Quantum Decoherence and Thermalization at Finite Temperatures of Non-Degenerate Spin Systems via Small Spin Environments

M.A. Novotny

Dept. of Physics and Astronomy and HPC^2 Center for Computational Sciences, Mississippi State U., Mississippi State, MS 39762, USA

F. Jin

Institute for Advanced Simulation, Jülich Supercomputing Centre,
Forschungszentrum Jülich, D-52425 Jülich, Germany

H. De Raedt

Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747AG Groningen, The Netherlands

K. Michielsen

Institute for Advanced Simulation, Jülich Supercomputing Centre,
Forschungszentrum Jülich, D-52425 Jülich, Germany
RWTH Aachen University, D-52056 Aachen, Germany

E-mail: `man40@msstate.edu`

Abstract. We study the case of a small quantum spin system S with a non-degenerate groundstate coupled to a small quantum spin bath. Finite temperature measures for both quantum decoherence and thermalization are studied. The computational results, obtained from exact diagonalization, compare well with a recent perturbation theory prediction, even when the system and bath are of comparable sizes.

1. Introduction

In quantum statistical mechanics a quantum system S is coupled to a quantum environment (or bath) E, and the time evolution of the entirety $S+E$ is governed by the time-dependent Schrödinger equation. A recent perturbation theory prediction [1] assumes that initially the entirety is in a canonical-thermal state [2, 3, 4], and makes predictions for both a measure σ for the decoherence and a measure δ for the thermalization. In this short paper the case of a non-degenerate ground state for S is examined for spin systems coupled to small spin baths. This study is performed in order to test the theoretical predictions for σ and δ for environments comparable in size to the system.

2. Theory and Results

The Hamiltonian of the entirety $S+E$ is taken to be

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_E + \lambda \mathcal{H}_{SE} \,, \tag{1}$$

where $\mathcal{H}_S$ and $\mathcal{H}_E$ are the system and environment Hamiltonian, respectively and $\mathcal{H}_{SE}$ describes the interaction between the system S and the environment E. We consider only time-independent Hamiltonians. The global system-environment coupling strength is λ.

In the normal fashion [5, 6, 7, 8], the quantum system S is described by the reduced density matrix $\widetilde{\rho}(t) \equiv \mathbf{Tr}_E \rho(t)$, where $\rho(t) = |\Psi(t)\rangle \langle \Psi(t)|$ is the density matrix of the entirety $S+E$ at time t, $\Psi(t)$ denotes the wavefunction of the entirety, and $\mathbf{Tr}_E$ denotes the trace over all degrees of freedom of the environment. We assume that $\widetilde{\rho}$ is expressed in the basis in which $\mathcal{H}_S$ is diagonal.

The degree of decoherence of the system is characterized by [9, 10]

$$\sigma(t) = \sqrt{\sum_{i=1}^{D_S-1} \sum_{j=i+1}^{D_S} |\widetilde{\rho}_{ij}(t)|^2} \,, \tag{2}$$

where $\widetilde{\rho}_{ij}(t)$ is the matrix element (i,j) of the reduced density matrix in the basis that diagonalizes H_S, and D_S is the dimension of the Hilbert space of $\mathcal{H}_S$. We also define a quantity measuring thermalization, namely the difference between $\widetilde{\rho}_{ii}$ and the canonical distribution as [9]

$$\delta(t) = \sqrt{\sum_{i=1}^{D_S} \left(\widetilde{\rho}_{ii}(t) - e^{-b(t)E_i^{(S)}} \Big/ \sum_{i'=1}^{D_S} e^{-b(t)E_{i'}^{(S)}} \right)^2} \,, \tag{3}$$

where $\{E_i^{(S)}\}$ denote the eigenvalues of $\mathcal{H}_S$ and $b(t)$ is a fitting parameter. For excellent fits to the canonical ensemble, the fitting parameter $b(t)$ should approach the inverse temperature $\beta = 1/T$ (in units $k_B = 1$) at large times.

Assuming that initially the entirety is in a canonical-thermal state, Ref. [1] gives a perturbation theory result valid for small $\beta\lambda$, for the expectation value for the decoherence measure of Eq. (2)

$$
\begin{aligned}
\mathcal{E}\left(\sigma^2\right) \;=\; & \frac{1}{2} \frac{Z_E(2\beta)}{Z_E^2(\beta)} \left(1 - \frac{Z_S(2\beta)}{Z_S^2(\beta)} \right) - \frac{2\,D}{(D+1)} \frac{Z_E(3\beta)}{Z_E^3(\beta)} \left(\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S(3\beta)}{Z_S^3(\beta)} \right) \\
& + \frac{3}{2} \frac{D}{(D+1)} \frac{Z_E^2(2\beta)}{Z_E^4(\beta)} \left(\frac{Z_S(2\beta)}{Z_S^2(\beta)} - \frac{Z_S^2(2\beta)}{Z_S^4(\beta)} \right) \,.
\end{aligned} \tag{4}
$$

Equation (4) is written in terms of partition functions for S and E at inverse temperature β, respectively $Z_S(\beta)$ and $Z_E(\beta)$. Here $D = D_S D_E = 2^{N_S+N_E}$ is the dimension of the Hilbert space of the entirety, with N_S (N_E) the number of spin-1/2 particles in the system (environment with Hilbert space dimension D_E). It is important to remember that even when $\lambda=0$ (no part of the Hamiltonian coupling the system to the environment) the assumption that the entirety is in a canonical-thermal state [1] means that the entirety wavefunction is not a direct product of wavefuctions from S and E. The groundstate degeneracy of the system (environment) is g_S (g_E). In this paper we concentrate on non-degenerate groundstates for S, so $g_S=1$. We restrict ourselves to $g_S=1$ since in the limit of low temperatures [1] one has

$$\mathcal{E}\left(\sigma^2\right) = \frac{1}{2} \frac{g_S - 1}{g_E g_S} \left(1 - \frac{D}{(D+1)\,g_E g_S} \right) \tag{5}$$

and thus for low temperatures $\mathcal{E}(\sigma^2) \to 0$ for $g_S{=}1$.

We performed exact diagonalization on an entirety $S{+}E$ composed of a ring of spin-1/2 particles (spins). The exact diagonalization allows us to calculate exactly the partition functions Z_S and Z_E of Eq. (4). Therefore direct comparisons between the theoretical results and the numerical results could be performed with **no** adjustable parameters. All couplings within the ring are made randomly between $[-1,1]$, the explicit random values are listed in Table 1, for nearest-neighbor spin couplings in a ring of $N{=}N_S{+}N_E$ spins with periodic boundary conditions. The Hamiltonian between spins j and $j{+}1$ is $\mathcal{H}_{j,j+1} = -J^x_{j,j+1}s^x_j s^x_{j+1} - J^y_{j,j+1}s^y_j s^y_{j+1} - J^z_{j,j+1}s^z_j s^z_{j+1}$.

In this paper we keep $N_S{=}4$, and always keep the interactions in $\mathcal{H}_S$ as the couplings in Table 1 for $\mathcal{H}_{j,j+1}$ with $j = 1, 2, 3$. Specifically, $\mathcal{H}_S = \mathcal{H}_{1,2} + \mathcal{H}_{2,3} + \mathcal{H}_{3,4}$, and the degeneracy of the ground state is thus $g_S{=}1$ always. The system-environment Hamiltonian used in this paper is $\mathcal{H}_{SE} = \mathcal{H}_{4,5} + \mathcal{H}_{N,1}$, always with the values listed in Table 1 (note the periodic boundary conditions since we study a ring of spins).
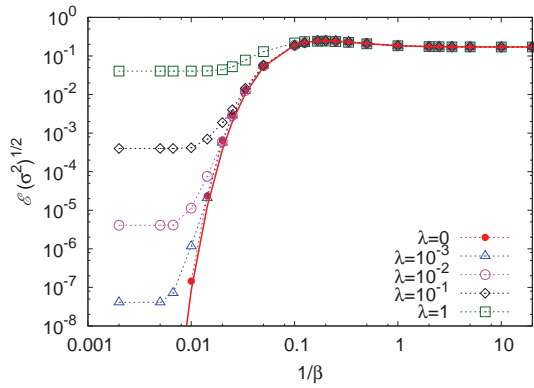
Figure 1. The square root of the expectation value for the decoherence measure σ^2 for a spin system with $N_S{=}4$ and $g_S{=}1$ coupled to a spin bath with $N_E{=}4$ and $g_E{=}1$ as a function of the temperature $1/\beta$ for various values of the global system-environment coupling strength λ. The solid line is obtained from Eq. (4). The dashed lines are guides to the eye.
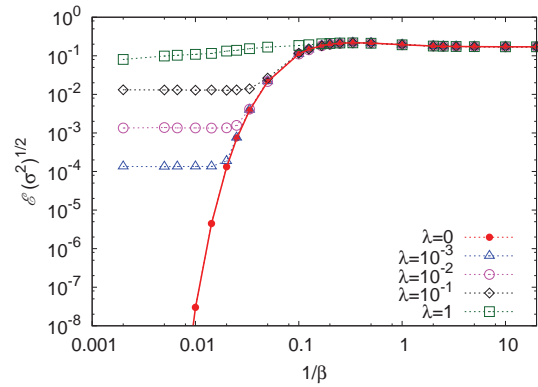
Figure 2. The same as in Fig. 1. Here, however, all interaction strengths in the $N_E = 4$ spin Hamiltonian $\mathcal{H}_E$ are set to -1, explicitly $\mathcal{H}_E = -\sum_{j=5}^{7}\left(s^x_j s^x_{j+1} + s^y_j s^y_{j+1} + s^z_j s^z_{j+1}\right)$, and therefore the environment degeneracy is $g_E = 5$. The solid line is the perturbation theory result from Eq. (4), while the dashed lines are guides to the eye.

Figure 1 shows results for the square root of the expectation value $\mathcal{E}(\sigma^2)$ as a function of temperature, $1/\beta$, for different strengths of the system-environment coupling strength λ. The groundstate degeneracies are $g_S{=}g_E{=}1$. Here there are four spins in both the system and the environment. The environment Hamiltonian here is $\mathcal{H}_E = \sum_{j=5}^{7}\mathcal{H}_{j,j+1}$ with the interaction strengths listed in Table (1). Figure 1 shows an extremely good agreement with the theory of Eq. (4), even though the dimensions of the Hilbert space of the environment and the system are equal $D_E{=}D_S{=} 2^4$. This is true for high temperatures, and continues to be true as long as $\beta\lambda{\ll}1$. Therefore, at all temperatures, it is not required to have a very large spin bath in order to obtain the predicted value for the decoherence measure σ.

The data points in all the figures are obtained by first picking uniformly at random a typical unit vector from the entirety Hilbert space. In particular, a unit vector $|\Psi_0\rangle = \sum_{j=1}^{D_S}\sum_{p=1}^{D_E} d_{j,p}|j,p\rangle$ is picked with the coefficients $\{d_{j,p}\}$ complex Gaussian random numbers

Table 1. The Hamiltonian $\mathcal{H}_{j,j+1}$ interaction strengths used in this paper.

j	$j+1$	$J^x_{j,j+1}$	$J^y_{j,j+1}$	$J^z_{j,j+1}$
1	2	0.99464	0.18950	-0.83949
2	3	0.66019	-0.74690	0.46002
3	4	0.87474	0.10580	-0.93014
4	5	0.76983	0.86751	0.29104
N	1	-0.35312	0.61078	0.17238
5	6	0.16682	-0.65712	-0.69131
6	7	-0.84125	-0.36024	0.97012
7	8	-0.30384	0.29020	0.77970
8	9	-0.99592	-0.33191	0.37434
9	10	0.49823	0.25744	-0.76540
10	11	0.64452	-0.99678	-0.78684
11	12	-0.65810	-0.89997	-0.41505

normalized so that $\sum_{j=1}^{D_S} \sum_{p=1}^{D_E} |d_{j,p}|^2 = 1$. The vectors $|j,p\rangle$ are any orthogonal basis that spans the D dimensional Hilbert space of the entirety. The associated canonical-thermal state, drawn uniformly from the ensemble of all canonical-thermal states at inverse temperature β, is given by

$$|\Psi_\beta\rangle = e^{-\beta\mathcal{H}/2} |\Psi_0\rangle \Big/ \langle\Psi_0| e^{-\beta\mathcal{H}} |\Psi_0\rangle^{\frac{1}{2}} \; . \tag{6}$$

This is called a canonical-thermal state because for any operator for an observable $\mathcal{A}$ one has

$$\langle\Psi_\beta| \mathcal{A} |\Psi_\beta\rangle \approx \mathrm{Tr}\left(\mathcal{A}e^{-\beta\mathcal{H}}\right) \Big/ \mathrm{Tr}\left(e^{-\beta\mathcal{H}}\right) \tag{7}$$

with the error in the approximation being of the order of $D^{-\frac{1}{2}}$. Each point in all the figures is an average over 10^3 vectors, as in Eq. (6), from the canonical-thermal-state ensemble.

Figure 2 shows results for the square root of the expectation value $\mathcal{E}(\sigma^2)$ as a function of temperature, $1/\beta$, for different strengths λ. Here the Hamiltonians $\mathcal{H}_S$ and $\mathcal{H}_{SE}$ are the same as in Fig. 1, but the environment has uniform, isotropic bond strengths

$$\mathcal{H}_E = -\sum_{j=N_S+1}^{N-1} \left(s^x_j s^x_{j+1} + s^y_j s^y_{j+1} + s^z_j s^z_{j+1}\right) \tag{8}$$

with N_E=4 and N=8. Consequently g_E=5. Again we observe that even though $N_S=N_E$=4 there is excellent agreement between the theory and the calculations as long as $\beta\lambda\ll1$.

Figure 3 shows results for the square root of the expectation value $\mathcal{E}(\sigma^2)$ as a function of temperature, $1/\beta$, for different strengths λ for the case N_E=8, again with random couplings drawn between $[-1,1]$ for the environment couplings. Again $\mathcal{H}_S$ and $\mathcal{H}_{SE}$ are unchanged from Fig. 1, but the environment Hamiltonian is now $\mathcal{H}_E = \sum_{j=5}^{11} \mathcal{H}_{j,j+1}$ with the interaction strengths listed in Table (1). Again we observe that even though $N_S=N_E/2$ there is excellent agreement between the theory and the calculations as long as $\beta\lambda\ll1$. In fact, there is very little difference that can be seen by eye in comparing Figure 1 and Figure 3. Note, however, that for high temperatures ($\beta\rightarrow0$) one has $\mathcal{E}\left(\sigma^2\right) \rightarrow (D_S - 1)/2(D_S D_E + 1)$ [10], which explains the slightly different infinite temperature asymptotic values between the two figures.
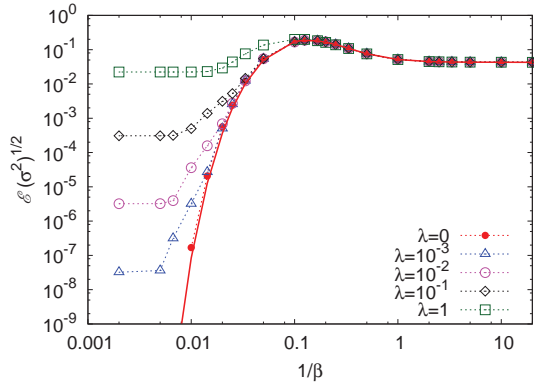
Figure 3. The same as in Fig. 1. Here, however, N_E=8 and again the environment degeneracy is g_E=1. The solid line is the perturbation theory result from Eq. (4), while the dashed lines are guides to the eye.
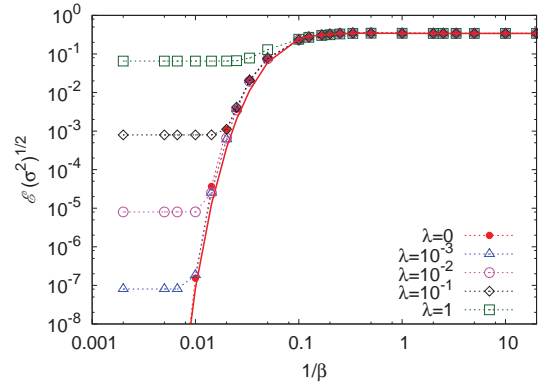
Figure 4. The same as in Fig. 1. Here, however, N_E=2 and again the environment degeneracy is g_E=1. The solid line is the perturbation theory result from Eq. (4), while the dashed lines are guides to the eye.

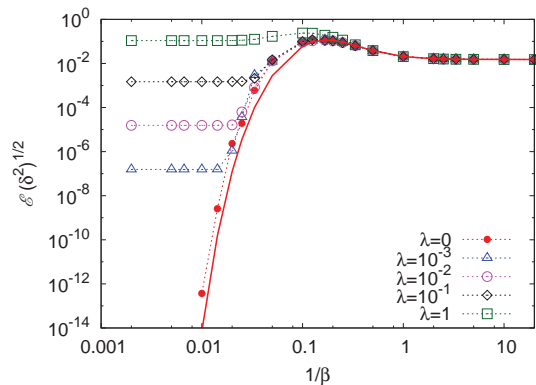Figure 4 shows results for the square root of the expectation value $\mathcal{E}(\sigma^2)$ as a function of temperature, $1/\beta$, for different strengths λ for the case N_E=2. Again $\mathcal{H}_S$ and $\mathcal{H}_{SE}$ are unchanged from Fig. 1, but the environment Hamiltonian is now $\mathcal{H}_E = \mathcal{H}_{5,6}$ with the interaction strength listed in Table (1). Again we observe that even though N_S=$2N_E$ and N_E=2, there is still agreement between the theory and the calculations as long as $\beta\lambda\ll1$. Now, however, there is a larger difference at temperatures below $1/\beta \approx 0.1$ between the perturbation theory and the results from Eq. (4). This suggests that higher order terms in the perturbation theory are relevant for small spin systems with N_S>N_E.

There is a related prediction for the expectation value of the measure of thermalization to that of Eq. (4) [1]. Figures 5 and 6 shows results for the square root of the expectation value of δ^2 for the same systems as studied in Fig. 3 and Fig. 4, respectively. We observe very nice agreement between the theory and the calculations as long as the temperature is higher than about $1/\beta\approx0.1$.

3. Discussion and Conclusions
We have studied decoherence and thermalization of quantum systems, focusing on the case where the groundstate of the system is non-degenerate and the bath is comparable to the system in terms of the sizes of the Hilbert spaces. This study, together with that of Ref. [1], may be of interest to the recently developing technology of adiabatic quantum computing [11, 12], as exemplified for example by D-Wave machines [12, 13, 14].

We have compared the theoretical predications of Ref. [1] with exact diagonalization calculations. We have concentrated on spin chains, with N_S=4 spins in the system and with N_E=2, 4, and 8 spins in the environment. In all cases at high temperatures excellent agreement is found between the exact diagonalization calculations and the perturbation theory predications of Ref. [1]. The same is true at low temperatures, excellent agreement is found, provided that $\beta\lambda\ll1$. At low temperatures, however, the N_E=2 case shows qualitative differences with the theoretical predictions. It is to be emphasized that there are no adjustable parameters in our comparison between the exact diagonalization calculations and the theoretical predictions.

Figure 5. The square root of the expectation value for the thermalization measure δ^2 for a spin system with $N_S=4$ and $g_S=1$ coupled to a spin bath with $N_E=8$ and $g_E=1$. The entirety is the same as in Fig. 3. The solid line is the perturbation theory result, while the dashed lines are guides to the eye.
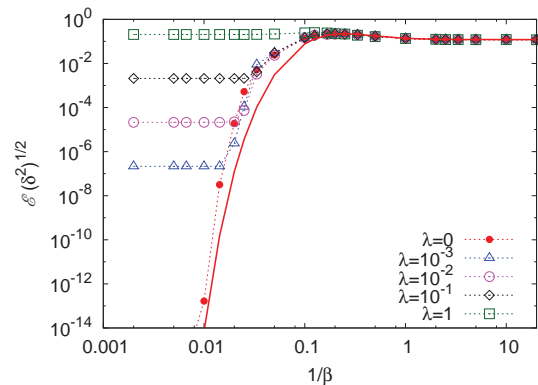
Figure 6. The square root of the expectation value for the thermalization measure δ^2 for a spin system with $N_S=4$ and $g_S=1$ coupled to a spin bath with $N_E=2$ and $g_E=1$. The entirety is the same as in Fig. 4. The solid line is the perturbation theory result, while the dashed lines are guides to the eye.

Acknowledgments

[1] Novotny MA, Jin F, Yuan S, Miyashita S, De Raedt H, and Michielsen K, 2016, *Phys. Rev. A* **93**, 032110.
[2] Hams A. and De Raedt H, 2000, *Phys. Rev. E* **62**, 4365.
[3] Jin F, De Raedt H, Yuan S, Katsnelson M.I, Miyashita S., and Michielsen K, 2010, *J. Phys. Soc. Jpn.* **79**, 124005.
[4] Sugiura S. and Shimizu A, 2013, *Phys. Rev. Lett.* **111**, 010401.
[5] Kubo R, Toda M, and Hashitsume N, *Statistical physics II: Nonequilibrium statistical mechanics*, (Springer-Verlag, 1985).
[6] Ponomarev A.V, Denisov S, and Hänggi P, 2011, *Phys. Rev. Lett.* **106**, 010405.
[7] Ponomarev A.V, Denisov S, Hänggi P, and Gemmer J, 2012, *Europhys. Lett.* **98**, 40011.
[8] Swendsen R.H, *An Introduction to Statistical Mechanics and Thermodynamics*, (Oxford University Press, 2012).
[9] Yuan S, Katsnelson M.I, and De Raedt H, 2009, *J. Phys. Soc. Jpn.* **78** 094003.
[10] Jin F, Michielsen K, Novotny M. A, Miyashita S, Yuan S, and De Raedt H, 2013, *Phys. Rev. A* **87**, 022117.
[11] Rieffel E and Polak W, *Quantum Computing: A Gentle Introduction*, (MIT Press, 2011).
[12] Boixo S, Rønnow T.F, Isakov S.V, Wang Z, Wecker D, Lidar D.A, Martinis J.M, and Troyer M, 2014, *Nature Physics* **10**, 218.
[13] Novotny M.A, Hobl Q.L, Hall J.S, and Michielsen K, 2016, *J. Physics: Conf. Series* **681**, 012005.
[14] D-Wave, The Quantum Computing Company, http://www.dwavesys.com