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Polynomial Scheme for Numerical Simulations of the Spin-bath Decoherence

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Polynomial Scheme for Numerical Simulations of the Spin-bath Decoherence (*Outline*)

- ***Introduction***
- ***Hamiltonian***
- ***Polynomial Expansion***
- ***Numerical Simulation***

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1. Introduction

For a quantum system prepared in a linear superposition of its eigenstates, some observables can oscillate with time. Interaction of the system with its environment leads to a decay of the system's initial pure state into a mixture of several states (**decoherence**): i.e, *nondiagonal elements of the density matrix vanish*.

$\because |\psi(0)>=(\sum_n C_n|n>)\bigotimes|e> \;\Rightarrow\; |\psi(t)>=(\sum_n C_n(t)|n>)\bigotimes|e_n>$

$\therefore \rho(0)=|\psi(0)><\psi(0)| \;\Rightarrow\; \rho_s(t)=\sum_n |C_n(t)|^2|n><n|$

Here we discuss decoherence of an open system made of several strongly coupled spins, $s_i = 1/2$, by a spin bath. That is to say we want to numerically solve the compound "system-plus-bath" time-dependent Schrödinger equation, using some types of polynomial expansion.

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2. Hamiltonian

Consider the system of two central spins $\mathbf{s}_1$ and $\mathbf{s}_2$ coupled by Heisenberg exchange: $H_s = 2J\mathbf{s}_1\mathbf{s}_1$. This system is coupled to a bath made of spins $\mathbf{I}_1$, ($I_k = 1/2$, $k = 1...N$) via Heisenberg interactions: $H_i = \sum_k (A_k^1 \mathbf{s}_1 \mathbf{I}_k + A_k^1 \mathbf{s}_1 \mathbf{I}_k)$. We consider only when $J \gg A_k^1, A_k^2$ and $A_k^1 = A_k^2$. So, $H = H_0 + H_i = H_s + H_b + H_i$, and here we talk about the case of "stacic" bath, with $H_b = 0$. Finally, we have:

$$\hat{H} = 2J\overrightarrow{s}_1 \cdot \overrightarrow{s}_2 + \sum_n (\overrightarrow{s}_1 + \overrightarrow{s}_2) \cdot \overrightarrow{I}_n$$

The time-dependent Schrödinger equation with the above $\hat{H}$ and its formal solution are given by

$$i\frac{\partial \psi(t)}{\partial t} = \hat{H}\psi(t), \psi(t) = e^{-i\hat{H}t}\psi(0)$$

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3. Polynomial Expansion

Recall that the Hermite polynomial is related to its generating function by

$$e^{-s^2+2sx} = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(x)$$

where $H_n(x)$ denotes the Hermite polynomial of order n. Next, rearrange the exponential operator $e^{-i\hat{H}t}$ into the form

$$e^{-i\hat{H}t} = e^{-(t/2\lambda)^2} e^{-(-it/2\lambda)^2 + 2\lambda H(-(\hat{i}t/2\lambda))}$$

here λ is an arbitrary parameter introduced for later convenience. By setting $s = -it/2\lambda$ and $x = \lambda\hat{H}$, we immediately obtain the Hermite expansion for $e^{-i\hat{H}t}$

$$e^{-i\hat{H}t} = e^{-(t/2\lambda)^2} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} (t/2\lambda)^n H_n(\lambda\hat{H})$$

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And thus the formal solution of the Schrödinger equation with time-independent Hamiltonian can be formulated as

$$\psi(t) = e^{-(t/2\lambda)^2} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} (t/2\lambda)^n \phi_n$$

where $\phi_n = H_n(\lambda \hat{H})\psi(0)$. It is easy to see that when n is enough big, the term $\frac{1}{n!}(t/2\lambda)^n$ will decay exponentially.

Likewise, the Hermite polynomial can produce an recursive algorithm for expansion, i.e:

$$\begin{aligned} \phi_0 &= \psi_0 \\ \phi_1 &= 2\lambda \hat{H} \psi_0 \\ \phi_{n+1} &= 2(\lambda \hat{H})\phi_n - 2n\phi_{n-1} \end{aligned}$$

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3.1. Chebyshev Polynomial Expansion

Another effective way of calculation of evolution operator $e^{-i\hat{H}t}$ is to expand it in a series of the Chebyshev polynomials($T_k(x) = cos(k \cos\ x)$). One point which should be noticed is $T_k(x)$ are defined for $x \in [-1, 1]$. Thus $hotH$ must be rescaled by the factor E_0 and E_c:

$$
\begin{aligned}
E_0 &= E_{max} - E_{min} \\
E_c &= \frac{1}{2}(E_{max} + E_{min}) \\
E_{min} &= min < \Phi|\hat{H}|\Phi > \\
E_{max} &= max < \Phi|\hat{H}|\Phi >
\end{aligned}
$$

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In this way, the rescaled operator $\tilde{H} = 2(\hat{H} - E_c)/E_0$ is also bounded by -1 and 1. And the expansion is

$$e^{-i\tilde{H}\tau} = \sum_{n=0}^{\infty} c_n T_n(\tilde{H})$$

where $\tau = E_0 t/2$, $c_n = a_n(-i)^n J_n(\tau)$, $J_n(\tau)$ is the Bessel function of kth order, $a_0 = 1, a_{n\neq 0} = 2$, and the successive terms can be determined using the recuision

$$\begin{aligned} T_0(\tilde{H}) &= 1 \\ T_1(\tilde{H}) &= \tilde{H} \\ T_{n+1}(\tilde{H}) &= 2\tilde{H}T_n(\tilde{H}) - T_{n-1}(\tilde{H}) \end{aligned}$$

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3.2. Laguerre Polynomial Expansion

Apparently, comparing with the Chebyshev expansion, the method of Hermite polynomial gain the advantage over it by no needing to scale the Hamiltonian into a special norm. And the Laguerre expansion has the same character, whose generating function is:

$$(1-s)^{-\alpha-1}e^{\frac{xs}{s-1}} = \sum_{n=0}^{\infty} L_n^{\alpha}(x)s^n$$

and the recursion process is:

$$\begin{aligned} L_0^{\alpha}(x) &= 1 \\ L_1^{\alpha}(x) &= \alpha+1-x \\ (n+1)L_{n+1}^{\alpha}(x) &= (2n+\alpha+1-x)L_n^{\alpha}(x)-(n+\alpha)L_{n-1}^{\alpha}(x) \end{aligned}$$

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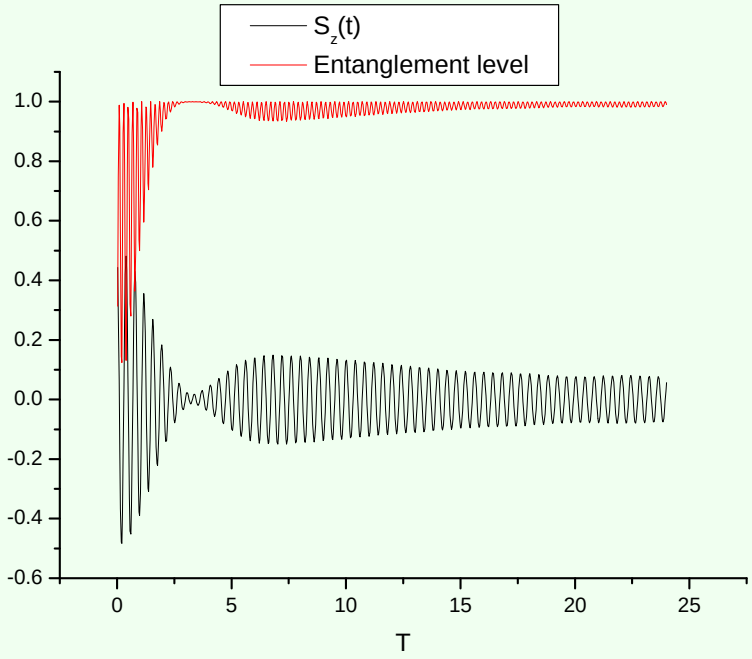
4. Numerical Simulation



"S_z" is the z component of one of the two spins which consist the open system, and "Entanglement level" is the von Neumann's entropy ($S = -Tr\rho\, ln\rho$), which characterizes how strongly mixed is the state of the system.

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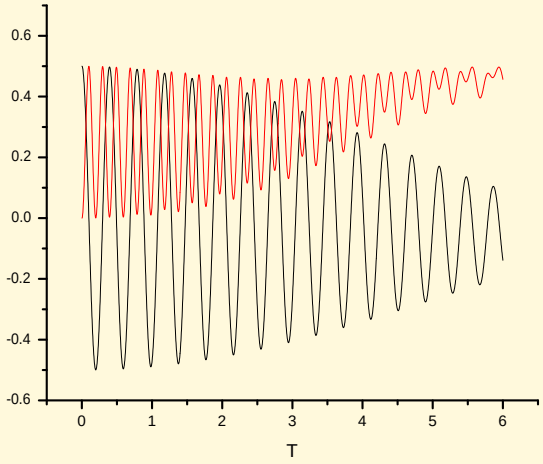
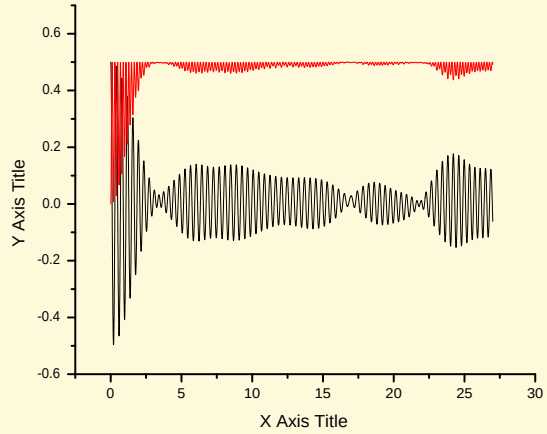
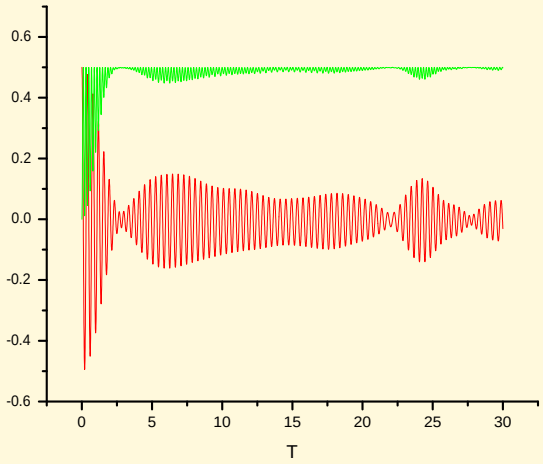
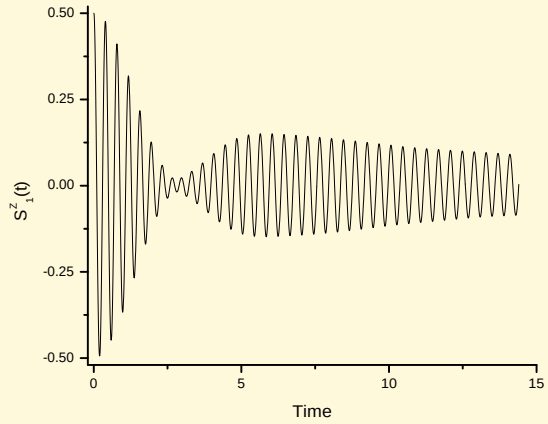
5. Other Results









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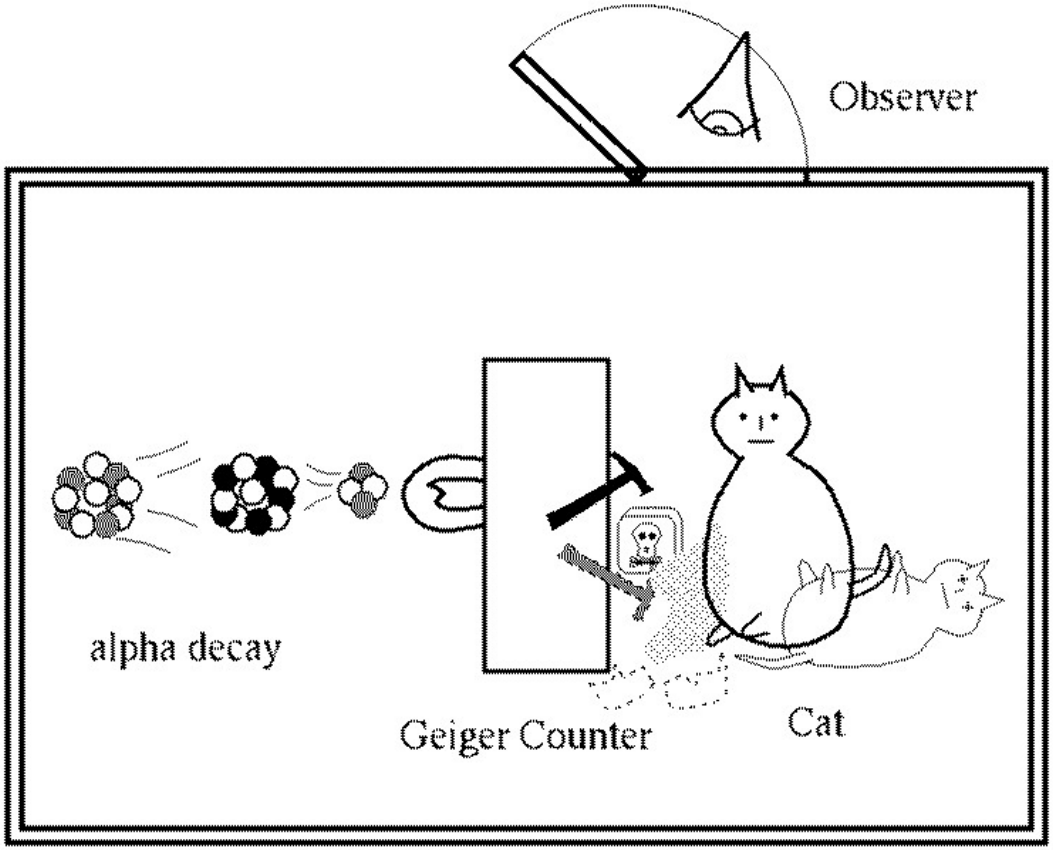

Thank you!

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