Macroscopic quantum coherence of chirality of a domain wall in ferromagnets

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The possibility of macroscopic quantum-mechanical coherent oscillation between two chirality states of a domain wall separated by the energy barrier due to a transverse anisotropy is quantitatively discussed. The frequency of the oscillation is calculated for the case of weak transverse anisotropy. The chirality variable is shown to be canonically conjugate to the position of the domain wall. The stronger the pinning of the domain wall is, the more strongly the chirality fluctuates and the larger the frequency becomes. [S0163-1829(96)00637-6]

I. INTRODUCTION

A domain wall in a ferromagnet contains a (semi-)macroscopic number of spins, the width of the wall being $10 \sim 1000$ Å, depending on the material. Being macroscopic, the wall has usually been treated as a classical object. For instance, the depinning of a wall from a pinning center at high temperatures is described as a classical process of the wall overcoming the pinning energy by the thermal fluctuation. However, even for a macroscopic wall there should be a finite probability of depinning due to the quantum fluctuation. In fact this quantum depinning was theoretically studied four years ago and was shown to be probable at sufficiently low temperatures.^{1,2} Experimental studies such as measurements of magnetic relaxation³ and magnetoresistance⁴ suggest that this phenomenon indeed occurs at temperatures typically below a few Kelvin. The quantum depinning has the significance of being a tunneling of a macroscopic object.^{5,6} Possibility of a coherent tunneling through a periodic pinning potential has also been discussed recently.

In addition to the translational motion, a domain wall can have internal degrees of freedom because it has a spatial structure. In the presence of a transverse anisotropy, two types of stable walls are possible; right-handed and lefthanded walls in which the spins rotate in the opposite senses. These configurations are separated by the energy barrier due to the transverse anisotropy. This *chirality* is not a true internal degree of freedom such as the spin of a particle, since as we shall see it is conjugate to the position of the wall. Nonetheless, if a strong pinning is present, the chirality behaves as if it were a true internal degree of freedom of a particle (i.e., the wall) fixed at the pinning center. In this case macroscopic quantum coherence (MQC) between the two chiralities will occur, which is the subject of this paper. It turns out that a strong pinning and weak transverse anisotropy lead to strong fluctuation of chirality; observation of the MQC will be easier in such cases. In particular experiments with magnetic junctions where a thin layer of magnetic material with strong anisotropy (such as SmCo₅) is inserted between magnets with moderate anisotropy (such as Ni) would be interesting. In the opposite case of weak pinning and strong transverse anisotropy, the position of the wall may tunnel through a barrier owing to its large fluctuation; this is the quantum depinning.

II. FORMULATION

We consider a ferromagnet consisting of a spin S of magnitude S at each site of a quasi-one-dimensional crystal, say cubic, of lattice constant a. The magnet is assumed to have an easy axis and a hard axis in the z and the x direction, respectively, and to be described by the Hamiltonian

$$\hat{H} = -\sum_{\langle i,j \rangle} \tilde{J}\hat{S}_{i} \cdot \hat{S}_{j} - \frac{1}{2} \sum_{i} (K\hat{S}_{z,i}^{2} - K_{\perp}\hat{S}_{x,i}^{2}) + V_{\text{pin}}(\{\hat{S}_{z,i}\}),$$
(1)

where the index *i* runs over the lattice sites, $\langle i,j \rangle$ runs over nearest-neighbor pairs, and \tilde{J} is the exchange coupling constant, and *K* and K_{\perp} are longitudinal and transverse anisotropy constants, respectively, which incorporate the effect of the demagnetizing field⁸ (see the caption of Fig. 1); \tilde{J}, K , and K_{\perp} are all positive. The last term V_{pin} denotes an additional localized anisotropy energy to be specified later. We shall work with the functional-integral formalism^{9,10} by use of the spin coherent state.¹¹ The latter is denoted by

$$|\boldsymbol{n}\rangle = (1+|\boldsymbol{\zeta}|^2)^{-1/2} \exp(\boldsymbol{\zeta}\hat{\boldsymbol{S}}_{-})|\boldsymbol{S}\rangle, \qquad (2)$$

where **n** is a unit vector $(n_x = \sin\theta \cos\phi, n_y = \sin\theta \sin\phi, n_z = \cos\theta), \zeta \equiv e^{i\phi} \tan(\theta/2)$, and $|S\rangle$ is the eigenstate of \hat{S}_z with eigenvalue S. These states form an overcomplete set and possess, among others, the following properties:

$$\langle \boldsymbol{n}|\hat{\boldsymbol{S}}|\boldsymbol{n}\rangle = S\boldsymbol{n}$$
, (3)

$$\frac{\langle \boldsymbol{n}' | (\hat{\boldsymbol{S}} \cdot \boldsymbol{e})^2 | \boldsymbol{n} \rangle}{\langle \boldsymbol{n}' | \boldsymbol{n} \rangle} = \left(1 - \frac{1}{2S} \right) \left(\frac{\langle \boldsymbol{n}' | \hat{\boldsymbol{S}} \cdot \boldsymbol{e} | \boldsymbol{n} \rangle}{\langle \boldsymbol{n}' | \boldsymbol{n} \rangle} \right)^2 + \frac{S}{2}, \quad (4)$$

where e is an arbitray unit vector. The last equation can be derived, for instance, from Eq. (6.15) of Ref. 11, or can be

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FIG. 1. Domain walls with three chiralities; (a) right-handed wall $(\phi_0 = \pi/2)$, (b) left-handed wall $(\phi_0 = -\pi/2)$, and (c) wall with no chirality $(\phi_0 = 0)$. Circles in (a) and (b) drawn to guide the eye lie in the yz plane, while the spins lie in the zx plane in (c). The quasi-one-dimensional direction of the crystal is here aligned with the spin hard axis for ease of visualization. A different alignment, which may be the case for a real magnet, does not affect the content of the text; for instance, one would rotate all the spins by $\pi/2$ around the y axis if the dominant anisotropy originates from the demagnetizing field.

read off the Appendix of Ref. 10. We shall be interested only in those spin configurations whose scale of spatial variation is much larger than a. Accordingly we arrive at the continuum Lagrangian

$$L = \int \frac{d^3x}{a^3} \left[\hbar S \dot{\phi} (\cos \theta - 1) - \left\{ \frac{JS^2}{2} (\nabla \mathbf{n})^2 + \frac{1}{2} KS \left(S - \frac{1}{2} \right) \right. \\ \left. \times \sin^2 \theta + \frac{1}{2} K_\perp S \left(S - \frac{1}{2} \right) \sin^2 \theta \, \cos^2 \phi \right\} \right] - V_{\text{pin}}[\theta], \quad (5)$$

which is to be used in the functional integral. Here $J \equiv \tilde{J}a^2$, $(\nabla n)^2$ is to be read as $(\nabla \theta)^2 + \sin^2 \theta (\nabla \phi)^2$, and $V_{\text{pin}}[\theta]$ is a functional of θ which comes from the last term of \hat{H} . The factor of $(S - \frac{1}{2})$ in the anisotropy-energy terms ensures the vanishing of the anisotropy energy for the case of $S = \frac{1}{2}$; in that case $\hat{S}_x^2 = \hat{S}_y^2 = \hat{S}_z^2 = \frac{1}{4}$ in the operator formalism. A quasi-one-dimensional magnet being in consideration, we shall neglect the spatial variation over the cross section, which is taken to lie in the yz plane.

We consider only the case of weak transverse anisotropy, $\alpha \equiv K_{\perp}/K \ll 1$, and study the dynamics to the lowest order in α . To $O(\alpha^0)$ and in the absence of V_{pin} , our model has a static domain wall of width $\lambda \equiv \{JS/K(S-\frac{1}{2})\}^{1/2}$ as a classical solution. (Since we are considering a quasi-onedimensional magnet, it is a planar wall lying in the *yz* plane.) The solution centered at x=Q is given by $\theta = \theta_0(x-Q)$, $\phi = \phi_0$, where

$$\cos\theta_0(x) = \tanh \frac{x}{\lambda}, \quad \sin\theta_0(x) = \frac{1}{\cosh \frac{x}{\lambda}},$$
 (6)

and ϕ_0 is an arbitrary constant. ϕ_0 is a quantitative measure of the chirality of the domain wall with respect to the *x* axis; the wall is maximally right handed if $\phi_0 = \pi/2$ and maximally left handed if $\phi_0 = -\pi/2$, while it has no chirality if $\phi_0 = 0$ (Fig. 1). Fluctuation around θ_0 can be expanded in terms of the eigenmodes $\{\eta_n(x)\}$ obeying the Schrödinger-type eigenvalue equation

$$\left[-\lambda^2 \nabla^2 + \cos 2\theta_0(x)\right] \eta_n(x) = \omega_n^2 \eta_n(x), \tag{7}$$

with $\{\omega_n^2 | n = 0, 1, 2, ...\}$ being eigenvalues. The lowest mode $\eta_0(x)$ is a zero mode $(\omega_0 = 0)$ corresponding to the uniform translation of the wall, and is given by $\nabla \theta_0(x)$. Thus the field θ can be expressed in the form

$$\theta(x,t) = \theta_0[x - Q(t)] + \Sigma' c_n(t) \eta_n[x - Q(t)], \qquad (8)$$

where Σ' denotes summation over positive modes $(n \ge 1)$. The wall center Q as well as the real coefficients $\{c_n | n = 1, 2, ...\}$ are now regarded as dynamical variables.¹²

Similarly we decompose ϕ into a certain weighted spatial average ϕ_0 and fluctuation around it as

$$\phi(x,t) = \phi_0(t) + \varphi[x - Q(t),t], \qquad (9)$$

and regard ϕ_0 and φ as dynamical variables. The variable ϕ_0 is the collective coordinate representing the chirality of the domain wall. By the weighted spatial average, we mean that

$$\phi_0(t) \equiv \int \frac{dx}{a} \phi(x,t) \sin^2 \theta_0[x - Q(t)], \qquad (10)$$

or equivalently

$$\int \frac{dx}{a}\varphi(x,t)\sin^2\theta_0(x) = 0.$$
(11)

Use of an average weighted over the wall rather than a uniform average is reasonable, since the behavior of ϕ far away from the wall, where $\theta \sim 0$ or π , should be irrelevant. The virtue of the particular weight adopted above shall be explained shortly.

Putting Eqs. (8) and (9) in the Lagrangian and keeping terms up to the second order in fluctuations and the first order in α and V_{pin} , we obtain $L = L_0 + L_1$ with

$$L_0 = -\frac{\hbar SN}{\lambda} Q \dot{\phi}_0 - \frac{1}{2} KS \left(S - \frac{1}{2} \right) N \alpha \cos^2 \phi_0 - V_{\text{pin}}(Q),$$
(12)

$$L_{1} = -\frac{1}{4} KS \left(S - \frac{1}{2} \right) N\Sigma' \omega_{n}^{2} c_{n}^{2}$$

$$- \int \frac{d^{3}x}{a^{3}} \left[\hbar S \dot{\varphi}(x) \sin \theta_{0}(x) \Sigma' c_{n} \eta_{n}(x) + \frac{1}{2} JS^{2} [\nabla \varphi(x)]^{2} \sin^{2} \theta_{0}(x) + \hbar S \left\{ \frac{1}{2} \dot{\phi}_{0} [\Sigma' c_{n} \eta_{n}(x)]^{2} \cos \theta_{0}(x) - \dot{Q} \Sigma' c_{n} \eta_{n}(x) \times [\nabla \varphi(x)] \sin \theta_{0}(x) \right\} \right], \qquad (13)$$

where $V_{\text{pin}}(Q) \equiv V_{\text{pin}}[\theta_0(x-Q)]$, which acts as a pinning potential for the center of the domain wall, and

 $N \equiv \int (d^3x/a^3) \sin^2 \theta_0(x) = 2A\lambda/a^3$ (A being the cross sectional area of the wall) is the number of spins in the wall. Terms of the first order in φ and $\{c_n\}$ are absent by virtue of Eq. (11).

In so far as we are interested in low-frequency motions of ϕ_0 and Q, the last two terms of L_1 may be neglected. Thus L_0 and L_1 are mutually decoupled. Therefore the dynamics of Q and ϕ_0 can be discussed with L_0 alone.

The first term of Eq. (12) indicates that ϕ_0 and Q are canonically conjugate to each other. If the pinning is weak and the transverse anisotropy is strong, ϕ_0 may be integrated out by use of the Gaussian approximation to yield an effective Lagrangian for Q.^{1,2,5,7} By contrast in this article we focus attention on the opposite case of a strong pinning and a weak anisotropy. The inertial mass to be associated with the chirality variable ϕ_0 is then determined by the pinning potential for Q. Let us approximate the pinning potential as harmonic; $V_{\text{pin}}(Q) = (M_w/2) v^2 Q^2$, where ν is a positive constant of dimension of frequency and $M_w (\equiv \hbar^2 N/\alpha J)$ is the domain wall mass.^{2,5} Then the integration over Q results in

$$L = \frac{1}{2} M_{\phi} \dot{\phi}_0^2 - \frac{1}{2} M_{\phi} \nu^2 \cos^2 \phi_0, \qquad (14)$$

where $M_{\phi} \equiv NS(S-\frac{1}{2})K\alpha/\nu^2$. Due to the transverse anisotropy, there are two stable values of ϕ_0 , namely $\phi_0 = \pm \pi/2$, corresponding to the maximally right- and left-handed chirality, respectively. The instanton $\phi_0(\tau)$ that connects these two chilarities in the imaginary time τ is given by

$$\cos\phi_0(\tau) = \pm \frac{1}{\cosh\nu\tau}, \quad \sin\phi_0(\tau) = \tanh\nu\tau, \quad (15)$$

where $[\phi_0(-\infty), \phi_0(\infty)]$ is equal to $(-\pi/2, \pi/2)$ in the upper-sign instanton and to $(-\pi/2, -3\pi/2)$ in the lower-sign one. The frequency Δ of the quantum coherent oscillation between the two chiralities is calculated within the semi-classical approximation¹³ as

$$\Delta = \frac{8}{\pi} \left(\frac{\pi M_{\phi} \nu}{\hbar} \right)^{1/2} \nu \exp\left(-\frac{2}{\hbar} M_{\phi} \nu \right)$$
$$= \frac{8}{\pi} \left[\pi N S \left(S - \frac{1}{2} \right) \frac{K}{\hbar \nu} \alpha \right]^{1/2}$$
$$\times \nu \exp\left[-2N S \left(S - \frac{1}{2} \right) \frac{K}{\hbar \nu} \alpha \right]. \tag{16}$$

Thus a large ν is favorable to the quantum coherence, which is a consequence of the fact that the strong pinning of Qimplies a strong fluctuation of the conjugate variable ϕ_0 ; this behavior is similar to the case of depinning of the wall, where a large α (strong pinning of ϕ) leads to a strong fluctuation of the postion of the wall $Q^{1,2,14}$ Since the thermal hopping rate at temperature T is given by $\Delta_{\rm th} \sim \nu \exp(-\frac{1}{2}M_{\phi}\nu^2/k_BT)$ (k_B is the Boltzmann constant), the quantum coherence will be seen for $T \leq T_*$, where $T_*(\equiv \hbar \nu/4k_B)$ is the crossover temperature.

III. DISCUSSION

The result (16) is interesting from an experimental point of view; one can make the MQC of chirality easier to observe by choosing a strong pinning center. Strong pinning will be realized by putting a thin layer of impurities with a strong longitudinal anisotropy as seen as follows. Such a layer produces $V_{pin}(Q) = \int (d^3x/a^3) \frac{1}{2} [K'(x)S(S - \frac{1}{2})\cos^2\theta_0(x-Q)]$, where K'(x) is a positive function whose support is localized in the range much smaller than λ . If K'(x) is peaked at x=0 with the range $N_pa(\ll \lambda)$, we have $V_{pin}(Q) = [N_pNK'S(S-\frac{1}{2})a/4\lambda](Q/\lambda)^2$, where K' is the anisotropy energy of the impurity per site. The frequency ν in this case is given by

$$\nu = \frac{\sqrt{S(S-1/2)}}{\hbar} \sqrt{N_p K K' \alpha \frac{a}{2\lambda}}.$$
 (17)

The exponent is then of Δ given by $2N\sqrt{S(S-\frac{1}{2})}\sqrt{(K/N_{p}K')\alpha(2\lambda/a)}$. Therefore if, for instance, we put a layer of SmCo₅ ($K' \sim 10$ K) with thickness of $N_p \sim 100$ in Ni wire [$K \sim 0.1$ K, $\lambda \sim 500$ Å (Refs. 4 and 5) and a = 2.5 Å] and if $\alpha \sim 10^{-5}$, we have $\nu/2\pi \sim 23$ MHz and $2S(S - \frac{1}{2})K\alpha/\hbar\nu \sim 8.9 \times 10^{-4}$ (we have chosen S = 1). Hence for a mesoscopic wall of $N \sim 10^4$, we expect that $\Delta/2\pi$ ~0.093 MHz and T_{*} ~0.3 mK. In an actual experiment, it is preferable to apply an external magnetic field in the x direction, which will enhance Δ and increase T_* .¹⁵ This circumstance is the same as in the case of magnetization reversal.16

So far we have not considered the effect of geometrical phase which comes from the first term in Eq. (5). The phase associated with the instantons (15) turns out to be $\pm \pi S$ modulo $2\pi S$ if the wall center Q coincides with a lattice point of the crystal, while it vanishes modulo $2\pi S$ if Q is at a middle of two neighboring lattice points. In the former case the MQC frequency (16) has to be multiplied by $|\cos \pi S|$. Note that this is not a consequence of the Kramers theorem; the chiral doublet under consideration is not a time-reversal doublet.

In general MQC of magnetization may be affected by environment. However, the couplings of the magnetization to phonons are known to be so weak that their effect is negligibly small.¹⁷ Couplings to magnons are also expected to be small if $T < T_{gap}$,^{1,5,15} where $k_B T_{gap}$ is the anisotropy gap of the magnon spectrum; $T_{gap} = c/\lambda k_B$ (~0.2 mK) with $c \equiv (S - \frac{1}{2}) \alpha^{1/2} \lambda K/\hbar$ being the magnon velocity. In metallic magnets the electron environment gives rise to strong dissipation in the case of a thin domain wall with width of about a few times the lattice constant or less, but for a thicker wall the effect is negligible.¹⁴ On the other hand, nuclear spins have been claimed to suppress MQC significantly.^{18,19} Hence, to observe the MQC of chirality, isotopically purified samples with few nuclear spins (such as ⁵⁸Ni and ⁶⁰Ni) might be better.

In conclusion, we have pointed out a possibility of macroscopic quantum coherence (MQC) of the chirality of a domain wall in ferromagnets. The chirality variable is ϕ_0 , the azimuthal angle of the spin averaged over the wall, and the energy barrier for ϕ_0 is due to the transverse anisotropy. The effective inertial mass of ϕ_0 arises from the fluctuation of the position of the wall in the pinning potential. Hence, as the pinning of the wall becomes stronger the fluctuation of ϕ_0 becomes larger, and the tunneling rate increases. Thus this MQC will be easier to observe in a system with a weak transverse anisotropy and a strong pinning center.

Note added. We have become informed of Refs. 7 and 15, the latter of which also briefly discusses tunneling between opposite chiralities. Since this latter work does not give a derivation of the effective Lagrangian nor stipulates the definition of the chirality variable, we cannot make a detailed

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comment on it except that the effective mass for the chirality variable mentioned there appears to be different from ours.

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