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Dynamics of nonequilibrium thermal entanglement

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The dynamics of a simple spin chain (two spins) coupled to bosonic baths at different temperatures is studied. The analytical solution for the reduced density matrix of the system is found. The dynamics and temperature dependence of spin-spin entanglement is analyzed. It is shown that the system converges to a steady state. If the energy levels of the two spins are different, the steady-state concurrence assumes its maximum at unequal bath temperatures. It is found that a difference in local energy levels can make the steady-state entanglement more stable against high temperatures.

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I. INTRODUCTION

In describing real physical systems one should always take into account the influence of the surroundings. The study of open systems is particularly important for understanding processes in quantum physics [1]. Whereas in most cases the interaction with an environment destroys quantum correlations within the system, it is well known that in some situations it can also build up entanglement [2] and in principle even prepare complex entangled states [3]. The dynamics of entanglement in open systems provides many interesting insights into relaxation and transport situations, in particular if the system dynamics involves many-body interactions (such as spin chains; see [4] for a review). In order to understand the role of the various parameters that compete in this setup, it is useful to find exactly solvable models. Here we study the dynamics of a model that was recently introduced by Quiroga [5]. It consists of a simple spin chain in contact with two reservoirs at different temperatures. In such a nonequilibrium case, most studies are restricted to the steady state to which the system converges in the limit of long times [5–8]. The dynamics for the model in the zero-temperature limit was studied in [9]. In the following, we study the dynamics of this model for generic temperatures.

This paper is organized as follows. In Sec. II we describe the model of a spin chain coupled to bosonic baths at different temperatures as introduced in Ref. [5]. For completeness we follow [5] in deriving the master equation for the reduced density matrix in the Born-Markov approximation. In Sec. III we present the analytical solution for the system dynamics and show the convergence of the obtained solution to the density matrix of the nonequilibrium steady state solution.

One should note that in [5] this steady state was found only in the case when the energy levels of the spins are equal. Finally, in Sec. IV we discuss the results and conclude.

II. MODEL

We consider the simplest spin chain consisting of two spins, with each spin coupled to a separate bosonic bath. In the derivation of the master equation we follow the formalism suggested in Ref. [5]. The total Hamiltonian is given by

\[ \hat{H} = \hat{H}_S + \hat{H}_{B1} + \hat{H}_{B2} + \hat{H}_{SB1} + \hat{H}_{SB2}, \]

where

\[ \hat{H}_S = \frac{\epsilon_1}{2} \hat{\sigma}_1^z + \frac{\epsilon_2}{2} \hat{\sigma}_2^z + K(\hat{\sigma}_1^+ \hat{\sigma}_2^- + \hat{\sigma}_1^- \hat{\sigma}_2^+), \]

is the Hamiltonian describing spin-to-spin interactions and \( \hat{\sigma}_i^\pm \) are the Pauli matrices. In this paper units are chosen such that \( \hbar = 1 \). The constants \( \epsilon_1 \) and \( \epsilon_2 \) denote the energy of spins 1 and 2, respectively, whereas \( K \) denotes the strength of the spin-spin interaction. We will see later that the energy difference \( \Delta \epsilon = \epsilon_1 - \epsilon_2 \) has a crucial role in determining the entanglement of the thermal state. We refer to the case \( \Delta \epsilon = 0 \) studied in [5] as the symmetric case. Our study focuses on the nonsymmetric case \( \Delta \epsilon \neq 0 \). The Hamiltonians of the reservoirs for each spin \( j=1,2 \) are given by

\[ \hat{H}_{Bj} = \sum_n \omega_n \hat{b}^+_n \hat{b}_{n,j}. \]

The interaction between the spin subsystem and the bosonic baths is described by

\[ \hat{H}_{SBj} = \hat{\sigma}^+_j \sum_n \hat{b}^+_n \hat{b}_{n,j} + \hat{\sigma}^-_j \sum_n \hat{b}^+_n \hat{b}^-_n = \sum_{j=1,2} \hat{V}_{j,\mu} \hat{f}_{j,\mu}. \]

The operators \( \hat{V}_{j,\mu} \) are chosen to satisfy \([\hat{H}_S, \hat{V}_{j,\mu}] = \omega_{j,\mu} \hat{V}_{j,\mu}\), and the \( \hat{f}_{j,\mu} \) act on bath degrees of freedom (this is always
To find a solution we go to the basis of the eigenvectors of the whole system (spin chain with reservoirs) is described by the Liouville equation
\[ \frac{d}{dt} \hat{\alpha}(t) = -i[\hat{H}, \hat{\alpha}(t)]. \]

We assume that the evolution of the dynamical subsystem (coupled spins) does not influence the state of the environment (bosonic reservoirs) so that the density operator of the whole system \( \hat{\alpha}(t) \) can be written as
\[ \hat{\alpha}(t) = \hat{\rho}(t) \hat{B}_1(0) \hat{B}_2(0) \]
(irreversibility hypothesis), where each bosonic bath is described by a canonical density matrix \( \hat{B}_j = e^{-\beta_j \hat{H}_B}/Tr(e^{-\beta_j \hat{H}_B}) \) and \( \hat{\rho}(t) \) denotes the reduced density matrix of the spin chain.

In the Born-Markov approximation the equation for the evolution of the reduced density matrix [10] is
\[ \frac{d\hat{\rho}}{dt} = -i[\hat{H}_S, \hat{\rho}] + \mathcal{L}_1(\hat{\rho}) + \mathcal{L}_2(\hat{\rho}) \]
with dissipators
\[ \mathcal{L}_j(\hat{\rho}) = \sum_{\mu,\nu} f_{\mu,\nu}(\omega_{j,\mu})\left(\hat{\rho}_{j,\mu} - \hat{\rho}_{j,\mu}\right) \]
and the spectral density is given by
\[ f_{\mu,\nu}^{(j)}(\omega_{j,\mu}) = \int_0^\infty ds e^{i\omega_{j,\mu}s} \langle e^{-i\hat{H}_j t} \hat{\rho}_{j,\mu} e^{i\hat{H}_j t} \hat{\rho}_{j,\mu} \rangle. \]

To find a solution we go to the basis of the eigenvectors \( |\lambda_j\rangle \) with eigenvalues \( \lambda_j \) of the Hamiltonian \( \hat{H}_S \),
\[ |\lambda_1\rangle = |0,0\rangle, \quad \lambda_1 = -\frac{\epsilon_1 + \epsilon_2}{2}, \]
and transition operators
\[ \mathcal{L}_j(\hat{\rho}) = \sum_{\mu=1}^2 \sum_{\nu=1}^2 f^{(j)}(\omega_{j,\mu})\left(\hat{\rho}_{j,\mu} - \hat{\rho}_{j,\mu}\right) \]
with transition frequencies
\[ \omega_1 = \lambda_2 - \lambda_3, \]
\[ \omega_2 = \lambda_2 + \lambda_3, \]
where \( \kappa = \sqrt{K^2 + (\Delta \epsilon)^2}/4 \) and \( \tan \theta = 2K/(\Delta \epsilon) \). In this representation the dissipative operator \( \mathcal{L}_j(\hat{\rho}) \) becomes
\[ \mathcal{L}_j(\hat{\rho}) = \sum_{\mu=1}^2 \sum_{\nu=1}^2 f^{(j)}(\omega_{j,\mu})\left(\hat{\rho}_{j,\mu} - \hat{\rho}_{j,\mu}\right) \]
and transition operators
\[ C_\mu(T_M, \Delta T) \]
where \( T_M = (T_1 + T_2)/2 \) and temperature difference \( \Delta T = T_1 - T_2 \) in the symmetric case \( \epsilon_1 = \epsilon_2 = 3 \) with \( K = 1 \).
\[ \dot{V}_{1,1} = \cos(\theta/2) (|\lambda_1\rangle\langle\lambda_1| + |\lambda_2\rangle\langle\lambda_2|), \]
\[ \dot{V}_{1,2} = \sin(\theta/2) (|\lambda_1\rangle\langle\lambda_2| - |\lambda_2\rangle\langle\lambda_1|), \]
\[ \dot{V}_{2,1} = \sin(\theta/2) (|\lambda_1\rangle\langle\lambda_2| - |\lambda_2\rangle\langle\lambda_1|), \]
\[ \dot{V}_{2,2} = \cos(\theta/2) (|\lambda_3\rangle\langle\lambda_2| + |\lambda_4\rangle\langle\lambda_4|). \]

In this paper we consider the bosonic bath as an infinite set of harmonic oscillators, so the spectral density has the form \( J^{(j)}(\omega) = \gamma(\omega) n(\omega) \), where \( n(\omega) = (e^{\hbar/\omega} - 1)^{-1} \) and \( J^{(j)}(-\omega) = e^{\hbar/\omega} J^{(j)}(\omega) \). For simplicity we choose the coupling constant to be frequency independent, \( \gamma(\omega) = \gamma_1 \) and \( \gamma_2(\omega) = \gamma_2 \). In the basis \(|\lambda_i\rangle\) the equation for the diagonal elements of the reduced density matrix is given by

\[
\frac{d}{dt} \begin{pmatrix} \rho_{11}(t) \\ \rho_{22}(t) \\ \rho_{33}(t) \\ \rho_{44}(t) \end{pmatrix} = B \begin{pmatrix} \rho_{11}(t) \\ \rho_{22}(t) \\ \rho_{33}(t) \\ \rho_{44}(t) \end{pmatrix},
\]

where \( B \) is a 4×4 matrix with constant coefficients. The time dependence for the nondiagonal elements has the following form:

\[ \rho_{ij}(t) = e^{i\omega_{ij}t}\rho_{ij}(0), \]

where \( \omega_{ij} \) is a complex number. For the initial state of the system in the computational basis \(|00\rangle, |01\rangle, |10\rangle, |11\rangle\) we choose

\[
\hat{\rho}(0) = \rho_{00}|00\rangle\langle00| + \rho_{11}|01\rangle\langle01| + \rho_{22}|10\rangle\langle10| + \rho_{33}|11\rangle\langle11| + C_{12}|01\rangle\langle10| + C_{12}|10\rangle\langle01|.
\]

### III. EXACT SOLUTION

The analytical solution in the basis of eigenvectors \(|\lambda_i\rangle\) is given by

\[
\rho_{ii}(t) = \frac{1}{X_i Y_i} \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \begin{pmatrix} \rho_{11}(0) \\ \rho_{22}(0) \\ \rho_{33}(0) \\ \rho_{44}(0) \end{pmatrix},
\]

where the coefficients \( a_{ij} \) are given by

- \( a_{11} = (X_1^+ + X_1^+ e^{-i\theta})(Y_2^+ + Y_2^+ e^{-i\theta}), \)
- \( a_{12} = (1 - e^{-i\theta})(1 - e^{-i\theta})Y_1^+ Y_2^+, \)
- \( a_{13} = (1 - e^{-i\theta})X_1^+ (Y_2^+ + Y_2^+ e^{-i\theta}), \)
- \( a_{14} = (X_1^+ + X_1^+ e^{-i\theta})(1 - e^{-i\theta})Y_2^+, \)
- \( a_{21} = (1 - e^{-i\theta})(1 - e^{-i\theta})X_2^+ Y_2^+, \)
- \( a_{22} = (X_1^+ + X_1^+ e^{-i\theta})(Y_2^+ + Y_2^+ e^{-i\theta}), \)
- \( a_{23} = (X_1^+ + X_1^+ e^{-i\theta})(1 - e^{-i\theta})Y_2^+, \)
- \( a_{24} = (1 - e^{-i\theta})X_1^+ (Y_2^+ + Y_2^+ e^{-i\theta}), \)
- \( a_{31} = (1 - e^{-i\theta})X_1^+ (Y_2^+ + Y_2^+ e^{-i\theta}), \)
- \( a_{32} = (X_1^+ + X_1^+ e^{-i\theta})(Y_2^+ + Y_2^+ e^{-i\theta}), \)
- \( a_{33} = (X_1^+ + X_1^+ e^{-i\theta})(1 - e^{-i\theta})Y_2^+, \)
- \( a_{34} = (1 - e^{-i\theta})(1 - e^{-i\theta})X_1^+ Y_2^+, \)
- \( a_{41} = (1 - e^{-i\theta})(1 - e^{-i\theta})X_1^+ Y_2^+, \)
- \( a_{42} = (1 - e^{-i\theta})X_1^+ (Y_2^+ + Y_2^+ e^{-i\theta}), \)
- \( a_{43} = (1 - e^{-i\theta})(1 - e^{-i\theta})X_1^+ Y_2^+, \)
- \( a_{44} = (X_1^+ + X_1^+ e^{-i\theta})(Y_2^+ + Y_2^+ e^{-i\theta}). \)

Taking into account the initial conditions, the nonvanishing nondiagonal elements are

\[
\rho_{34}(t) = e^{-2\omega_3 t}(X_1^+ Y_2^+ e^{-i\theta})/\rho_{34}(0),
\]
\[
\rho_{43}(t) = e^{-2\omega_4 t}(X_1^+ Y_2^+ e^{-i\theta})/\rho_{34}(0).
\]

In the present solution we have introduced some constants:

\[
X_i^\pm = 2 \cos^2(\theta/2) J^{(j)}(\pm \omega_0) + 2 \sin^2(\theta/2) J^{(j)}(\pm \omega_0),
\]
\[
Y_i^\pm = 2 \sin^2(\theta/2) J^{(j)}(\pm \omega_0) + 2 \cos^2(\theta/2) J^{(j)}(\pm \omega_0),
\]

or

\[
X_i^\pm = [J^{(j)}(\pm \omega_0) + J^{(j)}(\pm \omega_0)] + \frac{\Delta \epsilon}{\sqrt{4 K^2 + (\Delta \epsilon)^2}} [J^{(j)}(\pm \omega_0) - J^{(j)}(\pm \omega_0)],
\]
\[
Y_i^\pm = [J^{(j)}(\pm \omega_0) + J^{(j)}(\pm \omega_0)] - \frac{\Delta \epsilon}{\sqrt{4 K^2 + (\Delta \epsilon)^2}} [J^{(j)}(\pm \omega_0) - J^{(j)}(\pm \omega_0)].
\]

One can easily see that this solution converges with increasing time to a diagonal density matrix which does not depend on the initial conditions:

\[
\lim_{t \to \infty} \rho_{ii}(t) = \frac{1}{X_i Y_i} \begin{pmatrix} X_i^+ Y_i^+ \\ X_i^+ Y_i^+ \\ X_i^+ Y_i^+ \\ X_i^+ Y_i^+ \end{pmatrix},
\]
the mean bath temperature \( T_M \) and the temperature difference \( \Delta T = T_1 - T_2 \) in the case \( \epsilon_1 = 3, \epsilon_2 = 1, K = 1 \).

\[
\lim_{t \to \infty} \rho_{34}(t) = 0.
\]

In the symmetric case (\( \Delta \epsilon = 0 \)) the above limit reproduces the result obtained by Quiroga in [5]. In order to quantify the entanglement between the spins we consider the concurrence [11]. In the steady state (\( t \to \infty \)) it is given by

\[
C_\infty = \frac{2}{X_1 Y_2} \max \left( 0, \frac{\sin \theta}{2} \left| X_1^* Y_2^* - X_1 Y_2 \right| - \sqrt{X_1^* Y_2^* X_1 Y_2} \right).
\]

**IV. RESULTS AND DISCUSSION**

The dynamics of entanglement is analyzed in Figs. 1 and 2. In Fig. 1 the dynamics of the concurrence between the two qubits is shown. For the model considered here, the spin chain Hamiltonian \( \hat{H}_S \) can entangle the qubits for specific times, which gives rise to the oscillations of concurrence one observes for short times (note that the initial state is chosen to be separable \( \rho_0 = |1, 0\rangle \langle 1, 0| \)). For large times, the system converges to its steady state. One can see the disappearance of entanglement with increasing temperatures of the bosonic baths which was shown for the steady state in [5]. In Fig. 2 the dynamics of the concurrence for different initial states of the qubits is shown. For all cases the system converges to one and the same value of entanglement. The plots in Figs. 1 and 2 show clearly the competition between unitary and dissipative dynamics. If the qubits start from a “symmetric state,” i.e., \(|1, 1\rangle\), no oscillations in the concurrence dynamics are observed and if the qubits start from a “nonsymmetric state,” i.e., \(|1, 0\rangle \langle 1, 0| \) or \(|1, 0\rangle \langle 0, 1| \)/\( \sqrt{2} \), one can see oscillations of the concurrence which correspond to the energy exchange between the qubits in the unitary evolution. Both figures reveal that after time of order \( t \sim 2/\gamma \) the concurrence “forgets” about initial conditions and converges to the same value, given by \( C_\infty \) from the end of Sec. III. The steady-state concurrence \( C_\infty(\epsilon_1, \epsilon_2, K, T_1, T_2) \) is analyzed in Figs. 3–6. In Figs. 3 and 4 we plot the steady-state concurrence for the symmetric and nonsymmetric cases as a function of the mean temperature \( [T_M = (T_1 + T_2)/2] \) and the temperature difference \( (\Delta T = T_1 - T_2) \) of the baths. In the symmetric case one can easily see that the maximal value of the entanglement is reached for equal bath temperatures (\( \Delta T = 0 \)).

\[
C_{\text{sym}}^{\text{eq}} = \frac{\sinh(1/T) - 1}{2 \cosh(\omega_1/2T) \cosh(\omega_2/2T)}.
\]

The critical temperature in units of \( K \) above which the steady state becomes separable is given by \( T_C = \text{arcsinh}(1)^{-1} \) (\( T_C \approx 1.136 \)) [5]. It is interesting to note that in the nonsymmetric case (Fig. 4) the maximal entanglement is reached in the nonequilibrium case (\( \Delta T \neq 0 \)). In particular, the maximal entanglement is larger than the corresponding nonsymmetric equilibrium concurrence

\[
C_{\text{nonsym}}^{\text{eq}} = \frac{\sin \theta \sinh((\omega_2 - \omega_1)/2T) - 1}{2 \cosh(\omega_1/2T) \cosh(\omega_2/2T)}.
\]

The temperature at which entanglement disappears is a function of the energy difference \( \Delta \epsilon \) between qubits.
$$T_C = \frac{\sqrt{\Delta \epsilon^2 / 4 + 1}}{\text{arcsinh} \sqrt{\Delta \epsilon^2 / 4 + 1}}.$$  

It is easy to see that this function reaches its minimum value in the symmetric case ($\Delta \epsilon=0$). In Figs. 5 and 6 we show the maximally reachable value of entanglement as a function of qubit energies in the strong- and weak-coupling cases. For every pair of energies ($\epsilon_1, \epsilon_2$) we maximize the value of the concurrence for the different temperatures of the baths ($T_1, T_2$). One can see that in the strong-coupling case ($\epsilon_1, \epsilon_2 < K$; Fig. 5) the maximal value of the entanglement corresponds to the symmetric case. In Fig. 6 one can see that in the weak-coupling case ($\epsilon_1, \epsilon_2 > K$) the maximal value of the entanglement is reached in the nonsymmetric case.

In conclusion, we have found an analytical solution for a simple spin system coupled to bosonic baths at different temperatures. We studied the dynamics of the system and showed that in the long term the system converges to the steady-state solution. Resolving the entanglement dynamics allowed us to distinguish between entanglement created by the system and by the bath. For the symmetric case ($\epsilon_1 = \epsilon_2$) we reproduced the steady state found in [5]. We focused on the nonsymmetric case ($\epsilon_1 \neq \epsilon_2$) where we found that the steady-state concurrence assumes its maximal value for unequal bath temperatures. This corresponds to a dynamical equilibrium, where the spin chain transfers heat between the baths. We also found that a difference in local energy levels can make the steady-state entanglement more stable against high temperatures. These analytical results motivate further numerical studies on longer spin chains.

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