Damping of a nanocantilever by paramagnetic spins

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We compute damping of mechanical oscillations of a cantilever that contains flipping paramagnetic spins. This kind of damping is mandated by the dynamics of the total angular momentum, spin + mechanical, and it does not require an external magnetic field. Rigorous expression for the damping rate is derived in terms of the imaginary part of the magnetic susceptibility. The effect of spins on the quality factor of the cantilever can be significant in cantilevers of small length that have large concentration of paramagnetic spins of atomic and/or nuclear origin.

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I. INTRODUCTION

Small cantilevers have various applications in atomic force microscopy (AFM), in micro- and nanoelectromechanical systems (MEMS and NEMS), and for biological chemical detection [1]. Submicron cantilevers have recently permitted spatial resolution of the AFM that is sufficient to visualize tiny details of the DNA double helix near physiological conditions [2]. Further miniaturization of cantilevers has the potential to revolutionize technology and medicine. The accuracy of detectors based upon nanocantilevers relies on the quality factor of the cantilever; see, e.g., Ref. [3]. Mechanical motion of the cantilever is related to the dynamics of the angular momentum. Coupling of the mechanical angular momentum and the angular momentum associated with the magnetic moment of a ferromagnetic body is described by the Barnett and Einstein–de Haas effects [4,5]. In a paramagnetic body that coupling is less transparent. The question is whether thermal flipping of atomic and nuclear angular momenta inside a nonmagnetic cantilever can affect its quality factor. For a relatively large cantilever, having high moment of inertia, it seems unlikely that tiny angular momenta of atoms and nuclei may have any significant effect on the cantilever. However, as we shall see, the effect scales inversely with the square of the length of the cantilever and it may become important for nanoscale cantilevers.

Coupling of cantilevers to classical magnetic moments has been studied in the past. The possibility to reverse the magnetic moment by mechanical motion [6,7]. The Einstein–de Haas effect in a magnetic cantilever has been measured [8] and explained [9] by the motion of a domain wall. Mechanical friction of the cantilever oscillating near the surface of a solid, which originates from the interaction between localized spins in the cantilever and localized surface spins, has been proposed in Ref. [10] as an explanation of the strong influence of the proximity to the surface on the cantilever damping observed in Ref. [11]. Coupling of cantilevers to the embedded quantum spins has been investigated theoretically [12–14]. Experiment has progressed to the measurement of a single molecular spin in a NEMS obtained by drafting of a single-molecule magnet on a carbon nanotube [15,16]. A theory of such an experiment that treats both the spin and the cantilever as quantum objects has been developed in Ref. [17].

In this paper we consider a nanoscale cantilever that consists of a sufficiently large number of atoms to be treated as a classical mechanical object. Paramagnetic spins of atomic or nuclear origin, or both, inside the cantilever will be treated as quantum spins flipping due to thermal effects and/or quantum tunneling. Damping of micromechanical structures by paramagnetic relaxation in the presence of strong external magnetic field has been studied experimentally and theoretically in Ref. [18]. It was argued that when the cantilever oscillates in the external magnetic field the oscillation of the crystal-field axes of Mn^{2+} ions generates the ac magnetic field that is proportional to the external field and the amplitude of the oscillations of the cantilever.

Our main result is the demonstration that paramagnetic spins cause damping of the mechanical oscillations of the cantilever even in the absence of the external field, and that this kind of damping can be universally expressed via the imaginary part of the magnetic susceptibility. One can understand this effect by noticing that oscillations of the cantilever generate the effective ac magnetic field, $\mathbf{h} = \mathbf{\Omega}/\gamma$, in the rotating coordinate frame of the cantilever, with Ω being the angular velocity and γ being the gyromagnetic ratio for the spin [19]. In the absence of the external fields, all solid-state interactions of the spins are defined in that coordinate frame. It is therefore natural to solve the problem in the moving frame of the cantilever. Switching to that frame cannot, of course, generate any new physical effects. It is merely a method that allows one to express the damping of the cantilever in terms of measurable parameters without having the explicit knowledge of microscopic interactions.

The paper is structured as follows: In Sec. II the physics of the effect is elucidated by considering a rigid oscillating beam that contains paramagnetic spins. The damping of the cantilever is expressed via the imaginary part of the magnetic susceptibility. The dynamics of a physical elastic cantilever with paramagnetic spins is studied in Sec. III. It introduces a correction factor to the damping rate and its dependence on the oscillation mode. Discussion of the results and estimates are given in Sec. IV.

II. RIGID BEAM

The kinematics of a physical cantilever shown in Fig. 2 is more complicated than that of a harmonic oscillator; see, e.g., Ref. [20]. To explain the physics of the effect we will start with a toy model in which the physical cantilever is replaced with a rigid beam that swings as a harmonic oscillator

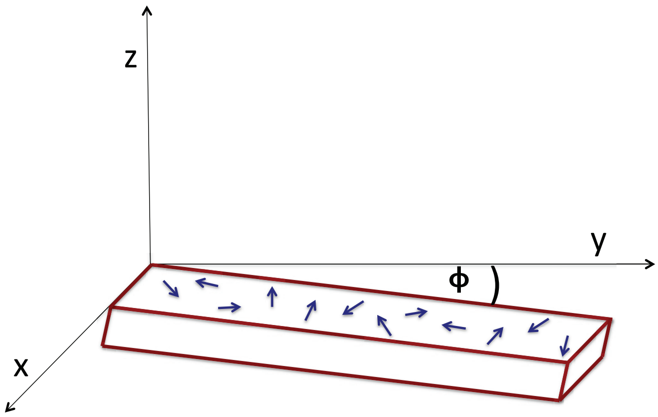

FIG. 1. (Color online) Rigid beam with paramagnetic spins.

by changing its orientation with respect to the y axis, with one end being at the origin of the coordinate frame; see Fig. 1. This crude approximation allows one to understand the physics of the effect in simple terms, as well as to obtain the estimate of the cantilever damping which serves as a test for the more involved computation with a physical cantilever. Note that the rigid beam approximation only applies to the motion of the cantilever as a whole and does not prohibit in our model the spin-phonon processes inside the beam.

The motion of the beam shown in Fig. 1 is characterized by the angle of rotation, $\phi(t)$, about the x axis. We shall approximate this motion by a harmonic oscillator with a returning torque $\tau_x = -\omega_0^2\phi$. The equation of motion of the beam is $dJ_x/dt = \tau_x$, where $J_x = L_x + S_x$ is the x component of the total angular momentum. The latter consists of the mechanical angular momentum $L_x = I\dot{\phi}$, with I being the moment of inertia, and the spin angular momentum $S_x = \sum_i S_x^i$, where the summation is over all spins in the beam. This leads to the following equation of motion:

$$I\frac{d^2\phi}{dt^2} + I\omega_0^2\phi = -\hbar\frac{dS_x}{dt}. \tag{1}$$

In most practical situations the mechanical oscillator would be a macroscopic object even for the smallest cantilevers. It makes sense, therefore, to average the above equation over thermal and quantum fluctuations of the spins,

$$I\frac{d^2\phi}{dt^2} + I\omega_0^2\phi = -\hbar\frac{d}{dt}\langle S_x\rangle. \tag{2}$$

The Hamiltonian of the spins, H_S, that reflects their interactions in a solid is always written in the coordinate frame that is rigidly coupled to the solid. It is therefore natural to solve the problem in that coordinate frame. As we shall see, the power of that method is that it provides the answer for cantilever damping in terms of the imaginary part of the susceptibility. The latter can be independently measured and, thus, does not require knowledge of the explicit form of H_S.

When the solid rotates the spin Hamiltonian becomes [19]

$$H = H_S - \hbar S_x\frac{d\phi}{dt}. \tag{3}$$

Consequently, the effect of the rotation on the spins is equivalent to the effect of the magnetic field $h = \dot{\phi}/\gamma$, where γ is the gyromagnetic ratio for the spin. Thus, using linear response theory, one can write

$$\hbar\gamma\langle S_x\rangle = \hat{\chi}\frac{\dot{\phi}}{\gamma}, \tag{4}$$

where χ is the magnetic susceptibility of the spins. Switching to Fourier transforms in Eqs. (2) and (4) one obtains

$$I\left(-\omega^2 + \omega_0^2\right)\phi_\omega = i\hbar\omega\langle S_x\rangle_\omega, \tag{5}$$

$$\langle S_x\rangle_\omega = -\frac{i\omega\chi(\omega)\phi_\omega}{\hbar\gamma^2}. \tag{6}$$

Substitution of Eq. (5) into Eq. (6) then gives

$$\omega^2 = \frac{\omega_0^2}{1 + \frac{\chi(\omega)}{\gamma^2 I}}. \tag{7}$$

Neglecting renormalization of the real part of the cantilever frequency by the spins and writing $\chi(\omega) = \chi'(\omega_0) + i\chi''(\omega_0)$, $\omega = \omega_0 - i\Gamma$, we get for the rate of damping of the mechanical oscillations

$$\Gamma = \frac{\omega_0\chi''(\omega_0)}{2\gamma^2 I}, \tag{8}$$

where χ'' is the imaginary part of the paramagnetic susceptibility.

We shall assume that temperature T is high compared to the energy scale of the spin Hamiltonian (3) and will neglect any resonant effects that may arise from the matching of the cantilever frequency and the spin energy levels (see discussion). Then the effect is dominated by the longitudinal susceptibility with [21]

$$\chi''(\omega_0) = f(\omega_0 T_1)\chi_0(T), \tag{9}$$

where $\chi_0(T)$ is the equilibrium static Curie susceptibility of N_S quantum spins of length S,

$$\chi_0(T) = \frac{N_S\hbar^2\gamma^2 S(S+1)}{3k_B T}, \tag{10}$$

and

$$f(\omega_0 T_1) = \frac{\omega_0 T_1}{1 + (\omega_0 T_1)^2} \tag{11}$$

is the factor depending on the longitudinal spin relaxation time T_1. Substituting this into Eq. (8) one obtains

$$\begin{aligned}\Gamma &= f(\omega_0 T_1)\left[\frac{N_S\hbar S(S+1)}{6I}\right]\frac{\hbar\omega_C}{k_B T}\\ &= f(\omega_0 T_1)\left[\frac{C_S\hbar S(S+1)}{2M_1 L^2}\right]\frac{\hbar\omega_C}{k_B T},\end{aligned} \tag{12}$$

where we have introduced $I = \frac{1}{3}NM_1L^2$ for the moment of inertia (with L being the length of the beam, N being the number of atoms in the beam, and M_1 being the mass of one atom) and $C_S = N_S/N$ for the number of spins per atom.

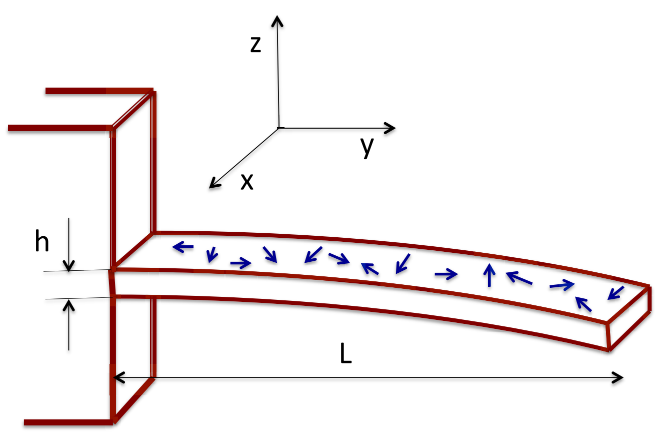

FIG. 2. (Color online) Elastic cantilever with paramagnetic spins.

III. PHYSICAL CANTILEVER

The physical elastic cantilever is shown in Fig. 2. Its motion is described by the displacement $u_z(y,t)$ from the equilibrium horizontal position. The dynamical equation for the displacement is [20]

$$\rho \frac{\partial^2 u_\alpha}{\partial t^2} = \frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta}, \tag{13}$$

where $\sigma_{\alpha\beta} = \delta H_{\rm tot}/\delta e_{\alpha\beta}$ is the stress tensor, $e_{\alpha\beta} = \partial u_\alpha/\partial x_\beta$ is the strain tensor, ρ is the mass density of the material, and $H_{\rm tot}$ is the total Hamiltonian of the system. It was shown in Ref. [9] that in the presence of the spins the stress tensor can be divided into two parts: the usual elastic part and the part coming from the local internal torques generated by the flipping of the spins. The equation that replaces Eq. (2) is [9]

$$\rho \frac{\partial^2 u_z}{\partial t^2} + \frac{h^2 E}{12(1-\sigma^2)} \frac{\partial^4 u_z}{\partial y^4} = \frac{\hbar}{2} \frac{\partial}{\partial y} \frac{\partial}{\partial t} S_x(y,t), \tag{14}$$

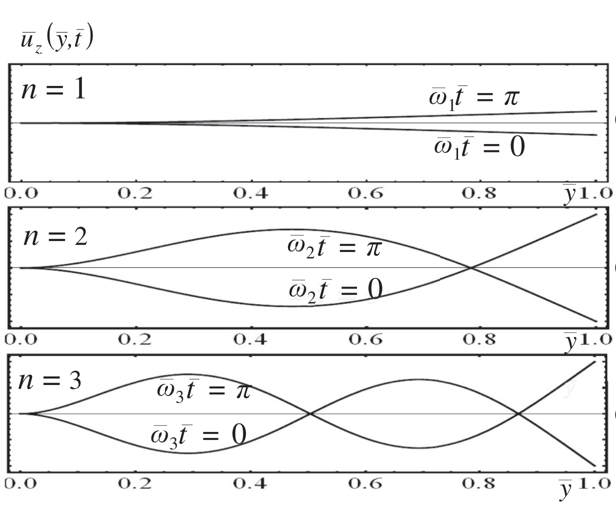

FIG. 3. Profiles of the oscillating cantilever at different moments of time for $n = 1,2,3$.

where ρ is the mass density of the cantilever, h is its thickness, E and σ are the Young's modulus and the Poisson elastic coefficient $(-1 < \sigma < 1/2)$, respectively, and S_x is the x component of the spin density.

Let us write as before $\langle S_x \rangle = \hat{\chi}\dot{\phi}/(\hbar\gamma^2)$, where $\hat{\chi}$ is now the susceptibility of the unit volume. Using the fact that $\phi = \partial u_z/\partial y$, one has

$$\langle S_x \rangle = \frac{1}{\hbar\gamma^2} \frac{\partial}{\partial t} \hat{\chi} \frac{\partial u_z}{\partial y}, \tag{15}$$

$$\rho \frac{\partial^2 u_z}{\partial t^2} + \frac{h^2 E}{12(1-\sigma^2)} \frac{\partial^4 u_z}{\partial y^4} = \frac{1}{2\gamma^2} \frac{\partial^2}{\partial t^2} \hat{\chi} \frac{\partial^2 u_z}{\partial y^2}. \tag{16}$$

It is convenient to switch to dimensionless variables,

$$\bar{u}_z = \frac{u_z}{L}, \quad \bar{y} = \frac{y}{L}, \quad \bar{t} = t\nu, \quad \nu \equiv \sqrt{\frac{Eh^2}{12\rho(1-\sigma^2)L^4}}, \tag{17}$$

where ν determines the scale of the eigenfrequencies of the cantilever. In terms of these variables Eq. (16) becomes

$$\frac{\partial^2 \bar{u}_z}{\partial \bar{t}^2} + \frac{\partial^4 \bar{u}_z}{\partial \bar{y}^4} = \frac{1}{2\gamma^2 \rho L^2} \frac{\partial^2}{\partial \bar{t}^2} \hat{\chi} \frac{\partial^2 \bar{u}_z}{\partial \bar{y}^2}. \tag{18}$$

This equation has to be solved with the boundary conditions $\bar{u}_z = 0$, $\partial \bar{u}_z/\partial \bar{y} = 0$ at $\bar{y} = 0$ and $\partial^2 \bar{u}_z/\partial \bar{y}^2 = 0$, $\partial^3 \bar{u}_z/\partial \bar{y}^3 = 0$ at $\bar{y} = 1$. The first two conditions correspond to the absence of the displacement and the absence of the bending of the cantilever at the fixed end, while the last two conditions correspond to the absence of the torque and the force, respectively, at the free end.

For the free oscillations of the cantilever in the absence of the spins one writes

$$\bar{u}_z(\bar{y},\bar{t}) = \bar{u}(\bar{y}) \cos(\bar{\omega}\bar{t}). \tag{19}$$

Substitution into Eq. (18) with $\hat{\chi} = 0$ then gives

$$\frac{\partial^4 \bar{u}}{\partial \bar{y}^4} - \kappa^4 \bar{u} = 0, \quad \kappa^2 \equiv \bar{\omega}. \tag{20}$$

Solution of this equation with the boundary conditions gives [20]

$$\bar{u}(\bar{y}) = (\cos\kappa + \cosh\kappa)\,[\cos(\kappa\bar{y}) - \cosh(\kappa\bar{y})] + (\sin\kappa - \sinh\kappa)\,[\sin(\kappa\bar{y}) - \sinh(\kappa\bar{y})]\,, \tag{21}$$

with

$$\cos\kappa \cosh\kappa + 1 = 0 \tag{22}$$

for the frequencies of the normal modes of the cantilever, $\bar{\omega}_n = \kappa_n^2$ [measured in the units of ν of Eq. (17)]. The fundamental (minimal) frequency is $\bar{\omega}_1 \approx 3.516$. The next two frequencies are $\bar{\omega}_2 \approx 22.03$ and $\bar{\omega}_3 \approx 61.70$. The profiles of the oscillations of the cantilever for the first three normal modes $(n = 1,2,3)$ are shown in Fig. 3.

Accounting for the term on the right-hand side of Eqs. (18) and (20) becomes

$$\frac{\partial^4 \bar{u}}{\partial \bar{y}^4} - \kappa'^4 \bar{u} = -\frac{\kappa'^4}{2\gamma^2 \rho L^2} \chi_\omega \frac{\partial^2 \bar{u}}{\partial \bar{y}^2}. \tag{23}$$

Since the right-hand side of this equation is small, to obtain the frequency $\bar{\omega}'^2 = \kappa'^4$ renormalized by the presence of the spins, one can safely substitute here the eigenmode of Eq. (21), for which $\partial^2\bar{u}/\partial\bar{y}^2 = -\kappa^2\bar{u}$, $\partial^4\bar{u}/\partial\bar{y}^4 = \kappa^4\bar{u}$. This gives

$$\omega'^2_n = \frac{\omega_n^2}{1 + \frac{\kappa_n^2\chi(\omega_n)}{2\gamma^2\rho L^2}}. \tag{24}$$

The imaginary part of the frequency is

$$\Gamma_n = \frac{\omega_n\kappa_n^2}{2\gamma_n^2\rho L^2}\chi''(\omega_n), \tag{25}$$

with

$$\chi''(\omega_n) = f(\omega_n T_1)\left[\frac{n_S\hbar^2\gamma^2 S(S+1)}{3k_B T}\right], \tag{26}$$

where $n_s = N_S/V = C_S(\rho/M_1)$ is the number of spin per unit volume. Consequently

$$\Gamma_n = f(\omega_n T_1)\left[\frac{C_S\kappa_n^2\hbar S(S+1)}{6M_1L^2}\right]\frac{\hbar\omega_n}{k_B T}. \tag{27}$$

For the first eigenmode, $\kappa_1^2 \approx 3.516$, the damping rate of the physical cantilever, given by Eq. (27), is greater than the damping rate of the rigid harmonic beam, given by Eq. (12), by a factor $3.516/3 = 1.172$. Notice, however, that the corresponding factor becomes significantly greater for higher modes, $\kappa_2^2/3 \approx 7.343$, $\kappa_3^2/3 \approx 20.57$, and so on. This is because $d\phi/dt$ and the corresponding effective magnetic field acting on the spins in the rotating frame, $\dot{\phi}/\gamma$, is greater for higher modes; see Fig. 3.

IV. DISCUSSION

We have computed the contribution of paramagnetic spins to the damping of the mechanical oscillations of the cantilever. The universal formula (25) has been obtained that expresses the damping via the imaginary part of the magnetic susceptibility that can be measured independently either in the cantilever or in the material it is made of. Thus, in principle, the damping due to spins can be obtained without the explicit knowledge of the concentration of spins or microscopic mechanisms of spin-lattice interactions.

The effect can be estimated with help of Eq. (27) that provides the damping rate of the nth mode in terms of the concentration C_S of spins of length S, flipping with the time constant T_1. Since Γ_n depends on parameters that are usually known in experiment, it can be easily assessed for a given cantilever. When different kinds of spins are present, they contribute to the damping additively in accordance with Eqs. (25) and (27). Note that $f(\omega_n T_1)$ has a maximum at $\omega_n T_1 = 1$. Thus, at comparable concentrations, the spins that flip at a rate comparable to ω_n provide the maximal damping. For ω_n in the kHz range these would normally be the nuclear spins, while for ω_n in the GHz range these would be the atomic spins. Here we have ignored resonant effects that may, in principle, exist in the coupling between cantilever and spin modes. The general formula (25) is correct, however, and accounts for resonant effects as well. Such effects have been studied in the context of, e.g., spin tunneling and decoherence in Ref. [14]. They require external fields to manipulate spin energy levels because cantilever modes are fixed.

As we have seen, up to a numerical factor the damping can be computed by replacing the physical cantilever with a rotating rigid beam. The study of a physical cantilever improves the result by introducing differential rotations along the length of the cantilever. This provides a clear picture of the mechanism of the damping studied in this paper. Oscillations of the cantilever generate an effective ac magnetic field in the coordinate frame of the rotating solid. This well-known phenomenon in the statistical mechanics of rotating bodies can also be viewed as a noninertial effect of rotating local crystal fields [19,22]. It couples the dynamics of the cantilever with the dynamics of the spins in the absence of any external fields. Thermal and/or quantum effects inside the cantilever make the spins flip. Spin flips transfer angular momentum to the cantilever, causing damping. At the end these are the internal interactions in a solid that are responsible for the damping; that is, responsible for the conversion of the mechanical kinetic energy of the cantilever into its thermal energy. The transition to the rotating frame is merely a useful mathematical method that allows one to express cantilever damping due to spins via the imaginary part of susceptibility, without invoking microscopic interactions.

The quality factor of the cantilever is $Q_n = \omega_n/\Gamma_n$. In practical situations one would want to know if the quality factor observed in experiment had anything to do with the spins. To answer this questions we notice that the maximal value of f is 1/2. Consequently, the spins cannot make the quality factor lower than

$$Q_{\min}^{(n)} = \frac{12M_1L^2k_BT}{\hbar^2k_n^2C_SS(S+1)}. \tag{28}$$

Resonant interaction of the oscillations of the cantilever with the spin energy levels would lower the quality factor significantly. However, as has been mentioned above, this would be an extraordinary situation because in the absence of the external fields neither spin levels nor cantilever modes can be easily manipulated. Notice the proportionality of $Q_{\min}^{(n)}$ to temperature. In the kelvin range one obtains from Eq. (28) $Q_{\min}^{(1)} \sim 10^5$ for the cantilever of length $L \sim 0.1$ μm and $Q_{\min}^{(1)} \sim 10^3$ at $L \sim 10$ nm and concentration of paramagnetic spins comparable to the number of atoms. The values of $Q_{\min}^{(n)}$ become progressively smaller at higher n and lower temperature. This suggests that paramagnetic spins should be suspect when the quality factor of a small cantilever becomes small upon decreasing the temperature. This mechanism of damping can also apply to the oscillations of nanowires and macromolecules. Recently, molecular-based cantilevers of length under 5 nm have been reported [23]. The effect described in this paper must be especially important in such small cantilevers.

ACKNOWLEDGMENT

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[1] K. Eom, H. S. Park, D. S. Yoon, and T. Kwon, Phys. Rep. **503**, 115 (2011).

[2] C. Leung, A. Bestembayeva, R. Thorogate, J. Stinson, A. Pyne, C. Marcovich, J. Yang, U. Drechsler, M. Despont, T. Jankowski, M. Tschöpe, and B. W. Hoogenboom, Nano Lett. **12**, 3846 (2012).

[3] J. P. Davis, D. Vick, D. C. Fortin, J. A. J. Burgess, W. K. Hiebert, and M. R. Freeman, Appl. Phys. Lett. **96**, 072513 (2010).

[4] S. J. Barnett, Phys. Rev. **6**, 239 (1915).

[5] A. Einstein and W. J. de Haas, Verh. Dtsch. Phys. Ges. **17**, 152 (1915); **18**, 173 (1916); **18**, 423 (1916).

[6] A. A. Kovalev, G. E. W. Bauer, and A. Brataas, Phys. Rev. Lett. **94**, 167201 (2005).

[7] A. A. Kovalev, G. E. W. Bauer, and A. Brataas, Phys. Rev. B **75**, 014430 (2007).

[8] T. M. Wallis, J. Moreland, and P. Kabos, Appl. Phys. Lett. **89**, 122502 (2006).

[9] R. Jaafar, E. M. Chudnovsky, and D. A. Garanin, Phys. Rev. B **79**, 104410 (2009).

[10] J.-H. She and A. V. Balatsky, Phys. Rev. Lett. **108**, 136101 (2012).

[11] K. Saitoh, K. Hayashi, Y. Shibayama, and K. Shirahama, Phys. Rev. Lett. **105**, 236103 (2010).

[12] R. Jaafar and E. M. Chudnovsky, Phys. Rev. Lett. **102**, 227202 (2009).

[13] A. A. Kovalev, L. X. Hayden, G. E. W. Bauer, and Y. Tserkovnyak, Phys. Rev. Lett. **106**, 147203 (2011).

[14] D. A. Garanin and E. M. Chudnovsky, Phys. Rev. X **1**, 011005 (2011).

[15] M. Ganzhorn, S. Klyatskaya, M. Ruben, and W. Wernsdorfer, Nat. Nanotechnol. **8**, 165 (2013).

[16] M. Ganzhorn, S. Klyatskaya, M. Ruben, and W. Wernsdorfer, ACS Nano **7**, 6225 (2013).

[17] M. F. O'Keeffe, E. M. Chudnovsky, and D. A. Garanin, Phys. Rev. B **87**, 174418 (2013).

[18] J. G. E. Harris, R. Knobel, K. D. Maranowski, A. G. Gossard, N. Samarth, and D. D. Awschalom, Appl. Phys. Lett. **82**, 3532 (2003).

[19] E. M. Chudnovsky, D. A. Garanin, and R. Schilling, Phys. Rev. B **72**, 094426 (2005).

[20] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon, New York, 1959).

[21] E. M. Chudnovsky and J. Tejada, *Macroscopic Quantum Tunneling of the Magnetic Moment* (Cambridge University Press, Cambridge, 1998).

[22] F. W. Hehl and W.-T. Ni, Phys. Rev. D **42**, 2045 (1990).

[23] S. Müllegger, M. Rashidi, K. Mayr, M. Fattinger, A. Ney, and R. Koch, Phys. Rev. Lett. **112**, 117201 (2014).