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Decoherence and entanglement in coherent quantum tunneling of magnetization with dissipation

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Abstract. We study the coherent quantum tunneling of magnetization, for example, in a biaxial molecular magnet with dissipation of the environment which results in the suppression of the tunneling and therefore the decoherence of superposition of macroscopic quantum states in terms of the general spin-boson model. The degree of entanglement between the magnet and the environment is evaluated explicitly with the help of reduced density matrix. We show an interesting relation that the degree of entanglement approaches maximum value when the coherent tunneling is suppressed completely.

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Quantum tunneling of the magnetization in a single-domain magnetic particle has attracted a great deal of theoretical and experimental interest because it may provide a signature of quantum mechanical behavior in macroscopic systems [1]. In particular, the coherent quantum tunneling between two degenerate orientations of the magnetization, which is called macroscopic quantum coherence [2], has stimulated considerable research activities in this field [3] because it may lead to the potential application in data processing [4]. In recent years, a series of experiments [5] on the crystals of magnetic molecules (for instance, Mn_{12} [6] and Fe_8 [7]) indicate that the molecular magnet is an ideal large spin system for investigating the coherent quantum tunneling of the magnetization. It is also demonstrated that the molecular magnet may be a candidate for realization of quantum computing [4,8]. Coherent quantum tunneling is susceptible to dissipative environment [2,9] and therefor a main obstacle for realizing experimentally quantum computing in magnetic grain is the unavoidable coupling of the qubit to the degree of freedom of external environment and the decoherence caused by coupling. Within the Caldeira-Leggett method treating the environment as a set of harmonic oscillators [10,11], the influence of the environment on the dynamics of two-level system is completely determined by a certain combination of oscillator parameter and coupling strength known as the spectral density. Later the method was extended to deal with the macroscopic quantum tunneling of magnetization with dissipation [12–14]. Reference [15] reported the first accurate numerical solution of a dissipative quantum mechanical model which exhibits steps in hysteresis loop and corresponding peaks in the relaxation rates. Coherent tunneling of magnetization has advantage in generating the coherent superposition of two macroscopically distinguishable states (i.e. the Schrödinger cat states) [4,16] required for quantum computing, however, is of disadvantage in information storage, where macroscopic quantum coherence would lead to information loss. It is, therefore, of importance to understand and furthermore to control the effect of the environment on the coherent tunneling. There is already a body of work concerning the various mechanisms of magnetization relaxation in the molecular magnets [17]; little work, however, is done on the quantitative study in the effect of environment on the coherent tunneling of magnetization, for example, in the decoherence and the entanglement. In this paper we shall study the coherent tunneling of the magnetization in a magnetic grain with dissipation resulted from a phonon-bath and show the suppression of the tunnel splitting by coupling to phonons by using the variational method which is a simpler way than most of preceding works. Our approach is based on the general spin-boson model in which the large spin system is approximated as a two-level system at low temperature. It is shown that tunnel splitting is suppressed by the dissipative environment which leads to decoherence of the Schrödinger cat states. Using the two trial gruond states, required by the variational method, which are two entangled states, we also

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investigate the entanglement between the giant spin and the environment and explore the intrinsic relation between the entanglement and the decoherence.

A biaxial anisotropy magnetic grain with XOY easy plane and the easy Y-axis can be described by Hamiltonian

$$H_0 = K_1 S_z^2 + K_2 S_x^2 \tag{1}$$

where K_1 and K_2 with $K_1 > K_2$ are longitudinal and transverse anisotropy constants, respectively. $|\psi_\pm\rangle$ denote the two macroscopically distinguishable quantum states, corresponding to two equilibrium orientations of the magnetization vector along positive and negative Y-axis, respectively. The quantum tunneling leads to the coherence between the degenerate state $|\psi_+\rangle$ and $|\psi_-\rangle$. At low temperature the tunneling rate between the degenerate state $|\psi_+\rangle$ and $|\psi_-\rangle$ is rather small and the tunnel splitting is much smaller than the level spacing. Thus the giant spin with dissipation may be approximated as a two-level system coupling to a phonon-bath and can be described by the effective Hamiltonian [11]

$$H = -\frac{\Gamma_0}{2}\sigma_x + \frac{1}{2}\sum_k \left(\frac{p_k^2}{m_k} + m_k\omega_k^2 x_k^2\right) + \sigma_z \sum_k C_k x_k, \tag{2}$$

where x_k, p_k, m_k and ω_k are, respectively, the coordinate, momentum, mass, and frequency of the kth harmonic oscillator in the heat bath, and C_k is the coupling strength between the two-level system and the kth oscillator. Γ_0 denotes the bare tunnel splitting and depends on the parameters K_1 and K_2. It has been shown, by using path-integral formalism [11], that the complete information of the effect of the heat bath on tunneling system is contained in the spectral density which is independent of the explicit form of the coupling strength. This concept is based on a fact that the bath degrees of freedom can be integrated out as Gaussian integrals with the displaced centres of phonon states. Later it was pointed out that the interaction between the bath and the tunneling system not only induces displacement, but also leads to deformation of phonon states because of the nonlinear interaction [18,19].

Using creation and annihilation operators the Hamiltonian (2) is expressed as

$$H = -\frac{\Gamma_0}{2}\sigma_x + \sum_k \omega_k b_k^+ b_k + \sum_k g_k \sigma_z \left(b_k^+ + b_k\right), \tag{3}$$

where $g_k = C_k \left(2m_k\omega_k\right)^{1/2}$ are effective coupling strength. In order to obtain the corresponding tunnel splitting in the dissipative environment the two lowest-energy eigenstates of the system-plus-environment may be assumed as

$$|\psi\rangle_\pm = \frac{1}{\sqrt{2}}\left(|\psi_+\rangle|\phi_+\rangle \pm |\psi_-\rangle|\phi_-\rangle\right) \tag{4}$$

which satisfy

$$H|\psi_\pm\rangle = E_\pm|\psi_\pm\rangle, \tag{5}$$

where $\sigma_z|\psi_\pm\rangle = \pm|\psi_\pm\rangle$ and $|\phi_\pm\rangle$ are the displaced phonon ground states, namely, the coherent states with $b_k|\phi_\pm\rangle = \pm\eta_k\ |\phi_\pm\rangle$, which are to be determined in terms of variational method. Inserting equations (3) and (4) into equation (5) and noting $\sigma_x|\psi_\pm\rangle = |\psi_\mp\rangle$ and $\langle\psi_i|\psi_j\rangle = \delta_{ij}(i,\ j = +,\ -)$ we obtain

$$E_\pm = \sum_k \left(\omega_k|\eta_k|^2 + 2g_k \operatorname{Re}\eta_k\right) \mp \frac{\Gamma_0}{2}\langle\phi_+|\phi_-\rangle. \tag{6}$$

The corresponding tunnel splitting is given by the expression

$$\Gamma = E_- - E_+ = \Gamma_0\langle\phi_+|\phi_-\rangle. \tag{7}$$

It is obvious that the effect of the heat-bath environment on tunnel splitting depends on the overlap $\langle\phi_+|\phi_-\rangle$. When the coupling between the tunneling system and the heat-bath environment and the interaction among phonons can be ignored, the Hamiltonian (3) reduces to $H_0 = -\frac{\Gamma_0}{2}\sigma_x + \sum_k \omega_k b_k^+ b_k$. The ground state of H_0 may be written as $|0\rangle|\psi_e\rangle$, where $|\psi_e\rangle = (|\psi_+\rangle + |\psi_-\rangle)/\sqrt{2}$ denotes the ground state of the two-level system and $|0\rangle = \prod_k |0\rangle_k$ is the ground state of phonon bath. For the weak coupling, the interaction between the tunneling system and the heat bath induces the displacement of phonon state which is dominating effect [18]. Thus the trial displaced ground state of the Hamiltonian equation (3) is written as

$$\begin{aligned} |\psi\rangle &= \prod_k \exp\left[-c_k\sigma_z(b_k^+ - b_k)\right]|0\rangle_k|\psi_e\rangle \\ &= \frac{1}{\sqrt{2}}\left(|\psi_+\rangle|\phi_+\rangle + |\psi_-\rangle|\phi_-\rangle\right), \end{aligned} \tag{8}$$

where $|\phi_\pm\rangle = \prod_k \exp\left[\mp c_k\left(b_k^+ - b_k\right)\right]|0\rangle_k$ are the phonon coherent states which we are looking for. c_k is the variational parameter determined from the equation $\delta E/\delta c_k = 0$ which minimizes the energy $E = \langle\psi|H|\psi\rangle$ and is given by $c_k = g_k/(\omega_k + \Gamma_0 K)$. The overlap between $|\phi_+\rangle$ and $|\phi_-\rangle$ is obtained [19] as

$$K = \langle\phi_-|\phi_+\rangle = \exp\sum_k\left(-2c_k^2\right). \tag{9}$$

By means of the simple power law for coupling strength $g_k = g_0\left(\omega_k/\omega_D\right)^\lambda$ with ω_D the upper cut-off frequency and replacing the sum over wave vector k by integral such that $\sum_k \sim \int \omega^{n-1}d\omega$ (n is the dimension of phonon bath), we have $\sum_k 2c_k^2 = \alpha\int_0^{\omega_D} d\omega J(\omega)/(\omega + \Gamma_0 K)^2$ with $J(\omega) = \omega^s/\omega_D^{s-1}(s = 2\lambda + n - 1)$ and $\alpha = 2g_0^2/\omega_D^2$ the dimensionless coupling strength. Thus for ohmic dissipation $(s = 1)$ we obtain

$$\Gamma = \Gamma_0 K = f(\Gamma),\quad f(\Gamma) = \Gamma_0\ \left(\frac{\Gamma}{\omega_D + \Gamma}\exp\frac{\omega_D}{\omega_D + \Gamma}\right)^\alpha. \tag{10}$$

It is seen that equation (10) has nonzero solution for Γ when $\frac{df(\Gamma)}{d\Gamma} > 1$, while only the trivial solution, $\Gamma = 0$, when $\frac{df(\Gamma)}{d\Gamma} < 1$. A critical value α_c is determined from

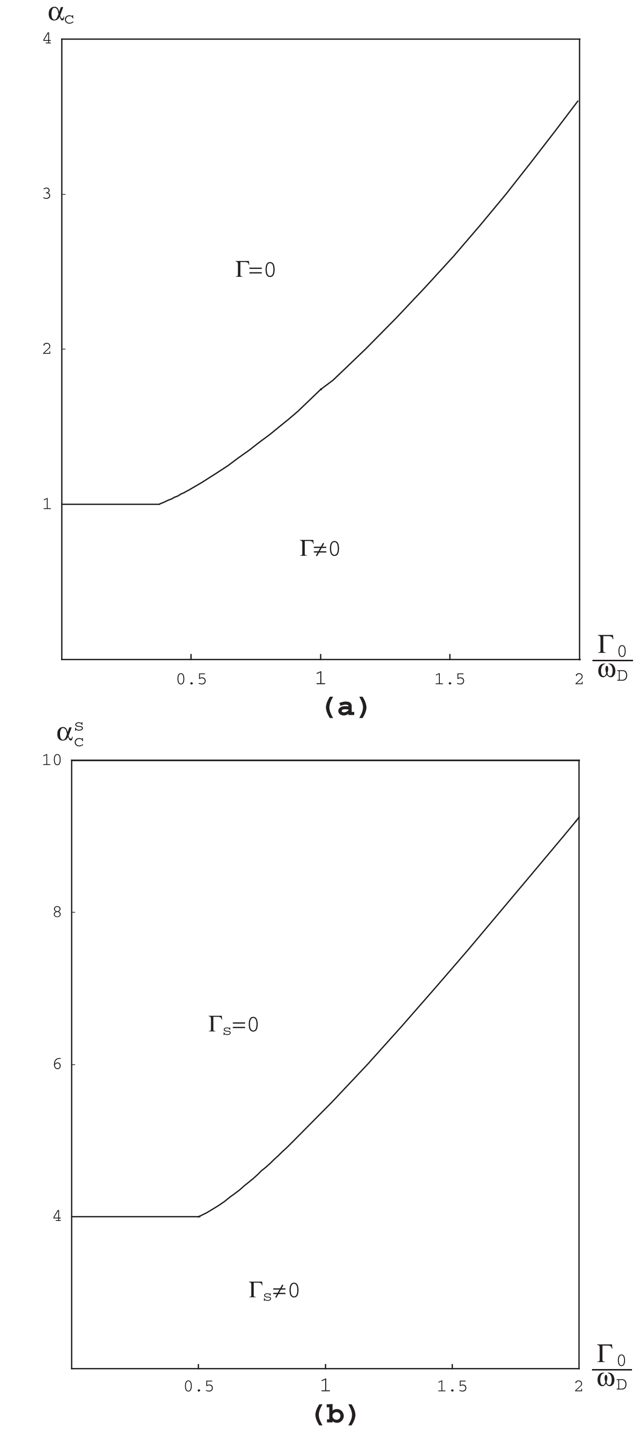

Fig. 1. The critical value α_c and α_c^s as a function of the ratio $\frac{\Gamma_0}{\omega_D}$.

the equation $\frac{df(\Gamma)}{d\Gamma} = 1$ along with equation (10) and is found to satisfy the equation

$$(\sqrt{\alpha_c} - 1)^{1-\alpha_c} = \frac{\Gamma_0}{\omega_D}\alpha_c^{-\alpha_c/2}e^{\sqrt{\alpha_c}} \tag{11}$$

with α_c depending on $\frac{\Gamma_0}{\omega_D}$. Figure 1a shows α_c as a function of the ratio $\frac{\Gamma_0}{\omega_D}$ and indicates that $\Gamma \neq 0$ in the region

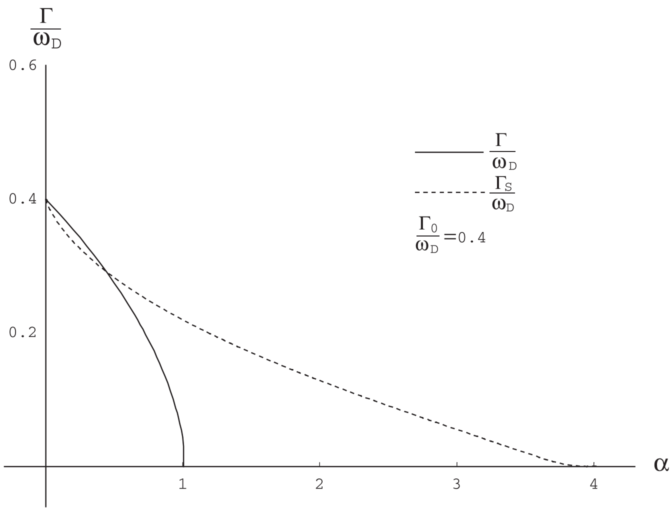

Fig. 2. The dimensionless tunnel splitting $\frac{\Gamma}{\omega_D}$ and $\frac{\Gamma_s}{\omega_D}$ as a function of the dimensionless coupling strength α for $\frac{\Gamma_0}{\omega_D} = 0.4$.

below the critical curve and $\Gamma = 0$ in the region above the critical curve. When $\frac{\Gamma_0}{\omega_D} \ll 1$, equation (11) gives critical value $\alpha_c = 1$, while equation (10) is approximated as $\Gamma = \Gamma_0\left(e\frac{\Gamma_0}{\omega_D}\right)^{\frac{\alpha}{1-\alpha}}$ for $\alpha < 1$ and $\Gamma = 0$ for $\alpha > 1$, which is just the results in references [11,20] where the cut off frequency ω_D is usually considered to be very large and all results referred to are in the lowest order of $\frac{\Gamma_0}{\omega_D}$. The critical value $\alpha_c = 1$ also is given by reference [9] where the finite temperature case is considered. The dimensionless tunnel splitting $\frac{\Gamma}{\omega_D}$ with dissipation is plotted in Figure 2 (solid line) as a function of α with scale $\frac{\Gamma_0}{\omega_D} = 0.4$. $\frac{\Gamma}{\omega_D}$ decreases with increasing α. When $\alpha \geqslant \alpha_c$, tunnel splitting vanishes and thus the coherent transition between two degenerate states $|\psi_\pm\rangle$ are completely suppressed.

For the strong coupling case, the displaced state approximation is no longer valid. In fact, the tunneling system not only induces the displacement of the oscillators in environment, but also leads to the deformation of the ground state of phonon bath because of the interaction among phonons. This deformation effect may be described by the squeezed state of phonon vacuum and thus variational state is assumed as

$$\begin{aligned}|\psi_s\rangle &= \prod_k \exp\left[-\sigma_z\frac{g_k}{\omega_k}\left(b_k^+ - b_k\right)\right] \\ &\quad\times \exp\left[-r_k\left(b_k^2 - b_k^{+2}\right)\right]|0\rangle_k|\psi_e\rangle \\ &= \frac{1}{\sqrt{2}}\left(|\psi_+\rangle|\phi_{s+}\rangle + |\psi_-\rangle\phi_{s-}\rangle\right),\end{aligned} \tag{12}$$

where $|\phi_{s\pm}\rangle = \prod_k \exp[\mp\frac{g_k}{\omega_k}(b_k^+ - b_k)]\exp[-r_k(b_k^2 - b_k^{+2})]|0\rangle_k$ is the displaced-squeezed coherent state of the phonon bath and r_k is variational parameter. Using variational method we obtain $r_k = \frac{1}{8}\ln(1 + 4g_k^2\Gamma_0 K_s/\omega^3)$. The overlapping integral between $|\phi_{s+}\rangle$ and $|\phi_{s-}\rangle$ satisfies the equation

$$K_s = \langle \phi_{s-}|\phi_{s+}\rangle = \exp\left[-\sum_k \frac{2g_k^2}{\omega_k^2}\exp(-2r_k)\right]. \quad (13)$$

The effective tunnel splitting in this case is denoted as $\Gamma_s = \Gamma_0 K_s$. With the same procedure we obtain

$$\Gamma_s = \Gamma_0\left(\frac{\sqrt{2\alpha\Gamma_s/\omega_D}}{1+\sqrt{1+2\alpha\Gamma_s/\omega_D}}\right)^{\alpha/2} \quad (14)$$

for ohmic dissipation. In Figure 2 (dashed line) $\frac{\Gamma_s}{\omega_D}$ as a function of α is shown for scale $\frac{\Gamma_0}{\omega_D} = 0.4$. $\frac{\Gamma_s}{\omega_D}$ decreases with increasing α and vanishes when $\alpha \geqslant \alpha_c^s$. The critical value α_c^s is determined by the equation

$$32\frac{\Gamma_0}{\omega_D}\alpha_c^s(\alpha_c^s-4)^{\alpha_c^s/4-1} = (\alpha_c^s+4)^{\alpha_c^s/4+1}. \quad (15)$$

The critical values α_c^s as a function of the ratio $\frac{\Gamma_0}{\omega_D}$ is plotted in Figure 1b. Including the nonlinear interaction among phonons which is described by squeezed coherent states the coherent tunneling seems to be expanded to a more wide region of value α. In both cases the tunnel splitting and therefore the macroscopic quantum coherence are suppressed by ohmic dissipation of the environment.

It is interesting to investigate the relation of decoherence to the entanglement between the giant spin and the environment. To this end we begin with the reduced density operator by performing the trace over Fock-space of phonons

$$\begin{aligned}\rho_p(\psi) &= \sum_n \langle n|\psi\rangle\langle\psi|n\rangle \\ &= \frac{1}{2}\left(|\psi_+\rangle\langle\psi_+| + |\psi_-\rangle\langle\psi_-| \right.\\ &\quad \left. + K|\psi_+\rangle\langle\psi_-| + K|\psi_-\rangle\langle\psi_+|\right) \end{aligned} \quad (16)$$

where $|n\rangle = \prod_k |n_k\rangle$ is the Fock-state of phonons. The reduced density operator has an obvious physical meaning that the quantum coherence between the degenerate states $|\psi_\pm\rangle$ is suppressed by the same suppressing factor K as the one appearing in tunnel splitting. Particularly when $K = 0$ the pure macroscopic quantum state $\frac{1}{\sqrt{2}}(|\psi_+\rangle + |\psi_-\rangle)$ reduces to a mixed state showing the complete decoherence. Using the von Nenmann entropy to measure the degree of entanglement between the giant spin and the environment, the degree of entanglement may be defined as [21]

$$E(\psi) = S[\rho_p(\psi)] = -\sum_{i=1}^m \lambda_i \log_2 \lambda_i, \quad (17)$$

where m is Schmidt number and $\{\lambda_i\}$ are nonzero eigenvalues of ρ_p. The degree of entanglement corresponding to the entangled state $|\psi\rangle$ is

$$E(\psi) = 1 - \frac{1}{2}\log_2\left[(1+K)^{K+1}(1-K)^{K-1}\right]. \quad (18)$$

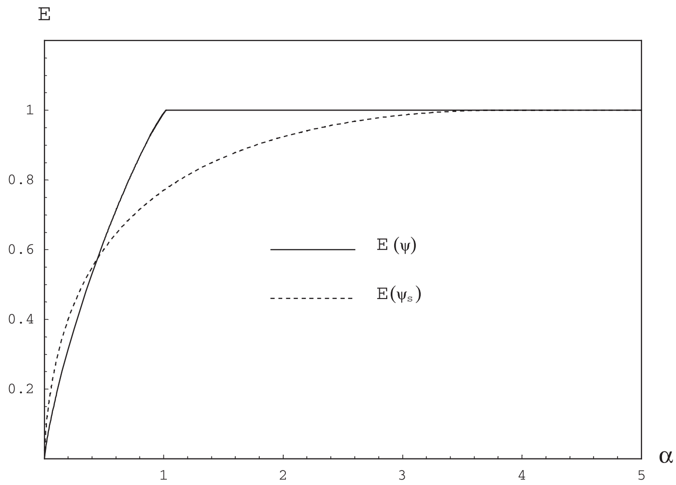

Fig. 3. Dependence of the entanglement degree on the dimensionless coupling strength α for $\frac{\Gamma_0}{\omega_D} = 0.4$.

When $K = 1$, the degree of entanglement is zero, while for $K = 0$, we have the maximum entanglement $E(\psi) = 1$. The entanglement depends on the dimensionless coupling strength α via K. The relation between K and α is found as

$$K = \left[\frac{\Gamma_0 K}{\omega_D + \Gamma_0 K}\exp\left(\frac{\omega_D}{\omega_D + \Gamma_0 K}\right)\right]^\alpha \quad (19)$$

for the state $|\psi\rangle$ in equation (8). For the case of considering the interaction among phonons the relation is replaced by

$$K_s = \left(\frac{\sqrt{2\alpha\Gamma_0 K_s}}{\sqrt{\omega_D}+\sqrt{\omega_D + 2\alpha\Gamma_0 K_s}}\right)^{\frac{\alpha}{2}}. \quad (20)$$

The dependence of the entanglement on the dimensionless coupling strength is shown in Figure 3 for $\frac{\Gamma_0}{\omega_D} = 0.4$. It is obvious that the decoherence occurs when the entanglement attains its maximum. From Figure 3 one can find that the degree of entanglement for the squeezed coherent state of phonons vacuum, $E(\psi_s)$, approaches its maximum value more slowly than $E(\psi)$ indicating a fact that interphonon interaction decreases the entanglement between the spin system and the environment and suppresses the decoherence (see Figs. 1 and 2), which is in favor of quantum computing.

In conclusion, the dissipation of environment consisting of phonon bath results in the suppression of tunnel splitting and therefore the decoherence in the magnetic grain. When the coupling strength is higher than its critical value, tunnel splitting is completely suppressed. In the case of considering the interaction between tunneling system and the environment, the interphonon interaction results in an effective decoupling of the spin system from the phonon bath and therefore decreases the decoherence and entanglement. When the effect of environment consisting of phonon bath is considered the molecular magnet (for instance Fe_8) is still a good candidate for the realization of qubits because Γ_0 may be far less than ω_D.

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