Dynamics of a Single Spin-1/2 Coupled to *x*- and *y*-Spin Baths: Algorithm and Results

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Abstract

The real-time dynamics of a single spin-1/2 particle, called the central spin, coupled to the *x*(*y*)-components of the spins of one or more baths is simulated. The bath Hamiltonians contain interactions of *x*(*y*)-components of the bath spins only but are general otherwise. An efficient algorithm is described which allows solving the time-dependent Schrödinger equation for the central spin, even if the *x*(*y*) baths contain hundreds of spins. The algorithm requires storage for 2×2 matrices only, no matter how many spins are in the baths. We calculate the expectation value of the central spin, as well as its von Neumann entropy $\mathcal{S}(t)$, the quantum purity $\mathcal{P}(t)$, and the off-diagonal elements of the quantum density matrix. In the case of coupling the central spin to both *x*- and *y*- baths the relaxation of $\mathcal{S}(t)$ and $\mathcal{P}(t)$ with time is a power law, compared to an exponential if the central spin is only coupled to an *x*-bath. The effect of different initial states for the central spin and bath is studied. Comparison with more general spin baths is also presented.

Keywords: Quantum Dynamics, Spin Bath, Decoherence, Thermalization

1. Introduction

Simulating the time development of any non-relativistic quantum system involves solving the Time-Dependent Schrödinger Equation (TDSE) [1],

$$\mathcal{H} \left| \Psi(t) \right\rangle = -\frac{\hbar}{i} \frac{\partial}{\partial t} \left| \Psi(t) \right\rangle, \tag{1}$$

where the Hamiltonian $\mathcal{H}$ is assumed to be independent of time and the initial wave function $\left| \Psi(0) \right\rangle$ is given. For example, to study the time-evolution of a model for a quantum computer the TDSE must be solved [2, 3, 4, 5, 6] for qubits, which are spin-1/2 objects. If the closed quantum system is composed of a subsystem S on which measurements will be taken, and an environment or bath B, then the Hamiltonian can be written as

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_B + \mathcal{H}_{SB}, \tag{2}$$

with the first term the Hamiltonian of the subsystem S, the second term the Hamiltonian of the bath B, and the third term the Hamiltonian for the coupling between the subsystem S and the bath B. In this paper we assume that the

subsystem S consists of a single spin-1/2 particle, also called the central spin, and that the bath B is composed of N_B spin-1/2 particles. The dimension of the Hilbert space of the bath is $D_B = 2^{N_B}$ and the dimension of the complete Hilbert space is $2D_B = 2^{N_B+1}$. Thus the dimension of the vector $|\Psi(t)\rangle$ in Eq. (1) is 2^{N_B+1}. The state of the subsystem S is described by the reduced density matrix

$$\rho(t) = \text{Tr}_B\left[\rho_{S+B}(t)\right], \tag{3}$$

where ρ_{S+B} is the density matrix of the complete $N_B + 1$ spin system, and the trace is over the N_B spins in the bath. Thus $\rho(t)$ is a 2×2 matrix. However, to calculate $\rho(t)$ one first needs to propagate with the TDSE

$$|\Psi(t)\rangle = \exp\left(-\frac{i\mathcal{H}t}{\hbar}\right)|\Psi(0)\rangle, \tag{4}$$

for all $N_B + 1$ spins, and then trace out the bath spins.

The dimension of $|\Psi(t)\rangle$ presents an enormous difficulty in computer calculations of spin systems. We need to have N_B large, but memory of computers is limited. For example, the most powerful computer on the November 2011 Top 500 list [7], the K computer at the RIKEN Advanced Institute for Computational Science in Japan, has 705,024 cores and has a Linpack benchmark of 10.5 Petaflop/s . Each compute node of the K computer has 16 Gbyte of memory, so the total memory of the K computer is about 1.2×10^{16} bytes, which means that the number of spins for the largest vector $|\Psi(t)\rangle$ that can be stored in the K computer is $N_B \approx 50$. The stated goal for exascale computing that the memory should be a few exabytes limits the size of the vector $|\Psi(t)\rangle$ to $N_B \approx 60$. The number of spins that can be included in TDSE computer calculations is small compared to the size of spin baths in laboratory experiments. For example, recent experiments studied a single electron coupled to a bath of about 10^9 spins [8, 9]. There are efficient algorithms to calculate the TDSE for any Hamiltonian for a small total number of spins, such as the efficient method based on Chebyshev polynomials [10, 11, 12, 13, 14]. A recent paper reported the use of Chebyshev-type algorithms to simulate the dynamics of up to 36 spin-1/2 particles to study decoherence and thermalization [15], storing the full vectors of size 2^{36} for the TDSE computation. Other studies have also used calculation of the TDSE to study the decoherence of quantum spin systems coupled to spin baths [16, 17, 18, 19].

In this paper we calculate the TDSE for a central spin-1/2 coupled to different types of N_B-bath spins. The paper has two goals. One goal is to introduce an efficient algorithm that only has to store matrices of size 2×2 (rather than vectors of size 2^{N_B+1}) to solve the TDSE for certain types of baths which we call x, y-baths. The second goal is to examine the decoherence and thermalization effects of x, y-baths. The x- and y-baths we compute are generalizations of baths studied analytically [20], with the quantum purity either decaying exponentially or as a power law, depending on the bath.

2. Model and Quantities Measured

We consider a single spin-1/2 particle coupled to a quantum bath of N_B spin-1/2 particles. The dimension of the Hilbert space is 2^{N_B+1}. Let the central spin be numbered spin 0, and the bath spins 1 through N_B. The Pauli spin matrices are

$$s^x = \frac{\hbar}{2}\sigma^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s^y = \frac{\hbar}{2}\sigma^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad s^z = \frac{\hbar}{2}\sigma^z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5}$$

We define spin operators which act on the Hilbert space of dimension 2^{N_B+1}

$$S_m^\ell = I_2 \otimes I_2 \otimes \cdots \otimes I_2 \otimes s^\ell \otimes I_2 \otimes \cdots \otimes I_2, \tag{6}$$

with I_2 the 2×2 identity matrix and s^ℓ the 2×2 Pauli spin matrix ($\ell \in \{x, y, z\}$) at the mth position in the Kronecker (direct) product of $N_B + 1$ matrices of size 2×2. From now on we set $\hbar = 1$.

The central spin Hamiltonian we consider is

$$\mathcal{H}_S = \omega_0 S_0^z, \tag{7}$$

where ω_0 denotes the strength of the external magnetic field that is applied to the central spin in the z-direction.

There are four quantities of interest that we measure. For any expectation value of the central spin, Eq. (3) gives the first class of quantities of interest,

$$\left\langle S_0^\ell(t) \right\rangle = \mathrm{Tr} \left[s^\ell \rho(t) \right] . \tag{8}$$

The second quantity of interest is the quantum purity for the central spin,

$$\mathcal{P}(t) = \mathrm{Tr} \left[\rho(t)^2 \right] . \tag{9}$$

Since $\rho(t)$ is a 2×2 matrix we can write it as $\rho(t) = a_\rho(t)I_2 + \vec{b}_\rho(t) \cdot \vec{\sigma}$, with the vector $\vec{b}_\rho(t)$ having components $\left(b_{\rho x}(t), b_{\rho y}(t), b_{\rho z}(t) \right)$ and $b_\rho(t) = \sqrt{b_{\rho x}^2(t) + b_{\rho y}^2(t) + b_{\rho z}^2(t)}$. With the identity $\left[\vec{b}_\rho(t) \cdot \vec{\sigma} \right]^2 = b_\rho^2(t)I_2$, one has for the quantum purity

$$\mathcal{P}(t) = 2a_\rho^2(t) + 2b_\rho^2(t) . \tag{10}$$

The third quantity of interest is the von Neumann entropy

$$\mathcal{S}(t) = -k_B \mathrm{Tr} \left[\rho(t) \log_2 \rho(t) \right] = -k_B \lambda_+(t) \log_2 \left[\lambda_+(t) \right] - k_B \lambda_-(t) \log_2 \left[\lambda_-(t) \right] , \tag{11}$$

where the eigenvalues of $\rho(t)$ are $\lambda_\pm(t) = a_\rho(t) \pm b_\rho(t)$. From now on we set Boltzmann's constant $k_B = 1$. The fourth quantity of interest, as defined in Ref. [15], is the sum of the off-diagonal elements of $\rho(t)$

$$\sigma(t) = \sqrt{\sum_{i=1}^{2^{N_s}-1} \sum_{j=i+1}^{2^{N_s}} \left| \rho_{ij}(t) \right|^2} , \tag{12}$$

if there were N_s spins in the subsystem. Note that $\sigma(t)$ should not be confused with the Pauli matrices σ^ℓ. For general N_s, thermalization toward a canonical distribution has the necessary condition that $\sigma(t)$ becomes very small [15]. For our single spin-1/2 system $N_s = 1$ so

$$\sigma(t) = \left| \rho_{12}(t) \right| . \tag{13}$$

3. Efficient Algorithm for x, y-baths

We assume that the N_B x, y-bath spins include N_x x-bath spins and N_y y-bath spins with $N_B = N_x + N_y$. The central-spin bath interaction Hamiltonian reads

$$\mathcal{H}_{SB} = S_0^x \left[\sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_{N_x}=0}^{1} J_{i_1,i_2,\cdots,i_{N_x}} \left(S_1^x \right)^{i_1} \left(S_2^x \right)^{i_2} \cdots \left(S_{N_x}^x \right)^{i_{N_x}} \right]$$
$$+ S_0^y \left[\sum_{j_1=0}^{1} \sum_{j_2=0}^{1} \cdots \sum_{j_{N_y}=0}^{1} K_{j_1,j_2,\cdots,j_{N_y}} \left(S_{N_x+1}^y \right)^{j_1} \left(S_{N_x+2}^y \right)^{j_2} \cdots \left(S_{N_x+N_y}^y \right)^{j_{N_y}} \right] , \tag{14}$$

where $J_{i_1,i_2,\cdots,i_{N_x}}$ denotes the coupling strength between the central spin and the N_x spins in the x-bath, while the $K_{j_1,j_2,\cdots,j_{N_y}}$ are the coupling strengths between the central spin and the N_y y-bath spins. The bath Hamiltonian is given by

$$\mathcal{H}_B = \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_{N_x}=0}^{1} \widetilde{J}_{i_1,i_2,\cdots,i_{N_x}} \left(S_1^x \right)^{i_1} \left(S_2^x \right)^{i_2} \cdots \left(S_{N_x}^x \right)^{i_{N_x}}$$
$$+ \sum_{j_1=0}^{1} \sum_{j_2=0}^{1} \cdots \sum_{j_{N_y}=0}^{1} \widetilde{K}_{j_1,j_2,\cdots,j_{N_y}} \left(S_{N_x+1}^y \right)^{j_1} \left(S_{N_x+2}^y \right)^{j_2} \cdots \left(S_{N_x+N_y}^y \right)^{j_{N_y}} , \tag{15}$$

where $\widetilde{J}_{i_1,i_2,\cdots,i_{N_x}}$ denotes the coupling strength between the N_x spins in the x-bath, and similarly $\widetilde{K}_{j_1,j_2,\cdots,j_{N_y}}$ denotes the coupling strength between the N_y y-bath spins. Note that the type of spin interaction (2-spin, 3-spin, $\cdots$) is specified

by the number of ones in the subscript of $\widetilde{J}$ or $\widetilde{K}$, since it follows from Eq. (6) that $\left(S_i^x\right)^0 = \left(S_j^y\right)^0 = I_F$ where I_F denotes the $2^{N_B+1} \times 2^{N_B+1}$ identity matrix. Similarly the type of spin interaction (2-spin, 3-spin, $\cdots$) is specified by one plus the number of ones in the subscript of J or K. When all x-bath two-body couplings are identical, for brevity we define these as a coupling strength J_2. Similarly for the x-bath the three-body interactions J are defined as J_3, the N_x-body interactions J_M (only one bath spin is not in the sum), and the $(N_x + 1)$-body interactions as J_A. We similarly define the coupling K_2 for the y-bath when all two-body couplings are identical, K_3 for all identical three-body couplings, K_M when all identical N_y-body couplings, and the $(N_y + 1)$-body coupling K_A.

We introduce the two matrices

$$p_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \qquad \text{and} \qquad p_y = \frac{1}{\sqrt{2}}\begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix}, \tag{16}$$

having the properties $p_x p_x^{-1} = I_2$ with $p_x^{-1} = p_x^T = p_x^\dagger$ and $p_y p_y^{-1} = I_2$ with $p_y^{-1} = p_y^\dagger$. The matrices p_x and p_y also exhibit the properties

$$p_x^\dagger s^x p_x = s^z \qquad \text{and} \qquad p_y^\dagger s^y p_y = s^z . \tag{17}$$

In addition

$$p_x^\dagger \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \text{and} \qquad p_y^\dagger \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{18}$$

We next introduce the matrix

$$P_p = I_2 \otimes p_x \otimes \cdots \otimes p_x \otimes p_y \otimes \cdots \otimes p_y , \tag{19}$$

with position zero in the product occupied by the 2×2 identity matrix, the positions 1 through N_x in the Kronecker product occupied by p_x, and the positions $N_x + 1$ through $N_B = N_x + N_y$ by p_y. It follows that $P_p^\dagger P_p = I_F$. We introduce the transformed Hamiltonian

$$
\begin{aligned}
\widetilde{\mathcal{H}} &= P_p^\dagger \mathcal{H} P_p \\
&= \omega_0 S_0^z + \sum_{i_1=0}^1 \sum_{i_2=0}^1 \cdots \sum_{i_{N_x}=0}^1 \widetilde{J}_{i_1,i_2,\cdots,i_{N_x}} \left(S_1^z\right)^{i_1} \left(S_2^z\right)^{i_2} \cdots \left(S_{N_x}^z\right)^{i_{N_x}} \\
&\quad + \sum_{j_1=0}^1 \sum_{j_2=0}^1 \cdots \sum_{j_{N_y}=0}^1 \widetilde{K}_{j_1,j_2,\cdots,j_{N_y}} \left(S_{N_x+1}^z\right)^{j_1} \left(S_{N_x+2}^z\right)^{j_2} \cdots \left(S_{N_x+N_y}^z\right)^{j_{N_y}} \\
&\quad + S_0^x \left[\sum_{i_1=0}^1 \sum_{i_2=0}^1 \cdots \sum_{i_{N_x}=0}^1 J_{i_1,i_2,\cdots,i_{N_x}} \left(S_1^z\right)^{i_1} \left(S_2^z\right)^{i_2} \cdots \left(S_{N_x}^z\right)^{i_{N_x}}\right] \\
&\quad + S_0^y \left[\sum_{j_1=0}^1 \sum_{j_2=0}^1 \cdots \sum_{j_{N_y}=0}^1 K_{j_1,j_2,\cdots,j_{N_y}} \left(S_{N_x+1}^z\right)^{j_1} \left(S_{N_x+2}^z\right)^{j_2} \cdots \left(S_{N_x+N_y}^z\right)^{j_{N_y}}\right].
\end{aligned}
\tag{20}
$$

The Hamiltonian $\widetilde{\mathcal{H}}$ is block diagonal with 2^N blocks of 2×2 matrices labeled by the index j and all having the form

$$\widetilde{\mathcal{H}}_j = \begin{pmatrix} \Omega_{zj} + \omega_0 & \Omega_{xj} - i\Omega_{yj} \\ \Omega_{xj} + i\Omega_{yj} & \Omega_{zj} - \omega_0 \end{pmatrix} = \Omega_{zj} I_2 + 2\vec{\Omega}_j \cdot \vec{s}, \tag{21}$$

with the vector $\vec{\Omega}_j$ having the components $\left(\Omega_{xj}, \Omega_{yj}, \omega_0\right)$ and $\left|\vec{\Omega}_j\right| = \sqrt{\Omega_{xj}^2 + \Omega_{yj}^2 + \omega_0^2}$. The eigenvalues of $\widetilde{\mathcal{H}}_j$ are $\Omega_{zj} \pm \left|\vec{\Omega}_j\right|$. The Hamiltonian $\widetilde{H}$ can thus also be written as

$$\widetilde{\mathcal{H}} = \widetilde{\mathcal{H}}_1 \oplus \widetilde{\mathcal{H}}_2 \oplus \cdots \oplus \widetilde{\mathcal{H}}_{2^{N_B}} . \tag{22}$$

Note that the Ω_{zj} depend on the $\widetilde{J}$ and $\widetilde{K}$ couplings only. Also the Ω_{xj} depend only on the J couplings while the Ω_{yj} depend only on the K couplings.

As in [15] we assume that the central spin is decoupled from the bath for times $t < 0$, and that the central spin and the bath spins are brought into contact at time $t = 0$. We assume that at time $t = 0$ the central spin has a wave function

$$|\psi(0)\rangle = \begin{pmatrix} \sin \alpha_0 \\ \cos \alpha_0 \end{pmatrix}, \tag{23}$$

so that if $\alpha_0 = 0$ the central spin initially is down, and is initially up for $\alpha_0 = \pi/2$. Note that the unitary transformation in Eq. (19) does not change the initial state of the central spin at time $t = 0$. After the unitary transformation by P_p at time $t = 0$ the state of the bath can be written as

$$\left|\widetilde{\Phi}(0)\right\rangle = \sum_{j=1}^{2^{N_B}} c_j |\varphi_j\rangle \qquad \text{with} \qquad \sum_{j=1}^{2^{N_B}} |c_j|^2 = 1, \tag{24}$$

with some complex coefficients c_j and $\{|\varphi_j\rangle\}$ the complete orthonormal set of states taken to be the usual direct products of the spin up and down states of the N_B bath spins. In practice one can regard the c_j as the coefficients obtained after starting with the $t = 0$ bath wave function $|\Phi(0)\rangle$ in the orthonormal basis of the eigenvectors of σ^x for the x-bath spins and the eigenvectors of σ^y for the y-bath spins, which with the unitary transformation by $P_p^\dagger$ gives the environment wave function of Eq. (24).

The expectation values $\langle S_0^\ell(t) \rangle$ are independent of the values of $\widetilde{J}_{i_1,i_2,\cdots,i_{N_x}}$ and $\widetilde{K}_{j_1,j_2,\cdots,j_{N_y}}$. With the initial wave function $|\Psi(0)\rangle = |\psi(0)\rangle \otimes |\Phi(0)\rangle$ this independence is because these terms only enter in Ω_{zj}, and furthermore,

$$\begin{aligned} \left\langle S_0^\ell(t) \right\rangle &= \langle \Psi(0)| \exp{(i\mathcal{H}t)} \left(s^\ell \otimes I_2 \otimes I_2 \otimes \cdots \otimes I_2 \right) \exp{(-i\mathcal{H}t)} |\Psi(0)\rangle \\ &= \left\langle \widetilde{\Psi}(0) \right| \exp{\left(i\widetilde{\mathcal{H}}t\right)} \left(s^\ell \otimes I_2 \otimes I_2 \otimes \cdots \otimes I_2 \right) \exp{\left(-i\widetilde{\mathcal{H}}t\right)} \left|\widetilde{\Psi}(0)\right\rangle, \end{aligned} \tag{25}$$

with $\left|\widetilde{\Psi}(0)\right\rangle = P_p^\dagger |\Psi(0)\rangle$. The reason is that

$$\mathcal{H} = P_p \widetilde{\mathcal{H}} P_p^\dagger, \quad \text{so} \quad \exp{[i\mathcal{H}t]} = P_p \exp{\left[i\widetilde{\mathcal{H}}t\right]} P_p^\dagger, \tag{26}$$

and the constant terms Ω_{zj} in each block cancel because they commute with everything. One Ω_{zj} term comes from each of the blocks $\widetilde{H}$ in Eq. (26), and $\exp{\left[i\Omega_{zj}t\right]} \exp{\left[-i\Omega_{zj}t\right]} = 1$. Therefore, without loss of generality we set all $\widetilde{J}$ and $\widetilde{K}$ to zero.

Next we want to trace out the bath spins to be left with the density matrix $\rho(t)$ for the central spin. At $t = 0$ the density matrix of the central spin is

$$\rho(0) = |\psi(0)\rangle\langle\psi(0)|. \tag{27}$$

Explicitly

$$\begin{aligned} \rho(t) &= \text{Tr}_B \left[e^{-i\mathcal{H}t} \left(\rho(0) \otimes \rho_B(0) \right) e^{i\mathcal{H}t} \right] \tag{28} \\ &= \text{Tr}_B \left[P_p e^{-i\widetilde{\mathcal{H}}t} P_p^\dagger \left(\rho(0) \otimes \rho_B(0) \right) P_p e^{i\widetilde{\mathcal{H}}t} P_p^\dagger \right] \tag{29} \\ &= \text{Tr}_B \left[e^{-i\widetilde{\mathcal{H}}t} \left(\rho(0) \otimes \widetilde{\rho}_B(0) \right) e^{i\widetilde{\mathcal{H}}t} \right]. \tag{30} \end{aligned}$$

Here $\widetilde{\rho}_B(0) = |\widetilde{\Phi}(0)\rangle\langle\widetilde{\Phi}(0)|$. Writing Eq. (30) in terms of the c_j of Eq. (24) and the block diagonal matrices $\mathcal{H}_j$ of Eq. (21) gives the final equation for the reduced density matrix for the central spin,

$$\begin{aligned} \rho(t) &= \left(|c_1|^2 \, e^{-i\widetilde{\mathcal{H}}_1 t} \rho(0) e^{i\widetilde{\mathcal{H}}_1 t} \right) + \left(|c_2|^2 \, e^{-i\widetilde{\mathcal{H}}_2 t} \rho(0) e^{i\widetilde{\mathcal{H}}_2 t} \right) + \cdots + \left(|c_{2^{N_B}}|^2 \, e^{-i\widetilde{\mathcal{H}}_{2^{N_B}} t} \rho(0) e^{i\widetilde{\mathcal{H}}_{2^{N_B}} t} \right) \\ &= |c_1|^2 \rho_1(t) + |c_2|^2 \rho_2(t) + \cdots + |c_{2^{N_B}}|^2 \rho_{2^{N_B}}(t). \end{aligned} \tag{31}$$

Equation (31) shows that the reduced quantum density matrix $\rho(t)$ for the central spin is the sum of 2^{N_B} different 2×2 density matrices $\rho_j(t)$. Notice that the initial state of the bath spins enters only in the terms $|c_j|^2$. The 2×2 matrix exponentials can easily be calculated using the relation $\exp{[\pm i (\vec{a} \cdot \vec{\sigma}) t]} = I_2 \cos{(at)} \pm i (\vec{a} \cdot \vec{\sigma}/a) \sin{(at)}$ with $a = |\vec{a}|$.

For any expectation value of the central spin, Eq. (31) gives

$$\left\langle S_0^\ell(t) \right\rangle = \sum_{j=1}^{2^{N_B}} \left| c_j \right|^2 \mathrm{Tr} \left[s^\ell \rho_j(t) \right] . \tag{32}$$

Thus the final result is that for the type of Hamiltonian defined in Eq. (20) (an x-bath plus a y-bath) the time dependence of the expectation value for any spin operator reduces to the sum over the expectation values of 2^{N_B} evolution equations with different Hamiltonians $\widetilde{\mathcal{H}}_j$. Equations (31) and (32) are the central results that will be exploited for our efficient algorithm. Note in particular that only 2×2 matrices must be worked with, and hence stored in memory. However, computationally we do not get something for nothing, in that we have to solve the TDSE for 2^{N_B} different Hamiltonians $\widetilde{\mathcal{H}}_j$ and then sum to get the final expectation value.

4. Symmetry of the Hamiltonian for x, y-baths

Equations (31) and (32) are the central results, and are very general. For the general case where all J and K values are different one has to sum over 2^{N_B} different density matrices $\rho_j(t)$ to obtain $\rho(t)$. If there is any symmetry in the couplings between the central spin and the x-bath spins or the central spin and the y-bath spins, then this symmetry can be exploited to reduce the number of terms that must be summed. The reduction comes because the symmetry in the Hamiltonian can make a number of the $\rho_j(t)$ identical. As long as some of the $\rho_j(t)$ are identical, the initial state of the bath does not need to have any symmetry in order to combine terms in the sum of Eqs. (31) or (32). For example, if all $\rho_j(t)$ are identical for $j \in \{i, \cdots, i + k\}$ then in Eq. (32) one can group together the terms that enter the sum to be

$$\left\langle S_0^\ell(t) \right\rangle = \cdots + \left\{ \left(\sum_{j=i}^{i+k} \left| c_j \right|^2 \right) \mathrm{Tr} \left[s^\ell \rho_{\mathrm{sym}}(t) \right] \right\} + \cdots \tag{33}$$

with the definition $\rho_j(t) = \rho_{\mathrm{sym}}(t)$ for $j \in \{i, \cdots, i + k\}$. Therefore in this example to calculate the term in curly brackets one only has to solve the TDSE for one block Hamiltonian, rather than for k different block Hamiltonians. Furthermore, the initial configuration of the bath spins only enters in the sum over j in parenthesis in Eq. (33).

In order to compare directly with the paper of Rao *et al* [20] we now make two additional assumptions. First, we assume that the initial state of all the spins (the central spin and all bath spins) is the down state, $|\Psi(0)\rangle = |\psi(0)\rangle \otimes |\Phi(0)\rangle = | \downarrow\downarrow \cdots \downarrow\rangle$. After the transformation with P_p this makes all the $|c_j|^2$ equally probable, so $|c_j|^2 = 2^{-N_x-N_y}$. Furthermore we assume that there are only 2-body interactions with all couplings identical, which are of strength J_2 and K_2. Therefore, we have equal couplings between the central spin and all spins in the x-bath and y-bath, respectively. Then we can organize the sum over the 2^{N_x} x-bath spins into ones that are identical, namely classified by the projection m_x onto the z-axis of the N_x spins. There are

$$\lambda_{N_x,m_x} = \begin{pmatrix} N_x \\ N_x/2 - m_x \end{pmatrix} = \frac{N_x!}{(N_x/2 - m_x)! \, (N_x/2 + m_x)!}, \tag{34}$$

identical vectors Ω_{N_x,m_x} for $-N_x/2 \le m_x \le N_x/2$ with m_x having integer steps. Similar definitions apply to the N_y spins of the y-bath. The Hamiltonian of each 2×2 block has the form of Eq. (21). The result for $\langle S_0^z(t) \rangle$ is thus the sum over 2^{N_B} terms that explicitly are

$$\begin{pmatrix} 0 & 1 \end{pmatrix} \exp \left[i\widetilde{\mathcal{H}}_j t \right] \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \exp \left[-i\widetilde{\mathcal{H}}_j t \right] \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{2} \frac{\omega_0^2 + \left(\Omega_{xj}^2 + \Omega_{yj}^2 \right) \cos \left[\sqrt{\Omega_{xj}^2 + \Omega_{yj}^2 + \omega_0^2} \, t \right]}{\Omega_{xj}^2 + \Omega_{yj}^2 + \omega_0^2}. \tag{35}$$

The initial central spin density matrix reads

$$\rho(0) = |\downarrow\rangle \langle\downarrow| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{36}$$

We define

$$\vec{\Omega}_{m_x m_y} = \left(m_x J_2, \ m_y K_2, \ \omega_0\right), \tag{37}$$

and $\Omega_{m_x m_y} = \sqrt{m_x^2 J_2^2 + m_y^2 K_2^2 + \omega_0^2}$. Then the result for the expectation value of the central spin is

$$\left\langle S_0^z(t)\right\rangle = \frac{1}{2^{N_x+N_y+1}} \sum_{m_x=-N_x/2}^{N_x/2} \sum_{m_y=-N_y/2}^{N_y/2} \lambda_{N_x,m_x} \lambda_{N_y,m_y} \frac{\left[\left(m_x^2 J_2^2 + m_y^2 K_2^2\right)\cos\left(\Omega_{m_x m_y} t\right)\right] + \omega_0^2}{\Omega_{m_x m_y}^2} . \tag{38}$$

As in reference [20], the quantum purity for the case $N_x = N_y = N$ and $K_2 = J_2$ becomes

$$2\mathcal{P}(t) - 1 = \left\{1 - \sqrt{\frac{\pi N J_2^2}{32}} t \exp\left[-\frac{N J_2^2 t^2}{32}\right] \text{Erfi}\left[\sqrt{\frac{N J_2^2 t^2}{32}}\right]\right\}^2 , \tag{39}$$

which asymptotically for $t \to \infty$ becomes

$$2\mathcal{P}(t) - 1 = \frac{128}{N^2 J_2^4 t^4} + \frac{24,576}{N^3 J_2^6 t^6} + \frac{2,555,904}{N^4 J_2^8 t^8} + O\left(t^{-10}\right) . \tag{40}$$

On the other hand when $K_2 = 0$ (or alternatively $N_y = 0$) then

$$2\mathcal{P}(t) - 1 = \exp\left(-\frac{N J_2^2 t^2}{4}\right) . \tag{41}$$

Thus, in the absence of disorder the quantum purity decays to its asymptotic value exponentially in $N J_2^2 t^2$ for one bath with only x-coupling, while for an x-bath and a y-bath it decays as a power law. We will test whether this is true also when there is disorder in the couplings J_i and K_j.

5. Decoherence and Thermalization with x, y- baths

We first show how the quantum purity $\mathcal{P}(t)$ and von Neumann entropy $\mathcal{S}(t)$ approach their asymptotic limit, Fig. 1. All $N_B + 1$ spins start in the down state. Fig. 1(A) shows that $2\mathcal{P}(t) - 1$ approaches zero as a power law in $N^2 t^4$, in agreement with the asymptotic result of Eq. (40) when there are only two-body interactions. Changing the number of x-baths or y-baths does not change that the approach to the $t \to \infty$ result is a power law, even if there is some 'disorder' in the couplings of the x, y-baths. This is very different from when there is no y-bath, only an x-bath (the orange stars, see also [21]). The power-law, rather than exponential, approach for $\mathcal{P}$ and $\mathcal{S}$ to their $t \to \infty$ value shows that the x, y-bath system decoheres much more slowly than does only an x-bath system. Fig. 1(B) shows that also the von Neumann entropy approaches unity as a power law for x, y-baths, compared to an exponential approach for only an x-bath. Note that in Fig. 1(B) the red line is only a guide for the eye, since there is no theoretical prediction of how $\mathcal{S}(t) \to 1$ as $Nt^2 \to \infty$. The largest number of bath spins in Fig. 1 is for $N = N_x = N_y = 300$ for x, y-baths, which has $N_B = 600$ so the Hilbert space is of dimension $2D_B = 2^{601} \approx 8 \times 10^{180}$, which certainly could not be computed storing an entire vector in the Hilbert space. The largest number of distinct 2×2 matrices calculated in the sum of Eq. (31) is $(60 + 1)^2(15 + 1)^4 \approx 2 \times 10^8$ for the baths with $60 + (2 \times 15) = 90$ spins in both the x-bath and y-bath.

Figure 2 shows how the quantum purity behaves when the starting state of the central spin is not down. Here all bath spins start down, and the x, y-baths have $N = N_x = N_y$. This figure illustrates a problem with the x, y-baths, namely that unless the central spin starts down (or up) decoherence is not complete in that $\mathcal{P}(t)$ does not approach its expected value of $1/2$ but rather saturates at some value which depends on α_0. The shown asymptotic value is the lowest order term from Eq. (40), and is valid only for $\alpha_0 = 0$ or $\alpha_0 = \pi/2$.

Fig. 3(A) shows the quantity $\sigma(t)$ from Eq. (12). If all spins start down, then $\sigma(t) = 0$ for all $t \geq 0$, which means that thermalization [as measured by $\sigma(t)$] occurs before decoherence [as measured by $\mathcal{P}(t)$ or $\mathcal{S}(t)$]. Figure 3(A) shows how $\sigma(t)$ decreases when the central spin is initially in the down state, but all bath spins start with the c_j of Eq. (24) uniformly distributed between zero and unity (and after assignment of all 2^{N_B} random c_j values they are
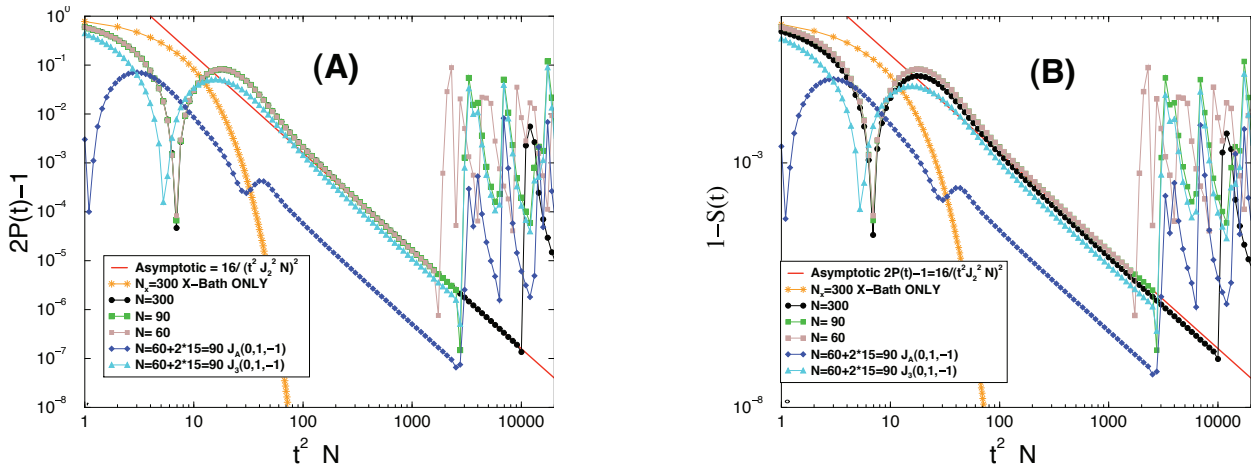
Figure 1: The quantity $2\mathcal{P}(t) - 1$ (A) and $1 - \mathcal{S}(t)$ (B) versus Nt^2. The starting state is down, $\alpha_0 = 0$. A single bath (orange, *, for $N_x = 300$ and $J_2 = 1$ and $N_y = 0$ and $K_2 = 0$) falls exponentially. The black, green, and brown curves are for $N_x = N_y = N$, $J_2 = K_2 = 1$, and agree with the asymptotic result (red line) of Eq. (40) for (A) [and is a guide for the eye in (B)]. The blue ($\diamond$) data points are for three x-baths, one with $N_x = 60$ and $(J_2, J_3, J_A) = (1, 0, 0)$ and two x-baths with $N_x = 15$ one with $(J_2, J_3, J_A) = (1, 1, 0)$ and one with $(J_2, J_3, J_A) = (1, -1, 0)$; with the same couplings and $N_y = N_x$ for the three y-baths, so $N_B = 180$. The cyan ($\triangle$) points are similar but for the $N_x = N_y = 60$ baths $(J_2, J_3, J_A) = (1, 0, 0)$ and the two $N_x = N_y = 15$ baths $(J_2, J_3, J_A) = (1, 0, 1)$ and $(J_2, J_3, J_A) = (1, 0, -1)$.

divided by $\sqrt{\sum_{j=1}^{2^{N_B}} |c_j|^2}$ so the vector $\widetilde{\Phi}(0)$ is normalized). Figure 3(A) shows that for random initial bath states the thermalization as measured by $\sigma(t)$ decreases as N increases. In Fig. 3(A) the x, y-baths have $N_x = N_y = N$. Note that the largest Hilbert space in Fig. 3(A) is for $N = 64$, and has a size of $2^{129} \approx 7 \times 10^{38}$, which could not be calculated by conventional algorithms.

Figure 3(B) shows the expectation value for $\langle S_0^z(t) \rangle$ for the listed couplings for two x-baths and two y-baths. The initial state of the central spin and all bath spins is down. The maximum number of bath spins is for $N = 64$, so $N_B = 256$ and the Hilbert space is $2^{257} \approx 2 \times 10^{77}$. The number of different 2×2 matrices calculated in Fig. 3(B) is only $65^4 \approx 1.8 \times 10^7$.
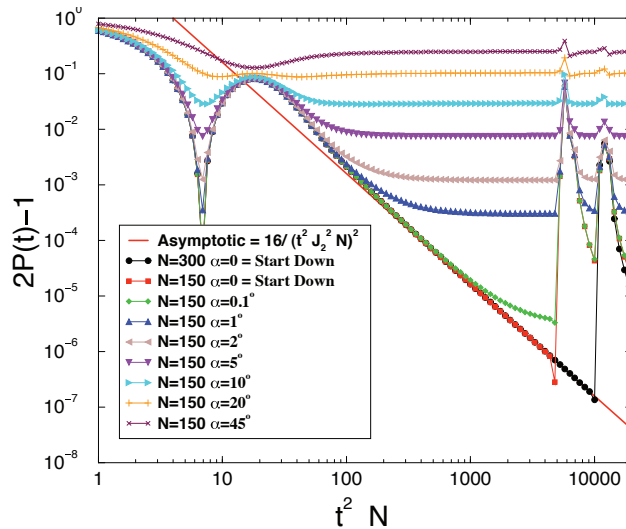

Figure 2: Comparison of the initial state of the central spin, with different initial angles α_0. All bath spins start down. These are all for x, y-baths with $N_x = N_y = N$ and $K_2 = J_2 = 1$ (with all other J and K couplings zero).

The x, y-baths are not the most general baths, in particular they do not have any intrinsic dynamics if they are not coupled to the subsystem. In order to test whether the power-law scaling persists with slightly generalized x, y-
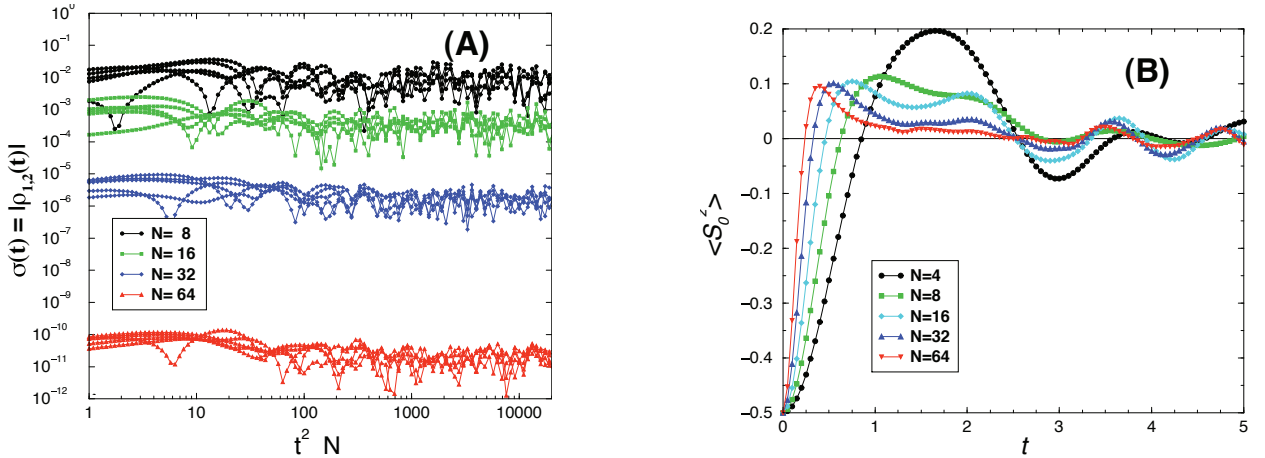
Figure 3: (A) The quantity $\sigma(t) = |\rho_{1,2}(t)|$ as a function of Nt^2 for different $N = N_x = N_y$, with $\alpha_0 = 0$, and $K_2 = J_2 = 1$ with all other J and K couplings zero. The bath spins are started in a random configuration, and five different random bath configurations are shown for each system size. (B) The expectation value $\langle S^z(t) \rangle$ for two x-baths and two y-baths, each with N spins so $N_B = 4N$. The two x-baths have couplings $(J_2, J_3, J_A) = (0.9, 0.1, 0.1)$ and $(J_2, J_3, J_A) = (1.1, -0.1, -0.1)$. The two y-baths have couplings $(K_2, K_3, K_A) = (0.9, -0.1, 0.1)$ and $(K_2, K_3, K_A) = (1.1, 0.1, -0.1)$.

baths with $N = N_x = N_y$, we performed Chebyshev polynomial calculations [13, 14] storing the entire 2^{N_B+1} vectors. The results are shown in Fig. 4. The coupling between the central spin and bath spins only has a coupling of the form $J_{2,i}S_0^x S_i^x$ with $J_{2,i}$ uniformly distributed in the range $[1 - r_x, 1 + r_x]$, and hence would qualify as an x-bath. However, here we do not limit ourselves to only x-baths, in that we allow intra-bath couplings of the form $\mathcal{H}_B = \sum_{i,j}^{N_x} \left(J_{ij}^x S_i^x S_j^x + J_{ij}^y S_i^y S_j^y + J_{ij}^z S_i^z S_j^z \right)$ with $J_{ij}^\ell \in [-r_x, +r_x]$ with $i = 1, \cdots, N_x$. Similarly, the coupling between the central spin and y-bath spins only has a coupling of the form $K_{2,i}S_0^y S_i^y$ with $K_{2,i}$ uniformly distributed in the range $[1 - r_y, 1 + r_y]$ and has intra-bath couplings of the form $\mathcal{H}_B = \sum_{i,j}^{N_y} \left(K_{ij}^x S_i^x S_j^x + K_{ij}^y S_i^y S_j^y + K_{ij}^z S_i^z S_j^z \right)$ with $K_{ij}^\ell \in [-r_y, +r_y]$ with $i = 1, \cdots, N_y$. Only if $r_x = r_y = r = 0$ do these baths reduce to an x, y-bath. Unfortunately, due to the restrictions imposed by computer memory on N, we are not able to penetrate the region where one might expect asymptotic behavior. Therefore the question of whether these generalized baths have a power-law decay to their asymptotic value is still an open question.

6. Conclusions and Discussion

We have presented an algorithm to efficiently calculate the real-time quantum dynamics of a single spin-1/2 subsystem coupled to x-bath and y-bath spins. The algorithm only requires that 2×2 matrices be stored in computer memory. This enables calculations for large numbers of bath spins. The largest number of bath spins shown in the figures had $N_B = 600$, which requires a Hilbert space of size $2^{601} \approx 8 \times 10^{180}$. Such a large Hilbert space could not be calculated even for the next generation of computers that should be capable of exascale computing.

When both an x-bath and y-bath are present, the decoherence as measured by the quantum purity $\mathcal{P}(t)$ and von Neumann entropy $\mathcal{S}(t)$ decay as a power law in $N^2 t^4$ if all spins start in the down state. This is in agreement with the analytical results of Rao *et al* [20]. This is illustrated in Fig. 1. However, as Fig. 2 shows if all bath spins start down but the central spin does not start up (or down), decoherence as measured by $\mathcal{P}(t)$ is not complete as $t \to \infty$. Figure 3(A) shows that thermalization as measured by $\sigma(t)$ depends on the number of bath spins and the initial state of the bath spins. Figure 3(B) shows how for many x, y-baths the expectation value $\langle S^z(t) \rangle$ can depend on the bath size. The results of Fig. 2 and Fig. 3(A) illustrate one difficulty with relying only on x, y-baths for decoherence and thermalization of the central spin.

Figure 4 was meant to test whether slight generalizations of x, y-baths would have a power-law dependence for $\mathcal{P}(t)$. Unfortunately, the number of bath spins that could be calculated are not sufficient currently to settle this question.

Future results of decoherence and thermalization of x, y-baths will be tested on subsystems of interest that are larger than a single spin. It is also of interest to see whether the algorithm can be generalized somewhat for baths that
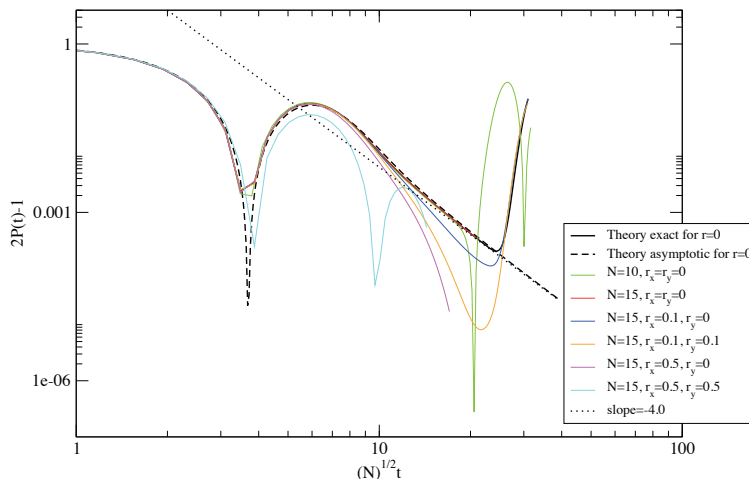
Figure 4: The quantity $2\mathcal{P}(t) - 1$ as a function of $t\sqrt{N}$ for two baths with only two-body couplings and $N_x = N_y = N$. If $r_x = 0$ ($r_y = 0$) the generalized bath is reduced to an x-(y-)bath. For non-zero r_x and r_y the bath is more general than an x- or y-bath. The theoretical exact value for $r=0$ is obtained from Eq. (39), and its lowest-order asymptotic result from Eq. (40).

have their own internal dynamics, unlike the x, y-baths treated here.

Acknowledgements

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