Simulation of non-Markovian dynamics of dipole-dipole interacting atoms

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Abstract. We investigate non-markovian dynamics of two interacting two-level systems by numerical solution of the stochastic Schroedinger equation (SSE). It is shown that non-markovian noises have significant influence on dynamics of atomic levels populations.

1. Introduction

All the models of open quantum systems can be divided into two classes: markovian and non-markovian ones [1]. In markovian case a state of an open systems in the present time depends only on the state in previous time. Oppositely, in non-markovian case, the evolution of a system depends on whole the past history.

The markovian approach is connected with negligibly small relaxation time of the environment. It means that the state of the environment is not significantly changed during the observation time. In non-markovian case the relaxation time is not small and cannot be neglected. In the non-markovian scenarios significant change of the dynamics can be observed [2]. Thus, the study of the dynamics of the two dipole-dipole interacting atoms is of great interest. Nevertheless, in the non-markovian approach, a solution of the master equation for an open system can be extremely difficult. In this regard, the solution can be found either perturbation [1] or non-perturbative asymptotic methods [3].

In this paper we derive a modified non-Markovian stochastic Schroedinger equation for the model of two interacting two-level systems. SSE is studied by direct numerical simulation.

2. Model

Let us consider the Hamiltonian of two interacting two-level atoms in separated thermostats:

\[ H = \hbar \omega_0 \sum_p \sigma^z_p + \hbar \sum_{k,p} \omega_{kp} b_{kp}^\dagger b_{kp} + \hbar \sum_{k,p} \left( g_{kp} b_{kp}^\dagger \sigma^+_p + g^*_{kp} b_{kp} \sigma^-_p \right) + \sum_{p \neq p'} V_{pp'} \sigma^+_p \sigma^-_{p'}, \]  

where \( \omega_0 \) is the atomic transition frequency, \( \sigma^z_p \) is the Pauli matrix of \( p \)th atom, \( \omega_{kp} \) is the frequency of the \( k \)th photon in \( p \)th thermostat, \( b_{kp}^\dagger, b_{kp} \) are the creation and annihilation operators of the \( k \)th photon in \( p \)th thermostat, \( g_{kp} \) is the atom-photon interaction constant, \( \sigma^+_p \) are lowering and raising operators of the \( p \)th atom, \( V_{pp'} \) is the dipole-dipole interaction constant.
Using the standard method we get the following master equation [1, 4]

\[
\frac{d\rho}{dt} = -\imath \Omega [\sigma_1^+ \sigma_2^- + \sigma_2^+ \sigma_1^- , \rho] - \frac{\gamma_0}{2} (\sigma_1^+ \sigma_1^- \rho - 2 \sigma_1^+ \rho \sigma_1^- + \rho \sigma_1^+ \sigma_1^-) - \frac{\gamma_0}{2} (\sigma_2^+ \sigma_2^- \rho - 2 \sigma_2^+ \rho \sigma_2^- + \rho \sigma_2^+ \sigma_2^-),
\]

(2)

where \( \Omega \) is the dipole-dipole interaction parameter including the influence of the thermostats, \( \gamma_0 \) is the damping constant, \( \rho \) is the reduced density matrix of the atomic system. Operators \( \sigma_1^\pm, \sigma_2^\pm \) have the following explicit form:

\[
\sigma_1^+ = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_1^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \sigma_2^+ = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_2^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.
\]

(3)

The two two-level atoms have in total four energy states. We use the following terminology: the first (upper) energy level corresponds to both atoms in the excited states, second and third correspond to one atom in the excited state and another in the ground state, and fourth (lower) corresponds to both atoms in the ground state.

3. **Markovian dynamics**

The standard procedure of the unravelling for equation (2) gives us the following stochastic Schrödinger equation:

\[
d|\psi\rangle = -\imath \Omega \sigma_1^+ \sigma_2^- |\psi\rangle dt - \imath \Omega \sigma_2^+ \sigma_1^- |\psi\rangle dt - \frac{\gamma_0}{2} \sigma_1^+ \sigma_1^- |\psi\rangle dt - \frac{\gamma_0}{2} \sigma_2^+ \sigma_2^- |\psi\rangle dt + \imath \sqrt{\gamma_0} \sigma_1^- |\psi\rangle dW_1 + \imath \sqrt{\gamma_0} \sigma_2^- |\psi\rangle dW_2,
\]

(4)

where \( |\psi\rangle \) is a four-component state vector that is connected to the initial density matrix (2) by \( \rho = E (|\psi\rangle \langle \psi|) \), where \( E \) means averaging over stochastic realizations; \( dW_i \) are increments of the two independent standard Wiener processes. We can rewrite this equation in more convenient form:

\[
d|\psi\rangle = A |\psi\rangle dt + B |\psi\rangle dW_1 + C |\psi\rangle dW_2.
\]

(5)

4. **Non-markovian dynamics**

For non-markovian description of the system A. Barchielli in [5] has suggested to replace markovian Wiener processes \( dW_i \) by some non-markovian noises. The simplest non-markovian relaxation corresponds to the Ornstein-Uhlenbeck process, which satisfies the following stochastic equation:

\[
dX = -kX + dW,
\]

(6)

where \( k \) is the environment relaxation constant. By substituting (6) into the equation (5), we get the following non-markovian SSE:

\[
d|\tilde{\psi}\rangle = A |\tilde{\psi}\rangle dt + B |\tilde{\psi}\rangle (\tilde{k}_1 X_1) dt + B |\tilde{\psi}\rangle dW_1 + C |\tilde{\psi}\rangle (\tilde{k}_2 X_2) dt + C |\tilde{\psi}\rangle dW_2.
\]

(7)

However this equation is not a Q-martingale (it doesn’t preserve an average normalization) and should be modified. After the little modification we finally derive the seeking non-markovian SSE:

\[
d|\bar{\psi}\rangle = A |\bar{\psi}\rangle dt + (B + B^t) |\bar{\psi}\rangle (\tilde{k}_1 X_1) dt + B |\bar{\psi}\rangle dW_1 + (C + C^t) |\bar{\psi}\rangle (\tilde{k}_2 X_2) dt + C |\bar{\psi}\rangle dW_2.
\]

(8)
It is clear, that the density operator \( \rho = \mathbb{E}(|\psi\rangle\langle\psi|) \) is a completely positive operator, and this is one of the key advantages of stochastic Schrödinger equations.

### 5. Computer simulation

Markovian (5) and non-markovian (8) stochastic equations we solve numerically with the explicit Euler method [6]. For the markovian equation we have four independent variables and two non-correlated noises, while for non-markovian case we have to add also two components \( X_{1,2} \) of non-markovian noises. The suggested approach to the non-markovian SSE is similar to one in [7, 8].

Initial conditions are \( |\psi\rangle = (1, 0, 0, 0)^T \), interaction and damping constants \( \Omega = 2.3, \gamma_0 = 1, k_1 = 0.8, k_2 = 1.6 \). The time interval of simulation is \( 4\gamma_0 \) (In that time frame the dynamic almost stabilizes at stationary values). The averaging is made over 50000 quantum trajectories. The relative error does not exceed 0.9%. The simulation of markovian (a) and non-markovian (b) is presented in figure 1.

![Figure 1. Results of numerical simulation.](image)

In figure 1 the blue line corresponds to the probability to find the system in the upper state, the black one — in lower state and the green and the red — in the second and the third, correspondingly. In the markovian case probabilities to find system in the second or the third state are absolutely identical. In non-markovian case one can see that the second and third level are not degenerate. Also the oscillations between the third and the second energy levels are clearly seen. Note that these oscillations are in opposite phases. The steady states of all four components are shifted in comparison to markovian case.

### 6. Conclusion

In this paper we had derived the stochastic Schrödinger equations for markovian and non-markovian relaxation of the system of two dipole-dipole interacting two-level atoms. The SSEs were numerically simulated and results of simulation were compared. It was shown that taking into account non-markovian character of the relaxation lead to substantial differences in dynamics and steady states of the system.
7. References
[1] Breuer HP 2002 The theory of open quantum systems (Oxford: Oxford University Press) p 640
[2] Vega I and Alonso D 2017 Dynamics of non-Markovian open quantum systems Rev. Mod. Phys. 89 15001
[3] Li Y, Zhou J, Guo H 2009 Effect of the dipole-dipole interaction for two atoms with different couplings in a non-Markovian environment Phys. Rev. A 79 012309
[4] Semin V and Gorokhov A 2009 Calculation of the fluorescence spectrum of two interacting atoms in external field Optics and Spectroscopy 107 586
[5] Barchielli A 2009 Quantum Trajectories and Measurements in Continuous Time (Berlin: Springer) p 325
[6] Platen E and Bruti-Liberati N 2010 Numerical Solution of Stochastic Differential Equations with Jumps in Finance (Berlin: Springer) p 856
[7] Semina I, Semin V, Petruccione F and Barchielli A 2014 Schroedinger Equations for Markovian and non-Markovian Cases Open Systems & Information Dynamics 21 1440008
[8] Semin V and Pavelev A 2017 Stochastic Non-Markovian Schroedinger equation for a three-level quantum system Proceedings of the Mathematical Modeling Session at the International Conference Information Technology and Nanotechnology (MM-ITNT) 263-265

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