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Sensitive chemical compass and quantum criticality at finite temperature

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ABSTRACT

We investigate the influence of a flip operation of the central spin on the quantum criticality of a radical pair system by employing the spin echo and its product yield. It is found that with echo control on the central spin, the critical behavior can be described by the product yield at very high temperatures. Moreover, we also study the short and long time behavior of the spin echo, and show that the decay factor of the short time evolution scales linearly. The long time evolution shows different statistics for varying chain lengths, temperature and external parameters of the Hamiltonian.

1. Introduction

Quantum phase transition (QPT) has been a topic that has attracted much research interest over the years [1]. QPT causes a qualitative change in the structure of the ground state properties of a quantum many-body system as some external parameters of the Hamiltonian are varied to a certain value, which is defined to be the critical point of the system. The behavior of many-body systems near the critical point is strongly influenced by the existence of a QPT, and it is associated with the divergence of correlation length of two-point correlation functions and the vanishing of the gap in the exciton spectrum. This change of phase is caused solely by quantum fluctuations, which exist at absolute zero temperature. In practice, we must work at low but finite temperatures, as close to the absolute zero as possible, and the finite-temperature QPT is important theoretically and experimentally [2–4].

The spin chain model has been a popular candidate for the study of QPTs due to the fact that many types of spin chains can be implemented experimentally and is soluble analytically [1,2,5–10]. Recently, the chain with spin chain environment have attracted much attention in the study of quantum phase transition [8,11,12] and quantum information processing [13]. The Loschmidt echo was introduced in NMR experiments to describe the hypersensitivity of the time evolution to the environmental effects [8]. It has been pointed out that nuclear environments surrounding electron spins in the radical pairs is crucial to the magnetic sensitivity of the chemical reaction, and the chemical product yield in cryptochrome is believed to affect the visual function of animals [14], which is given by the Laplace time-integral transform of the Loschmidt echo [9]. Moreover, the Loschmidt echo is shown to obey different probability distributions for different system setups [3,15], and the decaying behavior for short time evolution scales linearly with system size [16].

In this Letter we study how the flip operation of the central spin affects the quantum phase transition behavior of radical pair systems by means of the spin echoes and its product yield. It is shown that at very low temperatures, the product yield of the Loschmidt echo is able to pinpoint the critical points of the quantum phase transitions, but as the temperature gets higher, the Loschmidt echo fails to capture the critical points of quantum phase transitions due to thermal fluctuations. However, with echo control on the central spin, the critical behavior can be observed even at very high temperatures. Moreover, we also study the statistical distribution of the spin echo as well as the short and long time behavior of the spin echoes, and find that the product yield has very little dependence on the temperature, meaning the proposed echo control is very effective at removing the thermal fluctuations. It is demonstrated that the decay factor of the short time evolution scales linearly, and the echoes obey different short-time evolution behaviors. The long time evolution shows different statistics for varying chain lengths, temperature and external parameters of the Hamiltonian.

2. Loschmidt echo and the product yield at finite temperature

In a radical pair, there are two electrons, each of which is uniformly coupled to its own environment [9]. In this Letter, we made a generalization of the spin environment to allow anisotropic

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coupling of the environmental spins. The environment under an oblique external magnetic field can be described as

$$H_E = J\sum_{l=1}^{N}\left(\frac{1+\gamma}{2}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{2}\sigma_l^y\sigma_{l+1}^y + \lambda\cos\theta\sigma_l^z\right)$$

where γ is the anisotropic factor, λ is the external magnetic field strength, θ the oblique angle and σ is the Pauli operator. The central electron couples to this spin bath according to

$$H_I = \varOmega\sin\theta\tau^x + \varOmega\cos\theta\tau^z - Jg\tau^z\sum_{l=1}^{N}\sigma_l^z$$

where τ refers to the Pauli operator of the electron, $\varOmega$ is the electronic Zeeman energy splitting and Jg is the coupling strength. Similar to Ref. [9], we can obtain an effective Hamiltonian by making use of the Born–Oppenheimer approximation by first treating the environment operators in H_I as c-numbers as $H = |+\rangle\langle+|H_+ + |-\rangle\langle-|H_-$, where $H_\pm = H_E \mp Jg\cos\theta\sum_{l=1}^{N}\sigma_l^z$. This Hamiltonian, which only introduces dephasing into the system, can be diagonalized using the Jordan–Wigner transform followed by a Fourier transform [7,17]. Under the basis spanned by the electron state $\{|+\rangle, |-\rangle\}$, the diagonal elements of the electron's density matrix does not evolve with time, while the off-diagonal element decays according to $\rho_{+-}(t) = \rho_{+-}(0)\,\mathrm{Tr}[U^{(+)}\rho_E U^{(-)\dagger}]$, where ρ_E is the initial state of the environment and $U_t^{(\pm)} = \exp[-iH_\pm t]$. In the study of this decoherence effect, the Loschmidt echo is a very useful tool. The Loschmidt echo was introduced in NMR experiments to describe the hypersensitivity of the time evolution to the environmental effects and is defined as the squared modulus of the decay factor,

$$L(t) = \left|\mathrm{Tr}\left[U_t^{(+)}\rho_E U_t^{(-)\dagger}\right]\right|^2. \tag{1}$$

At finite temperature T, the initial state of the environment is chosen to be the Gibbs equilibrium state, $\rho_E = \exp[-\beta H_-]/Z$, where $\beta = 1/kT$ is the inverse temperature and $Z = \mathrm{Tr}(\exp[-\beta H_-])$ is the partition function. At zero temperature, this definition reduces to $L(t) = |\langle G|U_-^\dagger U_+|G\rangle|^2$, and has been studied extensively [8,15,16].

The Loschmidt echo, with the Hamiltonian diagonalized, can be readily calculated as [3]

$$L(t) = \left|\prod_k l_k(t)/Z_k\right|^2, \tag{2}$$

where

$$Z_k = 1 + \cosh\left[\beta\varLambda_k^{(-)}\right];$$
$$\Re\left[l_k(t)\right] = 1 + \cosh\left[\beta\varLambda_k^{(-)}\right]\left(\cos\left[t\varLambda_k^{(+)}\right]\cos\left[t\varLambda_k^{(-)}\right] + \cos\left[\theta_k^{(+)} - \theta_k^{(-)}\right]\sin\left[t\varLambda_k^{(+)}\right]\sin\left[t\varLambda_k^{(-)}\right]\right),$$
$$\Im\left[l_k(t)\right] = \left(\cos\left[\theta_k^{(+)} - \theta_k^{(-)}\right]\cos\left[t\varLambda_k^{(-)}\right]\sin\left[t\varLambda_k^{(+)}\right] - \cos\left[t\varLambda_k^{(+)}\right]\sin\left[t\varLambda_k^{(-)}\right]\right)\sinh\left[\beta\varLambda_k^{(-)}\right];$$
$$\epsilon_k^{(\pm)} = \cos(2\pi k/N) - (\lambda \mp g)\cos\theta;$$
$$\varLambda_k^{(\pm)} = 2\sqrt{\epsilon_k^{(\pm)2} + \gamma^2\sin^2(2\pi k/N)};$$
$$\theta_k^{(\pm)} = \tan^{-1}\left[\frac{\gamma\sin(2\pi k/N)}{\epsilon_k^{(\pm)}}\right],$$

where $\Re$ and $\Im$ refer to the real and imaginary part, respectively. The detailed steps needed for deriving the equations above are given in Appendix A.

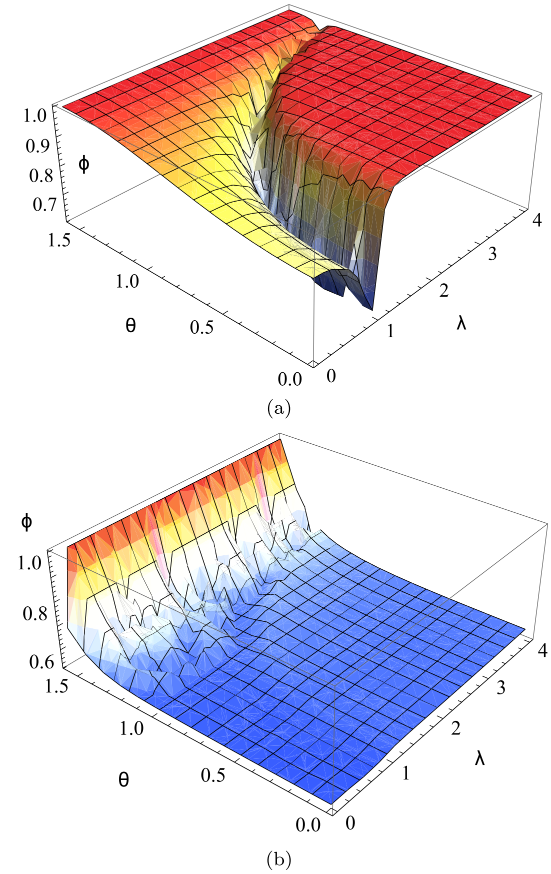

Fig. 1. (Color online.) Product yield of the Loschmidt echo at very low temperature $\beta = 200$ (Panel a) and high temperature $\beta = 0.2$ (Panel b) as a function of the angle θ and the magnetic field λ. As can be seen, along the critical points, the Loschmidt echo suffers a sudden drop at relatively low temperature, and the critical point is dependent on the magnetic field's strength as well as the angle. At higher temperatures, the sudden drop cannot be observed due to thermal fluctuations.

Recently, it has been pointed out that the Loschmidt echo is closely related to the sensitive chemical compass [9] by means of the product yield $\varPhi(t)$ given by

$$\varPhi(t) = \frac{1}{2} + \frac{s}{2}\int_0^t L(t)e^{-st}dt, \tag{3}$$

where s is the recombination rate. The ultimate product yield $\varPhi(\infty)$ in cryptochrome is believed to affect the visual function of animals [14]. In order to study the temperature effects, we plot the product yield at low and high temperatures as a function of the magnetic field strength and angle in Fig. 1 with $N = 80$, $g = 0.05$, $s = 0.1$ and $\gamma = 0.3$. It can be easily seen that while the product yield of the Loschmidt echo suffers a sudden drop along the critical points of QPT and is able to indicate the critical points at very low temperature, this ability is lost when the environment's temperature get higher due to high thermal fluctuations.

Now we study how the oblique angle affect the long-time and short-time evolution of the Loschmidt echo. In order to investigate the long-time evolution, we regard the values of the Loschmidt echo over a long observation time interval $[0, T]$ as a random variable [3,15] and investigate its statistical properties by calculating its probability distribution. We can obtain the probability distribution by discretely sampling the spin echo over a long period of time $[0, 10^{10}]$ and plot the statistical distribution of this sample. It is found that at low temperatures, the probability distribution of the echo is approximately exponential for long chains regardless of whether the bath is critical or not (Fig. 2), while for short