REDFIELD DYNAMICS OF A QUANTUM SPHERICAL SPIN

DINÁMICA DE REDFIELD DEL SPIN CUÁNTICO ESFÉRICO

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The temporal evolution of a quantum spherical spin in contact with a thermal bath is studied by solving the exact Redfield equation, in order to evaluate the effect of the frequently used Lindblad approximation. This simple model can be used as a starting point for the study of more complex open quantum systems. Significant discrepancies are observed for short times. In the equilibrium state both models give identical results, as expected.

Mediante la solución numérica de la ecuación exacta de Redfield, se estudia cuantitativamente el efecto de la aproximación de Lindblad sobre la dinámica temporal de un spin cuántico esférico en contacto con un baño térmico. Se utiliza este caso simple como punto de partida para el análisis de sistemas cuánticos abiertos más complejos. Se evidencian discrepancias notables para tiempos cortos, así como la coincidencia de los resultados para el estado de equilibrio.

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I. INTRODUCTION

It is well known that real quantum systems are not truly isolated from the environment. This implies that the comprehension of the properties of real quantum systems is connected with the proper understanding of the effects of dissipation and decoherence in quantum mechanics. This is a subject that goes beyond academic interest in the foundation of quantum mechanics and it is relevant to understand experimental works on qubits and quantum information processing.

Any theory for a quantum system that exchanges energy with its environment should lead to a master equation which satisfies three basic conditions: preserves the Hermiticity of the density matrix, preserves the trace of the density matrix and the probability of all possible states is positive [1, 2]. There are two main methods to find such master equations. The first one, Lindblad's approach, is phenomenological, and basically tries to build such master equation satisfying the conditions above. In the second approach, Bloch-Redfield's, one takes the evolution of a system and its environment and traces over the environment degrees-of-freedom. Unfortunately, in most cases one has to treat the system-environment interaction perturbatively.

In this work we compare the performance of both methods in a simple model. We first show, following a standard approach, how the Lindblad master equation can be understood as a special case of the Redfield master equation. We also make clear how the approximation made in going from the later to the first changes the behaviour of the model, specially on short time scales.

II. THE MODEL

The spherical spin model, in its classical form, was introduced by Berlin and Kac [3] as an alternative to the Onsager solution for the 2D Ising model. The classical spherical spin model is formally identical to the Ising model, with a global constraint to ensure the analytical result for the partition function. This model has been extended to different quantum versions [4, 5] in order to reproduce the right low-temperature behaviour. Both models are remarkable for having exact solutions in many settings and a non mean-field type critical behaviour.

In absence of magnetic field, the Hamiltonian can be written as

$$\hat{H} = \sum_n \left(\frac{g}{2}\hat{p}_n^2 + \frac{\mu(t)}{2}\hat{s}_n^2 - \sum_{j=1}^{d} J\hat{s}_n\hat{s}_{n+e_j} \right), \quad (1)$$

where the Lagrange multiplier $\mu(t)$ is chosen to satisfy the constraint

$$\left\langle \sum_n \hat{s}_n^2 \right\rangle = N. \quad (2)$$

The simplest possible approximation to deal with this problem, is the mean field one. It translates into the solution of the following one spin problem:

$$\hat{H} = \frac{g}{2}\hat{p}^2 + \frac{\mu(t)}{2}\hat{s}^2, \quad (3)$$

$$\left\langle \hat{s}^2 \right\rangle = 1. \quad (4)$$

Operators satisfy the commutation relation

$$[\hat{s}, \hat{p}] = i\hbar. \quad (5)$$

The Hamiltonian in (3) is equivalent to

$$\hat{H} = \hbar\omega(t)\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right), \tag{6}$$

where creation and annihilation operators are introduced in the usual way:

$$\hat{s} = \sqrt{\frac{\hbar g}{2\omega(t)}}\left(\hat{a}^{\dagger} + \hat{a}\right), \qquad \hat{p} = i\sqrt{\frac{\hbar\omega(t)}{2g}}\left(\hat{a}^{\dagger} - \hat{a}\right) \tag{7}$$

and

$$\omega(t) = \sqrt{\mu(t)g}. \tag{8}$$

Notice that equation (6) can be understood as a quantum harmonic oscillator with variable frequency. This is a problem that have been largely studied in the past. Indeed it is an archetypical problem in quantum optics, see for example [6] and references therein but also the particular solution to similar problems described in [7]. Historically, it is worth to mention the study by [8] of a decaying Fabry-Pérot cavity. In short, the usual motivation to study this kind of hamiltonians in quantum optics comes from the interest in the understanding of the interactions of an oscillator with an environment, that may act as a time dependent damping of the frequency, or alternatively by the presence of varying external fields that my act as controlled modulators of this frequency.

However, the spherical constraint (4) in this model implies that

$$\omega(t) = \frac{\hbar g}{2}\left(\left\langle\hat{a}^{\dagger}\hat{a}^{\dagger}\right\rangle + \langle\hat{a}\hat{a}\rangle + 2\left\langle\hat{a}^{\dagger}\hat{a}\right\rangle + 1\right). \tag{9}$$

and defines a model that differentiate from the ones usually studied in quantum optics. In summary, our work could be understood, starting directly from equation (6) as the study of the interaction with the environment of a very particular case of a quantum Hamiltonian with variable frequency, as usually done in quantum optics. But, alternatively, it may be understood as a mean field approximation to the quantum spherical spin defined in (1) and (2).

III. OPEN QUANTUM SYSTEMS

The temporal evolution of the density matrix $\hat{P}$ of a quantum system is given by the Liouville-von Neumann equation:

$$\dot{\hat{P}} = -\frac{i}{\hbar}\left[\hat{H}, \hat{P}\right], \tag{10}$$

where $\hat{H}$ is the Hamiltonian of the system.

Let us consider an open quantum system S in contact with another quantum system B, called the environment. The Hamiltonian of the total system $S + B$ is

$$\hat{H}(t) = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}, \tag{11}$$

where $\hat{H}_{SB}$ is the interaction Hamiltonian between S and B. From now on, we will call S the reduced system.

In the interaction representation, the density matrix $\hat{\tilde{\rho}}$ of the reduced system satisfies the Redfield equation

$$\frac{d\hat{\tilde{\rho}}(t)}{dt} = -\frac{1}{\hbar^2}\int_0^t dt' \,\mathrm{Tr}_B\left[\hat{\tilde{H}}_{SB}(t), \left[\hat{\tilde{H}}_{SB}(t'), \hat{\tilde{\rho}}(t') \otimes \hat{R}_0\right]\right], \tag{12}$$

where the well known Born approximation has been used [1,2], i.e., the coupling between the reduced system and the environment is weak. Here $\hat{R}_0$ is the density matrix of the environment.

A commonly used approximation is the substitution of the upper integration limit in Eq. (12) for infinity. The result is known as Lindblad equation:

$$\frac{d\hat{\tilde{\rho}}(t)}{dt} = -\frac{1}{\hbar^2}\int_0^\infty dt' \,\mathrm{Tr}_B\left[\hat{\tilde{H}}_{SB}(t), \left[\hat{\tilde{H}}_{SB}(t'), \hat{\tilde{\rho}}(t') \otimes \hat{R}_0\right]\right]. \tag{13}$$

This approximation is valid if the time scale over which the state of the reduced system varies substantially is large compared to the time scale over which the reservoir correlation functions decay appreciably [1]. If this condition does not hold, Eq. (13) is no longer valid and Eq. (12) must be used to describe the time evolution of the reduced system. For example, in photosynthetic complexes quantum coherence may play a fundamental role in the highly efficient transport of excitations, even in the presence of noise and high temperatures [9].

Equations (12) and (13) are difficult to solve, even for simple models. Instead, equations for the time evolution of some physical observables are solved [2]. The purpose of this work is to solve a set of equations derived from (12) in order to estimate the magnitude of the approximation in (13). We have chosen the quantum spherical spin model [4], whose Lindblad dynamics have been recently studied in [10].

IV. REDFIELD DYNAMICS

Following [2], in the limit of zero temperature equation (12) for a quantum harmonic oscillator of frequency $\omega(t)$ in an environment consistent of an infinite set of harmonic oscillators takes the form

$$\frac{d\hat{\tilde{\rho}}(t)}{dt} = -i\Delta(t)\left[\hat{a}^{\dagger}\hat{a}, \hat{\tilde{\rho}}\right] + \frac{\gamma(t)}{2}\left(2\hat{a}\hat{\tilde{\rho}}\hat{a}^{\dagger} - \hat{a}^{\dagger}\hat{a}\hat{\tilde{\rho}} - \hat{\tilde{\rho}}\hat{a}^{\dagger}\hat{a}\right), \tag{14}$$

where

$$\gamma(t) = 2\,Re\,\{\alpha(t)\}\,, \quad \Delta(t) = Im\,\{\alpha(t)\} \tag{15}$$

and

$$\alpha(t) = \alpha_L + \alpha_R(t), \tag{16}$$

with,

$$\alpha_L = \int_0^\infty d\tau \int_0^\infty d\omega' \exp\left[-i\left(\omega' - \omega(\tau)\right)\tau\right] g(\omega')|\kappa(\omega')|^2 \tag{17}$$

and,

$$\alpha_R(t) = -\int_t^{\infty} d\tau \int_0^{\infty} d\omega' \exp\left[-i\left(\omega' - \omega(\tau)\right)\tau\right] g(\omega')|\kappa(\omega')|^2. \quad (18)$$

We have explicitly separated the Lindblad, α_L, and Redfield, α_R, contributions. We have also defined $\gamma_L = 2\, Re\{\alpha_L\}$, $\gamma_R(t) = 2\, Re\{\alpha_R(t)\}$, $\Delta_L = Im\{\alpha_L\}$, $\Delta_R(t) = Im\{\alpha_R(t)\}$.

In (17) and (18), $g(\omega)$ is the environment density of modes, and $\kappa(\omega)$ is the coupling constant from the interaction Hamiltonian $\hat{H}_{SB}$, which in the rotating wave approximation takes the form

$$\hat{H}_{SB} = \hbar \sum_j \left(\kappa_j^* \hat{a}\hat{b}_j^\dagger + \kappa_j \hat{a}^\dagger \hat{b}_j\right). \quad (19)$$

We have assumed $g(\omega)|\kappa(\omega)|^2$ linear in ω with a cutoff frequency ω_{max}:

$$g(\omega)\,|\kappa(\omega)|^2 = C\omega\,\theta(\omega_{max} - \omega), \quad (20)$$

where C is a constant (irrelevant after adimensionalization) and $\theta(x)$ is the Heaviside step function.

Due to the presence of $\omega(t)$ in the integrands of (17) and (18), this problem must be solved in self-consistent form, using Redfield equation (14) and the spherical constraint (4). Following [10], we have taken the constant value $\omega(t) = \omega_0$ in the evaluation of both integrals. This is equivalent to consider the spherical constraint coming from a second bath, whose relaxation time is much shorter than the thermal one. Anyway, in next section we present the results for another, non-trivial $\omega(t)$ dependence.

With the choice (20) and after some manipulation one can show that:

$$\gamma_L = 2\pi\omega_0, \qquad \Delta_L = -\omega_{max} - \omega_0 \ln\left(\frac{\omega_{max}}{\omega_0} - 1\right) \quad (21)$$

$$\gamma_R(t) = -2\omega_0\left[\pi - \mathrm{Si}\left((\omega_{max} - \omega_0)t\right) - \mathrm{Si}\left(\omega_0 t\right)\right] + \\ + \frac{4}{t}\sin\left(\frac{\omega_{max}t}{2}\right)\sin\left(\frac{(\omega_{max} - 2\omega_0)t}{2}\right) \quad (22)$$

$$\Delta_R(t) = \omega_0\left[\mathrm{Ci}\left((\omega_{max} - \omega_0)t\right) + \mathrm{Ci}\left(\omega_0 t\right)\right] + \\ +\frac{2}{t}\sin\left(\frac{\omega_{max}t}{2}\right)\cos\left(\frac{(\omega_{max} - 2\omega_0)t}{2}\right)], \quad (23)$$

where

$$\mathrm{Si}(z) = \int_0^z \frac{\sin t}{t}dt, \qquad \mathrm{Ci}(z) = -\int_z^{\infty} \frac{\cos t}{t}dt. \quad (24)$$

V. RESULTS AND DISCUSSION

From (14) the following temporal evolution equations are obtained:

$$\frac{\partial\langle\hat{a}\rangle}{\partial t} = -\left[\frac{\gamma(t)}{2} + i\left(\omega(t) + \Delta(t)\right)\right]\langle\hat{a}\rangle, \quad \frac{\partial\left\langle\hat{a}^\dagger\hat{a}\right\rangle}{\partial t} = -\gamma(t)\left\langle\hat{a}^\dagger\hat{a}\right\rangle \quad (25)$$

and

$$\frac{\partial\langle\hat{a}\hat{a}\rangle}{\partial t} = -2\left[\frac{\gamma(t)}{2} + i\left(\omega(t) + \Delta(t)\right)\right]\langle\hat{a}\hat{a}\rangle. \quad (26)$$

Numerical solutions of the system (25)-(26) are shown in Figure 1 for different values of $\Omega = \omega_{max}/\omega_0$ and $\Gamma = \hbar g/\gamma_L$. Frequency $\omega(t)$ (in units of $\hbar g/2$) and magnetization $m(t)$ are plotted as functions of time (in units of $1/\gamma_L$). The dashed line corresponds to Lindblad approximation, and the solid line to Redfield dynamics.

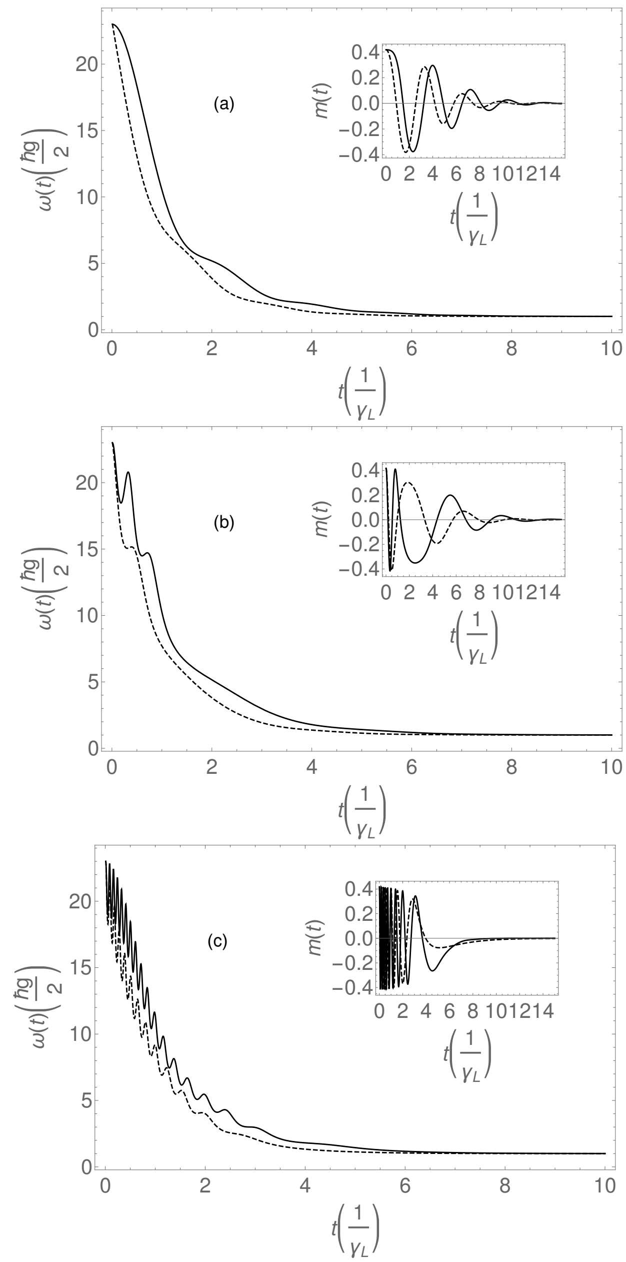

Figure 1. Frequency $\omega(t)$ (in units of $\hbar g/2$) and magnetization $m(t)$ vs time (in units of $1/\gamma_L$). Dashed line: Lindblad approximation, solid line: Redfield dynamics. (a) $\Gamma = 0.01$, $\Omega = 10$, (b) $\Gamma = 0.5$, $\Omega = 10$, (c) $\Gamma = 2$, $\Omega = 10$.

The long time behaviour of both approximations is the same, however, clear discrepancies appear at short time scales before the equilibrium. Remarkably, the longer relaxation times and the more pronounced oscillations of the Redfield dynamics.

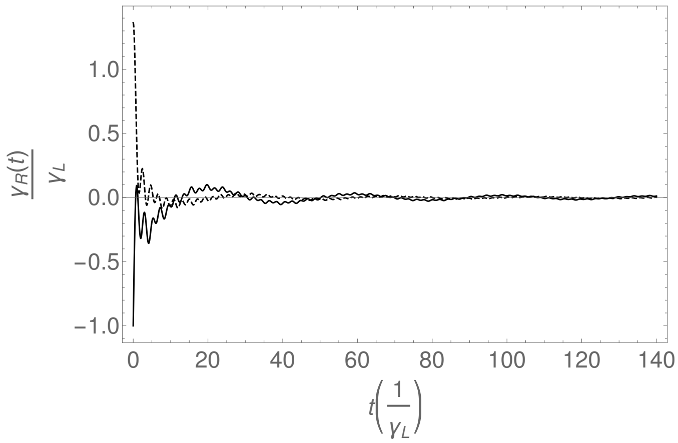

Figure 2. Magnitudes $\gamma_R(t)$ (solid line) and $\Delta_R(t)$ (dashed line) in units of γ_L vs time (in units of $1/\gamma_L$).

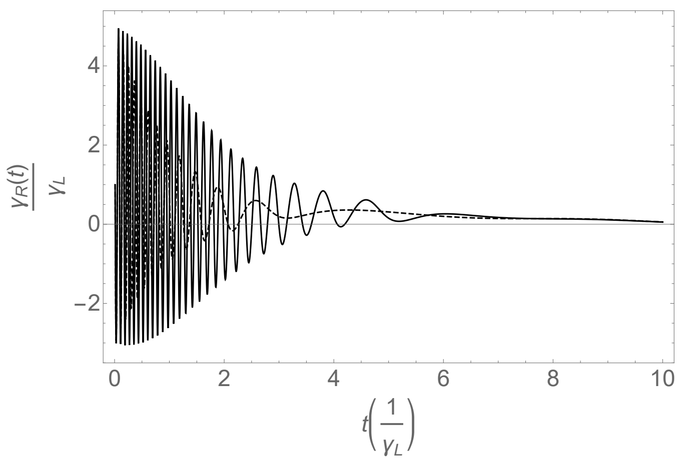

Figure 3. Decay coefficient $\gamma(t) - 4\, Im\, \langle \hat{a}\hat{a}\rangle$ for $\omega(t)$ in units of γ_L vs time (in units of $1/\gamma_L$). Solid line: Redfield dynamics, dashed line: Lindblad approximation.

The longer relaxation time can be traced back to the role of $\gamma(t)$ in the dynamics of the system. One must notice first that in the set of equations (25)-(26), $\frac{1}{\gamma(t)}$ defines a time dependent relaxation scale of the model. It follows that $\gamma(t) = \gamma_L + \gamma_R(t)$ where the behaviour of $\gamma_R(t)$ (in units of γ_L) as function of time (in units of $1/\gamma_L$) is shown in Figure 2. From the figure, it is evident that $\gamma_R(t)$ is negative in all the relevant time interval. This immediately implies that $\gamma(t) = \gamma_L + \gamma_R(t)$ is smaller than γ_L which is consistent with the larger relaxation time of the Redfield dynamics.

On the other hand, $\omega(t)$ satisfies the equation

$$\frac{\partial \omega(t)}{\partial t} = -\left[\gamma(t) - 4\, Im\, \langle \hat{a}\hat{a}\rangle\right] \omega(t) - \left[\gamma(t) - 4\Delta(t)\, Im\, \langle \hat{a}\hat{a}\rangle\right]. \quad (27)$$

Due to the temporal behaviour of $\gamma(t)$ and $\Delta(t)$, shown in Figure 2, the second term in the right hand side of (27) becomes small very fast, then

$$\frac{\partial \omega(t)}{\partial t} \approx -\left[\gamma(t) - 4\, Im\, \langle \hat{a}\hat{a}\rangle\right] \omega(t). \quad (28)$$

Therefore, the larger frequency for the oscillations of $\omega(t)$ observed in Redfield approach can be traced back to the more complex structure of the decay coefficient in (28), as shown in Figure 3.

In Figure 4 we show the results obtained when we calculate integrals in (17) and (18) using $\omega(t) = \omega_0\, e^{-a\,t}$, where a is a positive constant. We have taken the same parameters as in Figure 1c. Comparison between both graphics suggests the robustness of the results with respect to the choice of $\omega(t)$ in these integrals.

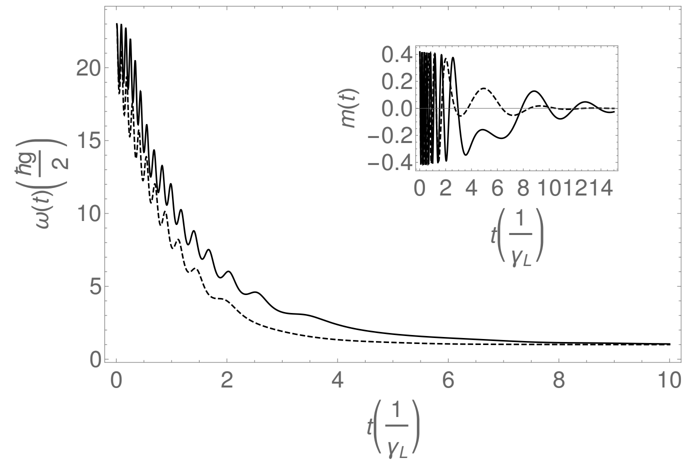

Figure 4. Frequency $\omega(t)$ (in units of $\hbar g/2$) and magnetization $m(t)$ vs time (in units of $1/\gamma_L$). Dashed line: Lindblad approximation, solid line: Redfield dynamics. The choice $\omega(t) = \omega_0\, e^{-a\,t}$ in Eqs. (17) and (18) has been used.

VI. CONCLUSIONS

We have quantitatively evaluated the effects of the Lindblad approximation in the simple case of the mean field quantum spherical spin model by considering the numerical solution of the exact Redfield equation. As expected, the long time predictions of both approximations is the same, however, important discrepancies are evident at short time scales. These discrepancies are explained unveiling the role of the Redfield contributions to the dynamical equations of the model. In particular, we can explain why Redfield approximation has longer time scales and more frequent oscillations.

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