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Quantum tunnelling and decoherence in nanomagnets

Z. Gedik[*] and **Ö. Bozat**

Sabanci University, Faculty of Engineering and Natural Sciences, Tuzla 34956, Istanbul, Turkey

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Starting from the observation that at very low temperatures an isolated nanomagnet can be treated as an effective two-state system, we introduce a model to study quantum tunnelling and decoherence phenomena. We assume that the total spin of the magnet interacts with a spin bath. We show that depending upon the interaction strengths the molecule can exhibit tunnelling with or without decoherence. We also investigate the case where the spin-spin interaction is mediated by phonons.

Quantum tunneling phenomena in nanomagnets have become a very attractive research area not only because of their potential applications like data storage and quantum computation but also due to the relevance of the problem to some fundamental issues in quantum mechanics like tunneling and decoherence [1]. Molecular magnets such as Mn_{12} and Fe_8, have been the most promising systems due to their well-defined structures with well-characterized spin ground states [2]. Generally nanomagnets can be modeled as a single large spin S with uniaxial anisotropy. In pure quantum regime the direction of magnetization changes when small transverse perturbation exist at the resonance between energy levels of spin states on opposite sides of the potential barrier. Then the spin Hamiltonian can be written as $H = -DS_z^2 + H_{trans}$, where D is uniaxial anisotropy constant and H_{trans} is the transverse term that does not commute with z-component of the spin. Tunneling between nearly degenerate levels can be understood by the Landau-Zener theory [3].

Quantum tunneling in these systems is important to understand the decoherence problem also [4]. Beside its connection to crossover from to quantum to classical world, decoherence is the main obstacle to built effective quantum information devices [5]. At very low temperatures it is possible to truncate the nanomagnet with large spin S to a two-level system [6]. Then Hamiltonian of the isolated system simply becomes $H = \Delta\sigma_x$, where σ_x is Pauli spin operator and Δ is the tunneling matrix element. This truncation is valid only if the tunneling splitting is small compared to energy gap between the lowest doublet spin states and the next excited states. Then it is easy to study decoherence phenomena due to the coupling of the two-state system to environmental degrees of freedom, such as nuclear spins [7] and phonons [8]. Although both of these couplings are well understood [9] there are still some discrepancies between experiment and theory [10]. For a consistent explanation of the experimental data, the two different baths, spin and phonon, which are considered to be effective at different time scales should be properly combined.

At low temperatures low temperatures local modes such as defects, impurity spins, and nuclear spins dominate the environmental quantum dynamics of molecular magnets. Therefore, we will first assume

[*] Corresponding author: e-mail: gedik@sabanciuniv.edu

that effective two-state system of the magnetic molecule interacts with bath of N spin-½ particles. For this purpose we will use the Hamiltonian

$$H = \sigma_x \left(\sum_{k=1}^{N} \hbar\omega_k \tau_{kx} \right) .$$

Here, τ_{kx} is the Pauli spin operator for the k^{th} spin of the bath and $\hbar\omega_k$ is the interaction strength. We will assume that the nanomagnet is initially in one of the degenerate ground states, say S = 10 corresponding to spin up state $|\uparrow\rangle$ in the two-state approximation so that

$$|\Psi(0)\rangle = |\uparrow\rangle \otimes \prod_{k=1}^{N} (\alpha_k |+_k\rangle + \beta_k |-_k\rangle)$$

where $|+_k\rangle$ and $|-_k\rangle$ are eigenstates of τ_{kx} with eigenvalues +1 and –1, respectively. We can easily find the state of the combined system at later times as

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}} |+\rangle \otimes \prod_{k=1}^{N} \left(\alpha_k e^{-i\omega_k t} |+_k\rangle + \beta_k e^{i\omega_k t} |-_k\rangle \right) + \frac{1}{\sqrt{2}} |-\rangle \otimes \prod_{k=1}^{N} \left(\alpha_k e^{i\omega_k t} |+_k\rangle + \beta_k e^{-i\omega_k t} |-_k\rangle \right)$$

where $|+\rangle$ and $|-\rangle$ are eigenstates of σ_x with eigenvalues +1 and –1, respectively. We observe that the nanomagnet and the bath spins, which are initially in a product state, become entangled as soon as the interaction is turned on.

Knowing the state vector $|\Psi(t)\rangle$ we can find the density matrix for the combined system as $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ however what we are interested in is the reduced density matrix $\rho_\sigma(t)$ which describes the nanomagnet. For this purpose we trace out bath spins so that $\rho_\sigma(t) = Tr_\tau |\Psi(t)\rangle\langle\Psi(t)|$, in σ_x-basis, is given by

$$\rho_\sigma(t) = \frac{1}{2} \begin{bmatrix} 1 & r \\ r^* & 1 \end{bmatrix}$$

where the decoherence factor is $r(t) = \prod_{k=1}^{N} \left(|\alpha_k|^2 e^{-i\omega_k t} + |\beta_k|^2 e^{i\omega_k t} \right)$. Here, $r = 1$ and $r = -1$ values correspond to $|\uparrow\rangle$ and $|\downarrow\rangle$ states, respectively. At $t = 0$, $r = 1$ and as t increases in general it decays to zero with a Gaussian time dependence [11]. When r vanishes, ρ_σ describes a classical ensemble of spin-1/2 systems where half of them are up and half of them are in the down state.

For the special case where $|\alpha_k|^2 = 1$ for all spin baths, the decoherence factor becomes $r(t) = \exp\left(-it \sum_{k=1}^{N} \omega_k \right)$ and there fore there is no decay and r simply traces the unit circle. In other words, the nanomagnet exhibits tunneling between $|\uparrow\rangle$ and $|\downarrow\rangle$ states back and forth.

Another special case is $|\alpha_k|^2 = |\beta_k|^2 = 1/2$. This time $r(t) = \prod_{k=1}^{N} \cos\omega_k t$ and if the interaction strengths are random we can show that $r(t) \cong \exp\left(-\frac{t^2}{2} \sum_{k=1}^{N} \omega_k^2 \right)$ so that r is always positive and hence the nanomagnet never goes to the state $|\downarrow\rangle$. The system undergoes decoherence before tunneling.

We can generalize the model to the case where the spin-spin interaction is mediated by phonons [12]. For this purpose, we introduce the harmonic oscillator operators a_k^+ and a_k and the Hamiltonian

$$H = \sigma_x \sum_{k=1}^{N} \hbar\omega_k \left(a_k^+ + a_k\right) \tau_{kx} + \sum_{k=1}^{N} \hbar\Omega_k a_k^+ a_k \ .$$

We assume that the nanomagnet, the spin bath and the phonon bath system is initially in the state

$$|\Psi(0)\rangle = |\uparrow\rangle \otimes \prod_{k=1}^{N} \left(\alpha_k |+_k\rangle + \beta_k |-_k\rangle \right) \otimes |\lambda_k\rangle$$

where $|\lambda_k\rangle$ denotes the coherent state corresponding to the annihilation operator a_k with eigenvalue λ_k so that $a_k |\lambda_k\rangle = \lambda_k |\lambda_k\rangle$. Coherent states describe classical harmonic oscillations: A Gaussian wave packet performs simple harmonic motion without loosing its shape. Therefore, if τ_{kx} is the nuclear spin operator, the model can be used to study decoherence in the presence of atomic vibrations. For te special case where $|\lambda_k\rangle$ is the gorund state of the k^{th} oscillator, decoherence factor becomes $r(t) \approx \exp\left(-2t^2 \sum_{k=1}^{N} \omega_k^2\right)$. Therefore, in this limit *r* is again a Gaussian function of time. It is possible to find *r(t)* for arbitrary $|\lambda_k\rangle$ and we can show that decoherence factor is always a decaying function.

In conclusion, using an effective two-state description of a nanomagnet we studied the decoherence and tunneling phenomena, We showed that except for a very special initial condition both spin and phonon baths cause the loss of coherence. In general, the nanomagnet undergoes decoherence before tunneling of magnetization. Decoherence of two nanomagnets is also an interesting problem. In this case entanglement of spins should properly be taken into account [13]. For example, if the two spins are prepared in properly chosen states, it is possible to obtain relatively longer coherence time.

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References

[1] D. Gatteschi and R. Sessoli, Angew. Chem. Int. Edit. **42**, 268 (2003).
[2] T. Lis, Acta Crystallogr. B **36**, 2042 (1980); K. Wieghardt, K. Pohl, I. Jibril, and G. Gunther, Angew. Chem. **96**, 63 (1984).
[3] L. D. Landau, Phys. Z. Sowjetunion **2**, 46 (1932), C. Zener, Proc. R. Soc. London, Ser. A **137**, 696 (1932).
[4] W. H. Zurek, Rev. Mod. Phys. **75**, 715 (2003).
[5] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, U.K., 2000).
[6] F. D. M. Haldene, Phys. Rev. Lett. **50**, 1153 (1983); D. Loss, D. P. di Vincenzo, and G. Grinstein, Phys. Rev. Lett. **69**, 3232 (1992).
[7] P. C. E. Stamp, Physica B **197**, 133 (1994); N. V. Prokof'ev and P. C. E. Stamp, J. Phys. CM Lett. **5**, L663 (1993).
[8] A. O. Calderia and A. J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1983); A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[9] N. V. Prokof'ev and P. C. E. Stamp, J. Low Temp. Phys. **104**, 143 (1996).
[10] M. Evangelisti, F. Luis, F. L. Mettes, N. Aliaga, G. Aromi, J. J. Alonso, G. Christou, and L. J. de Jongh, Phys. Rev. Lett. **93**, 117202 (2004); A. Morello, O. N. Bakharev, H. B. Brom, R. Sessoli, and L. J. de Jongh, Phys. Rev. Lett. **93**, 197202 (2004).
[11] W. H. Zurek, F. M. Cucchietti, and J. P. Paz, quant-ph/0312207.
[12] Ö. Bozat and Z. Gedik, preprint.
[13] Z. Gedik, quant-ph/0505176.

