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Le Modèle Spin-Boson: Décohérence, Localisation et Frustration Quantique

Résumé: Le Modèle Spin-Boson est traditionnellement un paradigme pour décrire la décohérence d'un bit quantique (qubit) exposé à une interaction avec l'environnement. Dans ce rapport on examine ses propriétés de bases et on applique un méthode diagrammatique originale basée sur les Fermions de Majorana, qui offre fiabilité à faible dissipation et facilite de mise en oeuvre par rapport aux méthodes traditionnelles. En appliquant l'analyse du groupe de renormalisation dans la méthode on retrouve les phases du modèle à température nulle. La transition de phase quantique du deuxième ordre entre l'état delocalisé et localisé est aussi capturé. Enfin on propose l'application de la méthode pour une variation du modèle avec deux environnements qui montre un phénomène dit de "frustration quantique".

Mots clés: Spin-Boson, Décohérence, Qubit, Dissipation Quantique, Frustration Quantique, Transition de Phase Quantique.

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The Spin-Boson Model: Decoherence, Localization and Quantum Frustration

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Introduction

Classical systems are described as a collections of physically measureable quantities whose value is well-defined at any stage of the evolution of the system by deterministic laws. Differently, in quantum theory the variables of the systems are not directly associated to definite observable values and at some stage it is necessary to introduce postulates (*wavefunction collapse*) in order to predict the possible outcomes of an experiment with their respective probability. Despite this artificial theoretical shortcut present in the application of the theory, the predictive power of quantum mechanics is not questionable, so until recently the advancements on this part of the theory has been mainly pursued for philosophical sake.

During the last 20 years technology allowed us to manipulate individual microscopic objects like atoms or single electrons with sufficient control to start exploring with precision the phenomenology of direct measurement of quantum evolving systems. The question on the interpretation of the measurement problem and the detailed description of the measurement operation is now an interest of the "applied physics" community, thanks mainly to the opportunity to exploit the quantum evolution for doing *quantum computation*.

At the time of writing the interpretation of wavefunction collapse is still an unsolved fundamental issue, but the treatment of measurement problem from the 'applied point of view' has a convincing theoretical framework, often evoked as the theory of *quantum decoherence*.

In this approach the observed system is seen as part of a larger system including the environment. The Hamiltonian of the total system provides a coupling between the a-priori factorized two Hilbert spaces of the system and the environment, so that quantum evolution usually determines *entanglement* of the subsystem's with the environment states. The environment is always "collapsed" (somewhen) so that the time evolution irreversibly breaks the purity of the subsystem state: the object becomes more and more classical.

In this approach, a key problem is then characterizing the environment and its full influence on the subsystem. For this reason it is of great interest to study at best models in which an *impurity* (i.e. a small system, for example a qubit, or a spin) is interacting somehow with a *bath* with many (maybe infinite and continuously dense) degrees of freedom. Due to the many-body nature of the interaction, understanding the ground state, the (equilibrium or non-equilibrium) dynamics or the relevant effects involving the subsystem it is often a formidable task, which requires advanced theoretical tools of Quantum Field theory as well as a phenomenological thinking as a guide.

In this research project we started to tackle an important model of decoherence named the *spin-boson* model (SB) with a technique valid at zero and finite temperature and at equilibrium, but easily extendible to non-equilibrium situation. In Section 1 the SB model and its phenomenology is presented. The diagrammatic technique employed for tackling the problem is introduced in Section 2. Weak coupling results for relevant quantities are introduced in that section. Section 3 presents the RG analysis of the model and the results concerning the quantum phase transitions in the SB model. Finally Section 4 concludes the report with a simple application of the diagrammatic theory to a recent extension to the SB model which exhibits a strong correlation effect of "frustration".

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1 The Spin-Boson Model

In technological application such as quantum computation we are mainly interested in two-level quantum systems, which are usually referred as *qubits*. The SB model describes a qubit coupled linearly to a continuum of bosonic modes. The actual importance of the model in practical systems can be quite general, since many fundamental environments with delocalized modes at low energy can be effectively described by a bath of harmonic oscillators. Typical applications involve Luttiger-liquid environments, magnons in spin-baths, phonons or photons baths. Moreover, since the model is an effective one valid a low energy, the central subsystem can be complicated at high energy; for example a "giant spin" or a particle tunneling in a doublewell potential or something else that can be reduced to a two-level system for the low energy description.

In practice, the SB model is used also as a microscopic phenomenological paradigm of the influence of noise in nanocircuits involving manipulation of qubits, where the observed (Gaussian) voltage fluctuations and the resulting decoherence are interpreted by the coupling of the two-level system with a properly-constructed bosonic bath. An example of this kind of applications are the Josephson junction qubits, where the pseudospin is represented the number of cooper pairs in a superconducting island, and the noise is provided by the voltage fluctuations at the tunnel junctions [1, 5].

We finally note that independently from the applications, the model is fundamentally interesting since despite its non-triviality it is one of the simplest completely non-classical model incorporating dissipation: it is thus important to fully understand its properties to interpret all open quantum systems.

1.1Definition of the model and notations

The Hamiltonian of the model reads:

$$H = \frac{\Delta}{2}\sigma_z + \frac{\lambda}{2}\sigma_x \sum_k \left(a_k + a_k^{\dagger}\right) + \sum_k \omega_k a_k^{\dagger} a_k \tag{1}$$

where σ_i are the Pauli matrices and refers to the Hilbert space of the two-level system, Δ is the magnetic field (or "tunnel splitting") of the model, λ the spin-bath coupling and ω_k are the energies of canonical boson modes represented by the creation/destruction operators a_k and a_k^{\dagger} (the commutation rule $\left|a_k^{\dagger}, a_{k'}\right| = \delta_{kk'}$ hold) [1, 2, 3].

Note that the ω_k may include k-dependent spin-bath coupling after a redefinition of the bosonic operators, so the bosonic energy distribution in k-space (or equivalently the density of states $\rho(\omega)$ in energy space) and the spin-bath coupling are sufficient to characterize completely the model.

 $\rho(\omega)$ may have a rich structure in principle, but it is quite general to assume that at sufficient low energy should go to zero with a power-law behavior. We will then assume that all high-energy properties of the model have been integrated out in the parameters λ , Δ and that we can consider a maximal (*cutoff*) energy Λ . In this situation, the resulting density of states is parametrized as:

$$\rho(\omega) = \sum_{k} \delta\left(\omega - \omega_{k}\right) = \frac{(s+1)}{\Lambda^{s+1}} \omega^{s} \Theta(\Lambda - \omega) \Theta(\omega)$$
(2)

Where $\Theta(x)$ is the Heaviside step function (in case it be replaced by another smooth cutoff function like an exponential function for example) and s is the exponent that dictates the distribution of the energies of the model (see figure 1).

For s < 1, the model is said to be *subohmic*, for s = 1 the model is *ohmic* while for s > 1 the model is superohmic.

The normalization is such that $\int_0^{+\infty} \rho(\omega) d\omega = 1$. It is convenient to define a new non-canonical bosonic field, corresponding to the the "displacement operator" coupled to the spin:

$$\phi = \sum_{k} \left(a_k + a_k^{\dagger} \right)$$

The density of states of this boson, odd in energy, is then:

$$\rho_{\phi}(\omega) = -\frac{s+1}{\Lambda^{s+1}} \left|\omega\right|^{s} \operatorname{sign}(\omega)\Theta(\Lambda^{2} - \omega^{2})$$
(3)

In order to provide a link with the existing literature, we note that it is usual to characterize the model by multiplying the density of states by the coupling, defining the *spectral function*:

$$J(\omega) = \pi \lambda^2 \sum_k \delta(\omega - \omega_k) = 2\pi \alpha \Lambda^{1-s} \omega^s \Theta(\Lambda - \omega) \Theta(\omega)$$

The chosen parametrization defines α as an adimensional constant $(\alpha = (s+1)\frac{\lambda^2}{\Lambda^2})$ which is interpreted as the *dissipation* strength.



Figure 1: density of states of canonical bosons for the subohmic, ohmic and superohmic case. The cutoff is taken as $\Lambda = 1.0$

1.2 Decoherence in the Spin-Boson Model

Spin- $\frac{1}{2}$ systems are "natural" qubits, and it is common to expand the Hamiltonian acting on a qubit in terms of the complete basis of *Pauli matrices* σ_x , σ_y , σ_z (plus the identity), the generators of the SU(2) algebra.

In our notations of the SB model the $|0\rangle$ and $|1\rangle$ states which are relevant for quantum computing are taken to be the eigenvectors of σ_z . The problem of the coherent manipulation of the single qubit is thus found in the ability of creating and preserving quantum superposition of the type $|\phi\rangle = a |0\rangle + b |1\rangle$.

An important question could be: given the state $|\Psi\rangle = |\phi\rangle \otimes |\psi_B\rangle$ at t=0, being $|\phi\rangle$ eigenvector of the operator σ_x ($|\phi\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$) with non degenerate eigenvalue ±1: what is the expectation value of σ_x at time t? In the Heisenberg Picture, and at zero temperature:

$$P(t) = \langle \Psi | \sigma_x(t) | \Psi \rangle \tag{4}$$

A related question is: what is the equilibrium expectation value of σ_x in the same situation supposing that the environment was already at equilibrium with the system in the state $|\phi\rangle$ at t = 0? This value will noted C(t), and it is a stationary, equilibrium property of the total system. Formally it is calculated as P(t), but projecting the initial state $|\Psi\rangle$ in the subspace where $\sigma_x |\Psi\rangle = \pm |\Psi\rangle$ (see later equation (5)).

In direct modeling of quantum manipulation of a qubit, P(t) seems to be the most important quantity, since we usually assume to have total control of the system at t=0 and to be able to prepare it in the state $|\phi\rangle$. But if the preparation time is negligible and the bath relaxes sufficiently fast with respect to the typical times of the subsystem's dynamics, C(t) should be equivalent to P(t).

1.2.1 Properties of the equilibrium correlation function

Noting $\mathcal{P} = \sigma_x \pm 1$ the projector into the subspace where the spin is in a given eigenstate of σ_x :

$$C(t) = \frac{1}{2} \langle \Psi | \mathcal{P}\sigma_x(t)\mathcal{P} | \Psi \rangle = \frac{1}{2} \left(\langle \sigma_x(t) \rangle \pm \langle \sigma_x \sigma_x(t) \rangle \pm \langle \sigma_x(t) \sigma_x \rangle + \langle \sigma_x \sigma_x(t) \sigma_x \rangle \right)$$

The first and the last term are zero due to the symmetry $(\sigma_x \to -\sigma_x, a_k \to -a_k, a_k^{\dagger} \to -a_k^{\dagger})$ of the Hamiltonian so we find that C(t) is the equilibrium symmetrized correlation function:

$$C(t) = \pm \frac{1}{2} \left\langle \left\{ \sigma_x, \ \sigma_x(t) \right\} \right\rangle \tag{5}$$

Given a perturbation to the spin-boson Hamiltonian of the form $\delta H(t) = \sigma_x f(t)$, the Kubo's formula holds:

$$\delta \langle \sigma_x(t) \rangle = \frac{i}{\hbar} \int_0^t dt' \left\langle \left[\sigma_x(t), \ \sigma_x(t') \right] \right\rangle f(t) = \int_{-\infty}^{+\infty} dt' \chi(t-t') f(t)$$

 $\chi(t)$ is called the *dynamical transverse spin-susceptibility* and it imaginary part $\chi''(\omega)$ has a relation with the energy change (dissipation) of the system due to the perturbation. Physically speaking, in our problem the "perturbations" on σ_x are induced by the spin-bath interaction term of the Hamiltonian, so the susceptibility is also related to the energy dissipated into the environment.

Indeed, the following *fluctuation-dissipation* relations are valid and useful (ω is the conjugate variable of t after Fourier transform) [3, 2]:

$$\chi^{''}(\omega) = \frac{1}{2\hbar} \left(1 - e^{-\omega\hbar\beta} \right) \int_{-\infty}^{+\infty} e^{i\omega t} \left\langle \sigma_x(t)\sigma_x(0) \right\rangle dt = \frac{1}{2\hbar} \int_{-\infty}^{+\infty} e^{i\omega t} \left\langle \left[\sigma_x(t), \ \sigma_x(0)\right] \right\rangle dt \tag{6}$$

$$C(\omega) = \frac{1}{2} \int_{-\infty}^{+\infty} e^{i\omega t} \left\langle \left\{ \sigma_x(t), \ \sigma_x(0) \right\} \right\rangle dt = \hbar \coth\left(\frac{\omega\hbar\beta}{2}\right) \chi''(\omega) \tag{7}$$

So we see that C(t) is straightforwardly linked to $\chi(t) = \frac{i}{\hbar}\Theta(t) \langle [\sigma_x(t), \sigma_x] \rangle = \frac{2}{\hbar}\Theta(t) \mathbb{I}m \langle \sigma_x(t)\sigma_x \rangle$, where $\Theta(t)$ is the Heaviside unit-step function.

We also note that, if $\langle \sigma_x(t)\sigma_x(0)\rangle = \int_{-\infty}^{+\infty} A(\omega)e^{-i\omega t}\frac{d\omega}{2\pi}$, exploiting the relation $\frac{d}{dt}\sigma_x = -\frac{\Delta}{\hbar}\sigma_y$ and the properties of quantum correlation functions we find the following sum-rules [4]:

$$\int_{-\infty}^{\infty} A(\omega) d\omega = 2\pi \qquad \qquad \int_{-\infty}^{\infty} \omega A(\omega) d\omega = 2\pi \frac{\Delta}{\hbar} \langle \sigma_z \rangle \tag{8}$$

Which imply sum rules on $\chi(\omega)$ because the fluctuation-dissipation theorem gives us $C(\omega) = \operatorname{sign}(\omega) \frac{1}{2}A(\omega)$ at T=0 and of course the probability at t = 0 to have an eigenstate of σ_x must be $C(0) = \int \frac{d\omega}{2\pi} C(\omega) = 1$.

It is finally worth of noting that the more usual *static susceptibility* of the spin, i.e. the linear response of the magnetization to a constant magnetic field ϵ in the x-direction, is obtained by:

$$\chi_0 = -\left.\frac{\partial^2 F}{\partial \epsilon^2}\right|_{\epsilon=0} = \lim_{\omega \to 0} \mathbb{R} e \chi(\omega) = -\frac{1}{\pi} \int \frac{\chi''(\omega)}{\omega} d\omega \tag{9}$$

 $(F \text{ is the free-energy of the system. We used the Kramers-Kronig relations, see later eq. <math>(24)$

1.2.2 The appearance of decoherence

By analyzing the limiting cases when one of the parameters of the SB model (Δ or λ) dominates over the other, we can have some hints about the dynamics of the system in the general case. Thus we are now going to have a glance at the limiting cases. For notational simplicity from now on we are working with the units where $\hbar = 1$.

 $\lambda = 0$: Rabi oscillations The trivial case with $\lambda = 0$ represents an isolated spin in a magnetic field. Given an initial "delocalized" state $|\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$ we get a unitary spin-evolution with a P(t) which oscillates periodically between the eigenvalues ± 1 :

$$P(t) = \langle \psi | e^{i\frac{\Delta}{2}\sigma_z t} \sigma_x e^{-i\frac{\Delta}{2}\sigma_z t} | \psi \rangle = \cos\left(\Delta t\right) \tag{10}$$

Evaluating C(t), the thermodynamical quantity $Tr\left(e^{-\beta H}\left\{\sigma_x(t), \sigma_x\right\}\right)$ we still get the same result, independent on temperature, simply because for $\lambda = 0$ $\{\sigma_x(t), \sigma_x\} = 2\cos(\Delta t)$. Of course the corresponding $C(\omega)$ is just two symmetric delta-peaks, centered on frequency Δ :

$$C(\omega) = \frac{1}{2} \left(\delta \left(\omega - \Delta \right) + \delta \left(\omega + \Delta \right) \right)$$

These oscillations are called *Rabi oscillations* and are a clear signature of quantum mechanical evolution, and thus of quantum coherence.

 $\Delta = 0$: Pure dephasing Also for $\Delta = 0$ the SB model (known as the *independent boson model* or the *pure dephasing* case) is exactly solvable.

To have a clearer notation it is convenient to rotate the spin-basis $(\sigma_x \to \sigma_z)$ and consider just the Hamiltonian:

$$H = \lambda \sigma_z \sum_k \left(a_k + a_k^{\dagger} \right) + \sum_k \omega_k a_k^{\dagger} a_k = H_{int} + H_B$$

which can be diagonalized by a unitary transformation (*polaronic transformation*) implemented by: $U = e^{-\sigma_z \sum_k \frac{\lambda}{\omega_k} (a_k - a_k^{\dagger})} = e^{-i\sigma_z \frac{\Phi}{2}}$:

$$UHU^{-1} = \lambda \sigma_z \left(\sum_k \left(a_k + a_k^{\dagger} \right) - 2 \sum_k \frac{\lambda}{\omega_k} \sigma_z \right) + \sum_k \omega_k \left(a_k^{\dagger} - \frac{\lambda}{\omega_k} \sigma_z \right) \left(a_k - \frac{\lambda}{\omega_k} \sigma_z \right) = \sum_k \omega_k a_k^{\dagger} a_k - \lambda^2 \sum_k \frac{1}{\omega_k}$$

(The identity operator for the spin Hilbert-space is implicit).

If we now compute $\langle \sigma^+(t) \rangle$, we are physically looking at the possibility for the spin to be flipped after a time t, we have:

$$\langle \sigma^+(t) \rangle = \operatorname{Tr} \left[U \rho_s \otimes \rho_B U^{-1} e^{-i\Phi(t)} \sigma^+ \right] = \operatorname{Tr}_S \left[\rho_s \sigma^+ \right] \operatorname{Tr}_B \left[U \rho_B U e^{i\Phi(t)} \right]$$

We used $U\sigma^+U^{-1} = UU\sigma^+ = e^{-i\Phi}\sigma^+$, and we assumed an initially spin-bath factorized density matrix, which can be taken, for example as:

$$\rho(0) = \left|+\right\rangle \left\langle+\right| \otimes e^{-\frac{\left\langle+\right|H\right|+\right\rangle}{k_{B}T}} = \left|+\right\rangle \left\langle+\right| \otimes \mathcal{Z}^{-1} e^{-\frac{\left\langle1\right|H\left|1\right\rangle+\left\langle0\right|H\left|0\right\rangle}{2k_{B}T}} = \left|+\right\rangle \left\langle+\right| \otimes e^{-\frac{H_{B}}{k_{B}T}}$$

 $(|+\rangle)$ is the σ_x eigenstate, and the projection $\langle +|H|+\rangle$ in the bath-density matrix implies that the whole system is at equilibrium at t = 0, so we are computing C(t); we omitted the usual normalization factor \mathcal{Z}^{-1}).

We are left with:

$$\left\langle \sigma^{+}(t) \right\rangle = \operatorname{Tr}_{B} \left[e^{-\frac{H_{B}}{k_{B}T}} e^{-i\frac{\Phi(0)}{2}} e^{i\Phi(t)} e^{-i\frac{\Phi(0)}{2}} \right] = \left\langle e^{i\Phi(t) - i\Phi(0)} \right\rangle = e^{\frac{1}{2}\sum_{k} \frac{4\lambda^{2}}{\omega_{k}^{2}} \left\langle \left(\left(1 - e^{-i\omega_{k}t}\right)a_{k} - \left(1 - e^{i\omega_{k}t}\right)a_{k}^{\dagger} \right)^{2} \right\rangle} = e^{-K(t)}$$
(11)

The exponent is real in this case, and is simply

$$K(t) = 4\lambda^2 \int d\omega \frac{\rho(\omega)}{\omega^2} \left(1 - \cos(\omega t)\right) \coth\left(\frac{\beta\omega}{2}\right)$$
(12)

(We used the useful formula for the bosonic average found in the Appendix D)

At short-time and at T = 0 this exponent is $-4\lambda^2 t^2$ which indicates a rapid decrease of coherence, while at long times, performing an asymptotic time expansion, the exponent depends on the spectrum and has a general power-decay of the form $t^{-2\alpha}$ plus an eventual exponential decay for the subohmic case. A computation of $\langle \sigma^-(t) \rangle$ by symmetry leads to the same result so at the end we can say that $C(t) = \frac{1}{2} \left(\langle \sigma^+(t) \rangle + \langle \sigma^-(t) \rangle \right)$ is rapidly vanishing with time.

 $\Delta, \lambda \neq 0$: General case In light of these results we can argue that in the complete SB model (1) the magnetic field term drives the coherent oscillations, while the bath with time kills the opportunity for the spin to oscillate, leading eventually to a statistical mixture of spin eigenstates of the component of the spin coupled to the bath. The combination of the two parameters usually leads to damped Rabi oscillations in P(t) and C(t), which is usually interpreted as the visual signature of the presence of decoherence.

We note that the naive diagonalization of the full Hamiltonian (1) is a numerically impossible task, since bosonic modes can allocate any number of quantas, so even at low energy the size of the Hilbert space is enormous. Advanced numerical techniques (see section 3.2.2) can obtain reliable results at low energy but for practical situation simpler, less justified approaches that recover some parts of the qualitative behavior of decoherence are usually applied.

1.2.3 Bloch equations

One very practical way to roughly characterize the action of decoherence on a two level system is to define its relaxation time (usually noted as T_1) and its decoherence time (usually noted as T_2). They physically represents the characteristic times associated to the evolution of (respectively) $\langle \sigma_z(t) \rangle$ and $\langle \sigma_z(t) \rangle$ towards their equilibrium long-time value.

The usual way to obtain these parameters is to set up the *Quantum Master Equation* (QME) of the problem, i.e. to study the time-dependence of the reduced density matrix of the system.

In fact:

$$\langle \sigma_i(t) \rangle = \operatorname{Tr}_s \left\{ \rho_s(t)\sigma_i \right\} = \operatorname{Tr}_s \left\{ \operatorname{Tr}_B \rho_{tot}(t)\sigma_i \right\}$$
(13)
$$\frac{d}{dt} \langle \sigma_i(t) \rangle = \operatorname{Tr}_s \left\{ \dot{\rho}_s(t)\sigma_i \right\} = \operatorname{Tr}_s \left\{ \operatorname{Tr}_B \dot{\rho}_{tot}(t)\sigma_i \right\}$$

Under the hypothesis of weak coupling (or *Born approximation*: $\rho_{tot}(t) = \rho_s(t) \otimes \rho_B$) and of *Markovian* evolution (obtained by "time coarsing": the evolution of the system at time t does not depend on previous times), we obtain the *Bloch equations* of the two-level system:

$$\frac{d}{dt} \langle \sigma_x(t) \rangle = -\Delta \langle \sigma_y(t) \rangle$$

$$\frac{d}{dt} \langle \sigma_y(t) \rangle = \Delta \langle \sigma_x(t) \rangle - \frac{1}{T_2} \langle \sigma_y(t) \rangle$$

$$\frac{d}{dt} \langle \sigma_z(t) \rangle = -\frac{1}{T_1} \langle \sigma_z(t) \rangle$$
(14)

The decoherence time T_2 in naive Markov calculations is the same as the relaxation time T_1 and it depends linearly in magnitude with the dissipation:

$$T_2^{-1} = \frac{\lambda^2}{2} \pi \rho_\phi \left(\Delta\right) \coth\left(\frac{\beta \Delta}{2}\right) \tag{15}$$

If we solve the system of equations for $\langle \sigma_x(t) \rangle = P(t)$ we have $\frac{dP(t)}{dt^2} + \frac{1}{T_2}\frac{dP}{dt} + \Delta^2 P = 0$, with the initial conditions P(0) = 1 and P'(0) = 0 we have:

$$P(t) = e^{-\frac{|t|}{2T_2}} \left(\cosh\left(\frac{|t|\delta}{2T_2}\right) + \frac{1}{\delta} \sinh\left(\frac{|t|\delta}{2T_2}\right) \right)$$
(16)

$$P(\omega) = \int e^{i\omega t} P(t) dt = \frac{T_2 \Delta^2}{\omega^2 + T_2^2 \left(\Delta^2 - \omega^2\right)^2}$$
(17)

The quantity $\delta = \sqrt{1 - T_2^2 \Delta^2}$ dictates whether P(t) oscillates or not: for $\Delta > \frac{1}{T_2}$ it is purely imaginary so in addition to the exponential decay $e^{-\frac{t}{2T_2}}$ we also have coherent oscillations. Note that for $\Delta < \frac{1}{T_2}$ oscillations do not occur: we are in the *overdamped* (or incoherent) regime.

It is clear the connection to the limits discussed in 1.2.2: for the free case $(T_2 = \infty, \Delta \neq 0) P(t)$ oscillates as (10); for the pure dephasing case $(\Delta = 0, T_2\Delta = \text{constant } \ll 1)$ we recover $P(t) = e^{-\frac{t+\delta t}{2T}}$ which is (11). Note that in (16) we symmetrized P(t), instead of putting a unit-step $\Theta(t)$ factor, since we want a real

Fourier transform, to compare to $C(\omega)$, as in the rest of this report we will be mainly interested in C(t).

Indeed, C(t) is a quantity more directly accessible within our diagrammatic approach described in the next section. Anyway we note that, although the Bloch equations are naturally adapted for calculating P(t), the Quantum Master Equation can be set up as well for the equilibrium correlation functions. The analytical results are more complicated to obtain, but in the Markovian approximation it is possible to show that Bloch relations like (14) exist also for $\langle \sigma_i(t)\sigma_i(0)\rangle$, and the resulting evolution is then similar for P(t) and C(t) in the spin-bath equilibrium limit [6].

1.3 A different approach for the dynamics of the SB model

It is important to bear in mind that despite their popularity, the Markovian QME are often incorrect in the sense that the approximations made are not well understood and the resulting evolution does not always preserve the complete positivity of the density matrix elements [7], which is a mathematical inconsistence that shows clearly that the validity of the approach is merely phenomenological. More importantly, this approach fails to capture the quantum phase transition of the SB model, which does have deep consequence for the physics of decoherence in the subohmic case (see section 3).

Going beyond these approximation is possible in the context QMEs (see for example [8]), but the resulting expressions are usually very complicated and analytically intractable. For this reason it would be valuable to find alternative calculation approaches that are more suitable for more transparent approximation and thus of assessable quantitative and qualitative value.

The method that will be developed in the following sections will allow us to have correct results for the weak coupling regimes (section 2.3), and it will be be able also to find the second order quantum phase transition (section 3) which is a typical non-perturbative phenomenon. So far, no one has clearly succeeded in the task of providing a correct description of all the physics of the SB model in all regimes, in particular of the subohmic case. One of the objectives of this study is to start to develop link between the physics of strong coupling and that of decoherence, by using a single approach with controllable approximations which directly work on the model, without exploiting any analogy to a different physical problem.

2 Diagrammatic Theory for the Spin-Boson Model

Spin- $\frac{1}{2}$ commutation relations are not fermionic nor bosonic, and it doesn't exist a simple *Wick theorem* (see **Appendix A**) for handling correlation functions of generators of the SU(2) algebra. To overcome this problem and treat spins with the standard theoretical tools for fermionic/bosonic particles, physicists have found several exact mappings linking on the formal level the action of spin-operators on the original Hilbert Space and the action of creation/annihilation operators of fermions/bosons on a new Hilbert space. In most of these *spin-representations* the dimensionality of the new Hilbert space must be reduced in order to get a full equivalence with the original problem, and this procedure gives often rise to technical difficulties.

In order to attack the spin-boson problem, we choose to exploit a mapping known as the *Majorana* fermions spin-representation, whose application to condensed matter problem is relatively recent ([9, 10]). This representation allows us to map the spin of our Hamiltonian on three real (Majorana) fermions, grants us simple calculation procedure for the dynamical susceptibilities, and doesn't suffer of the Hilbert space enlargement problem.

2.1 Majorana's Fermionic spin-representation

To be clear, the mapping between a spin- $\frac{1}{2}$ and real fermions follows the following correspondence rule:

$$\sigma_x = 2i\eta_2\eta_3$$
 $\sigma_y = 2i\eta_3\eta_1$ $\sigma_z = 2i\eta_1\eta_2$

where η_1 , η_2 , η_3 are fermionic Majorana creation/annihilation operators $(\eta_i = \eta_i^{\dagger}, \{\eta_i, \eta_j\} = \delta_{ij})$.

It is worth noting that the anticommutation of the fermions guarantees the preservation of spin commutation rules $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$. For example:

$$[\sigma_x, \sigma_y] = -4\eta_2\eta_3\eta_3\eta_1 - 4\eta_3\eta_1\eta_2\eta_3 = -4\eta_2\eta_1 = 2i\sigma_z$$

This representation is strictly related to the *drone-fermion* representation, which is obtained constructing the three Majorana fermions from two canonical Dirac fermions:

$$\eta_1 = \frac{1}{\sqrt{2}} \left(c + c^{\dagger} \right) \qquad \eta_2 = \frac{i}{\sqrt{2}} \left(c^{\dagger} - c \right) \qquad \eta_3 = \frac{1}{\sqrt{2}} \left(d + d^{\dagger} \right)$$

It is then clear that the new Hilbert space for the spin- $\frac{1}{2}$ in this representation is 4-dimensional. However, the spin-boson Hamiltonian acts on a two-dimensional subspace of this Hilbert space, so the increase in dimension is not a problem for us since the 4-dimensional Hilbert Space can be splitted in two equivalent and uncoupled 2-dimensional Hilbert space.

Indeed, the two sets of physical spin-states can be chosen as:

$$|\uparrow_A\rangle = |0\rangle \qquad |\downarrow_A\rangle = c^{\dagger}d^{\dagger}|0\rangle \qquad \text{or} \qquad |\uparrow_B\rangle = d^{\dagger}|0\rangle \qquad |\downarrow_B\rangle = c^{\dagger}|0\rangle$$

It is important to note that in this formalism:

$$\eta_i = \sigma_i \left(2i\eta_1\eta_2\eta_3 \right) = \sigma_i \Phi$$

where Φ is a "Hilbert-space-switching" ($\Phi | s_{A/B} \rangle = | s_{B/A} \rangle$) operator, that commutes with the Hamiltonian (and the η_i) and so it is time-independent.

This property is conveniently applied to express spin-spin correlation functions since:

$$\langle \sigma_i(t)\sigma_j(t')\rangle = \langle \eta_i(t)\Phi\eta_j(t')\Phi\rangle = \frac{1}{2} \langle \eta_i(t)\eta_j(t')\rangle$$

(we used $\Phi^2 = \frac{1}{2}$). So in this scheme the equilibrium expectation value of σ_x , C(t), is computed as a Majorana-fermionic correlator:

$$C(t) = \frac{1}{2} \left\langle \{\sigma_x(t), \ \sigma_x(0)\} \right\rangle = \frac{1}{4} \left\langle \{\eta_1(t), \ \eta_1(0)\} \right\rangle$$
(18)

2.2 Computing observables

The formal Hamiltonian derived from the mapping is the following:

$$H = H_0 + H_{int} = -i\frac{\Delta}{2} \left(\eta_1 \eta_2 - \eta_2 \eta_1\right) + H_B - \lambda i \phi \eta_2 \eta_3$$
(19)

In order to set up a path-integral representation of the physical quantities, we switch to the interaction picture, and we evaluate the action in the formal basis of the fermionic coherent states, where fermionic Majorana operators can be replaced by the corresponding anti-commuting Grassman fields. We also allow the boson operator ϕ to act on the physical bosonic coherent state basis so to replace the operators with commuting fields (we indicate the fields as η and ϕ as their operators). A review of the many-body path-integral technique is found in **Appendix A**).

2.2.1 Calculation of the spin-spin equilibrium correlation function

The formulas (18) allows us to express *exactly* the physical spin-spin correlation function in terms of the two-fermions Green's functions, which can be expressed in terms of free (bare) fermion/boson propagators at the desired order in our λ -perturbation theory.

Given the action S_0 in eq. (34), the bare fermionic propagators (G_{ij}^0 i, j=1, 2, 3 indicates the Majorana fermions) are found in the Matsubara-frequency formalism from (34):

$$G_{ij}^{0}(i\omega_{n})^{-1} = \partial_{\tau} - 2H_{ij} = \begin{pmatrix} i\omega_{n} & i\Delta & 0\\ -i\Delta & i\omega_{n} & 0\\ 0 & 0 & i\omega_{n} \end{pmatrix}$$

$$G_{ij}^{0}(i\omega_{n}) = \int_{0}^{\beta} e^{-i\omega_{n}\tau} \left\langle \mathcal{T}_{\tau}\eta_{i}(\tau)\eta_{j}(0)\right\rangle_{0} d\tau = \begin{pmatrix} \frac{-i\omega_{n}}{\Delta^{2}+\omega_{n}^{2}} & \frac{i\Delta}{\Delta^{2}+\omega_{n}^{2}} & 0\\ \frac{-i\Delta}{\Delta^{2}+\omega_{n}^{2}} & \frac{-i\omega_{n}}{\Delta^{2}+\omega_{n}^{2}} & 0\\ 0 & 0 & \frac{1}{i\omega_{n}} \end{pmatrix}$$

$$(20)$$

We see that the poles at $i\omega_n = \Delta$ reflect the perfect Rabi oscillations in the delocalized limit $\lambda = 0$ (see eq. (10)).

Diagrammatically it is clear that the fermionic self-energy matrix $\Sigma_{ij}(i\omega_n) \equiv \Sigma_{ij}$ is non-zero only for i=j=2, i=j=3 (it is not possible to construct diagrams for the other self energies given the vertex (37)). Here follow for example the simplest self-energies (the bosonic propagator will be discussed later in this paragraph):

$$\begin{split} \Sigma_{22}\left(\tau\right) &= -\lambda^2 G^0_{33}\left(\tau\right) G^0_{\phi}\left(\tau\right) = \underbrace{\frac{2}{2} \underbrace{s}^{\ast} \underbrace{s}^{\ast} \underbrace{s}^{\ast} \underbrace{s}^{\ast} \underbrace{s}^{\ast} + \dots \\ \Sigma_{33}\left(\tau\right) &= -\lambda^2 G^0_{22}\left(\tau\right) G^0_{\phi}\left(\tau\right) = \underbrace{\frac{3}{2} \underbrace{s}^{\ast} \underbrace{s}^{\ast} \underbrace{s}^{\ast} \underbrace{s}^{\ast} + \dots \end{split}$$

(The external lines are maintained for clarity, but of course they are not part of the self-energy)

By fully summing Dyson's expansion (eq. (36)) the *full* (or "dressed") fermionic propagators are then:

$$\mathcal{G}^{-1}(i\omega_n) = G^{0-1}(i\omega_n) - \Sigma_{\eta}(i\omega_n) = \begin{pmatrix} i\omega_n & i\Delta & 0\\ -i\Delta & i\omega_n - \Sigma_{22} & 0\\ 0 & 0 & i\omega_n - \Sigma_{33} \end{pmatrix}$$
$$\mathcal{G}_{ij}(i\omega_n) = \begin{pmatrix} \frac{\Sigma_{22} - i\omega_n}{\Delta^2 + i\omega_n(\Sigma_{22} - i\omega_n)} & \frac{i\Delta}{\Delta^2 + i\omega_n(\Sigma_{22} - i\omega_n)} & 0\\ -\frac{i\Delta}{\Delta^2 + i\omega_n(\Sigma_{22} - i\omega_n)} & \frac{-i\omega_n}{\Delta^2 + i\omega_n(\Sigma_{22} - i\omega_n)} & 0\\ 0 & 0 & \frac{1}{i\omega_n - \Sigma_{33}} \end{pmatrix}$$
(21)

Analogously the bare bosonic propagators are readily expressed in terms of their density of states $\rho_{\phi}(\epsilon)$ eq. (3) by means of the *spectral representation* (see **Appendix D**):

$$G^0_{\phi}(i\nu_n) = \int_{-\infty}^{+\infty} d\epsilon \frac{\rho_{\phi}(\epsilon)}{i\nu_n - \epsilon} = 2\frac{(s+1)}{\Lambda^{s+1}} \int_0^{\Lambda} d\epsilon \frac{\epsilon^{s+1}}{\nu_n^2 + \epsilon^2}$$

We can of course also define diagrammatically the associated self-energy for the full propagators $\mathcal{G}_{\phi}^{-1}(i\omega) =$ $G_{\phi}^{0-1}(i\omega) - \Sigma_{\phi}(i\omega)$:

$$\Sigma_{\phi} = \frac{1}{\beta} \sum_{i\omega_n} G_2 \left(i\nu_n - i\omega_n \right) G_3 \left(i\nu_n + i\omega_n \right) =$$

$$(22)$$

$$(22)$$

$$(22)$$

$$(22)$$

We are interested in $C(\omega)$, which is proportional to the imaginary part of the analytical continuation on the real axis:

$$G_{11}(i\omega) \to G_{11}^R(\omega + i0^+) = -2i\int \Theta(t)C(t)e^{i\omega t}dt = -\frac{1}{\pi}\int \frac{C(\omega)}{\omega}d\omega - iC(\omega)$$

 $G_{11}^R = -i\Theta(t) \langle \{\eta_1(t), \eta_1(0)\} \rangle$ is also called *retarded Green's function* of the Matsubara propagator $\mathcal{G}_{11}(i\omega)$. Indeed, noting:

$$\Sigma_{22}^R(\omega) = \gamma(\omega) + i\Gamma(\omega)$$

where $\Sigma_{22}^{R}(\omega)$ is the analytical continuation on the real axis of $\Sigma_{22}(i\omega)$, we then have:

$$C(\omega) = -\mathbb{I}mG_{11}^{R}(\omega) = -\frac{\Delta^{2}\Gamma(\omega)}{\left(\Delta^{2} + \omega\gamma(\omega) - \omega^{2}\right)^{2} + \omega^{2}\Gamma(\omega)^{2}}$$
(23)

It is immediately clear the link with the Bloch-equation results (17) if we assume that $\gamma(\omega) = 0$ and $\Gamma(\omega) = \Gamma_0$: the T_2 term of (17) is represented by the (usually called *lifetime*) Γ_0^{-1} .

Analytical expressions of the self-energy for weak dissipation 2.2.2

We start by noting that, being $\Sigma(\omega + i0^+)$ an analytic function in the upper-half complex plane, the Kramers-Kronig relations (K-K) state that $\Gamma(\omega)$ and $\gamma(\omega)$ are not independent:

$$\gamma(\omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\Gamma(\epsilon)}{\epsilon - \omega} d\epsilon$$

$$\Gamma(\omega) = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\gamma(\epsilon)}{\epsilon - \omega} d\epsilon$$
 (24)

(\mathcal{P} stands for the *Cauchy's principal value* distribution).

neglecting Σ_{ϕ} and considering the first-oder expression of Σ_{22} :

$$\begin{split} \Sigma_{22}(i\omega_n) &= -\lambda^2 \frac{1}{\beta} \sum_{i\nu_n} G^0_{33}(i\nu_n - i\omega_n) G^0_{\phi}(i\nu_n) = -\frac{\lambda^2}{\beta} \int d\epsilon \rho_{\phi}(\epsilon) \sum_{i\nu_n} \frac{1}{i\nu_n - i\omega_n} \frac{1}{i\nu_n - \epsilon} = \int d\epsilon \frac{-\frac{1}{\pi} \mathbb{I}m \Sigma_{22}(\epsilon)}{i\omega_n - \epsilon} \\ \Gamma(\omega) &= \mathbb{I}m \Sigma_{22}(\omega) = \lambda^2 \pi \rho_{\phi}(\omega) \left[\frac{1}{2} + n_B(\omega) \right] = -\frac{\lambda^2}{\Lambda^{s+1}} \pi(s+1) |\omega|^s \operatorname{sign}(\omega) \Theta(\Lambda^2 - \omega^2) \left[\frac{1}{2} + n_B(\omega) \right] \\ \gamma(\omega) &= \mathbb{R}e \Sigma_{22}(\omega) = -\frac{\lambda^2}{\Lambda^{s+1}_0} (s+1) \mathcal{P} \int_{-\Lambda}^{+\Lambda} d\epsilon \frac{|\epsilon|^s \operatorname{sign}(\epsilon) \left[\frac{1}{2} + n_B(\epsilon) \right]}{\epsilon - \omega} \end{split}$$

(we applied the Matsubara sum formulas (**Appendix D**), the spectral representation of Green's functions (40) and the K-K relations (24) for the self-energy).

This approximation negligees all terms proportional to α^2 and superior orders, so it is certainly justified for $\alpha \ll 1$.

The results of the calculations and their comparison to the QME results are found in **Appendix B**.

2.3 Weak Coupling Results

In order to test our machinery, we prepared a computer program which is capable to perform Green's function operations and derive the correlation functions and the susceptibilities, following our approach. More details on the code and the problematics associated to its implementation can be found in **Appendix C**.

2.3.1 The ohmic case

We already noted that at sufficiently weak coupling we can be satisfied with a self energy truncated at first-order in the Dyson's series, as those pictured in section 2.2.2. Numerically, we can compute $C(\omega)$ for any s and plot its behavior, iterating the loop only once. The reliability of the results has been tested by performing different runs with different interpolation parameters and moreover checking the sum rules (8). For the calculation of $\langle \sigma_z \rangle$ in the second sum rule (8) we note that:

$$\langle \sigma_z \rangle = 2i \langle \eta_1 \eta_2 \rangle = 2i \mathcal{G}_{12}(\tau = 0) = \frac{1}{\beta} \sum_{i\omega_n} \frac{-2\Delta}{\Delta^2 + i\omega_n \left(\Sigma_{22} - i\omega_n\right)}$$

(we used (21))

The results of the numerical code are in a very good agreement with all these checks, bearing in mind the Pade' approximation and the finite temperature.

Figure 2 shows $C(\omega)$ and C(t) for the ohmic case for $\alpha \ll 1$, so to be sure to work in the perturbative regime. The increase in dissipation triggers a broadening of the peak in the frequency domain, and a renormalization of the position of the peak that becomes centered on $\Delta_R < \Delta$. The inverse temperature has been set to $\beta = 3000$.

Correspondingly to the peak broadening, C(t) shows a reduction of the T_2 time as expected from the phenomenological Bloch analysis (15). We emphasize that, being at very weak coupling, our results are *quantitatively* correct. If we increase the dissipation beyond the perturbation regime with the bare formula we obtain a strong renormalization of Δ , as expected, but a narrower peak which predicts an unphysical longer T_2 time. This means that bare perturbation theory is probably insufficient also for intermediate couplings.



Figure 2: Equilibrium Correlation function for ohmic spin boson model calculated with bare perturbation theory (first order self-energy)

2.3.2 The subohmic case

Changing the spectrum from ohmic to subohmic, while maintaining the same dissipation increase the decoherence, as shown in figure 3 (note that the sum rules are still respected, but the spectral weight is distributed at low frequency and in the tail). As $\omega \to 0$ and at T = 0, the correlation function goes to zero rapidly as ω^s , and the characteristic frequency at which this behavior begins defines a new scale in the problem (see section 3.1). At finite temperature, the appearance of sharp peaks at very low frequencies makes it difficult to appreciate this power-law behavior $(C(\omega) \simeq \frac{T}{\omega} \chi''(\omega))$ for $\omega \ll k_B T$, because of eq. 7, so $C(\omega)$ diverges as ω^{s-1} at zero frequency). For this reason we introduced a $\tanh\left(\frac{\beta\omega}{2}\right)$ factor, thus plotting the symmetrized $\chi''(\omega)$, which corresponds to $C(\omega)$ at zero-temperature (in practice for our simulations the curves are indistinguishable apart from the sharp peaks mentioned). For the examples in figure 3, the inverse temperature has been fixed to $\beta = 5000$.



Figure 3: Varying the spectrum of the baths affects coherence. For the subohmic case is visible an additional structure at low frequency.

In conclusion we note that a weak dissipation induces decoherence of the qubit, but the ground state remains non-degenerate (since it is adiabatically connected to the limit $\alpha = 0$ at Δ finite). We will ask in the next section: what happens to the qubit when the dissipation is further increased? Most of traditional methods are not controlled in this regime, and bare perturbation theory of our diagrammatics is certainly not justified. However our approach is not approximate in nature, and can be exploited to understand some properties of the limit of strong dissipation and of all the intermediate regime.

3 Localized/Delocalized Phases of the Qubit

The spin-boson model in various forms and applications has a long and untraceable history, but despite its long study the analysis of its basic formulation is still a very active subject of research (over 50 specific papers in the Physical Review journals since 2005, to give an idea!).

The complete model has not been exactly solved; the current situation is that its properties have been extracted by many different techniques valid in different regimes: a comprehensive physical picture of problem, especially for the subohmic case, is still influenced by subjective points of view [7].

3.1 Quantum phase transitions in the SB model

For what concerns the equilibrium-phases of the model, starting from an uncoupled spin and increasing the dissipation, it is well established that the spin subsystem undergoes a quantum phase transition (QPT) for $\alpha > \alpha_c$ [12]. This means that at zero temperature, the ground state of the subsystem changes its properties, switching between two completely deconnected phases. At weak coupling we encounter a *delocalized* non-degenerate state where Rabi oscillations are visible. This is the limit discussed so far. After the phase transition we switch to a *localized* ground-state which is two times-degenerate like if the system was trapped in one eigenstate of a spin operator.

The characterization of QPTs follow closely the framework developed for their classical counterparts. So we can define $P(t \to \infty)$ as an *order parameter* (something which is non-zero only in the localized phase) for the delocalization/localization transition, and we can distinguish classes of phase transition (first order, second order, infinite order) on the basis of the behaviour of correlation functions at the transition.

First order phase transitions usually exhibit a discontinuous jump in the order parameter at the critical coupling which corresponds to a "level crossing point" in which the energy of an excited state of the system becomes lower than the (ex-)ground-state. In second order phase transitions the order parameter varies continuously at the transition, and its correlation function diverges with vanishing frequency at the transition point. At this point the whole system configuration is unstable with respect to fluctuations at the transition point and the system is said to be *critical*. In our model criticality implies that the functional expression of the correlation function C(t) depends on a time-scale which becomes infinite at the critical coupling (or correspondingly to an energy scale T^* that vanishes at criticality).

A similar situation is found for *infinite-order* phase transitions (or *Kosterlitz-Thouless*) where the system is critical, even if the order parameter is discontinuous at the transition point.

Understanding the characteristic time scales of the model is of course of great importance for the practical application of the SB model, since they defines the different regimes of coherent/decoherent behavior of the qubit.

Signatures of Criticality on $C(\omega)$ At T = 0 and s < 1, detailed calculations [12, 17] show that $C(\omega \to 0)$ should diverge at criticality as ω^{-s} , and be regular following ω^{s} in the disordered phase.

The sharp boundary between the phases of a quantum phase transitions can't be observed at finite temperature, so our Matsubara formalism can't capture directly the QPT. However we expect crossover effects (i.e. smooth signatures of scaling invariance and critical behaviour) on the physical quantities at low temperature when the disordered phase is induced both by thermal energy excitations and by quantum fluctuations [13]. The scheme in figure 4 shows the region in the T- α diagram (at fixed Δ) where the effect of the quantum critical point is detectable: the quantum critical region separates the localized/delocalized phases and due to its typical shape the region is commonly called the quantum critical fan.

The existence of this crossover temperature, is a clear manifestation of the appearance of the energy scale T^* in addition to the renormalized level splitting scale Δ_R in the structure of the correlation function.

One way to observe the signature of this second order phase transition is to look at the behavior of the *static* impurity susceptibility χ_0 (9) with temperature, as it crosses the quantum critical region.

When the pseudo-spin is "localized", so that the ground state is two times degenerate and adiabatically linked (by varying α) to an eigenstate of σ_x , from simple arguments the static spin-susceptibility at low temperature is known to follow *Curie's Law* for free spins: $\chi \sim \frac{\langle \sigma_x \rangle^2}{T}$. This means that at very strong dissipation we expect an asymptotic decay with temperature of $\frac{2}{T}$. Crossing the critical fan, in the crossover region, from NRG results we are expecting a power law behaviour of the form $\chi \sim \frac{1}{T^s}$. Finally, when the ground state is unique, in the delocalized phase, where even at T=0 there is some energy splitting between the levels, χ is expected to saturate to a constant.



Figure 4: the quantum critical fan. Decreasing the temperature the susceptibility switches from quantum criticality to delocalized or localized behavior

3.2 QPT around the localized limit

3.2.1 Perturbative renormalization group analysis

Today, the most powerful theoretical techniques to find and understand continuous phase transitions are the ideas developed in the context of the *Renormalization Group Analysis* (RG). Here is the idea: we look for a physical quantity F, a function of the system variables Ω (for example the frequency, and/or some length in momentum, time, or spatial domain) which is dependent of a particular scale Λ (for example some energy cutoff, or the temperature.) and of several parameters (for SB model: α , Δ ...). The technique consist to find a mapping of the problem to a new and completely equivalent problem valid at a different cutoff. If we are able to find a mapping for any arbitrary lower scale Λ' in which $F[\Lambda', \alpha(\Lambda'), \Delta(\Lambda')](\Omega)$ is written in the same way with respect to Ω , but with different parameters α' , Δ' (and eventually a parameters/cutoff-dependent multiplication factor), then we can define the RG flow equations of the model: $\alpha = \alpha(\Lambda)$, $\Delta = \Delta(\Lambda)$. Physically speaking, the method allows us to find the effective theory of the system, since analyzing the flow energy physics of the original problem. i.e. of the possible quantum phases of the model.

We now apply the RG analysis to the diagrammatic theory we developed so far, bearing in mind that we want to be perturbative in both Δ and α , around the limit $\Delta = \alpha = 0$, corresponding to a free spin. This limit is adiabatically connected to the $\Delta = 0$ (with α arbitrary) line of pure dephasing in the sense that the ground state is two-fold degenerate, and thus corresponds to the localized phase of the qubit.

For this purpose it is convenient to redefine slightly our diagrammatic theory, introducing the *free* fermionic propagator $G_j^{free}(i\omega_n) = \frac{1}{i\omega_n}$ (j=1,2,3 all represented by a dashed line) and the second interaction, the Δ -vertex (pictured as a cross):

$$\cdots \cdot \overset{!}{\mathbf{X}} \cdots \overset{2}{\mathbf{X}} \cdots = -i\Delta \eta_1 \eta_2$$

Renormalization of α The *physical vertex corrections* to the dissipative interaction are (we first consider the ohmic case):



$$\Gamma_{V}(\omega,\Lambda) = \frac{\lambda}{\Lambda} + \frac{\lambda}{\Lambda}\Delta^{2}G_{0}(\omega)^{2} = \frac{\lambda}{\Lambda}\left[1 - \frac{\Delta^{2}}{\omega^{2}}\right] = \frac{\lambda}{\Lambda}\left[1 - \frac{h^{2}}{4}\exp\left(2\ln\frac{\Lambda}{\omega}\right)\right]$$

We introduced the adimensional parameter $h = \frac{2\Delta}{\Lambda}$ and we put this expression introducing the logarithmic form since from a merely mathematical point of view, the perturbative RG procedure is a way to sum logarithmically divergent contributions of the diagrams.

We now rescale Λ to $\Lambda' = \Lambda - d\Lambda$

$$\Gamma_{V}(\omega,\Lambda') = \frac{\lambda}{\Lambda'} \left(1 + \frac{d\Lambda}{\Lambda}\right) \left[1 - \frac{h^{2}}{4} \exp\left(2\ln\frac{\Lambda'}{\omega}\right) + \frac{h^{2}}{2}\frac{d\Lambda}{\Lambda}\right] =$$
$$= \lambda \left(1 - h^{2}\frac{(\Lambda')^{2}}{\omega^{2}}\right) \left(1 + \frac{d\Lambda}{\Lambda} + \frac{h^{2}}{2}\frac{d\Lambda}{\Lambda}\right)$$

By including in the coupling definition the frequency dependent vertex function, we arrive finally at the following RG-flow equation:

$$\lambda_R = \lambda \left(1 + \frac{d\Lambda}{\Lambda} + \frac{h^2}{2} \frac{d\Lambda}{\Lambda} \right) \longrightarrow \frac{d\lambda}{dl} = -\lambda - \frac{1}{2} \lambda h^2$$
(25)

which is expressed in terms of the logarithmic differential $dl = -\frac{d\Lambda}{\Lambda}$.

Eq. (25) is translated straightforwardly in a flow equation for $\alpha = 2\frac{\lambda^2}{\Lambda^2}$:

$$\frac{d\alpha}{dl} = -\alpha h^2$$

We also note that for the subohmic case, by means of equations (39) and (38) in Appendix B, we get a flow of α due to the term Λ^{1-s} appearing always "attached" to the dissipative coupling for dimensional considerations:

$$\alpha_R \Lambda^{1-s} = \alpha \Lambda^{1-s} \left(1 - (1-s) \frac{d\Lambda}{\Lambda} \right)$$
$$\frac{d\alpha}{dl} = -\alpha h^2 + (1-s) \alpha \tag{26}$$

Renormalization of Δ The physical vertex corrections to the "magnetic" interaction are:

$$---\frac{1}{2} \times \frac{2}{2} + -\frac{1}{2} \times \frac{2}{2} \times \frac{3}{2} \times \frac{2}{2}$$

We have seen that for $\omega \ll \Lambda$ and ohmic dissipation (see **Appendix B**)

$$\Sigma_{22}(\omega) = -\frac{\alpha}{2}\omega \ln\left(\frac{\Lambda^2 - \omega^2}{\omega^2}\right) - i\frac{\alpha}{2}\pi |\omega| \simeq -\frac{\alpha}{2}\omega \left(2\ln\left(\frac{\Lambda}{\omega}\right) - 2\frac{\omega^2}{\Lambda^2} + i\pi \mathrm{sign}\left(\omega\right)\right)$$

We note that the $-2\frac{\omega^2}{\Lambda^2}$ term is zero at low frequencies, so it is irrelevant with respect to the RG flow. So, the prefactor of the Δ is at order α :

$$\Delta \left(1 + \alpha \ln \left(\frac{\omega}{\Lambda} \right) - i \frac{\alpha}{2} \operatorname{sign} \left(\omega \right) \right)$$
(27)

We now rescale Λ and look for renormalization of the couplings in the real and imaginary part of this last expression.

It is clear that, since the imaginary part does depend on α but does not depend on the cutoff Λ , in this vertex correction there is no flow associated to the dissipative coupling $\alpha_R = \alpha$ in the ohmic case. By reducing the cutoff from Λ to $\Lambda' = \Lambda - d\Lambda$, and including the generated terms in the magnetic-field Δ , for $\omega \to 0$ we obtain the flow equation for Δ :

$$\Delta \left(1 + \alpha \omega \ln \left(\frac{\omega}{\Lambda'} \right) + \alpha \pi \frac{d\Lambda}{\Lambda} \right) = \Delta_R \left(1 + \alpha \omega \pi \ln \left(\frac{\omega}{\Lambda} \right) \right)$$
$$\Delta_R = \Delta \left(1 + \alpha \frac{d\Lambda}{\Lambda} \right)$$

In terms of the parameter $h = \frac{\Delta}{\Lambda}$ we have $(\Delta_R - \Delta \simeq d\Delta \text{ and } \frac{dh}{dl} = \frac{1}{\Lambda} \frac{d\Delta}{dl} + \frac{\Delta}{\Lambda})$:

$$\frac{dh}{dl} = (1 - \alpha) h \tag{28}$$

Looking at this equation we can already say that, if we neglect the α flow, for $\alpha < 1$ the effective low-energy magnetic field flows towards $+\infty$ while for $\alpha > 1$, h flows towards 0. So it is clear that for $\alpha > 1$ the system at low energy will be in an *incoherent, localized* phase, since we effectively recover the pure dephasing case of section 1.2.2.

We finally note that the functions corresponding to the right hand side of eq. (28), (26) are called the *Callan-Symanzik beta functions* for the SB model.

3.2.2 Phase diagrams and known results

In order to interpret and assess the validity of the flow equations that we found, we are now going to review more clearly the understanding on the quantum phases of the SB model.

The ohmic case The s=1 case is the most understood, since a linear dispersion often allows analytical calculations up to a certain stage, and moreover an exact mapping between of the problem to the *anisotropic Kondo model* (AKM) has been demonstrated (see [16, 2]). Thanks to the works on the Kondo model we know that the critical dissipation is $\alpha_c = 1$ and the phase transition delocalized/localized is of Infinite order.

The flow equations obtained through the AKM, in the *h*-perturbative regime (but non-perturbative in α !) are the same we found:

$$\frac{d\alpha}{dl} = -\alpha h^2 \qquad \qquad \frac{dh}{dl} = (1 - \alpha) h \tag{29}$$

The flow trajectories generated by these equations are plotted in figure 5.



Figure 5: RG flow for ohmic SB model

The term in the α -flow $-\alpha h^2$ drives the dissipation to zero for $\alpha < 1$. When the *h*-flow goes to zero ($\alpha > 1$), α renormalize to $\alpha_R < \alpha$, and allows to identify in the RG equations the line of stable *fixed points* ($\alpha_c \ge 1$, $h_c = 0$) characteristic of the Kosterlitz-Thouless phase transition. For $\alpha > 1$ the RG equations flow beyond the validity of the Δ -perturbation approach, but numerical non perturbative calculations or more advanced techniques like the *Bethe Ansatz* confirm that the strong coupling fixed point is $\alpha = 0$, $h = +\infty$ [16].

Nonohmic case The Superohmic case is much easier than the ohmic, since for s > 1 there is no critical point, and all the coupling flow towards $h = +\infty$ and $\alpha = 0$: the qubit is always in the *delocalized* phase (see figure 6).



Figure 6: RG flow for superohmic (s=2) SB model

The subohmic case is the more complicated, since the SB-Kondo mapping is no more valid, and most of the results in the literature are approximate and phenomenological. A firm point has been set up very recently [18] when the model has been diagonalized at low-energy by means of the Numerical Renormalization Group non-perturbative technique. It has been established that a second order phase transition delocalized/localized occurs for all 0 < s < 1, with the associated critical behavior. As previously noted in section 3.1, this implies the appearance of an additional energy-scale T^* that should be visible in the structure of $C(\omega)$, which should diverge at criticality.

Despite its relevance for the possible application of the SB model, this result is not captured by common weak coupling approximations like those typical in the QME approach, and the phase transition is missed also by all variational treatments and path-integral techniques found in the classic literature of the SB model.

Like for the ohmic case, a clearer view of the phases is obtained by plotting the RG flow trajectories of the couplings. Using the equations:

$$\frac{d\alpha}{dl} = -\alpha h^2 + (1-s) \alpha$$
$$\frac{dh}{dl} = (1-\alpha) h$$

we obtain the flow plotted in figure 7, where it is easy to identify the fixed point $\alpha_c = 1$, $h = \sqrt{1-s}$. We see that at finite, small magnetic field the new scale T^* is necessary to parametrize when the flow will cross the critical line separating the delocalized phase to the localized phase, which occurs at $\alpha_c \simeq \Delta^{1-s}$. We note that these results from perturbative RG flow are valid just for the weakly subohmic case $1-s \simeq 1$, since otherwise the quantum critical point is possibly beyond the perturbative analysis. However for weak magnetic field the transition point occurs for weak dissipation and thus is affecting the physics of decoherence!



Figure 7: RG flow for subohmic SB model

In summary we have shown that the SB model has a QPT at small magnetic field in the ohmic and subohmic cases. In the ohmic case this occurs for strong dissipation only ($\alpha > 1$) and does not affect the practical physics of decoherence (at $\alpha \ll 1$). In the subohmic case, a QPT is not excluded at weak dissipation and may thus interplay with decoherence.

We will therefore consider in the next section the delocalized limit (Δ finite, α small) beyond the lowest order expansion in α (which was studied section 2.3, and corresponds to the red line in figure 8).



Figure 8: Regimes of validity of perturbation theory

3.3 QPT around the delocalized limit

We now focus on the delocalized limit $\Delta \neq 0$ and $\alpha = 0$ (corresponding to pure Rabi oscillations) and consider the possibility of a dissipation-induced QPT. As seen in section 2, dissipation is a regular perturbation (for $\omega \to 0$) at leading order in α , and while it introduces decoherence (i.e. a damping of the Rabi oscillations) the nature of the ground state is not affected. From previous discussion around the localized limit we are now convinced that a change of ground state should occur by increasing α , leading to a quantum phase transition. To capture this effect starting from the delocalized limit, it is thus necessary to consider higherorder corrections in α to the spin-spin correlation functions.

3.3.1 Beyond perturbation theory

The diagrammatic expansion is a formally correct expansion: if we were able to sum all the diagrams in the Dyson's series we should be able to compute the full non-perturbative result. The diagrams are infinite, but they can be grouped in *classes of diagrams* with common properties in terms of calculation procedure and magnitude of contribution.

It is sometimes possible to access to some qualitative properties (like a phase transition!) characteristic of the non-perturbative treatment (or just to have a better quantitative weak-coupling treatment) by summing all the diagrams in a given class, or by exploiting exact non-perturbative relations. However it is always necessary to have some guide on understanding which diagrams to sum and why, since it may often happen that high-order diagrams of different classes cancels each-others, so that a partial sum will include nonphysical contribution.

So we are interested in the self-energy diagrams. Starting on Σ_{η} , a typical distinction between these kinds of diagrams concerns whether the boson lines cross each other or not:



The choice of summing the first class of diagrams (also called *rainbow diagrams*) and neglecting the others is known as the *non-crossing approximation (NCA)*. It could be easily implemented in the codes by iterating the dressing (by Dyson's formula) of the propagators until a self-consistent solution for $\mathcal{G}_{22}(i\omega)$, $\mathcal{G}_{33}(i\omega)$, $\Sigma_{22}(i\omega)$, $\Sigma_{33}(i\omega)$ is found in the expression of $\mathcal{G}_{11}(i\omega)$ (23). However it is clear at the lowest order that all these corrections are *regular* at low frequency in the sense that they are not divergent for finite Δ : they are important for quantitative calculations but they can't cause the phase transition.

It is likely that including a self-energy Σ_{ϕ} will make us capable to capture the second order delocalization/localization QPT for the subohmic model. In fact, there exist a λ_c for which $\mathcal{G}_{\phi}(i\nu_n)$ is divergent as its denominator is zero at low frequencies:

$$G^{0}_{\phi}(i0) + \left(G^{0}_{\phi}(i\nu_{n}) - G^{0}_{\phi}(i0)\right)_{\nu_{n} \ll \Lambda} = 2(s+1)\frac{1}{s\Lambda} - 2(s+1)\frac{|\nu_{n}|^{s}}{\Lambda^{s+1}}\frac{\pi}{2}\frac{1}{\sin\left(\frac{\pi s}{2}\right)} \quad \propto \quad \frac{1}{s\Lambda^{s+1}}\frac{1}{s\Lambda^{s+1}} = \frac{1}{s\Lambda^{s+1}}\frac{1}{s\Lambda^{s+1}} = \frac{1}{s\Lambda^{s+1}}$$

$$\Sigma_{\phi} (i\nu = 0) = \frac{1}{\beta} \sum_{i\omega} \mathcal{G}_{22}(i\omega) G^{0}_{33}(i\omega - 0) = \frac{\lambda^{2}}{\beta} \sum_{i\omega_{n}} \frac{1}{\Delta^{2} + i\omega_{n} \Sigma_{22}(i\omega_{n}) + \omega_{n}^{2}} = R(\lambda)$$
$$\mathcal{G}_{\phi}^{-1} (\nu = 0) \simeq G_{\phi}^{0-1} (i0^{+}) - \Sigma_{\phi} (i0^{+}) \quad \propto \quad \Lambda s - R(\lambda)$$
(30)

and this translates to a divergence of the spin-susceptibility due to the exact relation (see Appendix D):

$$\mathcal{G}_{\phi}\left(i\nu_{n}\right) = \frac{\lambda^{2}}{8}G_{\phi}^{0}\left(i\nu_{n}\right) + \frac{\lambda^{2}}{16}G_{\phi}^{0}\left(i\nu_{n}\right)^{2}\chi\left(i\nu_{n}\right)$$
(31)

where the spin-correlator $\chi(\tau) = \langle \mathcal{T}\sigma_x(\tau)\sigma_x(0) \rangle$ is a bosonic Matsubara Green's function, and it corresponds to $\mathcal{G}_{11}(\tau)\operatorname{sign}(\tau)$ of the Majorana's formalism. In frequency domain, the imaginary part of its analytical continuation on the real axis corresponds directly to the previously defined $\chi''(\omega)$.

From (30) we see that $\Lambda s - R(\lambda)$ behaves as a bosonic "mass term" which goes to zero continuously at the transition point. It seems then a good choice for an order parameter of the continuous QPT.

3.3.2 Crossovers of the quantum phase transition

We computed $\chi_0 = \int_0^\beta d\tau \chi(\tau)$ for several temperatures and values of α , following the behavior of the static susceptibility through the critical fan. We set up the code to self-consistently sum all one-loop fermionic self-energies. In order to dress the bosonic propagator, we exploited the relation (31), effectively imposing an additional self-consistency in $G_{11}(i\omega)$. It is not clear what is the approximation made on \mathcal{G}_{ϕ} , but it is clear that we are considering some sort of self-energy in the propagator and that we maintain full-compatibility with our previous assumptions.

We note that we could have used the first classes of self-energies pictured in (22), the bare bubbles, doing then what is called the *random-phase-approximation* (RPA). Technically, in the code it is sufficient to write Dyson's equation for \mathcal{G}_{ϕ} in the iteration loop with the dressed \mathcal{G}_{22} , \mathcal{G}_{33} in order to perform our RPA selfconsistent calculation. Unfortunately our first attempts encountered some technical difficulties in the Pade' analytical continuation and in the interpretation of the results for the static susceptibility. Understanding what is the best class of diagrams to sum and why is one of the objectives of the future research.

The plot in figure 9 pictures the crossover phenomenon: when the susceptibility χ_0 is the quantum critical region, on logarithmic scale it should be a line of slope -s (orange region in the figure), following section 3.1.



Figure 9: Static Susceptibility vs. Temperature on logarithmic scale. At sufficient low temperature we are out of the critical fan and the Susceptibility either saturates or follow Curie's Law. In between we are close to the critical dissipation



Figure 10: The Dynamical Susceptibility for positive frequencies. Dissipation parameters and color code are the same as figure 9.

When we diminish the temperature, crossing the critical fan (see figure 4, and refer to the blue arrows), χ_0 either behaves as spin-localized (Curie's law, slope -1 on logarithmic scale), or as spin-delocalized (saturates to a constant). The α_c can be extracted this way as the value for which the Susceptibility changes behavior. We note that since χ_0 is proportional to $\langle \sigma_x \rangle^2$, this produces a shift in the origin of the lines for strong dissipation.

The signatures of criticality are recognizable in $C(\omega)$ as well, accordingly to section 3.1 (see also figure 10). The T^* energy scale, corresponding to the leftmost frequency "hill" in the curves, goes to zero as $\alpha \to \alpha_c$. For $\alpha \neq \alpha_c$, it is always recognizable the low frequency behaviour (verified on logarithmic scale).

We performed other tests, reproducing the parameters of some NRG calculation presented in [17]: all the results are encouraging since we find the correct critical dissipations (from visual considerations) and a structure of $C(\omega)$ at low frequency as expected. This is remarkable since the Majorana mapping is then the first method that captures the second order phase transition (some variational methods and other "infinitesimal transformation" approaches incorrectly find a first order QPT or cannot conclude on the nature of the transition. See [14] and references therein) which is in principle valid for computing observables at arbitrary frequency. This last feature is important for characterizing decoherence (quantum coherence in the SB model is a feature whose characteristic frequency is Δ).

4 Two Independent Bosonic Baths

The Spin-boson model can be easily extended to similar, more complicated models. Once again, the important scientific interest to study these problems consists in understanding the basics of many-body quantum dynamics of open systems. An interesting extension to (1) is found by adding a second independent bosonic bath, coupled linearly to an orthogonal spin-eigenstate with respect to the previous spin-bath coupling [19]. Unfortunately only weakcoupling results for the dynamic observables are reliable at this stage of the research, but its very likely that the technical issues arising for strong coupling situations can be overcome (see section 5.2).

4.1The two-baths frustrated spin-boson model

The model can be generalized to a two independent bath model by adding a term to the Hamiltonian, which then reads:

$$H = \Delta \sigma_z + \lambda_1 \sigma_x \sum_k \left(a_k + a_k^{\dagger} \right) + \lambda_2 \sigma_y \sum_k \left(b_k + b_k^{\dagger} \right) + \sum_k \omega_k a_k^{\dagger} a_k + \sum_k \epsilon_k b_k^{\dagger} b_k$$

We stress that this time the spin-bath coupling occurs also for the y-component of the spin. Intuitively we are expecting that this new term will increase the dissipation/decoherence rate with respect to the ordinary spin-boson case. However, when it comes to determine the ground state of the spin, and thus its character of being localized/delocalized, we are facing a *frustration* in the sense that it is impossible to find a common eigenstate of σ_x and σ_y so, at least for the completely boson-symmetric case ($\lambda_1 = \lambda_2$ and $\epsilon_k = \omega_k$) the system can't localize.

This model has been introduced by Novais et al. [19] to describe a spin- $\frac{1}{2}$ impurity embedded in an 3D environment of large spins: the spin-bath couplings represents the interaction of the impurity with spin waves, and the magnetic field Δ arise from molecular ferromagnetic coupling of the environment with the impurity. However, it is very likely that this simple model could have relevance also for qubit manipulation, where we usually have a certain degree of control on the environment. As a physical example for a realistic qubit system (such as the one based on the Josephson junctions), electronic voltage fluctuations are associated to ohmic (s = 1) noise, while random tunneling centers lead to the so-called 1/f noise (which can be modeled at finite temperature by a bosonic bath with exponent s = 0). Hence two independent noise sources (with different power spectra) can be possible in practice.

Since in principle we can avoid the dissipation-induced localization of the spin by *adding* an additional environmental mode coupled with the qubits, we can wonder whether we can reduce decoherence by exploiting the same principle. Apart from a recent study on a different, similar but much simpler model that exhibits this kind of frustration [20], no other research on the model has appeared since [19].

4.1.1**Diagrammatic Theory**

The diagrammatic theory in the Majorana-fermions formalism is a trivial extension of the simple spin-boson theory. Being perturbative in both λ_1 and λ_2 , we now have two vertex for our diagrams:



This means that we are now capable of building non-zero self energies Σ_{12} , Σ_{21} , Σ_{11} in addition to Σ_{33} , Σ_{22} . If we also assume that $\Delta \ll \Lambda$ we can drop terms proportional to $\alpha_1 \alpha_2 \frac{\Delta}{\Lambda}$ so that Σ_{12} , Σ_{21} appear only as higher-order contributions and thus we set them to zero as a first analysis.

We obtain the propagators in terms of the self-energies at order α_1 , α_2 and $\alpha_1 \alpha_2$:

$$\mathcal{G}_{ij}(i\omega_n) = \begin{pmatrix} \frac{\Sigma_{22} - i\omega_n}{\Delta^2 - (\Sigma_{11} - i\omega_n)(\Sigma_{22} - i\omega_n)} & \frac{i\Delta}{\Delta^2 - (\Sigma_{11} - i\omega_n)(\Sigma_{22} - i\omega_n)} & 0\\ -\frac{i\Delta}{\Delta^2 - (\Sigma_{11} - i\omega_n)(\Sigma_{22} - i\omega_n)} & \frac{\Sigma_{11} - i\omega_n}{\Delta^2 - (\Sigma_{11} - i\omega_n)(\Sigma_{22} - i\omega_n)} & 0\\ 0 & 0 & \frac{1}{i\omega_n - \Sigma_{33}} \end{pmatrix}$$
(32)

following the same steps as in section 2.2.1 we can arrive at the imaginary part of the dynamical transverse spin-susceptibility, whose form in terms of the real/imaginary part of the self-energies is quite complicated.

The self energies at order α_1 , α_2 have exactly the same form as those for the simple spin-boson model (pictured in section 2.2.1).

the $\alpha_1 \alpha_2$ order is represented by two rainbow diagrams which includes both bosonic propagators:



4.1.2 Perturbative RG flow and phase diagram

The same arguments on the vertex for the single-bath spin boson models in 3.2.1 apply for the frustrated model, leading immediately to the *h*-perturbative RG flow equations of the dissipative couplings: $\frac{d\alpha_i}{dl} = -h\alpha_i^2 + (1-s)\alpha_i$. The mixed rainbow diagrams of section (4.1.1) leads to a coupling to of the flow equations for the two dissipation parameters, since the associated vertex correction leads to $(G_{11} \simeq G_{33}$ when $\Delta \simeq 0$):



that is,

$$\frac{d\alpha}{dl} = -2\alpha_1\alpha_2$$

By including only this vertex correction in the flow, we immediately imply that the validity of the resulting flow equations will require that at least one of the coupling α_i is $\ll 1$, in such a way that the product with the other dissipation parameter will be small.

The renormalization of h is obtained as for the single bath (eq. 27 and following passages) by looking at the physical quantity $\mathcal{G}_{11}(\omega)$ from (32) for example. We note this time the need to introduce a renormalization factor Z for the Green's function itself, a procedure known under the name of *Wavefunction renormalization*:

$$G_{11}(\omega) = \frac{\Sigma_{22} - \omega}{\Delta^2 - (\Sigma_{11} - \omega)(\Sigma_{22} - \omega)} = \frac{1}{\frac{\Delta^2}{(\Sigma_{22} - \omega)} - (\Sigma_{11} - \omega)} = \frac{1}{(\Sigma_{11} - \omega)} \frac{1}{\frac{\Delta^2}{(\Sigma_{22} - \omega)(\Sigma_{11} - \omega)} - 1}$$
$$\implies \Delta_R = \Delta \left(1 + \alpha_1 \frac{d\Lambda}{\Lambda} \right) \left(1 + \alpha_2 \frac{d\Lambda}{\Lambda} \right) \qquad Z_R = \left(1 + \alpha_1 \frac{d\Lambda}{\Lambda} \right)$$

The final RG flow equations, perturbative both in $\frac{\Delta}{\Lambda}$ and in *one* dissipative coupling, are:

$$\frac{d\alpha_1}{dl} = -2\alpha_1\alpha_2 - \alpha_1h^2 + (1-s_1)\alpha_1$$

$$\frac{d\alpha_2}{dl} = -2\alpha_1\alpha_2 - \alpha_2h^2 + (1 - s_2)\alpha_2$$

$$\frac{dh}{dl} = (1 - \alpha_1 - \alpha_2)h$$
(33)

We note that the same RG equations can be obtained by means of a polaronic transformation and a α_2 -perturbative RG (or α_1 -perturbative) analysis on the partition function in the Kink-gas representation [19]. However our method is much simpler and more direct.

4.2 Results and quantum frustration

4.2.1 Phases of the model

Ohmic baths We start noting that for $s_1 = s_2 = 1$ the "frustrating" term $-2\alpha_1\alpha_2$ doesn't allow any fixed point apart from the ones of the classic SB model. Figure 11 shows some trajectories in the flow: for strong anisotropic dissipation the system may be localized by one of the two baths.



Figure 11: LEFT: RG flow for two independent ohmic baths. Cyan lines represent six different cases at non-zero magnetic field and nonzero coupling to both baths. The blue lines represent the flow on the h=0 plane RIGHT: projection of the flow for nonzero magnetic field in the $\alpha_1 \alpha_2$ plane. The flow is interrupted when h=1, when perturbation theory is certainly not valid. For strong anisotropic coupling the system flows towards the localized phase ($\alpha_R \neq 0$)

The flow behavior is particularly remarkable if we set $\alpha_1 = \alpha_2$, obtaining:

$$\frac{d\alpha}{dl} = -2\alpha^2 - \alpha h^2$$
$$\frac{dh}{dl} = (1 - 2\alpha)h$$

The important point is that in this case α always flows towards 0, while h always scales towards $+\infty$. This is the most evident manifestation of frustration: no matter how strong is the dissipation, the system is always *delocalized*, since its low energy behavior is that of the free decoupled spin. NRG results from [19] confirm this result also in the non-perturbative regime.

Nonohmic baths Fully understanding the consequences of (33), i.e. quantitatively evaluate the complete behavior of the two-bath model, seems overwhelmingly complicated. Nevertheless we can establish an intuition on the phase diagram by looking for fixed points in the RG flow. For the superohmic case, like for the ohmic case, we do not find any fixed point, and thus no phase separation. The flow of the dissipative coupling is always towards weak coupling and thus we are always in a delocalized phase.

The subohmic flow, with $s_1 < 1$ and $s_2 < 1$ has three non-trivial fixed points (α_1, α_2, h) instead: $(1, 0, \sqrt{s_1 - 1}), (0, 1, \sqrt{1 - s_2})$ and $(\frac{1 - s_2}{2}, \frac{1 - s_1}{2}, 0)$. Figure 12 should clarify a bit the situation and show the difficulty in the general definition of the phase diagram.

It is clear from the example that even in the subohmic case we can obtain the situation in which both dissipative couplings are strong, but the system remains delocalized.

Without entering the non-perturbative regime, we can check whether the Majorana diagrammatic theory allows us to obtain some signatures of the frustration effect.



Figure 12: LEFT: Flow diagram for the subohmic 2-bath case. The cyan lines depart at different dissipations for h=0.01. At strong dissipation, for not too different spin-bath couplings, the system flows towards the delocalized fixed point. RIGHT: Zoom near the non-dissipative case. The h=0 fixed point is shown as well as RG flows in the dissipation plane (the fixed point is stable, except in the h direction).

4.2.2 Weak coupling considerations

We note that in the two baths model the symmetrized σ_x -correlation function has not anymore directly the interpretation of the equilibrium σ_x value in the sense of section 1.2. However its oscillations are still a signature of quantum coherence, it is anyway a measure of spin dissipation into bath ϕ_1 (thanks to eq. (7)), and its long-time behavior is still a good order parameter to characterize the QPTs of the model.

In figure 13 we compare the results of the ohmic SB model with the associated ohmic two bath model, employing simple bare perturbation theory (self-energy diagrams are iterated only once in the code).

It is clear that adding a bath reduces coherence, but we note the "benefic" effect of the anti-localization diagrams of section 4.1.1: an increase in sharpness and height of the coherent peak in the correlation function with respect to the computation without these contributions.

However since the physics of frustration is produced at strong coupling in the ohmic model, we can conclude that the frustration effect is only slightly affecting the coherence properties of the model: for the two-baths case the qubit is more decoherent at weak coupling as naively expected.

Also for the subohmic case (figure 14) the coherence at weak coupling is not overrun by frustration. With bare perturbation theory we can't capture the localized phase, which occurs at weak coupling for the strongly subohmic case, so our plots have just an indicative value to check the effect of the $\alpha_1\alpha_2$ -diagrams in the delocalized phase.

For this reason, in the particular case of $s \simeq 0$ it will be important to achieve the non-perturbative regime for the two-bath case since the frustration effect is believed to be relevant also at weak coupling, and this





Figure 13: Bare perturbation theory applied to the two-bath ohmic s = 1 model for $\alpha \ll 1$. The pointed line corresponds to single bath SB model, the dashed line is the result for two equal baths without the "frustrating" diagrams, and the thick line is the bare result for $\alpha_1 = \alpha_2$ including the frustrating diagrams. Concerning the other parameters, $\Delta = 0.2$, $\Lambda = 1$ and $\beta = 3000$



Figure 14: Bare perturbation theory applied to the two-bath subohmic s = 0.1 model for $\alpha \ll 1$. The pointed line corresponds to single bath SB model, the dashed line is the result for two equal baths without the "frustrating" diagrams, and the thick line is the bare result for $\alpha_1 = \alpha_2$ including the frustrating diagrams. Concerning the other parameters, $\Delta = 0.2$, $\Lambda = 1$ and $\beta = 3000$. The peak at zero frequency in $C(\omega)$ is a finite-temperature effect. (note the difference in scale with respect to figure 13)

5 Remarks, Conclusions, Perspectives

During the four-month *stage* at Neel institute I familiarized with some of the most advanced methods in condensed matter field theory (spin fermionic representation, Matsubara diagrams, renormalization group) by applying them to an unsolved model, appreciating the limits of the different methods and trying to overcome the limitations of previous approaches.

Moreover, the huge literature on the spin-boson model, and its connection to other important fundamental paradigms of condensed matter theory allowed me to have a good bibliographical preparation on the subject of strong correlated systems. The numerical work has been an important experience as well, since it was for me the first time I had to practice advanced scientific programming for many-body quantum systems.

5.1 Summary

In this report we presented the application of Majorana's fermionic spin representation to the Spin-Boson model and to his two-baths extension. This diagrammatic technique has several advantages with respect to other approaches commonly used in strong correlation problems, but its usefulness in condensed matter has been recognized only recently [9, 10] so there is very little literature pertinent to our problem. The application of the representation allow us to find immediately Bloch-like analytical expressions for C(t) for arbitrary bosonic spectrum in the weak-coupling situation, which are qualitatively and quantitatively correct. The method is thus an immediate test-bed for phenomenological weak-coupling results like QME approaches, whose validity is often of difficult control.

The expressions found can be used to set up the perturbative RG analysis, and thus to discover the phases (localized/delocalized) of the system. The flow equations already presented in the literature [2, 12, 16] (mainly obtained thanks to the mapping of the SB model to the AKM) are recovered very easily with a vertex RG analysis, for arbitrary spectrum.

The technique allow us also to observe some signatures of the second order phase transition recently discovered for the subohmic case [18], since by summing classes of diagrams, or exploiting exact functional relations, we can enter in the non-perturbative regime. It is not clear the quantitative validity of the approach yet, but the critical exponents of the spin-susceptibility, divergent at low frequencies, can be extracted. It is important to note that we couldn't find any other approach in the literature that captures this continuous phase transition, except the recent NRG computer calculations.

The method has been proven to be applicable straightforwardly to the two bath case, and it is probably adaptable to many other extensions. The application of Majorana's representation to the two baths SB model gives immediately quantitatively correct results for the weak coupling case (which can be numerically computed for arbitrary spectrum of the two baths) and the RG analysis on correlation functions gives easily the flow equations already found in the literature [19], where they were obtained employing different, more complicated and less transparent methods. The quantum frustration effect recognized in [19] is believed to be identified by our approach, and some signatures for weak coupling expressions are presented and discussed.

In summary, we set up an approach that demonstrated to be able to compute the equilibrium dynamics of the SB model in a controllable way, and to capture to some extent the phenomena of decoherence, localization and quantum frustration present in this model.

5.2 Research directions

Some aspects remains unclear for the strong coupling regime. Unfortunately the Pade' numerical analytical continuation has proven to be instable at strong coupling, so a zero-temperature diagrammatics in which Matsubara's sums are integrals and the time and frequencies are taken to be real is desirable. Working from the origin at T=0 will also allow to capture the quantum phase transition, i.e. the delta peak at zero frequencies expected for C(t) in the localized phase.

We also note that the Matsubara Green's functions technique is easily extendible to non-equilibrium situation (Keldysh Technique, or contour Green's functions) so our approach can be adopted to compute P(t) and the non-equilibrium dynamics of the SB model, but the calculations are believed to be more quite cumbersome. Some simple weak-coupling expression for the ohmic case will be nevertheless investigated soon in order to detect the analytical difference between C(t) and P(t).

For what concerns the perturbative RG procedure, since we have some analytical formulas for observables like the susceptibility, we can now use the flow equations (29, 33) to compute the flow of the observable itself. This is performed by applying the *Callan-Symanzik Equation* which is a differential equation for the susceptibility involving the RG beta functions and the Z renormalization factors. The resulting function will allow us to have a useful, *exact* expression for the renormalized position and width of the peak at weak coupling, in contrast to order-of-magnitude approaches present in the literature.

Moreover, when the results in strong coupling and the critical regimes will be believed to be quantitatively or qualitatively trustable, a systematic study of the influence of strong dissipation and a careful comparison with NRG results for the subohmic case obtained in [18] will be made.

A more detailed investigation of the non-perturbative regime of the two-baths case is underway: the problem is a conceptual one on understanding what classes of diagrams to sum, and a technical one involving the convergence of the numerical code, whose self-consistency must now be verified between all fermionic and bosonic propagators. It would be also interesting to understand the application of the two-bath model to realistic situation involving nanodevices, in which it is pragmatic to assume that noise sources can be coupled to all spin-components (but it is not given that the baths can be treated as uncorrelated!). In such systems, a relevant question will be how the frustration effect or the interplay of different bath spectra can be eventually exploited.

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It would be in line with the Italian student tradition to conclude the report of the final project in my undergraduate studies with an epic series of thanks to all people, animals, computers, books and whatever has been important in my personal and academic life. However, bearing in mind the more contracted French style, I will limit myself to acknowledge as shortly as I can the important persons that made the difference for me in the last months.

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Appendix A: Formalism for Finite Temperature Green's Functions

Note on connection temperature-imaginary time

Introducing the temperature in a quantum problem reduces to consider a classical statistical mixture of possible states. The statistical weight of a given state of energy E is given by the Boltzmann factor $e^{-\beta E}$, where $\beta = \frac{1}{T}$ ($k_B = 1$). Formally, we apply a density matrix operator $e^{-\beta H}$ on the observable we are examinating and we trace over all states to get the seeked expectation value (see formula 13, for example).

The nice mathematical thing is that the time evolution operator and the temperature density matrix can be melted in a single operator provided we use an "artificial" imaginary time $\tau = it$:

$$\left\langle \mathcal{O}(t)\right\rangle = \sum_{n} \left\langle \psi_{n} \left| e^{-\beta H} e^{-iHt} \mathcal{O} \right| \psi_{n} \right\rangle = \sum_{n} \left\langle \psi_{n} \left| e^{-H(\beta+\tau)} \mathcal{O} \right| \psi_{n} \right\rangle$$

From a merely formal point of view all the machinery of Quantum Field Theory for the real time can be applied to the imaginary time, provided we take care of the properties of (anti-)*periodicity of the time-ordered correlation functions* in imaginary time-domain:

$$C(\tau) = -\langle \mathcal{T}A(\tau) B(0) \rangle = \pm \langle \mathcal{T}A(\tau + \beta) B(0) \rangle$$

(\mathcal{T} simply orders A, B in decreasent time, adding a -1 factor if it reverses fermionic operators). which implies that the integrals over τ will be bounded by β and that the quantity can be expanded in *Fourier series*, which means that the (Matsubara) frequencies are discrete:

$$C\left(n\right) = \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-\frac{i\pi n}{\beta}\tau} C\left(\tau\right)$$

The following relations can be demonstrated for two-point correlation functions of fermionic (c, c^{\dagger}) and bosonic (a, a^{\dagger}) operators:

$$C_{c}(\tau) = -\left\langle \mathcal{T}c(\tau)c^{\dagger}(0)\right\rangle \qquad C_{c}(i\omega_{n}) = \int_{0}^{\beta} d\tau C_{c}(\tau)e^{i\omega_{n}\tau} \qquad \omega_{n} = \frac{(2n+1)\pi}{\beta}$$
$$C_{a}(\tau) = -\left\langle \mathcal{T}a(\tau)a^{\dagger}(0)\right\rangle \qquad C_{a}(i\nu_{n}) = \int_{0}^{\beta} d\tau C_{c}(\tau)e^{i\nu_{n}\tau} \qquad \nu_{n} = \frac{2n\pi}{\beta}$$

We finally note that the analytical continuation on the real axis of the correlation function in the Matsubara frequency is directly connected with its real-frequency counterpart, the so called retarded Green's Functions (see section 2.2.1 for an application of this).

A complete treatment of the general formalism is found in any textbook on Finite Temperature Quantum Field Theory, for example in [11].

Path-integrals and correlation functions

We now apply from the basics the finite-temperature formalism to our Majorana fermion theory for the SB model.

The action corresponding to the SB Majorana-Hamiltonian in the imaginary-time formalism is:

$$S = S_0[\eta] + S_0[\phi] + S_{int}[\eta, \phi] + S_J[\eta] + S_{\theta}[\eta] =$$

$$= \frac{1}{2} \int_{0}^{\beta} d\tau \left(\sum_{i} \eta_{i}(\tau) \partial_{\tau} \eta_{i}(\tau) - i\Delta \eta_{1}(\tau) \eta_{2}(\tau) \right) + \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \left(\phi(\tau) G_{\phi}^{-1}(\tau - \tau') \phi(\tau') \right) + \int_{0}^{\beta} d\tau \left(-i\lambda \phi(\tau) \eta_{2}(\tau) \eta_{3}(\tau) \right) + \int_{0}^{\beta} d\tau \left(\sum_{i} J_{i}(\tau) \eta_{i}(\tau) \right) + \int_{0}^{\beta} d\tau \left(\theta(\tau) \phi(\tau) \right)$$
(34)

Where $G_{\phi}(\tau - \tau') \equiv G_{\phi}^{0}(\tau - \tau') \equiv \langle \mathcal{T}\phi(\tau)\phi(\tau') \rangle_{0}$ is the bare bosonic propagator. and it is defined through the relation $(\hbar = 1)$:

$$\frac{1}{2} \left(\partial_{\tau} - H_B \right) G_{\phi}^0 \left(\tau - \tau' \right) = \delta \left(\tau - \tau' \right) \tag{35}$$

The free-terms actions S_0 are, the fermion-boson term (interaction term S_{int}) of the action has been isolated since its treatment is not as simple as the quadratic terms, and the "source" terms S_J and S_{θ} are non-physical ones, useful for mathematical convenience. We can nevertheless develop a perturbation theory (diagrammatic theory) in λ (actually in α) by Taylor-expanding the exponential expressing the searched correlation function in terms of higher order boson-fermion correlation functions which can then be evaluated by means of Wick's theorem.

The path integral for $S_0 + S_J$ can be evaluated, giving the generator function of correlation-functions:

$$\mathcal{Z}[J] = e^{-\sum_{ij} \int_0^\beta d\tau \int_0^\beta d\tau' J_i(\tau) G^0_{ij}(\tau - \tau') J_j(\tau')} e^{-\int_0^\beta d\tau \int_0^\beta d\tau' \theta(\tau) G^0_\phi(\tau - \tau') \theta(\tau')}$$

Where $G_{ij}(\tau - \tau') \equiv G_{ij}^0(\tau - \tau') \equiv \langle \mathcal{T}\eta_i(\tau)\eta_j(\tau') \rangle_0$ is the bare fermionic propagator, which is defined through an analog equation as (35) for the free Hamiltonian H_0 in (19).

In this formalism, any fermionic correlation function (also called *Green's function*) may be expressed as:

$$\langle \mathcal{T} \eta_i(\tau_1) \dots \eta_k(\tau_n) \rangle = \int \int \mathcal{D}[\eta] \mathcal{D}[\phi] \eta_i(\tau_1) \dots \eta_k(\tau_n) e^{-S_{int}} \mathcal{Z}[J] \big|_{J,\theta=0}$$
$$= \frac{\delta}{\delta J_i(\tau_1)} \dots \frac{\delta}{\delta J_k(\tau_n)} \int \int \mathcal{D}[\eta] \mathcal{D}[\phi] e^{-S_{int}} \mathcal{Z}[J] \big|_{J,\theta=0}$$

For example for a two-fermions correlation function, using the rules of functional differentiation and the correspondence $\int \mathcal{D}[\eta]\eta(\tau)Z[J] = \frac{\delta}{\delta J(\tau)} \int \mathcal{D}[\eta]Z[J]$, and Taylor-expanding S_{int} :

$$\mathcal{G}_{ij}(\tau_{1}-\tau_{2}) = \langle T \eta_{i}(\tau_{1})\eta_{j}(\tau_{2})\rangle = \frac{\delta}{\delta J_{i}(\tau_{1})}\frac{\delta}{\delta J_{j}(\tau_{2})}\int \int \mathcal{D}[\eta]\mathcal{D}[\phi] \left(1+\lambda \int_{0}^{\beta} d\tau \eta_{1}(\tau)\eta_{2}(\tau)\phi(\tau) + \lambda^{2} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau \eta_{1}(\tau)\eta_{2}(\tau)\eta_{1}(\tau')\eta_{2}(\tau')\phi(\tau)\phi(\tau') + \mathcal{O}\left(\lambda^{3}\right)\dots\right) Z[J]\Big|_{J,\theta=0} = G_{ij}^{0}(\tau_{1}-\tau_{2}) + \lambda^{2} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau G_{i1}^{0}(\tau_{1}-\tau)G_{j2}^{0}(\tau_{2}-\tau)G_{12}^{0}(\tau-\tau_{1})G_{\phi}(\tau-\tau') + \dots$$
(36)

Where we developed up to second order and we assumed that $\langle \phi(\tau) \rangle = 0$. The fact that the complete correlation functions are expressed only as infinite convolutions of bare propagators is a result which is known as Wick Theorem. It allows us to simply predict the form of the infinite series of terms by assigning to each propagator a graphical element, and writing the expansions (36) (known as Dyson's expansion) in terms of diagrams whose structure is dictated by the multiple application of the interaction term S_{int} (or vertex) and whose calculation rules (or *Feynman's* rules) are straightforwardly derived from an expansion like (36).

For the SB model, the vertex is:

$$-i\lambda\eta_2\eta_3\phi =$$
(37)

So that:

 $\mathcal{G}_{ij}(\tau) = G_{ij}^0(\tau) + \sum_{lk} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_{il}^0(\tau - \tau_1) \sum_{lk} (\tau_1 - \tau_2) \mathcal{G}_{kj}(\tau_2) = \underbrace{1}_{l} + \underbrace{1}_{3} \underbrace{1}_{3} \underbrace{1}_{l} + \cdots$ and the $\sum_{ij}(\tau)$ function is called the *fermionic self-energy*.

Appendix B: Some Analytical Results

Simple Results

At T = 0 we can obtain some simple analytical results for the cases s = 1, s = 2: s = 0

$$\Gamma(\omega) = -\frac{\lambda^2}{\Lambda} \frac{\pi}{2} \Theta \left(\Lambda^2 - \omega^2\right) = -\alpha \Lambda \frac{\pi}{2} \Theta \left(\Lambda^2 - \omega^2\right)$$
$$\gamma(\omega) = -\frac{\lambda^2}{\Lambda} \frac{1}{2} \ln \left(\frac{\Lambda - \omega}{\Lambda + \omega}\right) = -\alpha \frac{\Lambda}{2} \ln \left(\frac{\Lambda - \omega}{\Lambda + \omega}\right)$$

s = 1

$$\Gamma(\omega) = -\frac{\lambda^2}{\Lambda^2} \pi \left|\omega\right| \Theta \left(\Lambda^2 - \omega^2\right) = -\alpha \frac{\pi}{2} \left|\omega\right| \Theta \left(\Lambda^2 - \omega^2\right)$$
$$\gamma(\omega) = -\frac{\lambda^2}{\Lambda^2} \omega \ln\left(\frac{\Lambda^2 - \omega^2}{\omega^2}\right) = -\alpha \frac{1}{2} \omega \ln\left(\frac{\Lambda^2 - \omega^2}{\omega^2}\right)$$

s=2

$$\Gamma(\omega) = -\frac{3}{2} \frac{\lambda^2}{\Lambda^3} \pi |\omega|^2 \Theta \left(\Lambda^2 - \omega^2\right) = -\alpha \frac{\pi}{2\Lambda} |\omega|^2 \Theta \left(\Lambda^2 - \omega^2\right)$$
$$\gamma(\omega) = -3 \frac{\lambda^2}{\Lambda^2} \omega - \frac{3}{2} \frac{\lambda^2}{\Lambda^3} \omega^2 \ln \left(\frac{\Lambda - \omega}{\Lambda + \omega}\right) = -\alpha \left(\omega + \frac{1}{2\Lambda} \omega^2 \ln \left(\frac{\Lambda - \omega}{\Lambda + \omega}\right)\right)$$

We also note that for a generic s<1, assuming $\omega \ll \Lambda$, we have that :

$$\Gamma(\omega) = -\frac{\lambda^2}{\Lambda^{s+1}} \frac{\pi}{2} (s+1) \left|\omega\right|^s \Theta(\Lambda^2 - \omega^2) = -\frac{\alpha}{\Lambda^{s-1}} \frac{\pi}{2} \left|\omega\right|^s \Theta(\Lambda^2 - \omega^2)$$
(38)

$$\gamma(\omega) = -(s+1)\frac{\lambda^2}{\Lambda^{s+1}}\frac{1}{2}\omega^s \left(\pi \tan\left(\frac{\pi s}{2}\right) + \ln\left(\frac{\Lambda-\omega}{\Lambda+\omega}\right)\right) = -\frac{\alpha}{\Lambda^{s-1}}\frac{\omega^s}{2} \left(\pi \tan\left(\frac{\pi s}{2}\right) + \ln\left(\frac{\Lambda-\omega}{\Lambda+\omega}\right)\right)$$
(39)

We note that the s=0 case, for $\omega \ll \Lambda$ is perfectly fitting the Bloch equation result (15). For the other cases, the same analogy is perfect if we apply the condition $\omega = \Delta$.

Appendix C: Numerical Code and Pade' Approximation

In order to compute the equilibrium correlation function, it is necessary to set up a numerical code that performs the Matsubara sums, the integrals and the required Fourier transforms that are not known analytically. The code has been written in the C++ programming language, and exploits heavily the tested libraries for finite temperature Green's functions written by Olivier Parcollet and Serge Florens, as well as standard routines from Numerical Recipes C.

The program must basically perform the calculations defined in section 2, but it is clear that if we include the self-energy diagrams with *full* propagators we are facing a problem of *self-consistency* that needs to be solved by iteration. The iteration loop works like this: at each cycle the previous propagators are injected as if they where the bare ones, if they do not change considerably (a tolerance must be defined, for instance 10^{-7}) after the "dressing" we have reached the desired self-consistency.

Technically, it is important to note that the convergence of the self-consistent calculation is not guaranteed if the loop is implemented naively. So it has been often necessary to introduce some (well known) convergence tricks like a weighted update of the Green's functions from each iteration, and adiabatic switching of the coupling constants during the first iterations and a careful writing of the Dyson expansions in such a way to minimize the numerical instabilities due to vanishing denominator in a fraction.

The Matsubara Green's functions (21) can be considered as complex-valued functions of a complexvariable, $\mathcal{G}_{ij}(z) : \mathbb{C} \longrightarrow \mathbb{C}$. Indeed, we have exploited in section 2.2.1 the fact that once obtained $\mathcal{G}_{11}(i\omega)$ we can obtain the correlation function $C(\omega)$ by evaluating \mathcal{G}_{11} on the real axis and taking the imaginary part. This is easily performed by a substitution in the analytical formula of the Green's function: $i\omega \longrightarrow \omega + i0^+$. However, if we do not know an analytical formula for \mathcal{G}_{11} but we have a table of data of the values of the Green's function evaluated on the Matsubara frequencies, it is not trivial to find a way to get the value of the function on the real axis.

The idea of Pade' approximation is to interpolate the values of $\mathcal{G}_{11}(i\omega)$ on the imaginary frequency axis with a trial Green's function $\mathcal{G}_{ij}^P(z)$ that is chosen so to represent faithfully the actual unknown $\mathcal{G}_{ij}(z)$ over all the complex plane. Once the optimal function is found, it can be evaluated anywhere on the real axis in order to have access to $C(\omega)$. The trial function (a rational polynomial function) is called the *Pade' approximant*.

In principle if two complex analytical functions have equal values in an infinite (numerable) number of points, the two functions are equal everywhere on the complex plane. Nevertheless, it is a bad idea to interpolate the function over all Matsubara frequencies since the algorithm implementing Pade' approximation is very sensitive to numerical truncation errors, and given the form of the trial function it can be rigorously (and empirically!) demonstrated that there exist an optimal (and quite unpredictable) number of fit frequencies to be taken in order to have a reliable result.

Most of the plot in the sections have been obtained interpolating the first 100-1000 Matsubara frequencies on the real axis.

Appendix D: Useful Formulas

We now list some useful formulas used in the report and some reference or hints about their derivation.

Boson Averages Formula

In section 1.2.2 we made use of the well known formula for averaging over exponentials of bosonic fields:

$$\left\langle e^{\sum_{k} \left(x_{k} a_{k} + y_{k} a_{k}^{\dagger} \right)} \right\rangle = e^{\frac{1}{2} \sum_{k} \left\langle \left(x_{k} a_{k} + y_{k} a_{k}^{\dagger} \right)^{2} \right\rangle}$$

This property is easy to show by employing bosonic coherent states and the disentanglement lemma $e^{A+B} =$ $e^{-\frac{1}{2}[\overline{A},B]}e^{A}e^{B}$

The derivation of the formula is a little long, so we refer the reader to textbooks (for example a succinct derivation is found in Quantum Theory of the Electron Liquid - G. Giuliani and G. Vignale, Cambridge 2005, appendix 21).

Spectral Representation and Matsubara sums

By application of Cauchy's theorem for analytical complex functions, we can find the useful spectral representation valid for any function which vanishes sufficiently fast at infinity and whose poles are on the real axis:

$$G(z) = \int_{-\infty}^{+\infty} d\epsilon \frac{\rho(\epsilon)}{z - \epsilon} \qquad \qquad \rho(\epsilon) = -\frac{1}{\pi} \mathbb{I} m G(\epsilon) \qquad (40)$$

Summing over Matsubara frequencies is very easy when we are dealing with analytical functions with simple poles. Indeed, by using the spectral representation we can convert Matsubara Green's function in integrals of the density of states bringing the dependency on the Matsubara frequency on the denominator. For example, for a convolution of two Green's function (typical situation in the calculation of self-energies):

$$\frac{1}{\beta}\sum_{i\omega_1}G_1\left(i\omega_1\right)G_2\left(i\omega_2-i\omega_1\right) = \frac{1}{\beta}\int_{-\infty}^{+\infty}d\epsilon\int_{-\infty}^{+\infty}d\omega\rho_1\left(\epsilon\right)\rho_2\left(\omega\right)\sum_{i\omega_1}\frac{1}{i\omega_1-\epsilon}\frac{1}{i\omega_2-i\omega_1-\omega_1}$$

By recognizing that $\frac{1}{\beta}$ are the *Cauchy's residues* of the $n_{F/B}(x) = \frac{1}{e^{\beta\omega}\pm 1}$ in the points corresponding respectively to the fermionic or bosonic Matsubara's frequencies, we can define a contour in complex space for which it is easy to prove that any Matsubara sum over functions f(z) with simple poles reduces to a sum of the residues of f multiplied by $n_{F/B}$ evaluated in the poles of the function (see [11] for a pedestrian derivation).

As an example of this quick calculations we report the practical sum formulas useful to derive the expressions for the self-energies of **Appendix** B:

$$\frac{1}{\beta} \sum_{n} \frac{1}{(i\omega_n - \epsilon)(i\omega_n - \epsilon')} = \frac{n_F(\epsilon) - n_F(\epsilon')}{\epsilon - \epsilon'}$$
$$\frac{1}{\beta} \sum_{n} \frac{1}{(i\nu_n - \epsilon)(i\nu_n - \epsilon')} = -\frac{n_B(\epsilon) - n_B(\epsilon')}{\epsilon - \epsilon'}$$

Exact connection between \mathcal{G}_{ϕ} and $\chi^{''}$:

Being this relation a non-standard one, we sketch in this subsection the complete derivation.

Without introducing Majorana Fermions, we can start from the exact spin-boson action (with the artificial spin-source term):

$$S\left[\sigma, \phi, J\right] = \int_{0}^{\beta} d\tau \left(\frac{\Delta}{2}\sigma_{z}\left(\tau\right)\right) + S_{free} + \sum_{i} \int_{0}^{\beta} d\tau \left(J_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\right) + \frac{34}{2} \left(J_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\right) + \frac{34}{2} \left(J_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\right) + \frac{34}{2} \left(J_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\right) + \frac{34}{2} \left(J_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\sigma_{i}\left(\tau\right)\right) + \frac{34}{2} \left(J_{i}\left(\tau\right)\sigma_{i}\left(\tau$$

$$+\frac{\lambda}{2}\int_{0}^{\beta}d\tau\left(\sigma_{x}\phi\left(\tau\right)\right)+\int_{0}^{\beta}d\tau'\int_{0}^{\beta}d\tau\left(G_{\phi}^{-1}\left(\tau-\tau'\right)\phi\left(\tau\right)\phi\left(\tau'\right)\right)$$

Where S_{free} indicates the action relative to free spins, usually called the *Berry* action, which is not explicited since its simple form relies on spin coherent states, whose introduction and definition is beyond the interests of the present analysis.

We can perform the redefinition of the fields $\tilde{\phi} = \frac{J}{\lambda} + \phi$ without changing the path-integral partition function:

$$\mathcal{Z} = \int \mathcal{D}\phi \mathcal{D}\sigma e^{-S[\sigma, \phi, J]} = \int \mathcal{D}\tilde{\phi} \mathcal{D}\sigma e^{-S\left[\sigma, \tilde{\phi}, J\right]}$$

The spin-spin correlators are then found from the partition function as:

$$\chi\left(\tau\right) = \left\langle \mathcal{T}\sigma_{x}\left(\tau\right)\sigma_{x}\left(0\right)\right\rangle = \frac{1}{\mathcal{Z}}\left.\frac{\delta^{2}\mathcal{Z}}{\delta J\left(\tau\right)\delta J\left(0\right)}\right|_{J=0} =$$

$$= \frac{1}{\mathcal{Z}} \left. \frac{\delta^2}{\delta J(\tau)} \int \mathcal{D}\tilde{\phi}\mathcal{D}\sigma \int_0^\beta d\tau \left(G_\phi^{-1}(\tau - \tau') \left[\frac{-4\phi(\tau)}{\lambda} + \frac{8\phi(\tau)}{\lambda^2} \right] \right) e^{-S[\sigma, \,\tilde{\phi}, \, J]} \right|_{J=0} =$$

$$=\frac{8}{\lambda^{2}}G_{\phi}^{-1}(-\tau)+\frac{16}{\lambda^{2}}\int_{0}^{\beta}d\tau_{1}\int_{0}^{\beta}d\tau_{2}G_{\phi}^{-1}(\tau_{1}-\tau)G_{\phi}(\tau_{2})\langle\phi(\tau_{1})\phi(\tau_{2})\rangle$$

So, in frequency domain $(\langle \mathcal{T}\phi(\tau)\phi(0)\rangle = \mathcal{G}_{\phi}(\tau))$:

$$\chi\left(i\nu_{n}\right) = \frac{16}{\lambda^{2}} \frac{\mathcal{G}_{\phi}\left(i\nu_{n}\right)}{G_{\phi}\left(i\nu_{n}\right)^{2}} + \frac{8}{\lambda^{2}} \frac{1}{G_{\phi}\left(i\nu_{n}\right)}$$

which corresponds exactly to (31).

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