beta\Im\left\{\partial_\beta\langle N_\alpha|N_\mu\rangle+\langle\partial_\beta N_\alpha|N_\mu\rangle+\langle\partial_\alpha N_\beta|N_\mu\rangle\right\}\\
&+\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma\Im\left\{\partial_\gamma\langle\partial_\beta N_\alpha|N_\mu\rangle\right\}.
\end{aligned}
\tag{5.114}
$$

combining (5.113) and (5.114) together we get

$$\begin{aligned}
&\frac{d}{ds}\Im\left\{\sum_k{}'\left(-\frac{i}{\Delta_{nk}}\frac{d}{ds}\left[c_{kn}^{[1]}\right]+\frac{i}{\Delta_{nk}}\sum_l{}' c_{ln}^{[1]}\langle\dot{k}|l\rangle\right)\langle\,\partial_\mu n|k\rangle\right\}\\
&+\Im\langle\partial_\mu n_1^\perp|\dot{n}_1^\perp\rangle=\frac{d^3q_\alpha}{ds^3}\Im\langle N_\alpha|N_\mu\rangle\\
&+\ddot{q}_\alpha\dot{q}_\beta\Im\left\{\partial_\beta\langle N_\alpha|N_\mu\rangle+\langle\partial_\beta N_\alpha|N_\mu\rangle+\langle\partial_\alpha N_\beta|N_\mu\rangle+\langle\partial_\mu N_\beta|N_\alpha\rangle\right\}\\
&+\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma\Im\left\{\partial_\gamma\langle\partial_\beta N_\alpha|N_\mu\rangle+\langle\partial_\mu N_\beta|\partial_\gamma N_\alpha\rangle\right\}. \qquad (5.115)
\end{aligned}$$

working out these two terms of the third-order post-adiabatic force, after some algebra, we see that it can be produced by the following Lagrangian

$$\begin{aligned}
&\frac{d}{ds}\Im\left\{\sum_k{}'\left(-\frac{i}{\Delta_{nk}}\frac{d}{ds}\left[c_{kn}^{[1]}\right]+\frac{i}{\Delta_{nk}}\sum_l{}' c_{ln}^{[1]}\langle\dot{k}|l\rangle\right)\langle\,\partial_\mu n|k\rangle\right\}\\
&+\Im\langle\partial_\mu n_1^\perp|\dot{n}_1^\perp\rangle=\\
&\left[-\frac{d^2}{ds^2}\frac{\partial}{\partial\ddot{q}_\mu}+\frac{d}{ds}\frac{\partial}{\partial\dot{q}_\mu}-\frac{\partial}{\partial q_\mu}\right]\left(-z_{\alpha\beta}\ddot{q}_\alpha\dot{q}_\beta+\frac{1}{3}\lambda_{\alpha\beta\gamma}\,\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma\right), \qquad (5.116)
\end{aligned}$$

where we define the antisymmetric tensor $z_{\alpha\beta}$ as

$$z_{\alpha\beta}\overset{def}{=}\frac{1}{2}\Im\langle N_\beta|N_\alpha\rangle, \qquad (5.117)$$

and the symmetric tensor $\lambda_{\alpha\beta\gamma}$ as

$$\begin{aligned}
\lambda_{\alpha\beta\gamma}\;&\overset{def}{=}\;\frac{1}{4}\Im\Big\{\langle\partial_\beta N_\gamma|N_\alpha\rangle+\langle\partial_\beta N_\alpha|N_\gamma\rangle+\langle\partial_\alpha N_\gamma|N_\beta\rangle\\
&+\;\langle\partial_\alpha N_\beta|N_\gamma\rangle+\langle\partial_\gamma N_\alpha|N_\beta\rangle+\langle\partial_\gamma N_\beta|N_\alpha\rangle\Big\}\\
&=\;\frac{6}{4}\Im\langle\partial_\alpha N_\beta|N_\gamma\rangle. \qquad (5.118)
\end{aligned}$$

In obtaining the above result we employed:

$$\begin{aligned}
&\Im\langle\partial_\beta N_\mu|N_\alpha\rangle=\frac{1}{2}\Im\langle\partial_\beta N_\mu|N_\alpha\rangle+\frac{1}{2}\Im\langle\partial_\beta N_\mu|N_\alpha\rangle\\
&=\frac{1}{2}\Im\langle\partial_\beta N_\mu|N_\alpha\rangle-\frac{1}{2}\Im\langle N_\alpha|\partial_\beta N_\mu\rangle\\
&=\frac{1}{2}\Im\langle\partial_\beta N_\mu|N_\alpha\rangle+\frac{1}{2}\Im\langle\partial_\beta N_\alpha|N_\mu\rangle+\frac{1}{2}\partial_\beta\Im\langle N_\mu|N_\alpha\rangle. \qquad (5.119)
\end{aligned}$$

Combining the above results for the last two terms of the third-order post-adiabatic force (5.116) with those we got for the firs three terms given by (5.110) yields

$$\frac{F_\mu^{[3]}}{2} = \left[-\frac{d^2}{ds^2}\frac{\partial}{\partial\ddot{q}_\mu} + \frac{d}{ds}\frac{\partial}{\partial\dot{q}_\mu} - \frac{\partial}{\partial q_\mu}\right]\left(-z_{\alpha\beta}\ddot{q}_\alpha\dot{q}_\beta + \frac{1}{3}[h_{\alpha\beta\gamma} + \lambda_{\alpha\beta\gamma}]\,\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma\right). \tag{5.120}$$

Thus the third-order post-adiabatic force is purely Lagrangian though containing higher-order derivatives.[6] We can write the third order Lagrangian as

$$\mathcal{L}^{[3]}[q,\dot{q},\ddot{q}] = \epsilon^3\left[f_{\alpha\beta\gamma}(q)\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma - z_{\alpha\beta}(q)\ddot{q}_\alpha\dot{q}_\beta\right], \tag{5.121}$$

where $f_{\alpha\beta\gamma}(q)$ is defined as

$$f_{\alpha\beta\gamma}(q) = \frac{1}{2}\Im\{\langle n|\partial_\gamma n\rangle\langle N_\beta|N_\alpha\rangle + \langle\partial_\gamma N_\beta|N_\alpha\rangle\}. \tag{5.122}$$

It is seen that besides the expected third-order polynomial in the velocities $f_{\alpha\beta\gamma}\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma$, the third-order Lagrangian $\mathcal{L}^{[3]}$ contains a linear dependence on the accelerations $\ddot{q}_\alpha$. The corresponding coupling matrix $z_{\alpha\beta}(q)$ is antisymmetric $z_{\alpha\beta}(q) = -z_{\beta\alpha}(q)$ as it should be, since any term $\phi_{\alpha\beta}\ddot{q}_\alpha\dot{q}_\beta$ with a symmetric $\phi_{\alpha\beta} = \phi_\alpha$, can be reduced (up to a total differential in time) to a third-order polynomial in the velocities.

The total Lagrangian describing the classical system including the higher-order terms up to ϵ^3, $\mathcal{L}_3[q,\dot{q},\ddot{q}]$, will include the previous order post-adiabatic Lagrangians and the bare classical Lagrangian,

$$\mathcal{L}_3[q,\dot{q},\ddot{q}] = -V(q) - E_n(q) + \epsilon A_\alpha(q)\dot{q}_\alpha + \frac{\epsilon^2}{2}[M\delta_{\alpha\beta} + G_{\alpha\beta}(q)]\dot{q}_\alpha\dot{q}_\beta$$
$$+\epsilon^3\left[f_{\alpha\beta\gamma}\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma - z_{\alpha\beta}\ddot{q}_\alpha\dot{q}_\beta\right], \tag{5.123}$$

[6] Let we are given a classical system with action $\int_0^S ds\mathcal{L}[\,\dot{q}(s), q(s)\,]$, where $\mathcal{L}$ is the Lagrangian, q is the vector of (generalized) coordinates, and $\dot{q} = \frac{dq}{ds}$. The Euler-Lagrange variational equations of motion $\frac{d}{ds}\frac{\partial\mathcal{L}}{\partial\dot{q}_\mu} - \frac{\partial\mathcal{L}}{\partial q_\mu} = 0$, are obtained when varying the action over the the coordinate-path $q(s)$ assuming that the end-points are fixed: $\delta q(0) = \delta q(S) = 0$. This well-known set-up has a straightforward generalization for a Lagrangian $\mathcal{L}[\,\ddot{q}(s), \dot{q}(s), q(s)\,]$ that depend on the acceleration [or more generally on higher-order derivatives of coordinates]. The corresponding Euler-Lagrange equations of motion read: $\frac{d}{ds}\frac{\partial\mathcal{L}}{\partial\dot{q}_\mu} - \frac{\partial\mathcal{L}}{\partial q_\mu} - \frac{d^2}{ds^2}\left[\frac{\partial\mathcal{L}}{\partial\ddot{q}_\mu}\right] = 0$, where now we assume that $\delta q(0) = \delta q(S) = \delta\dot{q}(0) = \delta\dot{q}(S) = 0$.

while the equations of motion it generates is [see Footnote 6]

$$\left[\frac{d}{ds}\frac{\partial}{\partial\dot{q}_\mu} - \frac{d^2}{ds^2}\frac{\partial}{\partial\ddot{q}_\mu} - \frac{\partial}{\partial q_\mu}\right]\mathcal{L}_3[q,\dot{q},\ddot{q}] = 0. \tag{5.124}$$

These equations of motion contain third-order time-derivatives $q_\alpha^{(3)}$ of coordinates, i.e., they can be written as

$$2\epsilon^3 z_{\alpha\beta} q_\beta^{(3)} = \varphi_\alpha(q,\dot{q},\ddot{q}). \tag{5.125}$$

Thus when the determinant of the matrix $z_{\alpha\beta}(q)$ is non-zero—and this is generically the case for even number of classical coordinates— the third-derivatives can be expressed through $(q,\dot{q},\ddot{q})$. This means that the dynamics described by (5.124) needs three independent sets of initial conditions at the initial (slow) time $s_{\rm i} = \epsilon t_{\rm i}$:

$$(\, q(s_{\rm i}),\, \dot{q}(s_{\rm i}),\, \ddot{q}(s_{\rm i})\,). \tag{5.126}$$

For an odd number K of classical coordinates, the determinant of $z_{\alpha\beta}$ vanishes, since $z_{\alpha\beta}$ is anti-symmetric. Generically, the matrix $z_{\alpha\beta}(q)$ will only have one eigenvalue equal to zero. Let us denote the related eigenvector by $y_\alpha^{[0]}$, where

$$y_\alpha^{[0]} z_{\alpha\beta} = 0, \tag{5.127}$$

and let $y_\alpha^{[\gamma]}$ with $\gamma = 1,\ldots,K-1$ be the eigenvector of $z_{\alpha\beta}$ with non-zero eigenvalues $\lambda^{[\gamma]}$. Eq. (5.125) produces

$$2\epsilon^3\lambda^{[\gamma]}\, y_\beta^{[\gamma]} q_\beta^{(3)} = y_\alpha^{[\gamma]}\varphi_\alpha(q,\dot{q},\ddot{q}), \quad \text{for} \quad \gamma = 1,\ldots,K-1, \tag{5.128}$$

$$0 = y_\alpha^{[0]}\varphi_\alpha(q,\dot{q},\ddot{q}). \tag{5.129}$$

Now the initial conditions $(\, q(s_{\rm i}),\, \dot{q}(s_{\rm i}),\, \ddot{q}(s_{\rm i})\,)$ at the initial time $s_{\rm i}$ cannot be anymore taken independently from each other, because (5.129) imposes a constraint on them. Provided that $(\, q(s_{\rm i}),\, \dot{q}(s_{\rm i}),\, \ddot{q}(s_{\rm i})\,)$ satisfy this constraint, (5.128) gives $K-1$ equations for components of $q_\alpha^{(3)}$. Another equation for components of $q_\alpha^{(3)}$ can be obtained by differentiating (5.129) over time t and taking $t \to t_{\rm i}$.

The construction described by (5.128), and (5.129) is conceptually not very different from its simplest analog: Consider two classical degrees of

freedom with coordinates x and q. Let the corresponding Lagrangian be $\frac{\dot{q}^2}{2} - V(q,x)$. Note that this Lagrangian does not contain the kinetic energy for the x-particle, i.e., the kinetic energy matrix is degenerate. The Lagrange equations of motion read: $\ddot{q} = -V'_q(q,x)$ and $V'_x(q,x) = 0$. The second equation is a constraint on admissible values of q and x at any time. In particular, it confines their initial values. Now the initial conditions amount to $q(s_{\rm i})$, $\dot{q}(s_{\rm i})$ and $x(s_{\rm i})$ provided that the constraint is satisfied. One is not free in choosing the initial velocity $\dot{x}(s_{\rm i})$. The latter is determined from differentiating the constraint over time s and taking $s \to s_{\rm i}$.

Before closing this discussion on the initial conditions let us note the following aspect. The quantum-classical equations (5.2, 5.5) have the following well-defined initial conditions at the initial moment $t = 0$ of the fast time t: $|\Psi(0)\rangle$, $q(0)$ and $\dot{q}(0)$. On the other hand, as we saw above, the autonomous classical dynamics starts to depend on higher-derivatives of the coordinate(s). The reason of this difference is that the initial conditions of the autonomous classical dynamics are to be imposed at an initial value $s_{\rm i} = \epsilon t_{\rm i}$ of the slow time, where $t_{\rm i}$ should be still sizable larger than $t = 0$. The difference between the original initial conditions of the slow variables and their effective initial conditions after eliminating the fast variables is known as the initial slip problem. It is well recognized in theories dealing with elimination of fast variables [107–109]. There also exist more or less regular procedures of relating the original initial conditions to effective ones [107–109]. In this work, we are interested in autonomous classical dynamics for sufficiently large (fast) times, where the precise relation with the original initial conditions is not directly relevant.

5.6.1 Kinematics

The dependence of $\mathcal{L}_3[q,\dot{q},\ddot{q}]$ on accelerations implies conceptual changes in the kinematics of the classical system, as we now proceed to show.

First we note that the momentum of the classical system is defined via the response of $\mathcal{L}_3$ to an infinitesimal coordinate shift $q_\mu \to q_\mu + \delta q_\mu$, where δq_μ does not depend on time [99]:

$$\delta\mathcal{L}_3 = \frac{\partial\mathcal{L}_3}{\partial q_\mu}\delta q_\mu = \delta q_\mu \frac{d}{ds}\left[\frac{\partial\mathcal{L}_3}{\partial\dot{q}_\mu} - \frac{d}{ds}\frac{\partial\mathcal{L}_3}{\partial\ddot{q}_\mu}\right], \tag{5.130}$$

where we used (5.124). Thus the momentum is defined as

$$p_\mu = \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} - \frac{d}{ds}\frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu}, \tag{5.131}$$

implying that the equations of motion can be written as $\dot{p}_\mu = \frac{\partial \mathcal{L}_3}{\partial q_\mu}$.

If $\mathcal{L}_3$ would not depend on q_μ (which is generically not the case), the corresponding momentum p_μ would be conserved in time. We note that p_μ consists of the usual part $\frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu}$ and the anomalous part $-\frac{d}{ds}\frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu}$ that comes solely from the dependence of the Lagrangian on the acceleration. Using (5.123) we get for the momentum

$$\begin{aligned} p_\mu &= \epsilon A_\mu + \epsilon^2[M\dot{q}_\mu + G_{\mu\alpha}\dot{q}_\alpha] + 3\epsilon^3 f^{(\mathrm{sym})}_{\mu\alpha\beta}\dot{q}_\alpha\dot{q}_\beta \\ &+ 2\epsilon^3 z_{\mu\alpha}\ddot{q}_\alpha + \epsilon^3\left[\partial_\gamma z_{\mu\beta}\right]\dot{q}_\gamma\dot{q}_\beta, \end{aligned} \tag{5.132}$$

where $f^{(\mathrm{sym})}_{\alpha\beta\gamma}$, defined as

$$f^{(\mathrm{sym})}_{\alpha\beta\gamma} \stackrel{def}{=} \frac{1}{6}\sum_{\Pi} f_{\Pi[\alpha\beta\gamma]}, \tag{5.133}$$

is the completely symmetrized expression (5.122); the sum is taken over all six permutations Π of three elements. It is seen that the expression for the momentum does depend linearly on the acceleration. One half of the acceleration-dependence comes from usual part $\frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu}$, while another half comes through the anomalous part $-\frac{d}{ds}\frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu}$, resulting altogether in $2\epsilon^3 z_{\mu\alpha}\ddot{q}_\alpha$ in (5.132).

The energy corresponding to the Lagrangian $\mathcal{L}_3[q,\dot{q},\ddot{q}]$ is obtained via looking at the total time-derivative of $\mathcal{L}_3[q,\dot{q},\ddot{q}]$:

$$\frac{d}{ds}\mathcal{L}_3[q,\dot{q},\ddot{q}] = \frac{\partial \mathcal{L}_3}{\partial q_\mu}\dot{q}_\mu + \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu}\ddot{q}_\mu + \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu}\frac{d^3 q_\mu}{ds^3}, \tag{5.134}$$

where we noted that $\mathcal{L}_3[q,\dot{q},\ddot{q}]$ does not have any explicit time-dependence. Employing equations of motion $\dot{p}_\mu = \frac{\partial \mathcal{L}_3}{\partial q_\mu}$, (5.134) results into energy conservation:

$$\frac{dE}{ds} = 0, \qquad E \equiv p_\mu\dot{q}_\mu + \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu}\ddot{q}_\mu - \mathcal{L}_3. \tag{5.135}$$

Thus the energy of the classical particle reads:

$$E = \frac{\epsilon^2}{2}[M\delta_{\alpha\beta} + G_{\alpha\beta}]\dot{q}_\alpha\dot{q}_\beta + 2\epsilon^3 f_{\alpha\beta\gamma}\dot{q}_\alpha\dot{q}_\beta\dot{q}_\gamma + 2\epsilon^3 z_{\mu\alpha}\ddot{q}_\alpha\dot{q}_\mu + V(q) + E_n(q). \tag{5.136}$$

Note that the vector-potential $A_\alpha(q)$ expectedly drops out from the expression of energy [99]. However, the acceleration-dependent part of the Lagrangian does contribute directly into the energy. In fact, the whole third-order Lagrangian (5.121) is multiplied by a factor 2 and enters into the energy expression.

Let us now turn to the generalized angular momentum tensor, which is defined via the response of $\mathcal{L}_3$ to an infinitesimal rotation (i.e., a distance conserving linear transformation) [99]: $q_\mu \to q_\mu + \omega_{\mu\sigma}\delta q_\sigma$, where $\omega_{\mu\sigma} = -\omega_{\sigma\mu}$:

$$\delta\mathcal{L}_3 = \omega_{\alpha\beta}\left[\frac{\partial\mathcal{L}_3}{\partial q_\alpha}q_\beta + \frac{\partial\mathcal{L}_3}{\partial\dot{q}_\alpha}\dot{q}_\beta + \frac{\partial\mathcal{L}_3}{\partial\ddot{q}_\alpha}\ddot{q}_\beta,\right] = \omega_{\alpha\beta}\frac{d}{ds}\left[p_\alpha q_\beta + \frac{\partial\mathcal{L}_3}{\partial\ddot{q}_\alpha}\dot{q}_\beta\right], \tag{5.137}$$

where we again used (5.124). The full angular momentum tensor is now defined as [recalling $\omega_{\mu\sigma} = -\omega_{\sigma\mu}$] :

$$M_{\alpha\beta} = p_\alpha q_\beta - p_\beta q_\alpha + \frac{\partial\mathcal{L}_3}{\partial\ddot{q}_\alpha}\dot{q}_\beta - \frac{\partial\mathcal{L}_3}{\partial\ddot{q}_\beta}\dot{q}_\alpha \tag{5.138}$$

$$= L_{\alpha\beta} + S_{\alpha\beta}, \tag{5.139}$$

so that when $\mathcal{L}_3$ is rotationally invariant, $M_{\alpha\beta}$ is conserved in time. One part of this tensor is the usual orbital momentum $L_{\alpha\beta} = p_\alpha q_\beta - p_\beta q_\alpha$. The remainder—non-orbital momentum, or spin— arises due to the dependence of the Lagrangian on the accelerations, and it is a second-order polynomial over the velocities:

$$S_{\alpha\beta} = \frac{\partial\mathcal{L}_3}{\partial\ddot{q}_\alpha}\dot{q}_\beta - \frac{\partial\mathcal{L}_3}{\partial\ddot{q}_\beta}\dot{q}_\alpha \tag{5.140}$$

$$= \epsilon^3[\, z_{\beta\gamma}\dot{q}_\gamma\dot{q}_\alpha - z_{\alpha\gamma}\dot{q}_\gamma\dot{q}_\beta\,]. \tag{5.141}$$

In the simplest two-coordinate situation $S_{12} = -S_{21} = \epsilon^3 z_{21}(\dot{q}_1^2 + \dot{q}_2^2)$, which means that the spin tensor is proportional to the velocity square.

Zitterbewegung effect

From the expression of the momentum given by (5.132) and the expression for the spin given by (5.140,5.141) and using the fact that $z_{\alpha\beta}$ is antisymmetric, we can write

$$p_\mu = \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} + \frac{d}{ds}\left[\frac{S_{\alpha\mu}\dot{q}_\alpha}{\dot{q}^2}\right], \qquad \dot{q}^2 \equiv \dot{q}_\beta \dot{q}_\beta, \tag{5.142}$$

which means that the anomalous part $p_\mu - \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu}$ of the momentum is driven by the time-derivative of the velocity-projected spin-tensor.

An expression similar to (5.142)—relating the momentum to the projected time-derivative of the spin—appears in the (relativistic) Dirac electron theory [110]. There the fact that the total angular momentum is a sum of the orbital part and the spin part, as well as the fact that the velocity and the momentum are different objects and are not simply proportional to each other via the mass, are the consequence of the relativistic invariance for the electron. The very effect of the spin time-derivative contributing into the momentum was named *zitterbewegung*, since for the free Dirac electron this contribution brings in an additional oscillatory motion [110]. In a more recent literature, the zitterbewegung effect is also derived via Lagrangians containing the higher-order derivatives of coordinates [111, 112].

There are, however, several aspects that distinguish (5.142) from the zitterbewegung effects already known in literature.

- First, we do not have a relativistic invariant theory; for us relation (5.142) emerges due to the fact that the classical system is open.

- Second, we do not have to have the conservation of momentum and of angular momentum for deriving (5.142). Both these quantities are generically non-conserved in our situation (ultimately since the system is open), but relation (5.142) still holds generally due to the specific, anti-symmetric form (5.121) of the acceleration-dependent part of the Lagrangian.

We close this part by emphasizing its main findings: due to interaction with the fast quantum system the classical system gets a spin [non-orbital angular momentum], which is related to its momentum via zitterbewegung effect.

5.6.2 Hamiltonian description

In this section we study the Hamiltonian description. Within the order ϵ^2 the Hamiltonian description is straightforward. However, the third-order dynamics has a non-trivial Hamiltonian structure, as seen below.

Let us first explicitly separate out the higher-derivative term of the Lagrangian given by (5.123). Thus we have

$$\mathcal{L}_3[q, \dot{q}, \ddot{q}] = L_3[q, \dot{q}] - \epsilon^3 z_{\alpha\beta} \ddot{q}_\alpha \dot{q}_\beta. \tag{5.143}$$

In general, we can introduce three sets of variables

$$q = (q_1, \ldots, q_K), \qquad v = (v_1, \ldots, v_K), \qquad \pi = (\pi_1, \ldots, \pi_K), \tag{5.144}$$

and instead of (5.143) introduce the following extended Lagrangian:

$$L[q, v, \pi] = L_3(q, v) - \epsilon^3 z_{\alpha\beta} \dot{v}_\alpha v_\beta + \pi_\alpha (\dot{q}_\alpha - v_\alpha). \tag{5.145}$$

It should be clear that if we treat q, v and π as coordinates, then the Lagrange equations generated by $L[q, v, \pi]$ are equivalent to those generated by $\mathcal{L}_3[q, \dot{q}, \ddot{q}]$. At this point π is considered as a part of the overall set of coordinates. It may be equivalently viewed as Lagrange multipliers. If $L[q, v, \pi]$ were not dependent on $\dot{v}$—that is, $\mathcal{L}_3[q, \dot{q}, \ddot{q}]$ would not depend on $\ddot{q}$—we would write the velocities $v = v(q, \pi)$ as functions of the coordinates and momenta, and end up with the usual Hamiltonian description with q and π being the canonical coordinates and momenta, respectively. Though $L[q, v, \pi]$ does depend on $\dot{v}$, it can be still related to a Hamiltonian in the following way [113].

Once the triplet q, v, π is considered as coordinates, we introduce a separate notation for it

$$Q = (Q_1, \ldots, Q_{3K}) = (q_\alpha, v_\alpha, \pi_\alpha). \tag{5.146}$$

Now the Lagrangian (5.145) reads

$$L[Q] = L_3[Q] + A_a[Q] \dot{Q}_a, \qquad a = 1, \ldots 3K, \tag{5.147}$$

where

$$A[Q] = (\pi_\alpha, \epsilon^3 z_{\beta\alpha}, 0). \tag{5.148}$$

Below we shall show that the expression $L_3[Q]$ plays the role of the Hamiltonian.

Eq. (5.147) generates the following Lagrange equations of motion:

$$\Omega_{ab}(Q)\,\dot{Q}_b = \frac{\partial L_3}{\partial Q_a}, \tag{5.149}$$

$$\Omega_{ab}(Q) \stackrel{def}{=} \frac{\partial A_a}{\partial Q_b} - \frac{\partial A_b}{\partial Q_a}. \tag{5.150}$$

In block-matrix notations Ω reads

$$\Omega = \begin{pmatrix} 0 & Y & I \\ -Y^T & Z & 0 \\ -I & 0 & 0 \end{pmatrix}, \tag{5.151}$$

where each element in the above matrix is a $K \times K$ matrix, with K being the number of classical degrees of freedom:

$$Y_{\alpha\beta} = \epsilon^3 v_\gamma \partial_\alpha z_{\gamma\beta}, \qquad Z_{\alpha\beta} = -2\epsilon^3 z_{\alpha\beta}, \qquad I_{\alpha\beta} = \delta_{\alpha\beta}, \tag{5.152}$$

and where I is the $K \times K$ unit matrix. Provided Z is invertible, the inverse of Ω reads [block-matrix notations]

$$\Omega^{-1} = \begin{pmatrix} 0 & 0 & -I \\ 0 & Z^{-1} & -Z^{-1}Y^T \\ I & -YZ^{-1} & YZ^{-1}Y^T \end{pmatrix}. \tag{5.153}$$

For an even K the matrix Z is generically invertible; as we discussed before. In this case Ω_{ab} is invertible and antisymmetric. Moreover, from its definition given by (5.150) we see that

$$\frac{\partial}{\partial Q_c}\Omega_{ab} + \frac{\partial}{\partial Q_b}\Omega_{ca} + \frac{\partial}{\partial Q_a}\Omega_{bc} = 0. \tag{5.154}$$

Therefore it ensures that the Poisson brackets defined via Ω_{ab} does not change in time [114]. In fact, Ω_{ab} defines a symplectic structure [114].
Then $L_3[Q]$ plays the role of the Hamiltonian.

Now for any two functions $C(Q)$ and $D(Q)$ the Poisson bracket is defined as

$$\{C(Q), D(Q)\}_{PB} = \Omega^{-1}_{ab}\frac{\partial C}{\partial Q_a}\frac{\partial D}{\partial Q_b}. \tag{5.155}$$

The equations of motion (5.149) can now be written as

$$\dot{Q}_a = \{\, Q_a, L_3[Q] \,\}_{PB}. \tag{5.156}$$

In this case the Poisson brackets are non-linear. It is seen from (5.151, 5.155) that $z_{\alpha\beta}$ and its derivatives define a non-trivial symplectic structure for the system.

The matrix Z is not invertible for an odd K. The Hamiltonian description in this case is still possible, but it requires more care in explicitly accounting for constraints.

5.7 The Fourth order Lagrangian

In this section we discuss a specific example on the fourth-order Lagrangian. Since the calculations now become very complicated, we shall restrict ourselves to the situation where the classical system has just one single coordinate q. For further simplicity we assume the quantum system has real adiabatic eigenstates. In fact, the main purpose of this section is to illustrate that the fourth-order Lagrangian again depends linearly on the highest-order time-derivatives of the classical coordinate.

Following the same lines of calculation for the third order non-adiabatic force presented in section 5.6, and assuming a single coordinate classical system and real eigenstates for the quantum system, the non-adiabatic force acting on the classical system in the fourth order is described by the following Lagrangian

$$\begin{aligned} &\epsilon^4 F^{[4]} = \\ &\left(\frac{d^3}{ds^3}\frac{\partial}{\partial q^{(3)}} - \frac{d^2}{ds^2}\frac{\partial}{\partial \ddot{q}} + \frac{d}{ds}\frac{\partial}{\partial \dot{q}} - \frac{\partial}{\partial q}\right)\mathcal{L}^{[4]}[q,\dot{q},\ddot{q},q^{(3)}], \end{aligned} \tag{5.157}$$

where

$$\mathcal{L}^{[4]}[q,\dot{q},\ddot{q},q^{(3)}] = \epsilon^4\left[a\dot{q}^4 + b\ddot{q}\dot{q}^2 + w\dot{q}q^{(3)}\right], \tag{5.158}$$

where $q^{(3)}$ stands for the third order time derivative of q, and where $\mathcal{L}^{[4]}$ represents the fourth-order Lagrangian. We notice the same pattern in the higher-order Lagrangian, i.e., that the dependence on the higher-order time

derivatives $\ddot{q}$ and $q^{(3)}$ is linear. The coefficients a, b, and w are given as

$$a(q) = \sum_k{}' \frac{|\langle \partial_q N|k\rangle|^2}{\Delta_{nk}} - \langle N|N\rangle\langle \partial_q n|N\rangle, \tag{5.159}$$

$$b(q) = -\sum_k{}' \frac{|\langle k|\partial_q n\rangle|^2}{\Delta_{nk}^2}\ \partial_q[\Delta_{nk}^{-1}], \tag{5.160}$$

$$w(q) = -\sum_k{}' \frac{|\langle k|\partial_q n\rangle|^2}{\Delta_{nk}^3}, \tag{5.161}$$

where $|N\rangle$ is given by (5.109): $|N\rangle = \sum_k{}' \frac{\langle k|\partial_q n\rangle}{\Delta_{nk}}|k\rangle$.

Then the total Lagrangian describing the one dimensional classical system reads

$$\begin{aligned}\mathcal{L}_4[q,\dot{q},\ddot{q},q^{(3)}] &= -V(q) - E_n(q) + \frac{\epsilon^2}{2}(M+G)\dot{q}^2 \\ &+ \epsilon^4\left(a\dot{q}^4 + b\ddot{q}\dot{q}^2 + w\dot{q}q^{(3)}\right),\end{aligned} \tag{5.162}$$

where the first and the third order terms vanish due to the assumption of real eigenstates of the quantum system, and where a, b, and w are given by (5.159)-(5.161) and G is defined as

$$G \equiv -2\sum_k{}' \frac{\langle n|\frac{d}{dq}|k\rangle^2}{\Delta_{nk}}. \tag{5.163}$$

The kinematics of this Lagrangian can be developed along the same lines as in the previous section and represent the similar pattern.

5.8 Summary

We have studied the post-adiabatic equations of motion for a slow classical system which is coupled to a fast quantum system. The slow versus fast motion is controlled by a small ratio ϵ of the characteristic times. The general problem we addressed is to find an effective Lagrangian that describes the dynamics of the classical system. The post-adiabatic reaction force is proved to be Lagrangian up to the fifth order of ϵ. We conjecture that at every order of ϵ the effective dynamics of the classical system can be derived from a Lagrangian.

In the order ϵ^0 the effective Lagrangian differs from the bare one by the Born-Oppenheimer potential energy. In the first order correction the effective

Lagrangian corresponds to a magnetic field, which is related to the geometric phase [2].

In the order ϵ^2 the effective Lagrangian gets an additional kinetic energy term, which is a second-order polynomial over the classical velocities [3,100]. We showed that in the second order of ϵ, the motion generated by the effective classical Lagrangian can be mapped on to geodesic curves on a suitable Riemannian manifold. Operating with the simplest possible example—two classical coordinates interacting with a two-level quantum system—we show that the Riemannian manifold is essentially curved solely due to the kinetic energy generated by the fast quantum system. The scalar curvature is frequently negative indicating that the classical trajectories [geodesic curves] are unstable with respect to small variations of the initial conditions. The metric tensor generated by the fast quantum system can change its signature as a function of the two coordinates. Physically this means a transition from an Euclidean to pseudo-Euclidean manifold, emergence of a time-like coordinate.

Within the order ϵ^3 the effective Lagrangian linearly depends on the accelerations of the classical system.

We argued that this result is important, because it provides a physically well-motivated scenario for the emergence of higher-derivative Lagrangians for open classical systems. This result should be contrasted to the usual open-system approaches, which can also produce forces depending on higher-order derivatives (e.g., the Abraham-Lorentz force in electrodynamics), but those forces are dissipative (non-Lagrangian).

The presence of higher-derivative terms can be tested by essential influences they bring on the kinematics of the system. First, they modify initial conditions; in our case this means that the trajectory of the classical system on the slow (coarse-grained) time starts to depend on acceleration. Second, the conserved energy of the slow classical motion does depend on the acceleration. And third, the presence of higher-derivative terms naturally separates the total angular momentum into the sum of orbital momentum and spin. We show that this spin satisfies an exact analogue of the zitterbewegung relation.

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APPENDIX A

Numerical illustration of initial state determination within the Jaynes-Cummings model

In this appendix we give two concrete examples on the inversion of the matrix $\mathcal{M}$ in (2.86).

- Let us assume that the average number of photons inside the cavity is $\bar{n} = 2$, the coupling constant is $g = 50$ KHz, and the detuning parameter $\Delta = 10$ KHz. Looking at Fig. 2.1(a) one sees that the determinant is maximal at (approximately) $\tau = 20\mu$s. (Recall that the typical interaction time of a thermal atomic beam with the single mode of the field is of the order of 100μs [30, 33].) The elements of the matrix $\mathcal{M}$ and the vector $\mathcal{B}$ are worked in section 2.5. Inserting all these numbers into (2.80) - (2.85) one obtains

$$\mathcal{M}^{-1}|_{(\Delta=10\text{KHz})} = \begin{pmatrix} 15.183 & 5.59578 & 0.0456968 \\ 1.14077 & -1.3668 & -1.38923 \\ 1 & 1 & 0 \end{pmatrix}, \quad \text{(A.1)}$$

$$\mathcal{B}|_{(\Delta=10\text{KHz})} = \begin{pmatrix} -0.0557631 \\ 2.05576 \\ 0.0411884 \end{pmatrix}. \quad \text{(A.2)}$$

- For the second example we take a larger detuning: $\bar{n} = 2$, $g = 50$ KHz and $\Delta = 100$ KHz. The optima interaction time $t = 300\mu$s is read off from Fig. 2.1(b) (the interaction time $t \approx 18\,\mu$s gives somewhat smaller determinant; see Fig. 2.1(b)). The numerical calculation of $\mathcal{M}^{-1}$ and $\mathcal{B}$ produces:

$$\mathcal{M}^{-1}|_{(\Delta=100\mathrm{KHz})} = \begin{pmatrix} 3.18085 & 1.23251 & -1.15186 \\ 5.92052 & -4.20194 & -4.52702 \\ 1 & 1 & 0 \end{pmatrix}, \tag{A.3}$$

$$\mathcal{B}|_{(\Delta=100\mathrm{KHz})} = \begin{pmatrix} -0.0707962 \\ 2.0708 \\ -0.119635 \end{pmatrix}. \tag{A.4}$$

APPENDIX B

Numerical illustration of maximum likelihood method

Below we give a numerical example, where the constraint (2.93) may or may not be satisfied automatically. We take $\bar{n} = 2$, $g = 50$ KHz, $\Delta = 100$ KHz, and we have chosen the measurement time $t = 300\mu$s such that the corresponding determinant D is maximized; see Fig. 2.1(b). Then we construct the matrix $\mathcal{C}$ and the vector $\mathcal{B}$ in (2.93) [see (A.3, A.4)]. Neglecting the probabilities of having more than three photons inside the cavity, we assume that we are given the following six frequencies $\nu_{\pm 1}(m)$ $(m = 1, 2, 3)$. These frequencies are normalized according to $\sum_{m=1}^{3} \sum_{a=\pm 1} \nu_a(m) = 1$. For simplicity we additionally assume that these frequencies are related to each other as

$$\nu_1(1) = \nu_{-1}(1), \quad \nu_1(2) = \nu_{-1}(2), \quad \nu_1(3) = \nu_{-1}(3). \tag{B.1}$$

For different values of $\nu_1(1)$, $\nu_1(2)$ and $\nu_1(3)$ the numerical maximization of (2.91) over $p_a(m)$ under the constraint (2.93) produced a result different from (2.96) ($\sum_{m=1}^{3} \sum_{a=\pm 1} p_a(m) = 1$). An example follows: for

$$\nu_1(1) = 0.05, \quad \nu_1(2) = 0.25, \quad \nu_1(3) = 0.2 \tag{B.2}$$

	$\nu_1(1) = 0.05$	$\nu_1(1) = 0.15$	$\nu_1(1) = 0.25$	$\nu_1(1) = 0.30$
$\nu_1(2) = 0.05$	$\delta = 0.00989504$	$\delta = 0.0000494347$	$\delta = 1.1102 \times 10^{-16}$	$\delta = 0.00108428$
$\nu_1(2) = 0.15$	$\delta = 0.00318619$	$\delta = 0$	$\delta = 0.00140516$	$\delta = 0.0115233$
$\nu_1(2) = 0.25$	$\delta = 0.0000717018$	$\delta = 0$	$\delta = 0.0336704$	–
$\nu_1(2) = 0.30$	$\delta = 1.1102 \times 10^{-16}$	$\delta = 0.0000961022$	–	–

Table B.1: The distance $\delta[\nu||p]$ (given by (B.5)) between the set of frequencies $\nu_{\pm 1}(m)$ and the set of corresponding probabilities $p_{\pm 1}(m)$ obtained from maximizing Eq. (2.91) under the constraint Eq.(2.93). As in the main text, we assumed that the frequencies satisfy Eq. (B.1). Thus the third frequency (not shown in the table) is obtained from $\nu_a(3) = \frac{1}{2} - \nu_a(1) - \nu_a(2)$. The numerical values for the involved parameters are: $\bar{n} = 2$ (the initial average number of photons), $g = 50$ kHz (coupling constant), $\Delta = 100$ kHz (detuning) and $t = 300\mu$s (the interaction time). The matrix $\mathcal{M}$ and the vector $\mathcal{B}$ in this case are given by Eqs. (A.3), and (A.4). Three places in the table are empty, because the corresponding frequencies are unphysical (their sum is larger than one due to the assumption Eq. (B.1)

the probabilities are:

$$\begin{aligned} p_1(1) &= 0.05148118, \quad p_{-1}(1) = 0.05087771, \\ p_1(2) &= 0.24811809, \quad p_{-1}(2) = 0.254403426, \\ p_1(3) &= 0.19158279, \quad p_{-1}(3) = 0.20353679. \end{aligned} \tag{B.3}$$

Employing these probabilities in (2.95) and in (2.86) we get for the initial spin density matrix:

$$\hat{\rho}_S = \frac{1}{2}\left[1 - (0.187183)\,\hat{\sigma}_x - (0.942992)\,\hat{\sigma}_y + (0.275121)\,\hat{\sigma}_z\right]. \tag{B.4}$$

In this context we need to quantify the difference between the input frequencies $\nu_a(m)$ and the probabilities $p_a(m)$ which result from maximizing (2.91) under the constraint (2.93). In particular, this difference will quantify the relevance of the constraint (2.93) in maximizing (2.91). A good measure of distance between two probability sets is provided by [52]

$$\delta[\nu||p] = 1 - \sum_{a=\pm 1}\sum_{m=1}^{3}\sqrt{\nu_a(m)p_a(m)}. \tag{B.5}$$

This quantity is equal to its minimal value zero if (and only if) $\nu_a(m) = p_a(m)$ (i.e., when the constraint (2.93) holds automatically), and it is equal to its maximal value 1 for $\nu_a(m)p_a(m) = 0$.

In Table B.1 we calculated the distance $\delta[\nu||p]$ between the frequencies and the corresponding probabilities. It is seen that in some cases this distance is just equal to zero, while for other cases it is rather small.

APPENDIX C

Properties of the back reaction factors $G_r(t)$ and $F_r(t)$

In this appendix we work out the back reaction factor $F_r(t)$ which appears in the expression of the collective bath coordinate as Let us first

$$\begin{aligned}\hat{X}^{(1)}(t) &= \sum_k g_k \left[\hat{a}_k^\dagger(0) e^{i\left(\frac{kr}{2}\cos\theta_k+\omega_k t\right)} + \hat{a}_k(0) e^{-i\left(\frac{kr}{2}\cos\theta_k+\omega_k t\right)}\right] \\ &- \hat{\sigma}_z^{(1)} \sum_k \frac{g_k^2}{\omega_k}\left(1-\cos\omega_k t\right) \qquad \text{(C.1)} \\ &- \hat{\sigma}_z^{(2)} \sum_k \frac{g_k^2}{\omega_k}\left[\cos(kr\cos\theta_k) - \cos\left(\omega_k t + kr\cos\theta_k\right)\right]. \qquad \text{(C.2)}\end{aligned}$$

where we define

$$G_r(t) \stackrel{def}{=} \sum_k \frac{g_k^2}{\omega_k}\left[\cos(kr\cos\theta_k) - \cos\left(\omega_k t + kr\cos\theta_k\right)\right], \qquad \text{(C.3)}$$

$$G(t) \stackrel{def}{=} \sum_k \frac{g_k^2}{\omega_k}\left[1-\cos\left(\omega_k t\right)\right]. \qquad \text{(C.4)}$$

In the same analogy, working out $\hat{X}_r^{(2)}(t)$ yields

$$\begin{aligned}\hat{X}_r^{(2)}(t) &= \sum_k g_k \left[e^{i\left(-\frac{kr}{2}\cos\theta_k+\omega_k t\right)}\hat{a}_k^\dagger(0) + e^{-i\left(-\frac{kr}{2}\cos\theta_k+\omega_k t\right)}\hat{a}_k(0)\right] \\ &- \hat{\sigma}^{(1)}\sum_k \frac{g_k^2}{\omega_k}\left[\cos\left(kr\cos\theta_k\right) - \cos\left(\omega_k t - kr\cos\theta_k\right)\right] \\ &-\hat{\sigma}_z^{(2)}\sum_k \frac{g_k^2}{\omega_k}\left(1-\cos\omega_k t\right). \end{aligned} \tag{C.5}$$

Averaging $G_r(t)$ over θ_k and denoting the result by $\bar{G}_r(t)$ amounts to

$$\bar{G}_r(t) = \frac{1}{2}\sum_k \frac{g_k^2}{\omega_k}\int_0^\pi \sin\theta_k d\theta_k \left\{\cos\left[kr\cos\theta_k\right] - \cos\left[kr\cos\theta_k + \omega_k t\right]\right\}. \tag{C.6}$$

This integral can be straight forwardly performed and as a result we have

$$\bar{G}_r(t) = \frac{1}{2}\sum_k \frac{g_k^2}{\omega_k}\frac{1}{kr}\left[\sin kr - \frac{1}{2}\sin(kr+\omega_k t) - \frac{1}{2}\sin(kr-\omega_k t)\right]. \tag{C.7}$$

We notice that $\bar{G}_r(t)$ is symmetric in r, i.e. $\bar{G}_{-r}(t) = \bar{G}_r(t)$.
Inserting the inverse dispersion relation

$$k = \frac{\omega_k}{c}, \tag{C.8}$$

where c is the velocity of the oscillation modes, into (C.7) we have

$$\bar{G}(t) = \sum_k \frac{g_k^2}{2\omega_k^2\tilde{t}}\left\{2\sin\omega_k\tilde{t} - \sin\left[\omega_k(t+\tilde{t})\right] + \sin\left[\omega_k(t-\tilde{t})\right]\right\}, \tag{C.9}$$

where $\tilde{t}$ is defined as

$$\tilde{t} \stackrel{def}{=} \frac{r}{c}. \tag{C.10}$$

Inserting the spectral density in $\bar{G}_r(t)$ yields

$$\bar{G}(t) = \int_0^\infty d\omega\, \frac{J(\omega)}{2\omega^2\tilde{t}}\left\{2\sin\omega\tilde{t} - \sin\left[\omega(t+\tilde{t})\right] + \sin\left[\omega(t-\tilde{t})\right]\right\}. \tag{C.11}$$

In the ohmic regime where we are interested in $J(\omega)$ reads

$$J(\omega) = \gamma\omega e^{-\omega/\Gamma}. \tag{C.12}$$

Thus $\bar{G}_r(t)$ reads

$$\bar{G}(t) = \gamma \int_0^\infty d\omega \, \frac{e^{-\omega/\Gamma}}{2\tilde{t}\omega} \left\{ 2\sin(\omega\tilde{t}) - \sin\left[\omega(t+\tilde{t})\right] + \sin\left[\omega(t-\tilde{t})\right] \right\}. \quad \text{(C.13)}$$

We know that

$$\int_0^\infty e^{-px} \sin(qx) \frac{dx}{x} = \arctan(q/p), \qquad p > 0. \quad \text{(C.14)}$$

Thus implying (C.14) into (C.15) we get

$$\bar{G}_r(t) = \quad \text{(C.15)}$$
$$\frac{\gamma}{2\tilde{t}} \left\{ 2\arctan(\Gamma\tilde{t}) - \arctan\left[\Gamma(t+\tilde{t})\right] + \arctan\left[\Gamma(t-\tilde{t})\right] \right\}.$$

Integrating $\bar{G}_r(t)$ given by (C.15) over time yields the back reaction factor $F_r(t)$ in the ohmic regime as

$$\bar{F}_r(t) = \int_0^t ds \, \bar{G}_r(s). \quad \text{(C.16)}$$

The time integral of $\arctan[\Gamma(t \pm \tilde{t})]$ can be taken using integrating by parts as

$$\int_0^t ds \, \arctan[\Gamma(t \pm \tilde{t})] = t \arctan[\Gamma(t \pm \tilde{t})] - I, \quad \text{(C.17)}$$

where I is defined as

$$I \stackrel{def}{=} \int_0^t ds \, \frac{s\Gamma}{1 + \left[\Gamma(s \pm \tilde{t})\right]^2}. \quad \text{(C.18)}$$

This integral can be easy taken by changing the variable $s \pm \tilde{t}$ to u. Thus

$$I = \frac{1}{2\Gamma} \ln\left(\frac{1 + \left[\Gamma(t \pm \tilde{t}\right]^2}{1 + (\Gamma\tilde{t})^2} \right) \mp \tilde{t} \arctan\left[\Gamma(t \pm \tilde{t})\right] + \tilde{t} \arctan(\Gamma\tilde{t}). \quad \text{(C.19)}$$

Substituting I in (C.17), for $\bar{F}_r(t)$ we have

$$\begin{aligned} \bar{F}_r(t) &= \frac{\gamma}{2\tilde{t}} \Bigg\{ \frac{1}{2\Gamma} \ln\left(\frac{1 + \left[\Gamma(t+\tilde{t})\right]^2}{1 + \left[\Gamma(t-\tilde{t})\right]^2} \right) + 2t \arctan\left(\Gamma\tilde{t}\right) \\ &- (t+\tilde{t}) \arctan\left[\Gamma(t+\tilde{t})\right] + (t-\tilde{t}) \arctan\left[\Gamma(t-\tilde{t})\right] \Bigg\}. \end{aligned} \quad \text{(C.20)}$$

$G(t)$ in the ohmic regime reads [66]

$$\begin{aligned} G(t) &= \gamma \int_0^\infty d\omega e^{-\omega/\Gamma} \left[1 - \cos(\omega t)\right] \\ &= \gamma\Gamma \left(1 - \frac{1}{1+\Gamma^2 t^2}\right) \end{aligned} \tag{C.21}$$

which then yields

$$F(t) = \gamma \left[\Gamma t - \arctan\left(\Gamma t\right)\right]. \tag{C.22}$$

Therefore $\chi(\tau, t)$ which is defined as

$$\chi(\tau, t) = F(t) + F(\tau) - F(t+\tau), \tag{C.23}$$

reads

$$\chi(\tau, t) = \gamma \left[\arctan\left(\Gamma(t+\tau)\right) - \arctan\left(\Gamma t\right) - \arctan\left(\Gamma\tau\right)\right]. \tag{C.24}$$

In the limit $\Gamma t \gg 1$ where the initial stat preparation is irrelevant, $\chi(\tau, t)$ reads

$$\chi(\tau, t) = -\gamma \arctan\left(\Gamma\tau\right). \tag{C.25}$$

We also need to calculate $\bar{\chi}_r(\tau, t) - \bar{F}_r(\tau)$. This can be done by using the fact that

$$\bar{\chi}_r(\tau, t) - \bar{F}_r(\tau) = \bar{F}_r(t) - \bar{F}_r(t+\tau). \tag{C.26}$$

Now implying (C.20) we get

$$\begin{aligned} \bar{\chi}_r(\tau, t) - \bar{F}_r(\tau) &= \frac{\gamma}{2\tilde{t}} \Bigg\{ - 2\tau \arctan\left(\Gamma\tilde{t}\right) \\ &- \tau \left[\arctan\left(\Gamma(t+\tau+\tilde{t})\right) - \arctan\left(\Gamma(t+\tau-\tilde{t})\right)\right] \\ &- t\left[\arctan\left(\Gamma(t+\tilde{t})\right) - \arctan\left(\Gamma(t-\tilde{t})\right)\right. \\ &- \left.\arctan\left(\Gamma(t+\tau+\tilde{t})\right) + \arctan\left(\Gamma(t+\tau-\tilde{t})\right)\right] \\ &- \tilde{t}\left[\arctan\left(\Gamma(t+\tilde{t})\right) + \arctan\left(\Gamma(t-\tilde{t})\right)\right. \\ &- \left.\arctan\left(\Gamma(t+\tau+\tilde{t})\right) - \arctan\left(\Gamma(t+\tau-\tilde{t})\right)\right] \\ &+ \frac{1}{2\Gamma} \ln\left(\frac{1 + \left[\Gamma(t+\tilde{t})\right]^2}{1 + \left[\Gamma(t-\tilde{t})\right]^2}\right) \\ &- \frac{1}{2\Gamma} \ln\left(\frac{1 + \left[\Gamma(t+\tau+\tilde{t})\right]^2}{1 + \left[\Gamma(t+\tau-\tilde{t})\right]^2}\right) \Bigg\}. \end{aligned} \tag{C.27}$$

We set $\Gamma t \gg 1$ to ensure that the final results are independent of the details of the state preparation. Thus in this limit $\bar{\chi}_r(\tau, t) - \bar{F}_r(\tau)$ reads

$$\bar{\chi}_r(\tau, t) - \bar{F}_r(\tau) = -\frac{\gamma\tau c}{r} \arctan\left(\frac{\Gamma r}{c}\right). \tag{C.28}$$

We notice that in the limit when r approaches to zero, (C.28) reads

$$\lim_{r\to 0}\left(\bar{\chi}_r(\tau, t) - \bar{F}_r(\tau)\right) = -\gamma\tau\Gamma. \tag{C.29}$$

APPENDIX D

Properties of the quantum noise operator

In this appendix we calculate the correlator and the anitcorrelator of $\hat{\eta}_r(t)$ which is given by

$$\hat{\eta}_r(t) = \sum_k g_k \left[e^{\frac{i}{2}kr\cos\theta_k}\, e^{i\omega_k t}\hat{a}_k^\dagger(0) + e^{-\frac{i}{2}kr\cos\theta_k}\, e^{-i\omega_k t}\hat{a}_k(0) \right]. \tag{D.1}$$

Calculation of $\hat{\eta}_r(t)\hat{\eta}_r(t')$ yields

$$\begin{aligned}
\hat{\eta}_r(t)\hat{\eta}_r(t') &= \sum_{k,l} g_k g_l \big[e^{\frac{ir}{2}(k\cos\theta_k + l\cos\theta_l)}\, e^{i(\omega_k t + \omega_l t')}\, \hat{a}_k^\dagger \hat{a}_l^\dagger \\
&+ e^{\frac{ir}{2}(k\cos\theta_k - l\cos\theta_l)}\, e^{i(\omega_k t - \omega_l t')}\, \hat{a}_k^\dagger \hat{a}_l \\
&+ e^{-\frac{ir}{2}(k\cos\theta_k - l\cos\theta_l)}\, e^{-i(\omega_k t - \omega_l t')}\, \hat{a}_k \hat{a}_l^\dagger \\
&+ e^{-\frac{ir}{2}(k\cos\theta_k + l\cos\theta_l)}\, e^{-i(\omega_k t + \omega_l t')}\, \hat{a}_k \hat{a}_l \big],
\end{aligned} \tag{D.2}$$

while $\hat{\eta}_r(t')\hat{\eta}_r(t)$ reads

$$\begin{aligned}\hat{\eta}_r(t')\hat{\eta}_r(t) &= \sum_{k,l} g_k g_l \big[e^{\frac{ir}{2}(k\cos\theta_k + l\cos\theta_l)}\, e^{i(\omega_k t+\omega_l t')}\, \hat{a}_l^\dagger \hat{a}_k^\dagger \\ &+ e^{-\frac{ir}{2}(k\cos\theta_k - l\cos\theta_l)}\, e^{-i(\omega_k t-\omega_l t')}\, \hat{a}_l^\dagger \hat{a}_k \\ &+ e^{\frac{ir}{2}(k\cos\theta_k - l\cos\theta_l)}\, e^{i(\omega_k t-\omega_l t')}\, \hat{a}_l \hat{a}_k^\dagger \\ &+ e^{-\frac{ir}{2}(k\cos\theta_k + l\cos\theta_l)}\, e^{-i(\omega_k t+\omega_l t')}\, \hat{a}_l \hat{a}_k \big]. \end{aligned} \tag{D.3}$$

The commutation of $\hat{\eta}_r(t)$ and $\hat{\eta}_r(t')$ then can be derived by subtracting (D.3) from (D.2)

$$[\hat{\eta}_r(t), \hat{\eta}_r(t')] = -2\, i\, \mathrm{sign}(t-t') \sum_k |g_k|^2 \sin\left[\omega_k (t-t')\right], \tag{D.4}$$

where $\mathrm{sign}(t-t')$ is $+1$ when $t > t'$ and is -1 when $t < t'$. In deriving (D.4) we implied the commutation rule between the bath creation and annihilation operators

$$\begin{aligned}\left[\hat{a}_k^\dagger, \hat{a}_l^\dagger\right] &= 0 = \left[\hat{a}_k, \hat{a}_l\right], \\ \left[\hat{a}_k, \hat{a}_l^\dagger\right] &= \delta_{kl}. \end{aligned} \tag{D.5}$$

We notice that the commutator of $\hat{\eta}_r(t)$ and $\hat{\eta}_r(t')$ is a complex number independent of r.

Adding (D.2) and (D.3) together we get the anticommutator of the quantum noise operator as the following

$$\begin{aligned}\{\hat{\eta}_r(t), \hat{\eta}_r(t')\} &= \sum_{k,l} g_k g_l \Bigg[e^{\frac{ir}{2}(k\cos\theta_k + l\cos\theta_l)}\, e^{i(\omega_k t+\omega_l t')}\, \left\{\hat{a}_k^\dagger, \hat{a}_l^\dagger\right\} \\ &+ e^{-\frac{ir}{2}(k\cos\theta_k - l\cos\theta_l)}\, e^{-i(\omega_k t-\omega_l t')}\, \left\{\hat{a}_k, \hat{a}_l^\dagger\right\} \\ &+ e^{\frac{ir}{2}(k\cos\theta_k - l\cos\theta_l)}\, e^{i(\omega_k t-\omega_l t')}\, \left\{\hat{a}_k^\dagger, \hat{a}_l\right\} \\ &+ e^{-\frac{ir}{2}(k\cos\theta_k + l\cos\theta_l)}\, e^{-i(\omega_k t+\omega_l t')}\, \left\{\hat{a}_k, \hat{a}_l\right\} \Bigg]. \end{aligned} \tag{D.6}$$

Averaging (D.6) over the initial thermal state of the bath yields

$$\langle \{\hat{\eta}_r(t), \hat{\eta}_r(t')\} \rangle = 2 \sum_k |g_k|^2 \left\langle \left\{\hat{a}_k, \hat{a}_k^\dagger\right\} \right\rangle \cos\left[\omega_k (t-t')\right]. \tag{D.7}$$

Since the bath initially in a Gibbs state

$$\left\langle \left\{ \hat{a}_k, \hat{a}_k^\dagger \right\} \right\rangle = \coth\left(\frac{\beta\hbar\omega_k}{2}\right). \tag{D.8}$$

Thus we have

$$\langle\{\hat{\eta}_r(t), \hat{\eta}_r(t')\}\rangle = 2\sum_k |g_k|^2 \coth\left(\frac{\beta\hbar\omega_k}{2}\right) \cos\left[\omega_k(t-t')\right]. \tag{D.9}$$

The time evolution of the quantum noise operator reads

$$\mathcal{E}_t\hat{\eta}_r(s) = \sum_k g_k \left[e^{\frac{i}{2}kr\cos\theta_k}\, e^{i\omega_k s}\hat{a}_k^\dagger(t) + e^{-\frac{i}{2}kr\cos\theta_k}\, e^{-i\omega_k s}\hat{a}_k(t) \right]. \tag{D.10}$$

Let us recall the expression for $\hat{a}_k(t)$

$$\begin{aligned} \hat{a}_k(t) &= e^{-i\omega_k t}\hat{a}_k(0) + \frac{g_k}{2\omega_k}\,\hat{\sigma}_z^{(1)}\, e^{(i/2)kr\cos\theta_k}\left(e^{-i\omega_k t} - 1\right) \\ &+ \frac{g_k}{2\omega_k}\,\hat{\sigma}_z^{(2)}\, e^{-(i/2)kr\cos\theta_k}\left(e^{-i\omega_k t} - 1\right). \end{aligned} \tag{D.11}$$

Inserting $\hat{a}_k(t)$ and its complex conjugate, $\hat{a}_k^\dagger(t)$, in (D.10) we get

$$\begin{aligned} &\mathcal{E}_t\hat{\eta}_r(s) = \\ &\sum_k g_k \left[e^{\frac{i}{2}kr\cos\theta_k}\, e^{i\omega_k(t+s)}\hat{a}_k^\dagger(0) + e^{-\frac{i}{2}kr\cos\theta_k}\, e^{-i\omega_k(t+s)}\hat{a}_k(0) \right] \\ &+\hat{\sigma}_z^{(1)} \sum_k \frac{g_k^2}{\omega_k}\left\{\cos\left[\omega_k\left(t+s\right)\right] - \cos\left(\omega_k t\right)\right\} \\ &+\hat{\sigma}_z^{(2)} \sum_k \frac{g_k^2}{\omega_k}\left\{\cos\left[kr\cos\theta_k + \omega_k\left(t+s\right)\right] - \cos\left(kr\cos\theta_k + \omega_k t\right)\right\}, \end{aligned} \tag{D.12}$$

which can be written as

$$\begin{aligned} &\mathcal{E}_t\hat{\eta}_r(s) = \hat{\eta}_r(t+s) + \\ &\hat{\sigma}_z^{(1)}\left[G(t) - G(t+s)\right] + \hat{\sigma}_z^{(2)}\left[G_r(t) - G_r(t+s)\right]. \end{aligned} \tag{D.13}$$

In the same analogy for $\mathcal{E}_t\hat{\eta}_{-r}(s)$ we get

$$\begin{aligned} &\mathcal{E}_t\hat{\eta}_{-r}(s) = \hat{\eta}_{-r}(t+s) + \\ &\hat{\sigma}_z^{(1)}\left[G_{-r}(t) - G_{-r}(t+s)\right] + \hat{\sigma}_z^{(2)}\left[G(t) - G(t+s)\right]. \end{aligned} \tag{D.14}$$

Summary

One of the main tasks in quantum information theory is to determine the initial state of a qubit, i.e. a two-level system that can be described by the Pauli matrices. Quantum state tomography provides a useful method for this aim. Quantum state tomography is the process of reconstructing the quantum state (density matrix) of an ensemble of quantum systems by performing measurements on it. In order to be able to uniquely identify the state, the measurements must be tomographically complete. That is, the measured operators must form an operator basis in the Hilbert space of the system, providing all the information about the state. However since in general different operators do not commute with each other, one needs to perform successive measurements of non-commuting observables to recover the initial state of the system. In chapter 2 we show that one can completely reconstruct the initial state of a qubit by means of simultaneous measurement of commuting observables. The price to be paid is to introduce another system called assistant of which the state is known. The assistant need not necessarily be another qubit. It may for example also be a single near resonance cavity mode. By letting the system and the assistant interact with each other, and after a some time laps performing measurements on one observable of each system it is possible to make a linear map between the measurement results and the initial state of the qubit. The suggested observables are the easiest ones to measure.

Usually it is very difficult to isolate a quantum system from its surrounding environment. Therefore studying the influence of the surrounding envi-

ronment on the state of an open quantum system, i.e. a quantum system that is interacting with its environment, is crucial in quantum processes. Depending on the type of environment, there are different conditions under which one can study the influence of the environment on a quantum system. A group of methods categorized by the name of system-bath interaction are based on the assumption that the reaction of the system on its surrounding environment is weak. One of the main consequences of this approach is the Langevin equation, which supplements the Newton equation of motion for the small system by two additional forces: random conservative force and non-conservative (i.e., non-Lagrangian), velocity-dependent friction force. Chapter 3 is devoted to specific application of this model with which one can study the dynamics of the polarization of an open qubit. Two non-interacting qubits are considered to be surrounded by a common environment. Inducing sharp and strong pulses on one of them makes the polarization transfer from the other one mediated by the common environment.

There is another set-up that allows studying the dynamics of an open system. Here the essential condition is that the time scale of the evolution of the quantum system is much faster than that of its classical environment. This is one the most used set-ups for coupling quantum and classics variables. In chapter 4 we consider the Hamiltonian governing the evolution of the quantum system as a function of slowly varying parameters of its surrounding environment. By employing the adiabatic perturbation theory, which is described in this chapter, we derive the state of the quantum system beyond the adiabatic regime where the transition to other energy levels is not forbidden.

In chapter 5 we turn our focus on the dynamics of the slow classical environment which experiences an average force exerted by the fast quantum system. We show that the back reaction force in contrast to the system-bath type of interaction is a conservative force that can be generated by a Lagrangian. The Lagrangian describing the situation depends on the classical slow parameters, and their higher order time derivatives. Several interesting aspects of the Lagranigan are discussed in chapter 5.

Samenvatting

Een van de belangrijkste opgaven in quantuminformatietheorie is de begintoestand van een qubit, een twee-niveau systeem dat kan worden beschreven door Pauli matrices, te bepalen. Quantum state tomography is een bruikbare methode om dit doel te bereiken. Met dit proces kan de quantumtoestand (de dichtheidsmatrix) van een ensemble van quantumsystemen gereconstrueerd worden door verschillende herhaalde metingen te doen. Echter, commuteren verschillende operatoren niet met elkaar dan moet men in principe meerdere opeenvolgende metingen van niet-commuterende observabelen doen om de begintoestand van het systeem te bepalen. In hoofdstuk 2 laten we zien hoe de begintoestand van een qubit volledig gereconstrueerd kan worden door het gelijktijdig meten van een aantal commuterende observabelen. Dit vereist de hulp van een ander systeem, de zogenaamde assistent, die in een bekende toestand is. De assistent kan bijvoorbeeld een andere qubit zijn of een bijna-resonante mode van het fotonveld. Na een wisselwerking tussen het systeem en de assistent gedurende een bepaalde tijd kunnen we zowel een observabele van het systeem als van de assistent meten waardoor het mogelijk wordt om de begintoestand van de qubit te bepalen. Dit is mogelijk doordat er een lineaire afbeelding bestaat tussen de meetresultaten en de begintoestand van een qubit. In tegenstelling tot quantumstatetomografie hoeven we geen metingen te doen aan niet-commuterende observabelen, dit maakt onze methode effectiever.

Een quantumsysteem dat wisselwerkt met de omgeving wordt een open quantumsysteem genoemd. Om zo'n systeem te bestuderen is het van cru-

ciaal belang om de invloed van de omgeving op de toestand van dit open quantumsysteem te achterhalen. Er zijn twee manieren om een open quantumsysteem te bestuderen. Een groep van methoden gecategoriseerd door de zogeheten systeem-bad wisselwerking is gebaseerd op de veronderstelling dat de reactie van het systeem op de omgeving zwak is. Hieruit volg dat de dynamica van het systeem beschreven wordt door de Langevin vergelijking. Deze vergelijking is analoog aan de Newton vergelijking voor de beweging van een klein systeem maar deze beschrijft twee extra krachten: een willekeurige conservatieve kracht en een niet-conservatieve (niet-Lagrangiaanse), snelheidsafhankelijke wrijvingskracht. In hoofdstuk 3 bestuderen we de specifieke toepassing van dit model, waarmee we de dynamica van de polarisatie van een open quantumsysteem kunnen bepalen. We beschouwen twee niet-interagerende spin-$\frac{1}{2}$ systemen die dezelfde omgeving hebben. Wanneer we één van hen blootstellen aan scherpe en sterke pulsen zien we dat de polarisatie van de andere wordt overgedragen op de eerste via de gemeenschappelijke omgeving.

Er is een tweede groep van methoden die het mogelijk maakt om de dynamica van een open systeem te bestuderen. In dit geval is de essentiële voorwaarde dat de tijdschaal van de evolutie van het quantumsysteem veel kleiner is dan die van de klassieke omgeving. Dit is één van de meest gebruikte manieren om quantum en klassieke variabelen te koppelen. In hoofdstuk 4 beschouwen we de Hamiltoniaan die de ontwikkeling van het quantumsysteem beschrijft als functie van de langzaam variërende parameters van de omgeving. Door toepassing van de adiabatische perturbatietheorie, die wordt beschreven in dit hoofdstuk, leiden we de toestand van het quantumsysteem af buiten het adiabatische regime, waarin de overgang naar andere energieniveaus niet verboden is.
In hoofdstuk 5 concentreren we ons op de dynamica van de langzame klassieke omgeving. Deze wordt veroorzakt door een gemiddelde kracht die het snelle quantumsysteem uitoefent op de omgeving. We laten zien dat, in tegenstelling tot het geval van systeem-bad interacties, de terugkoppeling leidt tot een conservatieve kracht die gegenereerd kan worden door een Lagrangiaan. De Lagrangiaan is een functie van de klassieke langzame parameters, en hun hogere orde tijds afgeleiden. Verschillende interessante aspecten van de Lagrangiaan worden besproken in hoofdstuk 5.

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