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Effective Hamiltonian approach to the non-Markovian dynamics in a spin bath

E Ferraro¹, H-P Breuer², A Napoli¹ and A Messina¹

¹ CNISM and Dipartimento di Scienze Fisiche ed Astronomiche, Università di Palermo, via Archirafi 36, 90123 Palermo, Italy
² Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany

E-mail: ferraro@fisica.unipa.it and breuer@physik.uni-freiburg.de

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Abstract
We investigate the dynamics of a central spin that is coupled to a bath of spins through a non-uniform distribution of coupling constants. Simple analytical arguments based on master equation techniques as well as numerical simulations of the full von Neumann equation of the total system show that the short-time damping and decoherence behaviour of the central spin can be modelled accurately through an effective Hamiltonian involving a single effective coupling constant. The reduced short-time dynamics of the central spin is thus reproduced by an analytically solvable effective Hamiltonian model.

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1. Introduction
Recent years have seen a growing interest in spin systems, particularly in connection with serious efforts in attempting to build scalable quantum computers [1–6]. Electron spins in semiconductor structures are indeed ideal candidates to realize the basic element in quantum information processing, namely a qubit [7]. In this sense it is extremely important to understand qualitatively and quantitatively all aspects of electron spin decoherence in solids that represent the main obstacle in quantum computing and information processing. A serious possible limitation of spin coherence in semiconductors is the hyperfine interaction with the surrounding nuclear spins [8]. It can lead to spin decoherence either through direct electron–nuclear spin flips or through an effective intra-bath interaction.

In this paper we consider a system composed of a single electron spin non-uniformly coupled to a bath of $N$ nuclear spins that is modelled by the Hamiltonian

$$H = \frac{\omega_0}{2}\sigma_3 + \sum_{k=1}^{N} \frac{\omega}{2}\sigma_k^3 + \sum_{k=1}^{N} \alpha_k \vec{\sigma} \cdot \vec{\sigma}_k,$$  

(1)

where the Pauli operators $\vec{\sigma}$ and $\vec{\sigma}_k$ act on the Hilbert space of the central spin and of the $k$th bath spin, respectively. The coefficients $\alpha_k$, $k = 1, \ldots, N$, take into account the strength of the spin–bath coupling and $\omega_0$ (\omega) quantifies the Zeeman splitting due to an external magnetic field acting on the central spin (bath spins). The interest towards the model (1), witnessed by the numerous papers that appeared in the literature during the last few years [9–12], undoubtedly stems from its versatility in describing very different systems in various physical scenarios with many applications. In the case of a non-uniform distribution of the coupling constants $\alpha_k$, the analysis of the physical properties of the system is however extremely difficult and several efficient numerical simulation techniques [13, 14] and analytical methods based on non-Markovian master equation and projection operator techniques [15–17] have been developed.

The aim of this paper is to develop a rather different strategy, namely to explore the possibility of reproducing the dynamical behaviour, resulting from the Hamiltonian (1) with a non-uniform distribution for the couplings, through the use of an effective Hamiltonian involving a single suitably chosen effective coupling $\alpha_{\text{eff}}$. The question is thus whether it is possible to reproduce the short-time dynamics of the populations and coherences of the central spin by means of an effective Hamiltonian model. In particular, the effective Hamiltonian approach should be able to model correctly the short-time damping and decoherence behaviour of the...
central spin. The great advantage of such an approach is obviously given by the fact that the model corresponding to the Hamiltonian (10) with uniform couplings is exactly solvable analytically.

2. Time-local master equation

Hamiltonian (1) can be written as \( H = H_0 + H_1 \), where

\[
H_0 = \frac{\omega_0}{2} \sigma_3^z + \sum_{k=1}^{N} \frac{\omega}{2} \sigma_3^k + 2\sigma_3 K_3
\]

(2)

represents the unperturbed part, and

\[
H_1 = 2 (\sigma_3 K_- + \sigma_+ K_+)
\]

(3)

is the interaction Hamiltonian [2]. \( \sigma_\pm \) are the raising and lowering operators of the central spin and

\[
K_3 = \frac{1}{2} \sum_{k=1}^{N} \alpha_k \sigma_3^k,
\]

\[
K_{\pm} = \sum_{k=1}^{N} \alpha_k \sigma_\pm^k.
\]

(4)

In the following we work in the interaction picture with respect to \( H_0 \) and denote by \( \Pi_m \) the bath projection operator that projects onto the eigenspace of the three-component of the total spin of the bath belonging to the eigenvalue \( m = -\frac{N}{2}, \cdots, +\frac{N}{2} \). The density matrix \( \rho_0(t) \) of the central spin can then be decomposed as \( \rho_0(t) = \sum_m \rho_m(t) \), where \( \rho_m(t) = \text{Tr}_B[\Pi_m \rho(t)] \) with \( \rho(t) \) denoting the density matrix of the total system and \( \text{Tr}_B \) the partial trace over the spin bath. Employing the correlated projection operator technique described in detail in [15–17], one derives the following system of coupled equations of motion for the dynamical variables \( \rho_m(t) \),

\[
\frac{d}{dt} \rho_m(t) = \int_0^t \sum_{\alpha, \alpha'} \left[ f_m(t) + g_m(t) \right] \rho_{\alpha \alpha'} \left[ \sigma_+ \rho_{\alpha'-1}(t) \sigma_- \right.
\]

\[
+ \left[ f_{m-1}(t) + g_{m+1}(t) \right] \sigma_- \rho_{\alpha'-1}(t) \sigma_+ \right.
\]

\[
- f_m(t) \sigma_+ \sigma_- \rho_{\alpha-1}(t) - f_{m-1}(t) \sigma_- \rho_{\alpha-1}(t) \sigma_+ \sigma_- \right.
\]

\[
- g_m(t) \sigma_- \sigma_+ \rho_{\alpha-1}(t) - g_{m+1}(t) \rho_{\alpha-1}(t) \sigma_- \sigma_+ \right].
\]

(5)

The quantities \( f_m(t) \) and \( g_m(t) \) represent certain two-point correlation functions of the spin bath and are given explicitly by [17]

\[
f_m(t) = 4 \sum_k \alpha_k^2 \langle \sigma_3^k \sigma_3^k e^{i(\omega_0 - \omega \Delta) K_3 + 2\sigma_3 \tau} \rangle_m,
\]

(6)

\[
g_m(t) = 4 \sum_k \alpha_k^2 \langle \sigma_3^k \sigma_3^k e^{i(-\omega_0 + \omega \Delta) K_3 + 2\sigma_3 \tau} \rangle_m,
\]

(7)

where \( \langle \cdot \rangle_m \) denotes the bath average under the constraint of fixed value for the quantum number \( m \).

3. Effective Hamiltonian

Master equation (5) clearly shows that the reduced system dynamics of the central spin is strongly influenced by the structure of the bath correlation functions defined by equations (6) and (7), depending in a complicated way on the distribution of the coupling constants \( \alpha_k \). However, for small times \( \tau \) the exponential functions in these expressions may be replaced by 1 obtaining the simpler form

\[
f_m(t) \simeq 4 \sum_k \alpha_k^2 \langle \sigma_3^k \sigma_3^k \rangle_m = 4 \frac{1}{N} \sum_k \alpha_k^2 \left( \frac{N}{2} - m \right) m \).
\]

(8)

\[
g_m(t) \simeq 4 \sum_k \alpha_k^2 \langle \sigma_3^k \sigma_3^k \rangle_m = 4 \frac{1}{N} \sum_k \alpha_k^2 \left( \frac{N}{2} + m \right) m \).
\]

(9)

The important point to note is that these approximate correlation functions coincide for small \( \tau \) with the correlation functions one obtains for the model of a uniform distribution of the coupling constants that is described by the Hamiltonian

\[
H_{\text{eff}} = \frac{\omega_0}{2} \sigma_3 + \sum_{k=1}^{N} \frac{\omega}{2} \sigma_3^k + \alpha_{\text{eff}} \sum_{k=1}^{N} \sigma_\cdot \sigma_\cdot^k,
\]

(10)

where we have introduced the effective coupling constant

\[
\alpha_{\text{eff}} = \sqrt{\frac{1}{N} \sum_k \alpha_k^2}.
\]

(11)

In fact, starting from the effective Hamiltonian \( H_{\text{eff}} \), one obtains a second-order master equation [16] that is exactly of the structure of equation (5), where however the correlation functions take the form

\[
f_{\text{eff}}(t) = 4 \alpha_{\text{eff}}^2 \left( \frac{N}{2} - m \right) e^{i(\omega_0 - \omega \Delta + 4\alpha_{\text{eff}} m + 2\alpha_{\text{eff}} \tau)},
\]

(12)

\[
g_{\text{eff}}(t) = 4 \alpha_{\text{eff}}^2 \left( \frac{N}{2} + m \right) e^{i(-\omega_0 + \omega \Delta + 4\alpha_{\text{eff}} m + 2\alpha_{\text{eff}} \tau)}).
\]

(13)

Analyzing the short-time behaviour of the two-point correlation functions in the two different models, it thus appears reasonable to suppose that the short-time dynamics of the central spin is essentially unaffected by the non-uniformity of the distribution of the coupling constants. We therefore expect that the short-time behaviour of the central spin coupled to a non-uniform spin bath can be modelled through the effective Hamiltonian (10) with a single effective coupling constant that is defined by means of relationship (11). This simple prescription leads to an efficient treatment of the short-time dynamics because the uniform spin bath model with Hamiltonian (10) can easily be solved analytically (see e.g. [16]).

4. Numerical results

In the following we compare the dynamics corresponding to Hamiltonian (1) with the dynamics given by the effective Hamiltonian (10) with coupling constant (11). In both cases we present the exact time evolution of the central spin, using the analytical solution for the effective Hamiltonian and...
shows the dynamics of a central spin coupled to a spin bath. An interesting result is that the decoherence behaviour of the central spin is very well predicted by the effective Hamiltonian, while for longer times an additional dephasing for stronger non-uniformity leads to the disappearance of the revivals of the coherences. Analogous conclusions can be drawn for polarized (finite-temperature) initial bath states. Figure 3 shows the temporal behaviour of the populations for the case of the initial bath state

\[
\rho_B(0) = \sum_m p^{N/2+m} (1-p)^{N/2-m} \Pi_m.
\]

Moreover, we have checked numerically that a similar behaviour is observed if one considers various other distributions for the coupling constants \(\alpha_k\), such as a linear or a Gaussian distribution.

5. Conclusions

We have developed an effective Hamiltonian approach to the non-Markovian damping and decoherence dynamics of a central spin coupled to a spin bath. An interesting extension of the present approach could be the development of a perturbation expansion that uses the dynamics given by the effective Hamiltonian as a starting point of zeroth
order. The perturbation parameter of such an expansion would not be given by the strength of the system–bath couplings, the $a_k$ in the example treated here, but by the degree of the non-uniformity of the distribution of the couplings, which is given in our example by quantity $A$ introduced in equation (14). The basic strategy underlying our approach could also be useful in the study of other relevant physical models featuring strong memory effects. The crucial ingredient is obviously to identify an appropriate class of effective Hamiltonian operators that is parameterized by a certain set of optimized effective variables.

References