

Ben-Gurion University of the Negev



*PhD Research Proposal*

דינמיקה ומעבר פאזה של מערכות דיסיפטיביות

**Dynamics and phase transition of dissipative systems**

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## תקציר

התחום של מערכות קוונטיות פתוחות עורר עניין רב בשנים האחרונות, עניין הנובע מצרכי יסוד וטכנולוגיה. מחקר בתחום זה התקדם רבות וענה על בעיות יסוד במכניקת הקוונטים כמו המעבר מקוונטי לקלאסי, בעיית הבסיס המועדף ובעיית המדידה. התובנות ממחקר זה עזרו לקדם וליישם טכנולוגיות עכשוויות כגון הקטנת טרנזיסטורים, הגדלת כח עיבוד ומימוש מחשוב קוונטי. מודל הספין-בוזון הוא אחד המודלים המרכזיים במערכות קוונטיות פתוחות המתאר את המערכת הקוונטית הקטנה ביותר (שתי רמות) שמצומדת לסביבה של אוסילטורים הרמוניים (אמבט תרמי); הסביבה גורמת למספר תופעות מעניינות כגון דה-קוהרנטיות, דיסיפציה, מעבר ממצב ממוקם למצב לא ממוקם ומעבר דינמי מאוסילציות קוהרנטיות ללא קוהרנטיות של המערכת. אחת ממטרות המחקר היא להבין את יחס הגומלין בין האינטראקציה לאמבט לבין האינטראקציה הרב גופית במערכת. לכן, ראשית נכליל את שיטת וריאצית הפולרון המדוייקת בטווח רחב של טמפרטורות ואינטראקציה בין המערכת לאמבט (עבור מודל הספין-בוזון). רוב המחקרים העכשוויים הוקדשו לתיאור מדוייק של מעבר בין מצב ממוקם ללא ממוקם כפונקציה של האינטראקציה עם האמבט, בעוד שהמחקר שלנו יתמקד בתלות בטמפרטורה; כיוון אשר קיבל פחות תשומת לב. אנו נמשיך בחקר מודל שני-ספין-בוזון כאשר בין שני הספינים יש אינטראקציה אייזינג. לבסוף, נשתמש בתוצאות שהתקבלו על מנת לחשב את הדינמיקה (כגון דיסיפציה ודה-קוהרנטיות) של מודל ספין-זכוכית שחקרנו בעבר. מודל הספין-זכוכית בנוכחות אמבט פונוני הוא מקרה פרטי של מודל  $N$ -ספין-בוזון המכיל גם אינטראקציה אייזינג דיפולרית בין הספינים; מודל זה מתאר אפקטיבית את הפיזיקה של חומרים אמורפיים ולא מסודרים בטמפרטורות נמוכות.

# Abstract

The field of open quantum systems (OQS) has been raising much interest in recent years, stemming from fundamental as well as technological purposes. Research in that field had large progress in addressing basic problems in quantum mechanics such as the quantum to classical transition, the preferred basis problem, and the measurement problem. The resulted insights helped push forward and implement cutting edge technologies e.g. scaling down and increasing the efficiency of transistors and realizing quantum computers. One of the central and well known models in OQS is the spin-boson model (SBM) which describes the smallest quantum system, i.e. two levels system (TLS), that interact with an environment of harmonic oscillators (thermal-bath). This introduces many interesting features such as decoherence, dissipation, localization-delocalization (LD) and coherent-incoherent (CI) transitions. One of this research goals is to investigate the interplay between system-environment coupling ( $\alpha$ ) and many-body interactions. Thus, first, we will generalize the variational polaron method (VP) which is accurate for a wide range of temperatures and spin-environment couplings for the SBM. Most recent efforts have been devoted to depict accurately the LD and CI transitions as a function of  $\alpha$  while our study will focus on the temperature dependence, which got less attention. Next, we continue to study the two-spin-boson model (two-SBM) for two Ising interacting spins. Ultimately, we apply our results on our previously studied TLS-glass (TG) model and explore its dynamics (decoherence and relaxation) more accurately than before. The TG model in the presence of a phonon bath is a specific case of the N-SBM with Ising dipolar interaction between the TLSs; it effectively describes the low temperature physics of amorphous and disordered solids.

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# Chapter 1

## Introduction

Every quantum system in nature ultimately interacts with its environment which leads to irreversible loss of energy and phase coherence. For the past three decades the theory of open quantum systems which depict these phenomena have had tremendous progress [1, 2, 3, 4]. One of the most studied archetypical models in this framework is the Spin-Boson model (SBM) [2, 5, 6]. The SBM describes a single tunneling two-level system (TLS) or a spin interacting with a large number of quantum harmonic oscillators which represents the environment. Realizations of the SBM, among many, are impurities in disordered materials or two-level systems in amorphous solids coupled to phonons [7, 8, 9, 10], superconducting qubits coupled to photons in transmission line or situated in a noisy environment [11, 12], atom in a cavity [13, 14] and, two impurity Kondo model [15, 2, 16]. Two of the most prominent and interesting physical aspects of the SBM are the coherent-incoherent (CI) transition and the localization-delocalization (LD) phase transition. The former represents the transition from underdamped (decay with oscillations) to overdamped (decay without oscillations) dynamics of the spin, and the latter represents the transition of the general system plus environment ground state with localized spin part to delocalized superposition. Both of the transitions are functions of temperature and system-environment coupling strength.

In this work we are interested in the dynamics of interacting spin-boson model

$$\mathcal{H} = \sum_i \left( \frac{\Delta_i}{2} \sigma_i^z + \frac{\Delta_{0i}}{2} \sigma_i^x \right) + \frac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i^z \sigma_j^z + \sum_{ik} g_{ik} \sigma_i^z (a_k^\dagger + a_k) + \sum_k \hbar \omega_k a_k^\dagger a_k \quad (1.1)$$

where  $i, j = 1, \dots, N$ ,  $\sigma^{x,z}$  are Pauli matrices which represent the spin or TLS, the boson degrees of freedom serves as the environment (heat bath) of harmonic oscillators with frequencies  $\omega_k$ ,  $a_k^\dagger$  and  $a_k$  are respectively the boson creation and annihilation operators of a given momentum  $k$ ,  $\Delta$  is the bias energy (also called asymmetry) and  $\Delta_0$  is the tunneling amplitude. The environment is characterized by the spectral function [2, 3, 4]

$$J(\omega) = \pi \sum_k |g_k|^2 \delta(\omega - \omega_k) = 2\pi \alpha \omega^s \omega_c^{1-s} \Theta(\omega_c - \omega) \Theta(\omega) \quad (1.2)$$

where  $\alpha$  is a dimensionless parameter that gives a scale for the strength of system-bath coupling,  $\omega_c$  is the cutoff frequency and  $\Theta(\omega)$  is the known step function. The spectral power,  $s$  sorts the bath into three types: sub-Ohmic ( $s < 1$ ), Ohmic ( $s = 1$ ) and super-Ohmic ( $s > 1$ ). Furthermore, the spectral function is assumed to be continuous since the bath is large and with level spacing small with respect to the system.

A relevant realization of the interacting spin-boson model are TLSs in amorphous solids, as mentioned above. An amorphous solid is a material that lacks long range order characteristic of crystalline solids giving rise to a rough low energy landscape comprising many local metastable states. Each TLS represents an atom or a group of atoms that occupy one of two localized configuration states that result from an approximated local potential in the shape of asymmetric double-well. The TLS's tunneling amplitude is given by  $\Delta_0 \sim e^\Gamma$  where  $\Gamma$  is a function of the height and width of the barrier. Given the random nature of the system,  $\Delta$  and  $\Gamma$  are assumed to be distributed uniformly, leading to the distribution [7, 8, 9]

$$P(\Delta, \Delta_0) = \frac{P_0}{\Delta_0}. \quad (1.3)$$

Furthermore, TLSs reach thermal equilibrium with a phonon bath through a linear coupling

to the local strain and also interact via acoustic and electric dipole interactions

$$J_{ij} = \frac{u_{ij}}{r_{ij}^3} \quad (1.4)$$

where  $u_{ij}$  is a random symmetric variable. Equations 1.3 and 1.4 together with the first two terms in Eq. 1.1 (for  $N \gg 1$ ) defines the TLS-glass (TG) Hamiltonian

$$H_{TG} = \sum_i \left( \frac{\Delta_i}{2} \sigma_i^z + \frac{\Delta_{0i}}{2} \sigma_i^x \right) + \frac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i^z \sigma_j^z \quad (1.5)$$

which is the effective low temperature model of amorphous solids [9, 10]. The glassy nature arises from the competition between disorder and interactions leading to a multiplicity of low-lying metastable states that are close in energy; in the low temperature regime,  $T < T_g$ , where  $T_g$  is the glass transition temperature, we get frustration, a situation in which the competition between all the interactions cannot be satisfied simultaneously in order to reach the equilibrium state. TLS-TLS interactions result in, e.g., spectral diffusion [17], delocalization of low energy pair excitations [18], and slow relaxation of dielectric and acoustic response at ultra low temperatures [19, 20] suggesting the formation of a TLS-glass. In some of our applications we will use the TG model as a system as well as a bath.

Our research generally concerns the dynamics of dissipative quantum systems and is comprised of two projects. The first deals with small tunnel junctions in an open quantum dot system (elaborated below). The second project will have two aspects (*i*) understanding the dynamical features as well as the coherent-incoherent and localization-delocalization transitions for the single and two-spin boson models, and (*ii*) using it to understand the dynamics of the TG model coupled to a phonon bath.

# Chapter 2

## Research Objectives

1. **Conductance of resonant level coupled to dissipative leads:** Recently it has been shown that the conductance peak of a quantum dot (resonant level) coupled to two dissipative leads reaches a full transmission for a symmetric coupling, and the resonance width scales as  $T^{r/(1+r)}$  where  $r$  is the dimensionless resistance of the two leads [34]. This conductance characteristic was also measured in Luttinger liquid Tunnel junction [35]. Using this correspondence between the two systems the resonant conductance of the quantum dot have been explained by mapping the dissipative leads to two Luttinger liquids, each with its own interaction parameter [36]. However, it seems that the bosonization procedure (mapping) can be applied on a 3D electron gas only under specific conditions which were not addressed. In order to understand better the nature of the measured conductance we plan to derive it directly from the original model.
2. **Generalised-polaron-ansatz (GPA) for finite temperatures:** The polaron ansatz is based on a unitary transformation done on the wave function of the entire spin-boson system and gives the ability to investigate the SBM in a much broader regime of the spin-bath coupling strength ( $\alpha$ ) than the perturbative Redfield and the full-polaron

master equations. As was previously shown [21, 22, 23], choosing the transformation correctly, based on physical arguments, reproduces accurately the LD quantum phase transition of the SBM deep inside the intermediate regime of the system-bath coupling at zero temperature. We would like to extend method to finite temperatures in order to investigate the CI and LD transitions as a function of temperature as well.

3. **Localization-delocalization and coherent to incoherent transition for the two-SBM:** Using our results found in objective (1) we extend the analysis for the two-SBM exploring the CI and LD transition as a function of temperature and using interaction between the two spins. Also, given the addition of the spin-spin interaction we can explore the possibility of finding new decoherence free subspaces of several initial state preparations and initial non zero correlations between the system and the bath, which might not occur in the single spin case.
4. **Dephasing of a TLS in TLS-glass environment:** Previous work [24] had much success in explaining the free induction signal and spin echo experiments done in NMR (Nuclear magnetic resonance), and phonon echo experiments in amorphous solids. The dephasing mechanism of the tagged spin/TLS was modeled as a classical fluctuating noise resulting from a spin/TLS bath. We are interested in including interaction between the bath TLSs and add explicitly the interaction of each bath TLS with a bath of phonons (which is the source of the flipping of the bath TLSs). First, we expect to find a regime where the inter-TLS interactions affect the dephasing of the tagged TLS. Second, by treating the TLS bath as quantum noise we can find under what circumstances classical noise can be assumed.
5. **Temperature dependence of the TLS-glass relaxation:** It is found in experiment that at low temperatures  $T < 1K$  the relaxation of non-adiabatic dielectric response of amorphous solids is temperature independent [25]. Our preliminary results (see

Sec 3) show the same behaviour under several simplifying approximations such as (i) postulating the response of the system can be expanded in spin occupations (ii) mean-field approximation, (iii) static density of states, i.e. the DOS approximately does not change from the external field and thus does not depend on time, (iv) the system is close to equilibrium (expanding to linear order in the deviation from equilibrium value). We would like to see if the temperature independence of the relaxation persist without these approximations using the master equation (ME) formalism to define and calculate accurately the response function.

## 2.1 Related work

### 2.1.1 The conductance of resonant level coupled to dissipative leads

A tunnel junction (TJ), in its simplest form, is a thin insulating layer (barrier) between two conducting materials; because of its small size, its charging energy ( $E_C = Q^2/2C$  where  $Q$  is the total charge in the junction and  $C$  is its capacitance) is large compared to the thermal energy and tunneling amplitude, giving rise to Coulomb blockade, a state where electrons can't tunnel through the barrier because of the Coulomb repulsion. In that regime Ohm's law of conductance is replaced by a staircase pattern [26, 27]. The small size of the TJ is also responsible for the high sensitivity to charge noise (caused by the coupling of the leads to electromagnetic (EM) environment) which results in a smearing of the staircase pattern and to a power law behaviour at low bias voltage ( $V$ ),  $G = dI/dV \propto \max(k_B T, eV)^{2r}$  [28, 29, 30, 31], where  $k_B$  is Boltzmann constant,  $T$  is the temperature,  $e$  is the electron charge and the power  $r = e^2 R/h$  is the dimensionless resistance of the junction and is dependent on the coupling to the EM environment. A similar power law is also seen in Luttinger liquid (LL) TJ [32, 33], where the power is proportional to the interaction between the electrons.

Recently, the analogy between these two different systems has been further extended to the case of resonant level (quantum dot) coupled to a dissipative leads with the same resistance  $r$ , where the conductance peak saturates at  $e^2/h$  for symmetric coupling and its resonance width scales as  $T^{r/(r+1)}$  at low temperatures [34, 35]. Using the correspondence to LL TJ the aforementioned conductance behaviour was explained by mapping the free electrons in the leads into an effective model which consists a resonant level coupled to two different LL's [36]. Yet, given the leads 3D structure and high resistance, it seems that the mapping to a LL by the conventional prescription, i.e. bosonization of electrons in 1D, generally can not be done. This implies that the current approach might not depict accurately the experimental system. In order to understand the microscopic origin of the conductance, it will be useful to use a direct approach applying nonperturbative methods on the original model.

### 2.1.2 Generalised-polaron-ansatzs (GPAs) for finite temperatures

The variational polaron ansatz method, developed by Silbey and Harris (SH) [37], opened a new avenue for analytical study of the spin boson model; it has seen much success in treating the SBM in a wide regime of the system-bath coupling which could not be treated by the perturbative Redfield equation or accurately enough in the full polaron master equation. SH method is comprised of two steps, first rotating the Hamiltonian (Eq. 1.1 for  $J = 0$ ) using a "partial" (not full) polaron transformation

$$U = \exp \left[ \sum_{ik} \frac{f_{ik}}{2\omega_k} (a_k^\dagger - a_{-k}) \sigma_{iz} \right]. \quad (2.1)$$

This unitary transformation displaces the harmonic-oscillator (HO) with momentum  $k$  by an amount proportional to  $f_{ik}$  (which depends on  $g_{ik}$ , see Eq.1.1); the full polaron transformation is then defined for  $f_{ik} = g_{ik}$ . The second step is calculating the Feynman-Bogoliubov free-energy upper-bound [38, 39] and minimize it with respect to  $f_{ik}$ . SH approach loses its accuracy for Ohmic and sub-Ohmic baths ( $0 < s \leq 1$ ) in the intermediate coupling regime

where the localization-delocalisation phase transition takes place [40, 41]. Thus, several new ansatzs have been done that generalize Eq.2.1 in order to capture accurately the phase transition and the spin dynamics in this coupling regime, at zero and finite (but low) temperatures [22, 21, 42, 43]. These ansatzs explained the breakdown of SH approach around the critical value ( $\alpha_c$ ) and are used as an analytic framework to compare and understand the results obtained by numerical approaches [5, 44, 23]. It is then left to study how the CI and LD transitions depends on temperature, which is not covered by aforementioned methods.

### **2.1.3 Localization-delocalization and coherent-incoherent transition for the two-SBM**

The two-SBM model is a natural generalization of the single-SBM which incorporates two-body interactions in presence of dissipative environment. The addition of bath-induced or direct spin-spin interactions that competes with the spin-bath coupling can lead to a different behaviour than obtained for the single spin case. For example, it has been shown that the presence of Ising interactions effectively acts as a bias in the frame of each spin which smooths the LD transition and shifts the cratical point ( $\alpha_c$ ) to lower values [45, 46], yet, intriguingly  $\alpha_c$  reaches a minimal value at a finite separation between the spins and retain this value for smaller separations (i.e. stronger interaction values) [45]. Also, it is found that the entanglement between the spins can be destroyed or generated by the bath, and the entanglement between the spins and the bath depend strongly on the initial preparation of the two-spin system [46, 47, 48].

### **2.1.4 Dephasing of a spin in spin-glass environment**

The seminal work of Klauder and Anderson [24] had much success in explaining the observed decay of an electron spin precession. They modeled the noise surce as thermal nuclear spins of the underlying material which are coupled to the tagged spin via dipolar interaction

[49, 50, 51]; one of the main results obtained is the Lorentzian spectral diffusion kernel rather than the speculated Gaussian shape. Using this mechanism Black and Halperin implemented a similar treatment for TLSs in amorphous solids [52] to explain the phonon echos measured in experiments. In this case the tagged TLS also has a dipole interaction with thermal TLSs, although phonon mediated. In both cases the tunneling amplitude of the tagged TLS is neglected and, more importantly, also are the interactions among the TLSs of the bath; these interactions are known to give a logarithmic gap in the single particle density of states of the TG model [53, 54, 55, 56] and might affect the dephasing of the tagged TLS. Furthermore, introducing the interaction among the bath TLSs might break (possibly in a narrow window of parameters) the approximation of classical noise. The comparison between quantum and classical noise was already addressed on a simpler model which showed that in some cases the coherence persists over longer time scales for quantum noise [57].

### 2.1.5 Temperature dependence of the TLS-glass relaxation

The effective dipolar interactions in amorphous solids have been found to be small in comparison to other energy scales of the system, in fact, given the energy density of non-interacting TLSs,  $P_0$ , and the typical interaction between TLSs,  $U_0$ , it is found that the dimensionless parameter  $\chi = P_0 U_0$  has a small almost constant value in all known amorphous materials. By using the dielectric response derived from the classical Bloch equations [58], Burin calculated a contribution to the dielectric relaxation (to first order in  $\chi$ ) that results from the time dependence of the dipole gap (nonadiabatic TLSs) [55]:

$$\delta\epsilon(\omega) = \frac{4\pi}{9} \chi (P_0 p_0^2) \log(\phi/T) \log(\alpha T^2 \phi/\omega) \log(\tau_{max}/t) \quad (2.2)$$

where  $k_B = 1$ ,  $T$  is the temperature,  $\phi = -p_0 E_{DC}$  is the energy of the dipole of the TLS,  $p_0$ , subjected to external AC field,  $E_{AC}$ , with frequency  $\omega$ ,  $\alpha = 10^8 K^{-3} s^{-1}$  and  $\tau_{max} \simeq 1/\alpha \Delta_{0min}^2 T$  is the approximate maximum relaxation time of a TLS due to phonons (given the lowest tunneling energy of the TLSs,  $\Delta_{0min}$ ). Eq.2.2 found to be in a good agreement with

experiment [59]. However, it is found also that the relaxation is temperature independent [25], where clearly Eq.2.2 is temperature dependent. More recent study [60] have shown a temperature independent relaxation for various glasses which seems to agree well with experiments, yet, they use rather general considerations. Thus, it would be interesting to derive the relaxation specifically for the TG model (see Eq. 1.5).

## 2.2 Significance of the Research

Understanding decoherence and the coherent to incoherent transition of a single quantum bit/TLS (qubit) subject to noise is of great importance for quantum computation and memory applications. The decoherence time sets the upper limit for computation; when exceeded the information stored in the phase of the qubit is irreversibly lost to the environment. Furthermore, just as classical processors are built from numerous bits also several qubits are usually used to build a quantum processor, which sets the stage for an effective qubit-qubit interactions resulting from, for example, common bath or noise source. Our research on the one and two spin boson model is set to obtain accurate analytical results in wide regime of qubit couplings and temperature. This might contribute to the long time effort of understanding and preventing qubit information loss in order to increase the computation time of quantum computers. The second part of the study concerns the TG model. Since the TG is a universal model that effectively describes all of the amorphous and disordered solids in nature (at low temperatures) it is of great fundamental importance to explore its physical behavior. Particularly, since the relaxation time scale of TG system is much larger than the typical time of the experiment, it is relevant to explore non-equilibrium features such as relaxation as proposed in one of our research objectives.

## 2.3 Research Methodology

### 2.3.1 Polaron Master-equation

The Time-convolutionless master-equation (TCL-ME) gives a unified and systematic framework for the dynamics of the reduced density matrix [61, 62, 63, 64]. To obtain the dynamics of the reduced dynamics one starts from the equation of motion for the state of the entire system; therefore, the Liouville von-Neumann equation in the interaction picture is:

$$\frac{d\rho(t)}{dt} = -i\alpha [V, \rho(t)] = \alpha \mathcal{L}(t)\rho(t), \quad (2.3)$$

given the Hamiltonian

$$\mathcal{H} = H_S + H_B + \alpha V = H_0 + \alpha V \quad (2.4)$$

where  $H_0 = H_S + H_B$  is assumed to have a known solution and is composed of the system and bath Hamiltonians respectively,  $V$  is the interaction between the system and the bath,  $\alpha$  is dimensionless parameter and  $\mathcal{L}(t)$  is called the Liouvillian operator. The dynamics of the relevant part of the Hilbert space is then obtained using the projection superoperator technique [64, 3],

$$\frac{d\mathcal{P}\rho(t)}{dt} = K(t)\mathcal{P}\rho(t) + I(t)\mathcal{Q}\rho(t_0) \quad (2.5)$$

where  $\rho(t)$  is the density matrix of the total system-bath in the interaction picture,  $\mathcal{P}\rho(t)$  is the relevant Hilbert subspace and  $t_0$  is the initial time. The TCL generator and the Inhomogeneous term presented in Eq.2.5 are defined as

$$\begin{aligned} K(t) &= \alpha \mathcal{P}\mathcal{L}(t) [1 - \Sigma(t)]^{-1} \mathcal{P}, \\ I(t) &= \alpha \mathcal{P}\mathcal{L}(t) [1 - \Sigma(t)]^{-1} \mathcal{G}(t, t_0) \mathcal{Q} \end{aligned} \quad (2.6)$$

given

$$\Sigma(t) = \alpha \int_{t_0}^t d\tau \mathcal{G}(t, \tau) \mathcal{Q}\mathcal{L}(\tau) \mathcal{P}\mathcal{G}(t, \tau), \quad (2.7)$$

where the forward and backward propagators are respectively

$$\begin{aligned} \mathcal{G}(t, t_0) &= T_{\rightarrow} \exp \left\{ \alpha \int_{t_0}^t \mathcal{Q}\mathcal{L}(t') dt' \right\}, \\ \mathcal{G}(t, t_0) &= T_{\leftarrow} \exp \left\{ -\alpha \int_{t_0}^t \mathcal{Q}\mathcal{L}(t') dt' \right\}, \end{aligned} \tag{2.8}$$

where  $\mathcal{Q} \equiv \mathcal{I} - \mathcal{P}$ ,  $\mathcal{I}$  is the unit superoperator and  $I(t)$  accounts for a correlation between the system and the bath at  $t = t_0$ . Generally, Eq.2.5 does not contain an integral over the history of the system which is much easier to handle analytically than other master equations that contain it, such as Nakajima-Zwanzig (NZ) equation [65, 66]. Nevertheless, the TCL and NZ have the same assumptions and approximations thus expected to have the same accuracy even when dealing with non-markovian dynamics, atleast in the weak system-bath coupling regime [3]. In some cases TCL might be even more accurate than NZ [67, 68, 69].

The exact calculation of the TCL master equation is as complicated as solving the Liouville von-Neumann equation, therefore one may resort to perturbation expansion of  $K(t)$  and  $I(t)$  in terms of  $\alpha$ . After substituting  $[1 - \Sigma(t)]^{-1} = \sum_{n=0}^{\infty} [\Sigma(t)]^n$  in Eq.2.6 and then expanding  $\mathcal{G}(t, t_0)$  and  $\mathcal{G}(t, t_0)$  in powers of  $\alpha$  one obtains:

$$\begin{aligned} K(t) &= \alpha \sum_{n=0}^{\infty} \mathcal{P}\mathcal{L}(t)[\Sigma(t)]^n \mathcal{P} = \sum_{n=1}^{\infty} \alpha^n K_n(t), \\ I(t) &= \sum_{n=1}^{\infty} \alpha^n I_n(t). \end{aligned} \tag{2.9}$$

Usually it is assumed that the bath average of odd moments of the interaction Hamiltonian vanish which gives only even powers of  $\alpha$ .

The TCL is considered a general Master-equation and thus a good starting point when deriving the dynamics for a new model system. In fact the Born-Markov ME is a special case of the TCL [3]; in order to obtain it, several approximations are in order: (i) choose projection operator in the form of  $\mathcal{P}\rho = \text{Tr}_B\{\rho\} \otimes \rho_B = \rho_S \otimes \rho_B$ , where  $\rho_S$  and  $\rho_B$  are the system and bath density operators, (ii) the system is prepared in an uncorrelated state:

$\rho(0) = \rho_s(0) \otimes \rho_B(0)$  (i.e.  $I(t) = 0$ ), (iii) the Markov approximation, (iv) expand  $K(t)$  up to 2nd order in  $\alpha$ . Also, the Lindblad positive form can be obtained by further making the secular approximation.

Even though the TCL approach reduces the number of approximations to just two (the Born approximation and weak coupling), as opposed to the perturbative Lindblad ME, there are many situations where they do not apply. For that reason we use the generalised polaron method that allow us to investigate the dynamics of the system in the region of intermediate to strong interactions.

The generalised polaron method is based on the principle that the bath oscillators are displaced as a result of their interaction with the system by an amount dictated by the transformation's free parameters (FP). The new interaction terms of the transformed Hamiltonian is then minimized by choosing the FP according to a given procedure; this results in a new system-bath interaction Hamiltonian which then can be treated as perturbation for a wide range of the coupling strengths in the original frame. Two known procedures are: (i) fluctuation-decoupling: the FP are found through the requirement that the average of the new interaction term vanishes [21, 42]. (ii) variation of the free energy or ground state energy with respect to the FP [37, 22, 23].

In this study we will use a generalised polaron method similar in nature to what presented in Refs. [21, 22]. Also, since procedure (i) is good only for low temperatures the FP will be determined by the minimisation of the free energy according to Silbey and Harris prescription [37], which allow an accurate treatment of the model also in finite temperatures.

### 2.3.2 Pauli Master-equation and the mean-field approximation

The combination of the Pauli ME with the mean-field approximation allow us to study relaxation and other dynamical features of the bulk material such as the  $N$ -SBM given in Eq.1.1 (and in our case the TG model coupled to a phonon bath). The method is based on

previous work done on the Electron-glass model [70] and the TLS-glass model [56]. Starting from the TLS-glass model we obtain the mean-field (MF) equations for the bias energy by variational derivative with respect to  $\sigma_z$ . The obtained self-consistent equations (SCE) are:

$$\Delta'_i = \Delta_i + \frac{1}{4} \sum_{j \neq i} \frac{u_{ij}}{r_{ij}^3} \tanh\left(\frac{\Delta'_j}{2T}\right) \quad (2.10)$$

where we set the Boltzmann constant to unity, reassign  $\Delta'_i = \langle \Delta'_i \rangle_T$  as the thermal average of the bias, and use  $\langle S_i^z \rangle_T = \frac{1}{2} \langle \sigma_i^z \rangle_T = -\frac{1}{2} \tanh\left(\frac{1}{2} \beta \Delta'_i\right)$ . The single TLS shifted Hamiltonian is then:

$$\mathcal{H}'_{TLS} = \sum_i (\Delta'_i S_i^z + \Delta_{0i} S_i^x) \quad (2.11)$$

and the equilibrium excitation energy of the  $i$ 'th TLS is:

$$E_i = \text{sgn}(\Delta'_i) \sqrt{\Delta_i'^2 + \Delta_{0i}^2} \quad (2.12)$$

Unlike the distribution given in the Standard-tunneling-model [7, 8],  $p(\Delta, \Delta_0) = \frac{P_0}{\Delta_0}$ , which is uniform in the asymmetry energies, we choose

$$p(\Delta, \Delta_0) = \frac{P_0}{\Delta_0} \frac{1}{\sqrt{2\pi W^2}} \exp\left(-\frac{1}{2} \frac{\Delta^2}{W^2}\right). \quad (2.13)$$

This choice eventually does not affect the qualitative physical outcome. However, it allows us to look at the effect of changing disorder.

The dynamics of the average occupation of state  $i$  at time  $t$  ( $p_i(t)$ ) is generally described by the Pauli ME. Given the transitions are allowed between states of the same TLS the Master equation reduces into two coupled rate equations of the occupations of the  $i$ 'th TLS. Using probability conservation in each TLS separately,  $p_1(t) + p_2(t) = 1$ , one can represent the rate equation in the pseudospin form by substituting  $\sigma_i = \langle \sigma_i^z \rangle = p_2^i - p_1^i$ :

$$\frac{d\sigma_i}{dt} = -2a_i \Delta_{0i}^2 E_i \left[ \sigma_i \left( N_i + \frac{1}{2} \right) + \frac{1}{2} \right] = -\lambda_i \sigma_i - a_i \Delta_{0i}^2 E_i \quad (2.14)$$

given the TLS-phonon relaxation rate in equilibrium [71, 9]

$$\lambda_i = -(\omega_-^i + \omega_+^i) = -a_i \Delta_{0i}^2 E_i \coth\left(\frac{E_i}{2T}\right). \quad (2.15)$$

where  $\omega_+^i$  and  $\omega_-^i$  are respectively the TLS upward and downward transition rates caused by the TLS interaction with the phonon bath (Fermi's golden rule [71, 9]),  $\sum_i \sum_k g_{ik} (a_{-k}^\dagger + a_k) S_i^x$ ,  $k$  represents phonon with momentum vector  $\mathbf{q}$  and polarization  $s$ , and  $g_{ik}$  is coupling constant which is proportional to the deformation potential constant.

For TLS occupations slightly out of equilibrium ( $\delta\sigma_i \equiv \sigma_i - \sigma_i^0 \ll 1$ ) we can expand the right-hand side of Eq. (2.14) to first order in  $\delta\sigma_i$  around the local equilibrium point. Neglecting a subdominant interaction term [56] we obtain

$$\frac{d\delta\sigma_i}{dt} \simeq -\lambda_i \delta\sigma_i. \quad (2.16)$$

Eq. 2.16 has a simple solution:

$$\delta\sigma_i(t) = c_i e^{-\lambda_i t} \quad (2.17)$$

where  $c_i \equiv \delta\sigma_i(0)$  is the initial deviation of TLS  $i$  at the moment the external strain driving force has stopped. To quantify the total relaxation of the system one can take the norm of the vector  $\delta\boldsymbol{\sigma}$  [70]:

$$|\delta\boldsymbol{\sigma}| = \sum_i c_i e^{-\lambda_i t} \quad (2.18)$$

and in the continuous limit,

$$|\delta\boldsymbol{\sigma}| \simeq c \int_{\lambda_{min}}^{\lambda_{max}} p(\lambda) e^{-\lambda t} d\lambda \simeq -c [\gamma_E + \log(\lambda_{min} t)], \quad (2.19)$$

where a uniform distribution of initial excitations  $c(\lambda) = c$  is assumed [70], we use  $\frac{1}{|\lambda|}$  rate distribution which is calculated numerically [56],  $\gamma_E$  is the Euler constant and the integral is approximated for  $1/\lambda_{max} < t < 1/\lambda_{min}$ . As can be seen, the right-hand side depends on the energy, i.e.  $\lambda_{min}(E_i)$ , which in turn depends on the interactions, disorder and out-of-equilibrium occupations of all the TLSs in the system, i.e.,  $E_i(\boldsymbol{\sigma}')$  where  $\boldsymbol{\sigma}'$  denotes all the elements of the pseudospin vector except the  $i$ th element. The linear response of the material (for example the time dependent dielectric response) is then approximately obtained by expanding it to linear order in  $|\delta\boldsymbol{\sigma}|$  [70].

# Chapter 3

## Preliminary Results

Our preliminary results are on the temperature dependence of TG relaxation. The TG DOS (Fig 3.1) and the rates distribution (Fig 3.2) were calculated using the method presented in Sec 2.3.2, for different temperatures. The calculation goes as follows: first we numerically solve the self-consistent equations (Eq. 2.10), then we use it to find the rate distribution according to equation 2.15. The lowest value of the plateau region in the rate distribution is then defined as the minimum rate (see Eq. 2.19). As can be seen, the gap in the DOS disappears gradually while the rate distribution plateau region does not shift as the temperature increases. This indicates that the system relaxation is temperature independent as been shown also in experiment [25]. It seems that this phenomenon comes from two opposing effects; as evident from Eq.2.15, the rate depends directly on the temperature and also indirectly through the mean-field energies; for increasing temperatures the direct dependence shifts the rates to higher absolute values while the energies (and thus the rates) are shifted to lower values as the gap in the DOS closes.

Given the approximations done in this approach (see Ch. 2) it would be interesting to see if the temperature independence persist for more accurate calculation. This can be done by defining the dielectric response for a TLS pair using the results we will obtain for

the two-SBM, then averaging over all possible pairs in order to get the bulk response.

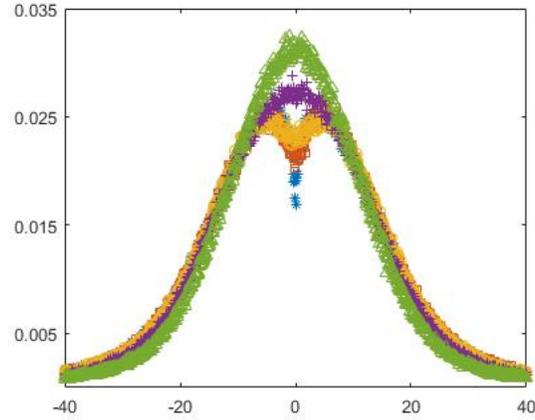
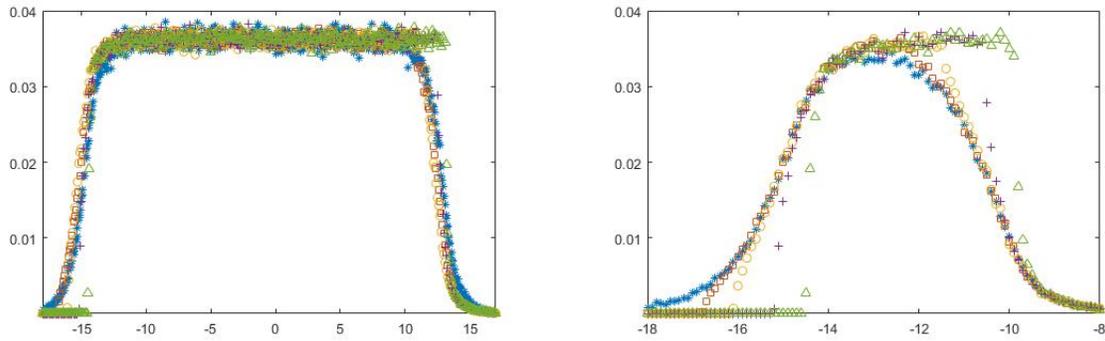


Figure 3.1: Density of States for  $T=0.1, 1, 2, 5, 10$ ,  $W=10$  and  $J=1$ .



(a)

(b)

Figure 3.2: Log scale of the the TLS rate distribution for  $T=0.1, 1, 2, 5, 10$ ,  $W=10$  and  $J=1$ .

(a) All the tunnelling amplitudes  $\Delta_0 \in [10^{-7}, 10^{-1}]$ . (b) Low tunnelling amplitudes  $\Delta_0 \in [10^{-7}, 10^{-6}]$ . The cutoff (defining  $\lambda_{min}$  in Eq. 2.19) is taken to be in the peak region on sub figure b.

### 3.1 Future Directions

Having set the stage for accurate treatment of the one and two-SBM in a wide range of parameters, the next step would be to take into account the effects of a non-equilibrium bath. Glassy systems are natural candidates for the exploration of this phenomena since they are known to have slow relaxation which can extend to time scales much longer than the typical duration of the experiment. Previous work done on this subject shows that an initial non-equilibrium preparation of the bath may cause suppression or enhancement of the spin oscillation dynamics depending on the temperature and system-bath coupling [72, 73] and also saturation of spin relaxation rates for large tunneling amplitudes in the strong system-bath coupling regime [74]. Under the framework of the TCL-ME we can investigate how the single TLS dynamics is affected by the slow relaxation of a TLS-glass bath by starting from a correlated initial state of the entire system i.e. a given inhomogeneity ( $I(t)$ , see Eq.2.6) representing some experimental initial setup done on the system.

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