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Quantum force of tunneling macrospins with a mechanical resonator

Gwang-Hee Kim

Department of Physics and Astronomy, Sejong University, Seoul 05006, Republic of Korea

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ABSTRACT

We study force dynamics of macropsin of molecular magnets coupled to a torsional resonator. In the presence of an ac field and a static field with a gradient, the force is shown to display various types of quantum oscillations which depend upon the coupling strength and the frequency of torsional oscillations. Optimal conditions for observing them will be discussed within the framework of experimentally controllable parameters.

1. Introduction

Investigations of the macroscopic quantum tunneling in magnetic systems have been a topical issue of intensive theoretical and experimental studies over the past few decades [1]. Especially, molecular magnets (MMs) have been at the forefront of research on quantum tunneling of magnetization at the nanoscale. These magnets exhibit particularly fascinating quantum effects, such as the topological interference [2], magnetic deflagration [3], and Rabi oscillation [4]. Such phenomena provide an ultimate limit of the miniaturization of magnetic memory and are promising candidates for qubits [5] and molecular devices [6]. Many efforts have been made to understand their mechanisms by considering the Landau–Zener-Stueckelberg model [7] in MMs. Among them, the tunnel splitting generated from the transverse anisotropy or field has been recognized as playing an important role in quantum force generated by the quantum dynamics of the magnetic moment in MMs.

The question of the force of a quantum nature in two-state systems was theoretically studied by Chudnovsky et al. [8]. They showed that mechanical forces of quantum origin could be observed in two-state systems with level splitting which depends on the space, and applied them to MMs in the presence of a microwave field when the magnets were placed in a static magnetic field with a gradient. A natural extension of the quantum force in two-level physics is the force in nanomagnets coupled to one or several quantized modes of a harmonic oscillator. In fact, placing the sample on a resonator is prevalent in nanomagnetic systems and molecular devices. The coupling of cantilevers to quantum spins has been theoretically studied in recent years in the context of the possibility of reversing the magnetic moment by using mechanical motion [9,10]. Experimental progress [11] has been made in characterizing MMs in a nanoelectromechanical system obtained by grafting MMs on a carbon nanotube or nanocantilever. Hence it is important to investigate how strongly such couplings make an effect on the quantum force dynamics before contemplating real experiments.

In this paper we consider mechanical forces of quantum origin in MMs that are coupled to a torsional resonator in the presence of an ac field and a transverse field. In the presence of the gradient of the level splitting created by the gradient of the transverse field we demonstrate that there are various force dynamics generated by four parameters: $p = \omega/\omega_R,\ \epsilon = S(L/L_c)(\omega/\omega_R),\ \gamma_0 = \omega_r/\omega$, and $\lambda = \sqrt{2\hbar S^2/I_z\omega_r}$. Here ω is a frequency of ac field, ω_R is the Rabi frequency associated with the amplitude of ac field, L is a thickness of sample, L_c is the characteristic length describing the field gradient, $\hbar S$ is the spin, I_z is the moment of inertia of the resonator, and ω_r is the fundamental frequency of torsional oscillations. With an eye on resonant experiments the magnitude of p and ϵ determine the possibility of the existence of a quantum force through the oscillation of the populations of the two-levels in time. The other two parameters, γ_0 and λ play crucial roles in the oscillatory structure of the force such as the shape of the force with nodes, i.e., quantum beat. Especially, the period of the beat strongly depends upon the coupling strength between the spin and oscillator. Based on the analytic expression of a quantum force obtained with the use of the rotating wave approximation, we provide the optimal condition for the appearance of quantum beat by controlling the parameters. In this respect, the quantum dynamics of the force in a spin-oscillator system is expected to be more diverse and experimentally measurable in molecular devices.

E-mail address: gkim@sejong.ac.kr

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This paper is organized as follows. The two-state model in MMs coupled to a mechanical resonator is reviewed in Section 2. The quantum force of spin-oscillator system is introduced in Section 3. Employing the rotating wave approximation, we present the approximate analytic form of the force in a weak coupling regime and analyze the period of its oscillating part which relies on four parameters. Section 4 contains conclusions and suggestions for experiment.

2. The two-state model in a spin-oscillator system

Consider a crystal of MM with the Hamiltonian

$$\mathscr{H}_{\mathrm{MM}} = -DS_z^2 + \mathscr{H}_{\perp}, \tag{1}$$

where $S_i(i = x, y, z)$ are three components of the spin operator, $D(> 0)$ is the second order longitudinal anisotropy constant. The second term is a small transverse term that does not commute with S_z and, thus, allows tunneling of **S** between states. Absence of $\mathscr{H}_{\perp}$ implies that $|\pm S\rangle$ eigenstates of S_z are degenerate ground states of $-DS_z^2$. The transverse operator $\mathscr{H}_{\perp}$ in the Hamiltonian (1) perturbs the $|\pm S\rangle$ and provides the quantum tunneling which results in the avoided level crossing between two states $|-S\rangle$ and $|S\rangle$. Then, the ground state and the first excited state are even and odd combinations of $|\pm S\rangle$, respectively, [12]

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|S\rangle \pm |-S\rangle). \tag{2}$$

with $E_- - E_+ = \Delta$ being the level splitting. Since the tunnel splitting Δ is generally many orders of magnitude less than the energy to the next spin level($\sim 2SD$), [13] it makes the two-state approximation very accurate at low energies. In this respect we can describe such a two-state system by a pseudospin 1/2 whose components are

$$\begin{aligned} \hat{\sigma}'_x &= |-S\rangle\langle +S| + |+S\rangle\langle -S|, \\ \hat{\sigma}'_y &= i|-S\rangle\langle +S| - i|+S\rangle\langle -S|, \\ \hat{\sigma}'_z &= |+S\rangle\langle +S| - |-S\rangle\langle -S|. \end{aligned} \tag{3}$$

Projecting $\mathscr{H}_{\mathrm{MM}}$ onto $|\pm S\rangle$ states and applying an ac field along the Z axis, one obtains the Hamiltonian

$$\mathscr{H}_{\sigma} = -\frac{\Delta}{2}\hat{\sigma}'_x - g\mu_B S B_{\mathrm{ac}} \sin(\omega t)\hat{\sigma}'_z, \tag{4}$$

where B_{ac} is an amplitude of ac field and ω is its frequency, with g being the gyromagnetic factor and μ_B being the Bohr magneton. Here the second term can be small compared to the first term as long as the magnitude of ac field satisfies $B_{\mathrm{ac}} \ll \Delta/(g\mu_B S)$. As this condition is fulfilled, the approximate eignestates of the problem are given by Eq. (2). Their energies are $\pm\Delta/2$ which correspond to the states $|\mp\rangle$. At $\omega \simeq \Delta/\hbar$, the second term produces transitions between these states, resulting in the Rabi oscillation [14].

Let now MMs be coupled to a mechanical resonator with torsional rigidity k. In the presence of a mechanical rotation of the oscillator that can rotate around the Z axis, [15] we perform the rotation of the Hamiltonian (4) by angle ϕ about the Z axis which leads to [9]

$$\begin{aligned} \mathscr{H}_{\sigma,\mathrm{osc}} = {} & \frac{\hbar^2 L_z^2}{2I_z} + \frac{1}{2}I_z\omega_r^2\phi^2 - g\mu_B S B_{\mathrm{ac}} \sin(\omega t)\hat{\sigma}'_z \\ & -\frac{\Delta}{2}\left[\hat{\sigma}'_x \cos(2S\phi) + \hat{\sigma}'_y \sin(2S\phi)\right], \end{aligned} \tag{5}$$

where I_z is the moment of inertia of the resonator about its rotation axis and $\omega_r(= \sqrt{k/I_z})$ is the fundamental frequency of torsional oscillations. The operator of the mechanical angular momentum, $L_z = -i\partial/\partial\phi$ and the angular displacement ϕ of the oscillator obey the commutation relation $[\phi, L_z] = i$. The first two terms in Eq. (5) describe mechanical rotation and the last term indicates the coupling of spin transition to the mechanical rotations. The limit $\omega_r = 0$ corresponds to the case where the system consists of a free nanomechanical body and a tunneling spin [16].

Since we are interested in the case where the states in Eq. (2) are coupled to nanoresonator which rotates in an oscillator fashion under a restoring torque, it is convenient to introduce the annihilation and creation operator, a and $a^\dagger$,

$$L_z = i\sqrt{\frac{I_z\omega_r}{2\hbar}}(a^\dagger - a), \phi = \sqrt{\frac{\hbar}{2I_z\omega_r}}(a^\dagger + a), \tag{6}$$

for the oscillator, and use the basis that is a direct product of the two basis states, $|\pm\rangle$, and the harmonic oscillator basis, $|m\rangle$. Then, the projection of the Hamiltonian in Eq. (5) onto $|m\rangle|\pm\rangle$ states gives

$$\begin{aligned} \mathscr{H} = {} & \hbar\omega_r\left(a^\dagger a + \frac{1}{2}\right) - \hbar\omega_R \sin(\omega t)\hat{\sigma}_x \\ & -\frac{\Delta}{2}\left[\hat{\sigma}_z \cos(2S\phi) - \hat{\sigma}_y \sin(2S\phi)\right], \end{aligned} \tag{7}$$

where $\omega_R = g\mu_B S B_{\mathrm{ac}}/\hbar$ is the Rabi frequency and $\hat{\sigma}_i$ $(i = x, y, z)$ has the same form as Eq. (3) by replacing $|\pm S\rangle$ by $|\pm\rangle$. In this case the wave function can be expressed as

$$|\Psi(t)\rangle = \sum_{m=0}^{\infty}\sum_{\alpha=+,-} C_{m\alpha}(t)|m\rangle|\alpha\rangle, \tag{8}$$

where the coefficients $C_{m\alpha}$ satisfy the time-dependent Schrödinger equation.

3. Force dynamics of tunneling macrospins with torsional oscillations of a mechanical resonator

Let us now consider a spin-oscillator system containing a macroscopic number of noninteracting two-state particles. The force on the systems is given by

$$\mathbf{F} = -\sum{}' \mathrm{Tr}(\rho\nabla\mathscr{H}), \tag{9}$$

where $\sum'$ indicates the summation over the systems and $\rho = |\Psi\rangle\langle\Psi|$ is the thermal-state one-particle density matrix.

In general, the level splitting is generated by the transverse anisotropy or field. For the gradient Δ, choosing a gradient of the transverse magnetic field that can be used as a controllable parameter in experiment is feasible. Because we are interested in the resonant state, the spatial change in Δ across a system of thickness L along the Y axis is small compared to Δ itself; that is, $|d\Delta/dy| \ll \Delta_0/L$, where Δ_0 is the tunnel splitting in the center of the system ($y = 0$). Such a condition indicates $S|dB/dy| \ll B_0/L$ by using the relation that [1] $\Delta \propto B^{2S}$, where $B(y)$ is the transverse external field along the medium or hard axis and $B(0) = B_0$. Writing $B(y) = B_0(1 + y/L_c)$, where L_c is the characteristic length describing the field gradient, we find the expression for Δ as a function of y expressed as

$$\Delta = \Delta_0\left(1 + \frac{2Sy}{L_c}\right) \tag{10}$$

with $S(L/L_c) \ll 1$.

With the help of Eq. (8), denoting the density matrix ρ as

$$\rho = \sum_{m,m'=0}^{\infty}\sum_{\alpha,\alpha'=+,-}|m\rangle|\alpha\rangle\rho_{mm'\alpha\alpha'}\langle m'|\langle\alpha'|. \tag{11}$$

one has a quantum force originated from the gradient of the tunnel splitting in a spin-oscillator system given by