Spin bosons and spin glasses

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Citation for published version (APA):

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3

Introduction

3.1 Motivation

A known feature of technological progress is the increase of human ability to control and design the microscopic world. Recent efforts in manipulating simple quantum systems, e.g., in the context of quantum computing or quantum chemistry, is one aspect of this general trend. Another aspect is the field of quantum thermodynamics whose main objective is in designing and studying thermodynamical processes in the domain where quantum features of small systems are relevant. In particular, this activity aims to improve our understanding of phenomenological thermodynamics by addressing its concepts from the first principles of quantum mechanics. The current activity in quantum thermodynamics includes quantum engines, general aspects of work extraction from quantum systems, thermodynamical aspects of quantum information theory and limits of thermodynamical concepts such as the second law and temperature. There were also much earlier applications concerning, in particular, thermodynamic aspects of lasers and masers.

Our present purpose is to study two complementary processes: work extraction from a two-temperature system and cooling at the expense of work, on the basis of the spin-boson model [BP02, L+87, Luc90, VL98]. The spin-boson model is one of the simplest models in the study of quantum open systems. By open quantum systems, we mean systems which are in contact with an environment, which for us will be a thermal bath. Closed systems, on the contrary, are systems which can be described on themselves, without giving any consideration to their surroundings, though for instance, external fields can act on them. Furthermore, one could speak over isolated systems where all dynamics is determined by the internal degrees of freedom without any external influence.

The study of an open quantum system consists in describing the dynamics of the system together with the dynamics of the environment. The latter can produce qualitative changes on the dynamics of the system. In our situation, the necessity of the bath has to be stressed since in the usual practice of quantum system manipulation,
the bath is a serious hindrance one cannot get rid of. In contrast, both processes
of work-extraction and cooling, when starting from an equilibrium situation, cannot
be achieved without external thermal baths.

- The second law in Thomson's formulation\footnote{Thomson's formulation of the second law: Starting from equilibrium, so \( \rho(0) = e^{-3H/Z} \), and having a cyclic process \( H(t) \), so \( H(0) = H(T) = H \), implies that the work is non-negative: \( W \geq 0 \).}—which can be derived as a theorem in quantum mechanics [Thi83, BK77, BK79, Bas78, PW78, Len78, AN02]—forbids work-extraction from an equilibrium system via cyclic processes generated by external fields. The easiest way to employ such an equilibrium system in work-extraction is to attach it to a thermal bath having a different temperature, which is the standard setting of heat engines. The entire system is then out of equilibrium and work-extraction is not forbidden, at least in principle, at the most general level.

- The no-cooling principle, which is related to the second law, states that an equilibrium system cannot be cooled that is for a two level system that the occupation of its ground state cannot be increased—by means of cyclic external fields [KP92]. It is, however, possible to cool in the presence of the thermal bath, even when having the same initial temperature. Then according to the above statement of the second law such a cooling process will be accompanied by a loss of work, which is the energy cost needed for cooling, that is, the principle of a refrigerator.

### 3.1.1 Work Extraction

The general restrictions just mentioned determined the way how standard quantum work extraction (also known as amplification or lasing/masing) processes are designed [Sie71]. The most traditional lasers and masers operate by extracting work from an ensemble of two-level systems having a negative temperature, in other words, population inversion, which is a strongly non-equilibrium state. More recent schemes of lasing without inversion employ non-equilibrium states of three (four, multi-) level systems without population inversion of energy levels, but, in contrast, they have initially sizable non-diagonal terms of the corresponding density matrix in the energy representation, usually called coherences [SZ97, Koc92]. These schemes attracted attention due to both their conceptual novelty and the fact that non-zero non-diagonal elements represent a weaker form of non-equilibrium compared to population inversion, and thus their preparation can be, in principle, an easier task.

### 3.1.2 Cooling of spins

Cooling, i.e. obtaining relatively pure states from mixed ones, is of central importance in fields dealing with quantum features of matter. Laser cooling of motional states of atoms is nowadays a known achievement [EMSKB03]. The related problem
of cooling spins is equally known: it originated as an attempt to improve the sensitivity of NMR/ESR spectroscopy [AG82, Sør89, Sli90, Lam68, C+90, H+97, A+03, B+02, I+03]. Since in experiments the signal strength is proportional to polarization. Recently it got renewed attention due to realizations of setups for quantum computers in NMR physics [GC97, War97]. The very problem arises since the most direct methods of cooling spins, such as lowering the temperature of the whole sample or applying strong dc fields, are not feasible or not desirable, e.g. in biological applications of NMR, where strong static fields or low temperatures may destroy the very studied material. Without any external influence the polarization is really low, for example, at temperature \( T = 1 \text{K} \) and magnetic field \( B = 1 \text{T} \) the equilibrium polarization of a proton is \( \tanh \frac{\mu B}{2k_B T} = 10^{-3} \) where \( \mu \) is the ratio \( \frac{\text{frequency}}{\text{field}} \) and it is equal to 42 MHz/T for a proton, \( 10^3 \) larger for electrons and 10 times smaller for \( ^{15}\text{N} \).

Over the years, several methods were proposed to attack the problem of small polarizations. The polarization is generally increased via a dynamical process and it is used before relaxing back to equilibrium [AG82, Sør89, Lam68, C+90, H+97, A+03, Sli90, I+03, B+02]. Especially known are methods where a relatively high polarization is transferred from one place to another, e.g. from electronic to nuclear spins [AG82, Sør89, Lam68, C+90, H+97, A+03, Sli90, I+03]. In this respect electronic spins play the same role as the zero-temperature bath of vacuum modes employed for laser cooling of atoms [EMSKB03] (this latter bath is typically useless for cooling spins). Polarization transfer was studied in various settings both theoretically and experimentally [AG82, Sør89, Sli90, Lam68, C+90, H+97, A+03, I+03]. However, this scheme is limited – besides requiring already existing high polarization by the availability and efficiency of the transfer interaction.

A related method, polarization compression, consists in manipulating a set of \( n \) spins, each having a small polarization, in such a way that the polarization of one spin is increased at the expense of decreasing the polarization of the remaining \( n - 1 \). These spoiled spins can be recycled and used again [B+02]. This method cools spins one by one, thereby taking a long time for cooling a large ensemble of spins, and requires carefully designed inter-spin interactions.

### 3.2 Open quantum systems and spin boson model

The following chapters are devoted to quantum open systems, in particular to the spin-boson model, more precisely, an exactly solvable limit of it. In this introduction we give the basic ingredients of the spin-boson model. Only a general background is given. In chapter 4, a concrete situation will be given, motivated and solved.

As already stated, in quantum open systems we describe the subsystem plus its environment. We can write then the full Hamiltonian as

\[
\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I
\]  

where \( \hat{H}_S \) corresponds to the Hamiltonian of the subsystem \( S \), \( \hat{H}_B \) corresponds to the Hamiltonian of the environment or reservoir (which is typically a heat bath) and
$\hat{H}_I$ correspond to the interaction between them. Then the Hilbert space where $\hat{H}$ works is composed in the tensorial product of the subsystem's Hilbert space with the bath's Hilbert space: $S \otimes B$.

The state of the subsystem $S$ will change as a consequence of its internal dynamics and of the interaction with the surroundings. The interaction with the environment can be such that the resulting state changes in the subsystem $S$ alone can no longer be represented by unitary, Hamiltonian dynamics. To get the subsystem's dynamics, one traces out the environment degrees of freedom ($\text{tr}_B \rho$), e.g. one sums over all possibilities for the environment. By doing this we get an effective description of the dynamics of the subsystem, the so-called reduced dynamics ($S$ is called the reduced system).

In the spin-boson model, the subsystem is a two-level system, thus a spin. By two-level system we can mean an intrinsic two-level system, i.e. a 1/2-spin, the polarization of a photon; but we can also consider a system having many levels where the two lowest ones are the only accessible ones or a system having a continuous degree of freedom subject to a potential energy function $V(q)$ with two separated minima, see fig.(3.1). If the height of the barrier $V_0$ is large enough compared with $\omega_+\omega_-$ the two minima can create an effective two-level system. The energy levels though, do not correspond to each of the minima but to a state which is a superposition of both. Examples of such a situation could be for instance some types of chemical reaction or the motion of defects in some crystalline solids. Effective two-level systems are also believed to be responsible for the linear specific heat of amorphous solids at low temperatures $\sim 1 \text{K}$ [Phi81, Esq98].

Therefore the motivation to use a two-level system is overwhelming, it is almost everywhere and it is the minimal model having non-trivial quantum features. In the spin boson model [L+87], the Hamiltonian for the subsystem reads

$$\hat{H}_S = \frac{1}{2} \hbar \Delta \hat{\sigma}_x + \frac{1}{2} \varepsilon \hat{\sigma}_z$$  \hspace{1cm} (3.2)

where $\hat{\sigma}_x$, $\hat{\sigma}_y$ and $\hat{\sigma}_z$ are Pauli's matrices. In the picture of the two-wells potential, $\Delta$ is related with the transition probability between wells and $\varepsilon$ with their energy difference, see fig.(3.1). In the spin language, however, $\Delta$ and $\varepsilon$ correspond to magnetic fields acting on the $x$ or the $z$ direction respectively.

Furthermore, in the spin-boson model the environment is modeled by a set of harmonic oscillators, thus bosons. In some cases this may be taken in the literal sense, when harmonic oscillators represent phonons or photons. However, it is also

![Double well potential](image)
II.3.2 Open quantum systems and spin boson model

known that rather general classes of thermal baths can be effectively represented via harmonic oscillators. The motivation for that is the subject of sections and appendices of many papers, appendix C in Ref. [CL83] or section 2 in Ref. [MS80] to mention some.

The basic idea is that the bath is a macroscopic entity in a stable equilibrium state which is only weakly perturbed by the interaction with the system. Therefore, due to the weak perturbation noticed by the bath, the system sees only excitations which can be considered as the ones of harmonic oscillators.

The Hamiltonian of the bath is thus taken as

\[ \hat{H}_B = \sum_k \hbar \omega_k \hat{a}_k^\dagger \hat{a}_k, \quad [\hat{a}_l, \hat{a}_k^\dagger] = \delta_{kl}. \]  

(3.3)

where \( \hat{a}_k^\dagger \) and \( \hat{a}_k \) are boson creation and annihilation operators of the bath oscillator with the index \( k \) with frequency \( \omega_k \).

The last part of the Hamiltonian is the interaction between the system’s degrees of freedom and the environment surrounding it. According to the above assumptions of harmonicity of the bath, the interaction, up to this approximation, can be taken as linear in the variables of the bath. Due to the assumption that the bath is weakly perturbed, higher order terms, i.e. anharmonicities, can be neglected. A linear interaction suffices to bring the system in equilibrium to the temperature of the bath. For stronger arguments in this line, we refer the reader to [L+87, CL83]. Then in general

\[ \hat{H}_I = \frac{\hbar}{2} \sum_{a=x,y,z} \hat{\sigma}_a \hat{X}^a. \quad \hat{X}^a = \sum_k g_k^a (\hat{a}_k^\dagger + \hat{a}_k). \]  

(3.4)

where \( g_k^a \) is the strength of the coupling of the \( a \) component of the system to the \( k \) oscillator. The coupling only depends on the position and not the momenta of the oscillators. It can be proven that any linear coupling can, via appropriate canonical transformations, be expressed only in terms of position operators [Leg85]. Furthermore, this interaction couples the bath to all spin components. This is usually relaxed to couple the bath only to \( \hat{\sigma}_z \). The reason for that depends on the system studied. In the following chapter we will do so and motivate this approximation.

If the modes of the bath are dense enough, we can describe the effect of the interaction of the bath to the system via a single spectral function \( J(\omega) \). This is the case, for instance, when the thermodynamic limit is taken for the bath. Then the coupling to each of the harmonic oscillator \( g_k \) is not important and a global description for the interaction suffices to obtain all interesting physics. The spectral density function reads:

\[ J(\omega) = \sum_k g_k^2 \delta(\omega - \omega_k). \]  

(3.5)

All quantities involving the interaction with the bath will be composed by integrals of this function.
The problem is completely defined by the parameters $\Delta$, $\varepsilon$ and the function $J(\omega)$. However, this is untractable analytically. A lot of effort has been spent in the last two decades to find appropriate approximations that lead to reasonable physics, though maybe, in a restricted area of application, for instance, high temperatures or weak coupling strength to the heat bath. In the following chapter we will propose a simplification of this general model that ends up in an analytically tractable model for all temperatures and coupling strength to the heat bath. Further we will study how, via external perturbations, one can achieve cooling and work extraction in this setup.