The role of the initial system-bath correlations in the dynamics of open quantum systems

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Abstract. In the typical derivation of the master equation for the system interacting with a bath it is assumed that initially system and bath are uncorrelated. However, in many physical situations this is not the case. Here, we study the influence of the initial system-bath correlations on the dynamics of the system. As a toy model we will consider a particle with spin 1/2 interacting with a spin bath through an intermediate spin. On the one hand, we use the technique of correlated projection operators to construct a time convolutionless (TCL) master equation with an inhomogenous term and on the other hand we will solve exactly the equation for the evolution operator of the total system. This allows us not only to study the influence of the initial correlations on the system-bath dynamics, but also the influence of the initial system-bath correlations on the accuracy of TCL approach.

1. Introduction

In this paper, we study the reduced dynamics of a spin coupled to a spin bath through an intermediate spin. The main goals of this work are the following: Firstly, to use the exact solution of the studied model derived here to show the importance of initial system-bath correlations. Secondly, to demonstrate that in the case where initial system-bath correlations are present, a rigorously derived master equation will contain an inhomogeneous term which substantially affects the dynamics of the reduced system. Thirdly, by comparing the exact and approximate solutions of the master equation, to understand the limitations of the approximate correlated projector method in the presence of an inhomogeneous term in the quantum master equation.

2. Model

We consider the model of a central spin coupled to a spin bath through an intermediate spin. The interaction Hamiltonian is given by

$$H = H_{SI} + H_{IB}, \tag{1}$$

where

$$H_{SI} = \frac{\gamma}{2}\left(\sigma_+\tau_- + \sigma_-\tau_+\right)$$

is the Hamiltonian describing spin-spin interactions and $\sigma_\pm, \tau_\pm$ are the creation and annihilation operators for the central spin and the intermediate spin, respectively, while γ denotes the strength of the spin-spin interaction. In this work units are chosen such that $k_B = \hbar = 1$.

The interaction between the intermediate spin and the spin bath is described by

$$H_{IB} = \frac{\alpha}{2\sqrt{N}} \left(\tau_+ J_- + \tau_- J_+\right), \tag{2}$$

where $J_\pm = \sum_{i=1}^{N} \sigma_\pm^i$, where $\sigma_\pm^i$ are the creation and annihilation operators for the ith spin in the bath, α is the strength of interaction, and N denotes the number of bath spins. The factor $1/\sqrt{N}$ is introduced as usual [1] to obtain the correct behaviour in the thermodynamic limit $(N \to \infty)$.

3. Exact dynamics

To describe the exact dynamics of the total system we need to specify an initial state of the total system given by the density operator $\rho_{\rm tot}(0)$, and to find an evolution operator of the total system $U(t)$ in an explicit form, as

$$U(t) = \exp[-iHt]. \tag{3}$$

With the knowledge of the evolution operator and the initial state of the total system, the reduced dynamics of the central spin can be found as

$$\rho^S(t) = {\rm tr}_{IB}\{U(t)\rho_{\rm tot}(0)U^\dagger(t)\}. \tag{4}$$

In this work, we will consider an initially correlated state between the central spin and the intermediate spin, while the rest of the bath is assumed to be unpolarized.

The initial state of the total system reads,

$$\rho_{\rm tot}(0) = \rho_{SI}(0) \otimes \rho_B(0), \tag{5}$$

where the initial state $\rho_{SI}(0)$ is given by the generic X-like two-qubit density matrix, as

$$\rho_{SI}(0) = \begin{pmatrix} \rho_{11}^0 & 0 & 0 & \rho_{14}^0 \\ 0 & \rho_{22}^0 & \rho_{23}^0 & 0 \\ 0 & \rho_{32}^0 & \rho_{33}^0 & 0 \\ \rho_{41}^0 & 0 & 0 & \rho_{44}^0 \end{pmatrix}, \tag{6}$$

while $\rho_B(0)$ is the density matrix describing the bath of N unpolarized spin-1/2 particles, given by

$$\rho_B(0) = \frac{I_B}{2^N}. \tag{7}$$

The evolution operator can be found analytically from Schrödinger's equation $i\frac{\partial}{\partial t}U = HU$. Then, using Eq. (4), we derive the reduced density matrix of the central spin. The typical behaviour of the probability to find the central spin in the excited state for different initial correlations is shown in Fig. 1.

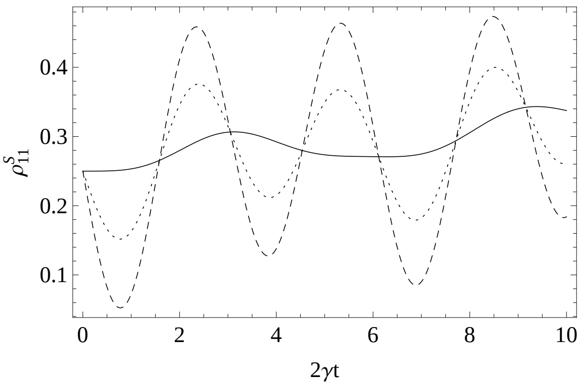

Figure 1. Exact solution for $\rho_{23}^0 = \rho_{32}^0 = 0$ (solid line), $\rho_{23}^0 = -\rho_{32}^0 = 0.2i$ (dashed line), $\rho_{23}^0 = -\rho_{32}^0 = 0.1i$ (dotted line). Other parameters: $N = 10$, $\rho_{11}^0 = 0$, $\rho_{22}^0 = 0.25$, $\rho_{33}^0 = 0.25$, $\rho_{44}^0 = 0.5$, $\alpha = \gamma/4$.

4. Time-convolutionless master equation

The idea behind applying projection operator techniques to open quantum systems is to consider the operation of tracing over the environment as a formal projection $\rho \mapsto \mathcal{P}\rho$ in the state space of the total system [2, 3]. The superoperator $\mathcal{P}$ has the property of a projection operator, that is $\mathcal{P}^2 = \mathcal{P}$, and the density matrix $\mathcal{P}\rho$ is said to be the relevant part of the density ρ of the total system. Correspondingly, a projector $\mathcal{I} - \mathcal{P}$ or $\rho \mapsto \mathcal{Q}\rho$ is defined as a projection onto the irrelevant part of the total density matrix.

An exact master equation for the relevant part of ρ is obtained by removing the dependence of the system's dynamics on the full history of the system, and formulating a time-local equation of motion, which is given by [2]

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t) + \mathcal{I}(t)\mathcal{Q}\rho(0). \tag{8}$$

This equation is called the time-convolutionless (TCL) master equation, and $\mathcal{K}(t)$ is a time-dependent superoperator, which is referred to as the TCL generator. In general, the term proportional to $\mathcal{Q}\rho(0)$ on the right-hand side of Eq. (8) is called the inhomogeneous term.

The TCL generator and inhomogeneous term can be perturbatively expanded in powers of H. The expansion to second order is given by

$$\mathcal{K}(t) = \mathcal{P}\mathcal{L}(t)\mathcal{P} + \int_0^t ds \mathcal{P}\mathcal{L}(t)\mathcal{L}(s)\mathcal{P}, \tag{9}$$

$$\mathcal{I}(t) = \mathcal{P}\mathcal{L}(t)\mathcal{Q} + \int_0^t ds \mathcal{P}\mathcal{L}(t)\mathcal{L}(s)Q. \tag{10}$$

It was shown Fisher and Breuer [4] that a general class of projection superoperators can be represented as follows:

$$\mathcal{P}\rho = \sum_i \mathrm{tr}_E\{A_i\rho\} \otimes B_i, \tag{11}$$

where $\{A_i\}$ and $\{B_i\}$ are two sets of linearly independent Hermitian operators on $\mathcal{H}_E$ satisfying the relations

$$\mathrm{tr}_E\{B_i A_j\} \quad = \quad \delta_{ij}, \tag{12}$$

$$\sum_i (\mathrm{tr}_E B_i) A_i = I_E, \tag{13}$$

$$\sum_i A_i^T \otimes B_i \geq 0. \tag{14}$$

Once $\mathcal{P}$ is chosen, the dynamics of the open system is uniquely determined by the dynamical variables

$$\rho_i(t) = \mathrm{tr}_E\{A_i \rho(t)\}. \tag{15}$$

The connection to the reduced density matrix is simply given by

$$\rho_S(t) = \sum_i \rho_i(t), \tag{16}$$

and the normalization condition reads

$$\mathrm{tr}_S\, \rho_S(t) = \sum_i \mathrm{tr}_S\, \rho_i(t) = 1. \tag{17}$$

In this way, the correlation projection operator for our model is chosen as

$$\mathcal{P}\rho = \sum_{j=0,\frac{1}{2}}^{N/2} \sum_{m=-j}^{j} \mathrm{tr}_{IB}\left(\Pi_{jm}^{+}\rho\right) \otimes \frac{\Pi_{jm}^{+}}{N_j} + \sum_{j=0,\frac{1}{2}}^{N/2} \sum_{m=-j}^{j} \mathrm{tr}_{IB}\left(\Pi_{jm}^{-}\rho\right) \otimes \frac{\Pi_{jm}^{-}}{N_j}, \tag{18}$$

where $\Pi_{jm}^{\pm} = |\pm\rangle\langle\pm| \otimes |j,m\rangle\langle j,m|$. The $|\pm\rangle$ are eigenvectors, τ_z and $|j,m\rangle$ are eigenvectors of the bath operators J_z and J^2, with corresponding eigenvalues m and $j(j+1)$. It is convenient to introduce the notation

$$N_j = \mathrm{tr}\Pi_{jm}^{\pm} = \frac{2j+1}{\frac{N}{2}+j+1} \frac{N!}{(\frac{N}{2}+j)!\frac{N}{2}-j)!}. \tag{19}$$

Then, the TCL master equation with projection operator (18) has the form of a system of coupled equations

$$\dot{r}_{jm} = -\frac{\alpha^2}{2N} b(j,-m)(r_{jm} - R_{jm-1})t - \frac{\gamma^2}{4}(r_{jm}\sigma^-\sigma^+ + \sigma^-\sigma^+ r_{jm} - 2\sigma^- R_{jm}\sigma^+)t + \Lambda_1 \tag{20}$$

$$\dot{R}_{jm} = -\frac{\alpha^2}{2N} b(j,m)(R_{jm} - r_{jm+1})t - \frac{\gamma^2}{4}(R_{jm}\sigma^+\sigma^- + \sigma^+\sigma^- R_{jm} - 2\sigma^+ r_{jm}\sigma^+)t + \Lambda_2, \tag{21}$$

where $b(j,m) = (j-m)(j+m+1)$, $R_{jm} = \mathrm{tr}_{IB}\left(\Pi_{jm}^{+}\rho\right)$, and $r_{jm} = \mathrm{tr}_{IB}\left(\Pi_{jm}^{-}\rho\right)$. The inhomogeneity is given by

$$\Lambda_1 = \begin{pmatrix} i\frac{\gamma}{2^{N+1}}(\rho_{23}^0 - \rho_{32}^0) & 0 \\ 0 & 0 \end{pmatrix}, \tag{22}$$

$$\Lambda_2 = \begin{pmatrix} 0 & 0 \\ 0 & -i\frac{\gamma}{2^{N+1}}(\rho_{23}^0 - \rho_{32}^0) \end{pmatrix}. \tag{23}$$

The exact dynamics of the probability to find the central spin in the excited state following from Eq. (21) and Eq. (22) is shown in Fig. 2.

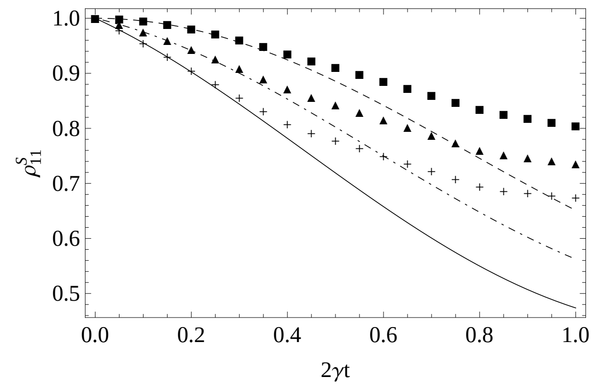

Figure 2. TCL 2 solution for $\rho_{23}^0 = 0.2i$, $\rho_{32}^0 = -0.2i$ (cross dot); for comparison, the solid curve is the exact solution; $\rho_{23}^0 = 0.1i$, $\rho_{32}^0 = -0.1i$ (triangle dot); for comparison, the dot-dashed curve is the exact solution; $\rho_{23}^0 = \rho_{32}^0 = 0$ (square dot); for comparison, the dashed curve is the exact solution. The other parameters are chosen as: $\alpha = \gamma/2$, $\rho_{11}^0 = \rho_{22}^0 = 0.5$, $\rho_{33}^0 = \rho_{44}^0 = 0$, $N = 30$.

5. Conclusion

We have found an exact solution for a simple spin system coupled to a spin bath through an intermediate spin. We have studied the dynamics of the system and have shown that the initial correlations between the central spin and the intermediate spin have a strong influence on the dynamics of the central spin. On the other hand, the dynamics of the central spin are weakly dependent on the number of bath spins. In addition to the exact solution, an approximate TCL2 master equation was derived with the help of the projection correlation operator technique. The derived equation explicitly takes into account initial correlations between the central spin and the intermediate spin. The solution of the master equation was compared with the exact solution. It is shown that the approximate technique gives good results for short time dynamics.

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