

# Global and local relaxation of a spin chain under exact Schrödinger and master-equation dynamics

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We solve the Schrödinger equation for an interacting spin chain locally coupled to a quantum environment with a specific degeneracy structure. The reduced dynamics of the whole spin chain as well as of single spins is analyzed. We show that the total spin chain relaxes to a thermal equilibrium state independently of the internal interaction strength. In contrast, the asymptotic states of each individual spin are thermal for weak but nonthermal for stronger spin-spin coupling. The transition between both scenarios is found for couplings of the order of  $0.1 \times \Delta E$ , with  $\Delta E$  denoting the Zeeman splitting. We compare these results with a master-equation treatment; when time averaged, both approaches lead to the same asymptotic state and finally with analytical results.

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## I. INTRODUCTION

Various attempts have been made to account for thermodynamical behavior of quantum systems [1,2]. Especially the relaxation into an equilibrium state in a pure quantum world does not seem to be feasible since Schrödinger dynamics is reversible like the classical Hamiltonian dynamics. By introducing irreversibility into quantum mechanics one thus has to face all the old difficulties.

One quite successful way to introduce relaxation behavior into quantum mechanical models is to consider open systems modeled by a quantum master equation [3,4] or the Lindblad formalism [5–7]. In these approaches the influence of the environmental system enters the Liouville–von Neumann equation for the considered system via incoherent damping terms. To deduce such a closed evolution equation several approximations are necessary, e.g., the Born-Markov assumption.

In the context of quantum thermodynamics irreversible behavior has recently been found in classes of very small bipartite quantum systems described by a pure Schrödinger evolution only [8,9]. This approach does not need those specific assumptions about the environment. Instead, system and environment are treated as a whole. Even in small bipartite systems, consisting of a two-level system (“gas system”) coupled to an environment (“container”) of no more than some hundred levels thermodynamical behavior is generic—relaxation occurs to a theoretically predicted equilibrium state (see [10]).

In the above mentioned scenarios the gas system was very small (from two to five levels) and coupled to an environment without any structure or selectivity. In a more complex situation the system under consideration (gas system) could be constructed from several identical subsystems, e.g., the

system could be a spin chain. For such bipartite systems with increased internal complexity the effect of the coupling topology is not yet completely understood: If we couple a chain of identical subsystems at one edge only to a quantum environment as before, the question arises whether the whole system will still relax into a thermal equilibrium state. Furthermore, we are interested in whether and when the individual subsystems are also in a thermal equilibrium state.

According to recent investigations on local temperature of modular systems [11,12], we expect the same global as well as local temperature in the system for weakly coupled chains. In cases of a stronger coupling this may no longer be the case (as shown by an open system approach [13]).

Those chain systems coupled to a quantum environment will be treated as a closed system subject to Schrödinger dynamics and will be compared to the modeling via a quantum master equation. In particular, we will analyze chains with different coupling types and strengths with respect to their local as well as global thermal or nonthermal properties.

## II. THEORETICAL BACKGROUND

### A. The considered system

We consider chains of three identical quantum systems described by the Hamiltonian

$$\hat{H}_s = \sum_{\mu=1}^3 \hat{H}_{\text{loc}}(\mu) + \frac{\lambda}{I} \sum_{\mu=1}^2 \hat{I}_s(\mu, \mu+1). \quad (1)$$

Here the first sum contains the local Hamilton operators  $\hat{H}_{\text{loc}}(\mu)$  of the site. In our case the local Hamiltonian of site  $\mu$  reads

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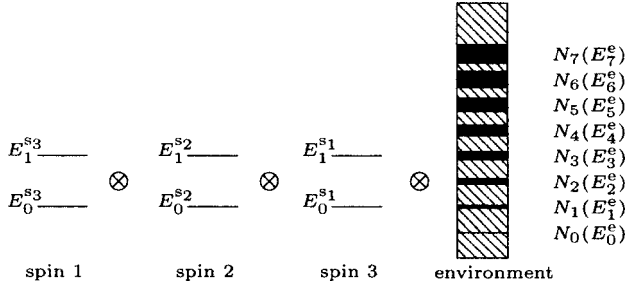


FIG. 1. Coupling topology of the spin chain to the quantum environment.

$$\hat{H}_{\text{loc}}(\mu) = \hat{1} + \frac{1}{2} \hat{\sigma}_z(\mu) \quad \text{with } \mu = 1, 2, 3, \quad (2)$$

where  $\hat{\sigma}_z$  denotes the Pauli spin operator. Here and in the following all energies are taken in units of the Zeeman splitting. The second sum refers to the next neighbor couplings between the subsystems normalized by

$$I = \frac{1}{n} \sqrt{\text{Tr}\{\hat{I}_s^2\}}, \quad (3)$$

where  $n$  is the Hilbert space dimension of the chain. Thus, it is possible to control the internal coupling strength by the single parameter  $\lambda$  [see Eq. (1)] only, irrespective of the type of coupling. In the following we compare two different interactions, a random coupling

$$\hat{I}_s^R(\mu, \mu + 1) = \sum_{i=1}^3 \sum_{j=1}^3 p_{ij} \hat{\sigma}_i(\mu) \otimes \hat{\sigma}_j(\mu + 1), \quad (4)$$

where the  $p_{ij}$  are normally distributed random numbers in the interval  $[-1, 1]$ , and a Heisenberg interaction,

$$\hat{I}_s^H(\mu, \mu + 1) = \sum_{i=1}^3 \hat{\sigma}_i(\mu) \otimes \hat{\sigma}_i(\mu + 1). \quad (5)$$

### B. The environment

The model system described in the last section is now coupled to an adequate environment:

$$\hat{H}_{\text{tot}} = \hat{H}_s + \hat{H}_e + \frac{\kappa}{I_{\text{se}}} \hat{I}_{\text{se}}. \quad (6)$$

The first term is the Hamiltonian of the chain,  $\hat{H}_e$  refers to the Hamiltonian of the environment and  $\hat{I}_{\text{se}}$  is the interaction between system and environment. After normalizing  $\hat{I}_{\text{se}}$  via  $I_{\text{se}} = (1/n) \sqrt{\text{Tr}\{\hat{I}_{\text{se}}^2\}}$  [compare Eq. (3)] the external coupling strength is controlled by the parameter  $\kappa$  only. This system environment coupling is taken to be small in all cases as a precondition to allow for thermodynamic behavior. The interaction will be chosen in such a way that it couples only to one boundary of the system (see Fig. 1), say to the third spin of the chain. Furthermore, the interaction should allow for energy exchange between system and environment.

In the following we will consider both a complete solution of the Schrödinger equation for system and environment according to  $\hat{H}_{\text{tot}}$  as well as a quantum master equation, simulating a corresponding bath coupling.

### C. Hilbert space average approach

Let us start with the complete model under Schrödinger dynamics. At first sight it may not seem clear how a totally time reversible equation like the Schrödinger equation could produce something like irreversible behavior. To clarify this point we introduce some aspects of quantum thermodynamics. A complete derivation of all aspects of this theory is beyond the scope of this paper. Therefore we only sum up some central aspects of this approach and refer the interested reader to [9,14].

According to quantum thermodynamics (see [9]), the system proper relaxes to a Gibbsian state whenever the density of states of the environment is an exponential function of energy; the latter is typical for many-body systems. We model such a quantum environment here by a system (Fig. 1; the width of the energy levels should indicate the degeneracy) of the eight energy levels  $E_i^e$  with degeneracies given by

$$N^e(E_i^e) = N_0^e 2^{E_i^e}. \quad (7)$$

This may seem rather artificial, but the idea is as follows: The environment may possess a continuous spectrum, but due to the weak coupling between system and environment the system couples only to the resonant levels. Thus we can neglect all the other levels. This environment is then expected to induce on the spin chain a canonical state with the reciprocal temperature  $\beta$ ,

$$\frac{1}{k_B T} = \beta = \frac{\partial}{\partial E} \ln N^e(E) \quad (8)$$

where  $k_B$  is the Boltzmann constant. With the special degeneracy structure (7) this leads to  $\beta = \ln 2$ .

For a numerical test and to avoid any bias we pick for  $\hat{I}_{\text{se}}$  a Hermitian random matrix from an ensemble with the distribution [15]

$$P(\hat{I}_{\text{se}}) = \frac{1}{\sqrt{4\pi}} e^{-\text{Tr}\{\hat{I}_{\text{se}}^2\}/4}. \quad (9)$$

### Theoretical predictions

In contrast to the master-equation approach, the dynamics of the closed system (spin chain and environment) is purely Schrödinger type. The von Neumann entropy of the completely closed system thus remains constant. But by splitting up the whole system into two parts, a small system taken to be the spin chain and a large one, the environment, the von Neumann entropy of the parts can change in time. As a matter of fact, the small system shows a thermodynamical behavior if two restrictions are met.

(a) The coupling between the small system and the environment should be small, i.e., the energy contained in the

interaction has to be much smaller than the local energies,

$$\langle \hat{I}_{se} \rangle \ll \langle \hat{H}_s \rangle, \langle \hat{H}_e \rangle \quad (10)$$

which guarantees that the spectrum of the environment is not disturbed too much.

(b) The Hilbert space of the environment should be very large compared to the Hilbert space of the small system. Conversely, all systems meeting these conditions may be called thermodynamical.

The concrete form of the interaction defines an accessible region within the whole Hilbert space, selected by the initial state. Using a model with full energy exchange between system and environment (canonical situation) only one supplementary condition remains active, the overall energy conservation defining the accessible region. By a topological investigation of the Hilbert space (see [9]), the details of which are beyond the scope of this paper, it is possible to show that the state of the complete system will enter a very large region (the dominant region) within the accessible region, for which the system under consideration is in a state with approximately maximum von Neumann entropy. The respective energy distribution of the small system in this dominant region, i.e., the probability to find the small system in an energy eigenstate  $E_i^s$  (no degeneracy) for an initial state with a sharp energy is then given by

$$W^d(E_i^s) = \frac{N_i(E_i^e)}{N_{\text{tot}}} \quad (11)$$

[for a complete derivation of Eq. (11) see [9,14]].  $E_i^s$  is the  $i$ th energy level of the spin system,  $E_i^e$  the corresponding energy level in the environment with the degeneracy  $N_i(E_i^e)$ , and  $N_{\text{tot}} = \sum_{i=1}^8 N_i(E_i^e)$  the total number of levels in the environment.

#### D. Master-equation approach

Master equation approaches describe the dynamics of open systems. They have been widely applied to describe system bath models, in particular in quantum optics [3]. Their derivation is standard and can be found in several textbooks. However, since our system, the spin chain, has an internal structure and since only one of the boundary spins directly couples to the bath, special care must be taken.

The entire dynamics of the system coupled to the bath is given by the Liouville-von Neumann equation, from which the Nakajima-Zwanzig equation can be derived [3]. Assuming that the bath is in a thermal state,

$$\rho_e = \frac{e^{-\beta H_e}}{Z_e}, \quad (12)$$

an expansion of the latter up to second order in the system-bath coupling reads

$$\frac{d\rho_s}{dt} = -i[\hat{H}_s, \rho_s] - \int_0^t dt' \text{Tr}_e[\hat{I}_{se}, [\hat{I}_{se}(t'-t), \rho_s \otimes \rho_e]], \quad (13)$$

where  $\rho_s$  is the reduced density matrix of the spin system and  $\hat{I}_{se}(t)$ , the system bath interaction in the interaction picture, reads

$$\hat{I}_{se}(t) = e^{i(\hat{H}_s + \hat{H}_e)t} \hat{I}_{se} e^{-i(\hat{H}_s + \hat{H}_e)t}, \quad (14)$$

the time dependence of which can be computed in the eigenbasis of  $\hat{H}_s$  and  $\hat{H}_e$ . Applying, as usual, the Markov approximation, the integral of (13) can be computed and the following form of the damping rates is found:

$$\frac{d\rho_s}{dt} = -i[\hat{H}_s, \rho_s] + (\hat{A}\hat{\Gamma}^a \rho_s) - (\hat{\Gamma}^a \rho_s \hat{A}) + (\rho_s \hat{\Gamma}^b \hat{A}) - (\hat{A} \rho_s \hat{\Gamma}^b), \quad (15)$$

where

$$\hat{A} = \hat{I}(1) \otimes \hat{I}(2) \otimes \hat{\sigma}_x(3). \quad (16)$$

As can be seen the environment has been locally coupled to spin 3 only.

Denoting the energy eigenvalues and eigenvectors of the spin system by  $E_i^s$  and  $|i\rangle$ , respectively

$$\hat{H}_s |i\rangle = E_i^s |i\rangle, \quad (17)$$

and defining  $\omega_{ij} = \hbar(E_i^s - E_j^s)$ , the transition matrices  $\Gamma^{ab}$  have the following matrix representation in the eigenbasis of  $H_s$ :

$$\langle i | \Gamma^a | j \rangle = \begin{cases} \kappa \frac{1}{e^{\omega_{ij}\beta_e - 1}} A_{ij} & \text{for } \omega_{ij} > 0, \\ \kappa \frac{e^{\omega_{ji}\beta_e}}{e^{\omega_{ij}\beta_e - 1}} A_{ji} & \text{for } \omega_{ij} < 0, \end{cases} \quad (18)$$

$$\langle i | \Gamma^b | j \rangle = \begin{cases} \kappa \frac{e^{\omega_{ij}\beta_e}}{e^{\omega_{ij}\beta_e - 1}} A_{ij} & \text{for } \omega_{ij} > 0, \\ \kappa \frac{1}{e^{\omega_{ji}\beta_e - 1}} A_{ji} & \text{for } \omega_{ij} < 0. \end{cases} \quad (19)$$

$$\langle i | \Gamma^b | j \rangle = \begin{cases} \kappa \frac{e^{\omega_{ij}\beta_e}}{e^{\omega_{ij}\beta_e - 1}} A_{ij} & \text{for } \omega_{ij} > 0, \\ \kappa \frac{1}{e^{\omega_{ji}\beta_e - 1}} A_{ji} & \text{for } \omega_{ij} < 0. \end{cases} \quad (20)$$

$$\langle i | \Gamma^b | j \rangle = \begin{cases} \kappa \frac{1}{e^{\omega_{ji}\beta_e - 1}} A_{ji} & \text{for } \omega_{ij} > 0, \\ \kappa \frac{e^{\omega_{ij}\beta_e}}{e^{\omega_{ij}\beta_e - 1}} A_{ij} & \text{for } \omega_{ij} < 0. \end{cases} \quad (21)$$

Note that by virtue of Eq. (14) the real damping rates of Eq. (18)–(21) only appear if the transition matrices  $\Gamma^{ab}$  are represented in the eigenbasis of  $\hat{H}_s$ . Therefore, simply writing down Lindblad damping terms [16] for spin 3, the one which directly couples to the bath, would in general, lead to wrong results [17]. However, if the coupling between the spins in the chain is small enough, additional approximations can be made and one will obtain the Lindblad type damping rates for spin 3 [18].

It should also be mentioned that the thermal state

$$\rho_s = \frac{e^{-\beta \hat{H}_s}}{Z_s} \quad (22)$$

is the stationary and therefore asymptotic solution of Eq. (15).

### III. NUMERICAL RESULTS

#### A. Spectral temperature

We will use as a measure to characterize the asymptotic state of the spin system and the single spins a “spectral temperature” defined as

$$\frac{1}{k_B T} := - \left( 1 - \frac{W_0 + W_M}{2} \right)^{-1} \sum_{n=1}^M \left( \frac{W_n + W_{n-1}}{2} \right) \frac{\ln W_n - \ln W_{n-1}}{E_n - E_{n-1}}, \quad (23)$$

where  $W_n$  is the probability to find the system at the  $n$ th energy level  $E_n$ , and  $M$  is the highest and 0 the lowest energy level. The main idea here is to assign a Boltzmann factor to each pair of neighboring energy levels. The spectral temperature then simply is the average over all these factors weighed by the corresponding occupation probabilities. This spectral temperature also exists in nonequilibrium situations but coincides with the standard definition of temperature (e.g., [19]) only for a canonical state.

For the calculation of the spectral temperatures according to Eq. (23) we insert for  $W_n$  the long time average  $\langle \rho_s^{nn}(t) \rangle_t$  of the respective occupation probability.

#### B. Schrödinger dynamics

To demonstrate the relaxation behavior of the spin chain under Schrödinger dynamics we have diagonalized the total Hamiltonian  $\hat{H}_{\text{tot}}$  [see Eq. (9)] and solved the exact Schrödinger equation

$$\frac{d}{dt} |\psi_{\text{tot}}(t)\rangle = - \frac{i}{\hbar} \hat{H}_{\text{tot}} |\psi_{\text{tot}}(t_0=0)\rangle. \quad (24)$$

The initial state  $|\psi_{\text{tot}}(t_0)\rangle$  has been taken as a product state of the spin chain and the environment. From the density matrix  $\rho_{\text{tot}}(t) = |\psi(t)\rangle\langle\psi(t)|$  we trace out the environment and transform the resulting reduced density matrix into the eigenbasis of the spin system. The time evolution of this reduced density matrix  $\rho_s(t)$  is plotted in Fig. 2 for an internal random coupling and in Fig. 3 for a Heisenberg coupling. (We restrict our analysis to  $\lambda > 0$ , the antiferromagnetic case. Corresponding results can be obtained for  $\lambda < 0$ .)

Both evolutions have been obtained with the coupling parameters  $\kappa=0.001$  and  $\lambda=0.4$ . The horizontal lines are the probabilities as expected from Eq. (11). As can be seen, for both internal couplings, the spin system relaxes into a state which is in accordance with Eq. (11). The probability fluctuations can be interpreted as a finite size effect of the environment.

##### 1. Global and local temperatures

Now that we have demonstrated the relaxation of the spin chain into a thermal equilibrium state, we want to analyze the relaxation behavior of the spinchain depending on the internal interaction strength  $\lambda$ . The approach of Sec. II C is independent of the internal structure of the small system. Thus the relaxation behavior should be independent of  $\lambda$  and the temperature of the spin chain should be identical to that

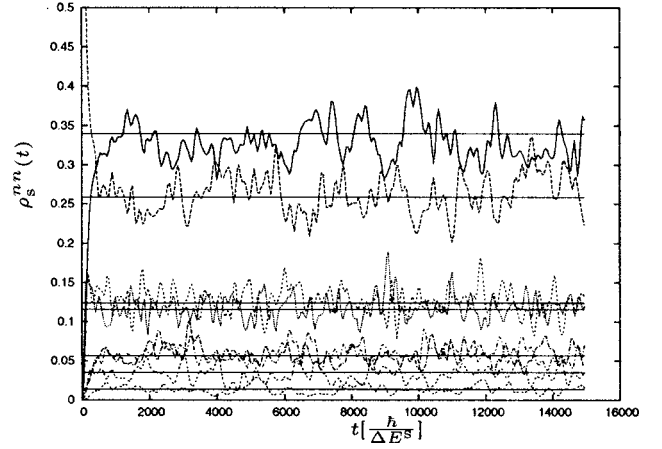


FIG. 2. Relaxation of the spin chain  $s$  into equilibrium under Schrödinger dynamics for  $\lambda=0.4$  and  $\kappa=0.001$  with a random interaction. The horizontal lines are the expected probabilities from (11) to find the system at the corresponding energies. These are in good accordance with the time-averaged values of  $\rho_s(t)$ .  $\lambda$  and  $\kappa$  are energies taken in units of the Zeeman splitting. [Note that  $W^d(E_4^s) = W^d(E_3^s)$ , Eq. (11).]

induced by the environment  $T^c = 1/\ln 2$  [see Eq. (7)]. To specify the temperature of the spin chain  $T^s$  we use the “spectral temperature” defined in (23). We compare the spectral temperature of the total spin chain to those of each individual spin. For the local spectral temperature  $T_\mu^{\text{loc}}$  of a single spin, (23) reduces to

$$T_\mu^{\text{loc}} = - \frac{E_1^\mu - E_0^\mu}{\ln(W_1^\mu) - \ln(W_0^\mu)}, \quad (25)$$

where  $W_i^\mu$  is the long time average of the probability to find the  $\mu$ th spin at the energy  $E_i^\mu$ . These quantities are plotted as a function of  $\lambda$  for a random interaction in Fig. 4 and for an antiferromagnetic Heisenberg interaction in Fig. 5.

The spectral temperature of the spin chain  $T^s$  approaches the temperature  $T^c$  imposed by the environment, irrespective of the internal coupling strength  $\lambda$ . However, the spectral temperature of each single spin is found to increase with

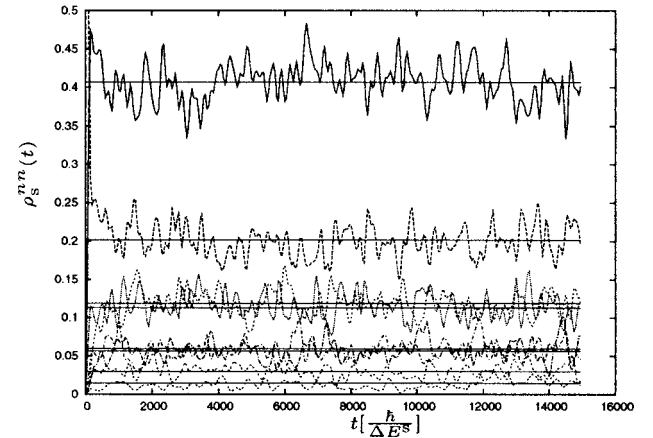


FIG. 3. Relaxation into equilibrium under Schrödinger dynamics as of Fig. 2 but with antiferromagnetic Heisenberg interaction.

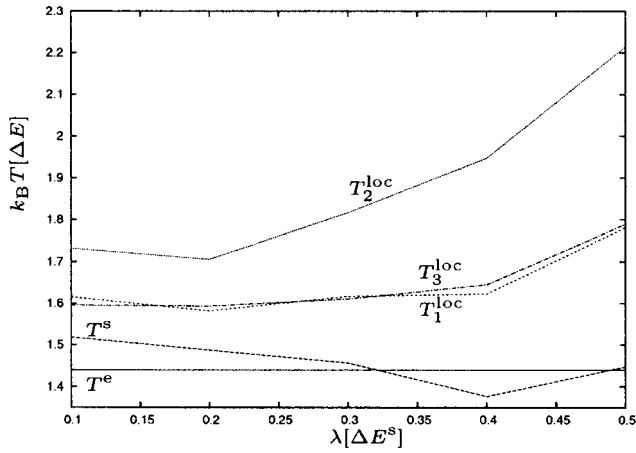


FIG. 4. Global and local temperatures as a function of  $\lambda$  for a random interaction.

increasing  $\lambda$ . The reason for this behavior is that the local spin system is disturbed more and more with increasing  $\lambda$  although the whole spin system continues to reach a canonical state [12].

Especially for a Heisenberg coupled spin chain one can verify analytically that for a canonical state with some respective temperature, the local temperatures deviate more and more with increasing  $\lambda$  (see Sec. IV). Note that for a ferromagnetic Heisenberg coupling the spectral temperatures of each spin show a different behavior: they decrease with increasing  $\lambda$ . In any case, they deviate from  $T^e$ .

To verify that the state of the total spin chain  $\rho_s$  is indeed canonical we test the off diagonal elements. All absolute values are smaller than  $10^{-4}$ . Therefore we argue that the state of the total spin chain is indeed a canonical one for all practical purposes and its spectral temperature can be identified as the thermodynamic temperature.

The deviation of the local spectral temperatures from the temperature of the whole spin chain can also be understood by analyzing the correlation  $C$  between the spins

$$C = \text{Tr}\{[\langle \rho_1(t) \rangle_t \otimes \langle \rho_2(t) \rangle_t \otimes \langle \rho_3(t) \rangle_t - \langle \rho_s(t) \rangle_t]^2\}. \quad (26)$$

The angular brackets  $\langle \rangle_t$  denote the time average of the density matrices of the single spins ( $\rho_\mu$ ) and the spin system

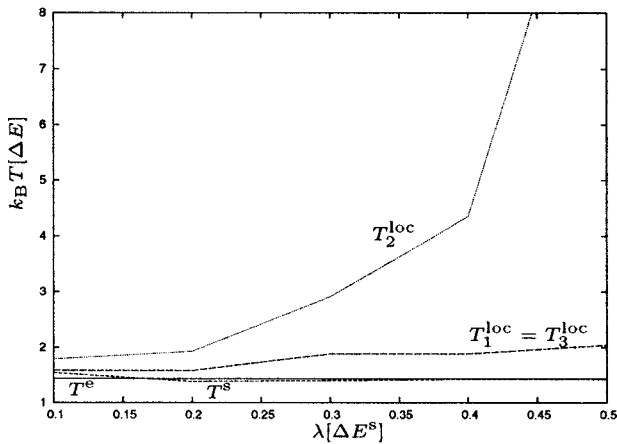


FIG. 5. Global and local temperatures as a function of  $\lambda$  for antiferromagnetic Heisenberg interaction.

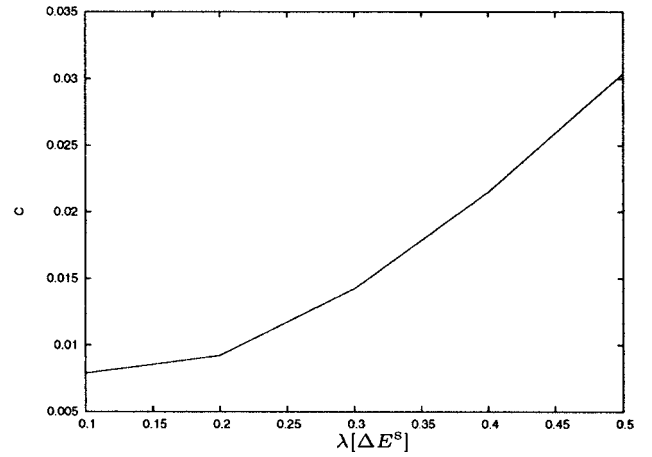


FIG. 6. Correlation  $C$  [Eq. (26)] as a function of  $\lambda$  for a random interaction.

( $\rho_s$ ). Due to increasing  $\lambda$  the spins are more and more correlated. This correlation causes an increase of the local entropy which leads to an increased spectral temperature of each individual spin. Figure 6 shows  $C$  as a function of  $\lambda$  for a random interaction and Fig. 7 for a antiferromagnetic Heisenberg interaction.

As can be seen from both figures, the correlations  $C$  increase with increasing  $\lambda$ . The ferromagnetic Heisenberg coupling also show increasing correlations in the considered ranges of  $\lambda$  and  $T^e$ .

## 2. Master equation

We have solved the master equation of Sec. II D with the same values for the parameters  $\lambda=0.4$  and  $\kappa=0.001$  as for the Schrödinger dynamics. The corresponding relaxation into equilibrium is shown in Fig. 8 for a random coupling and in Fig. 9 for the antiferromagnetic Heisenberg coupling.

The horizontal lines denote, again, the equilibrium state, which the spin system should reach according to Eq. (11). The state obtained via the master equation with only one spin coupled directly to the bath approaches the same equilibrium state as the Schrödinger dynamics. Also the off diagonal el-

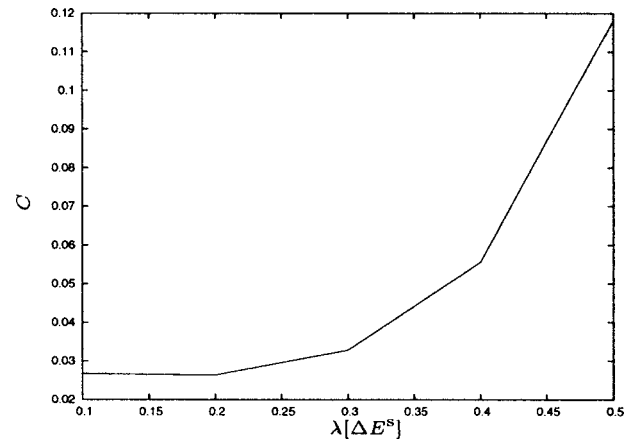


FIG. 7. Correlation  $C$  [Eq. (26)] as a function of  $\lambda$  for a Heisenberg interaction.

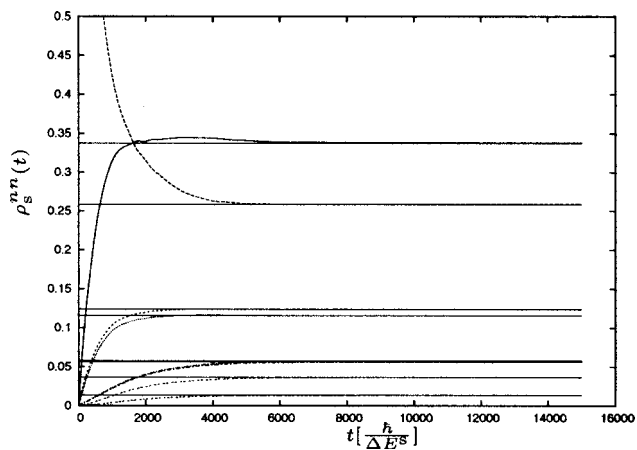


FIG. 8. Time evolution of  $\rho^s$  under a master equation with random interaction. The equilibrium reached is the same as that under Schrödinger dynamics (Fig. 2) and the one predicted by Eq. (11) (horizontal lines).

ements are damped away. Asymptotically both methods show, under the analyzed conditions, the same behavior whereas the short time behavior is difficult to compare.

### 3. Global and local temperatures

As for the Schrödinger dynamics we now study the global and local states of the spin chain in dependence of the parameter  $\lambda$ . We have calculated the spectral temperature (24) for the whole chain and for each individual spin (25). The results are plotted in Fig. 10 for a random interaction and in Fig. 11 for an antiferromagnetic Heisenberg interaction.

In both cases the temperature of the whole spin chain  $T^s$  reaches the same value as the temperature of the environment  $T^e = 1.44$ . For weak spin-spin coupling ( $\lambda \ll 1$ ) the local spectral temperature of each spin is approximately the same as the one of the whole chain. As for the Schrödinger dynamics with increasing  $\lambda$  the local spectral temperature of each spin rises. In particular, the local temperature of the spin in the middle of the chain, spin 2, increases more rapidly than those at the boundaries.

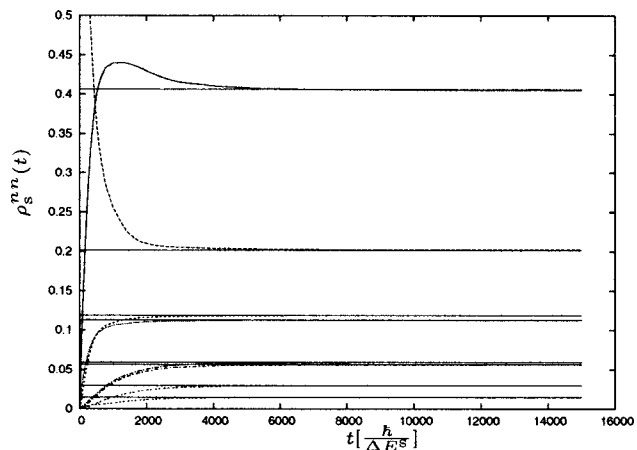


FIG. 9. Time evolution of  $\rho^s$  under a master equation with antiferromagnetic Heisenberg interaction. (compare Fig. 3).

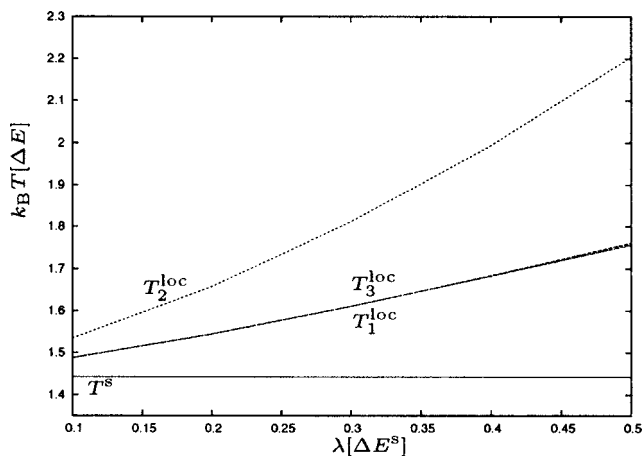


FIG. 10. Spectral temperatures under a master equation with random interaction as function of  $\lambda$ . The solid line is the spectral temperature  $T^s$  of the total spin chain. The dashed line is the local temperature  $T_1^{\text{loc}}$  of spin 1, the narrower dashed line  $T_2^{\text{loc}}$  the one of spin 2, and the dotted line  $T_3^{\text{loc}}$  the one of spin 3.

## IV. ANALYTICAL RESULTS

Finally we want to compare the numerical results shown before with the analytic solutions for the Heisenberg coupled spin chain. We start from a density matrix  $\rho_S(\beta, \lambda)$  for the whole spin chain in a canonical state. Transforming  $\rho_S(\beta, \lambda)$  into the product basis, one can get the reduced density matrices of the single spins  $\rho_\mu(\beta, \lambda)$ . We have calculated the local spectral temperature for each spin using Eq. (23) in dependence on  $\beta$  and  $\lambda$ . The result is shown in Fig. 12 (with the same global inverse temperature  $\beta = \ln 2$  as for the numerical calculations) and is in good agreement with our numerical results (compare with Figs. 5 and 11, respectively).

To analyze the analytical solution for the correlation measure  $C(\beta, \lambda)$  we have used again (26) with the analytical density matrices  $\rho_S(\beta, \lambda)$  and  $\rho_\mu(\beta, \lambda)$ . Figure 13 shows  $C(\beta, \lambda)$  for the global inverse temperature  $\beta = \ln 2$ . Again the analytical result is in very good accordance with our numeri-

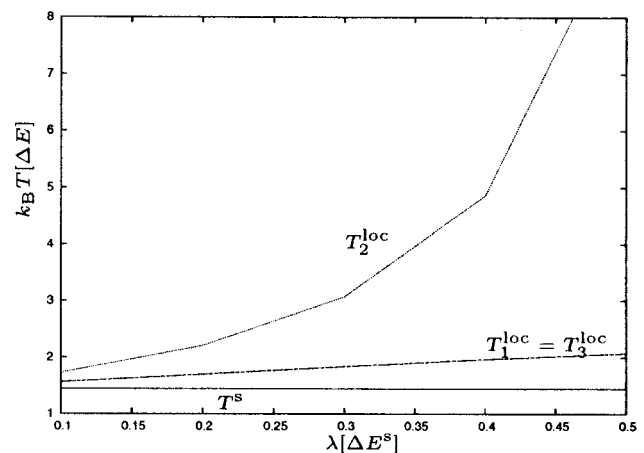


FIG. 11. Spectral temperatures under a master equation with antiferromagnetic Heisenberg interaction in dependence on  $\lambda$  (compare Fig. 10).

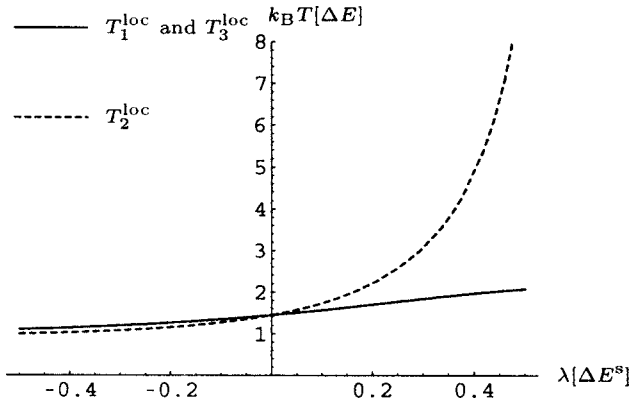


FIG. 12. Analytical results for local spectral temperatures with the global inverse temperature  $\beta = \ln 2$  as function of  $\lambda$  for ferromagnetic ( $\lambda < 0$ ) and antiferromagnetic ( $\lambda > 0$ ) Heisenberg coupling.

cal results (compare with Fig. 7). An interesting point is that the correlations  $C$  also increase in the ferromagnetic case although it is known that there exists no nearest neighbor entanglement [20].

Figure 14 shows  $C(\beta, \lambda)$  as a function of  $\beta$  and  $\lambda$ .  $C$  increases with increasing  $\beta$  and  $\lambda$  in the antiferromagnetic case as one would expect because of the entanglement in the spin chain for low temperatures. For the ferromagnetic coupling one can see a bump depending on  $\beta$  and  $\lambda$ . For low temperatures (large  $\beta$ )  $C$  decreases and vanishes for  $T=0$ .

Presently it is not quite clear why this bump occurs in the ferromagnetic case for intermediate temperatures. It can be shown, that the crest of the ferromagnetic bump is a function of  $\beta$  and  $\lambda$ . The behavior for high temperatures is the same for the ferromagnetic as well as the antiferromagnetic case:  $C$  is vanishing because the local states and the global state will be a totally mixed one.

Note that  $C$  is not an entanglement measure.  $C$  checks whether  $\rho_S(\beta, \lambda)$  is factorizable by the reduced density matrices  $\rho_\mu(\beta, \lambda)$ . Therefore  $C \geq 0$  in the ferromagnetic case for  $T > 0$  indicates on one hand that the product basis differs from the eigenbasis of the spin chain [11] (which is a pure quantum mechanical effect) and otherwise whether a local thermodynamical description is possible.

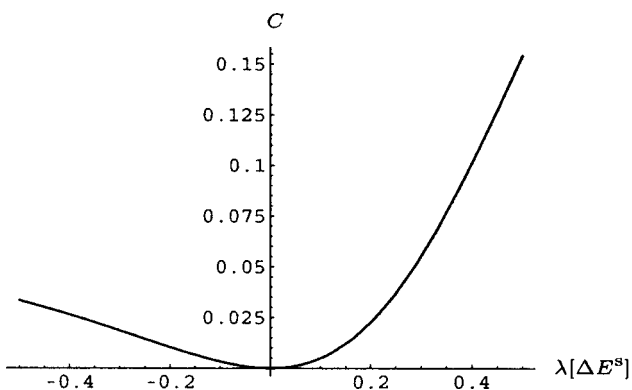


FIG. 13. Correlations  $C$  as function of  $\lambda(\beta = \ln 2)$  for ferromagnetic ( $\lambda < 0$ ) and antiferromagnetic ( $\lambda > 0$ ) Heisenberg coupling.

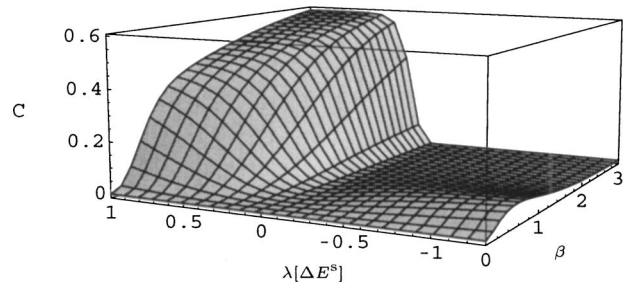


FIG. 14. Correlations  $C$  as a function of  $\beta$  and  $\lambda$  for ferromagnetic ( $\lambda < 0$ ) and antiferromagnetic ( $\lambda > 0$ ) Heisenberg coupling.

V. SUMMARY AND CONCLUSION

The main motivation of this paper has been to analyze the thermodynamic behavior of one part (“the system”) within a bipartite quantum system subject to Schrödinger evolution. Such effective relaxation to equilibrium is predicted to occur under rather general conditions. Nevertheless deviations are not excluded. Here we have been interested in (spatially) selective system-environment couplings and in the effect of further partitioning of the system under consideration.

For this purpose we have studied a spin chain consisting of three interacting spins coupled locally to a quantum environment. Two different spin-spin coupling types have been examined: a random and a Heisenberg coupling. For both we have solved the exact Schrödinger equation and analyzed the reached equilibrium states. We showed that the spin system relaxes into a thermal equilibrium state, which is in accordance with the state one would expect from quantum thermodynamics. Temporal fluctuations persist, though, and are a result of the still comparatively small environment.

The spin chain always reaches the predicted state independently of the internal coupling type and strength. Thus we can conclude that the internal structure of a small system as well as locality of the coupling to a quantum environment does not effect the relaxation behavior. The results also show that the overall state reached is a canonical one and thus the spectral temperature of the total spin chain can be identified as the “real” (thermodynamic) temperature of the system.

On the other hand, the spectral temperature of each individual spin does depend on the internal coupling strength, an effect which has been traced back to increased correlations of each spin with its neighbor(s). This causes an increase of the local entropy which mimics a higher spectral temperature. So our conclusion is that for stronger internal couplings the local spin states are nonthermal states [21], indicating that the global temperature ceases to be available also locally.

For the antiferromagnetic Heisenberg spin chain, we have found that single spins are approximately in thermal states up to coupling strengths  $\lambda \approx 1.5$ . This is in agreement with the results in [22]. Also the comparison with the analytical solution shows no differences with the numerical results for the reached equilibrium states.

A further motivation of this paper has been to compare the well-known Markovian master equation approach with the exact Schrödinger dynamics. We have found, that in all con-

sidered cases both approaches lead to the same asymptotic result, i.e., equilibrium states of canonical form. The analysis of the short time dynamics, e.g., the relaxation times, etc., for the considered approaches should be an interesting topic for future research.

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