Chirality tunneling in mesoscopic antiferromagnetic domain walls

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We consider a domain wall in the mesoscopic quasi-one-dimensional sample (wire or stripe) of weakly anisotropic two-sublattice antiferromagnet, and estimate the probability of tunneling between two domain wall states with different chirality, in the limits of weak and strong rhombicity. Topological effects forbid tunneling for the systems with half-integer spin S of magnetic atoms which consist of an odd number of chains $n_\perp$. External magnetic field yields an additional contribution to the Berry phase, resulting in oscillating field dependence of the tunneling rate with the period proportional to $\sqrt{JK}/n_\perp$, where J and K are exchange and anisotropy constants, respectively, and in the appearance of *two* different tunnel splittings in any setup involving a mixture of odd and even $n_\perp$. [S0163-1829(98)06242-0]

I. INTRODUCTION

In recent years, there has been much interest in the problem of quantum spin coherence in mesoscopic magnetic systems, mainly in nanoparticles[1] and high-spin molecular clusters.[2] Another possible way, proposed in Refs. 3 and 4, is to use *topologically nontrivial* magnetic structures: domain walls in quasi-one-dimensional (1D) systems (wires, stripes), vortices in 2D systems, etc. Such objects have mesoscopic scale, e.g., in materials with magnetic ions in s states the domain wall thickness is usually about 100 lattice constants, and since their shape is determined by the material constants they are to a high extent identical.

Classically, magnetic domain wall (DW) has certain ''chirality,'' an internal degree of freedom characterizing the way of rotation of magnetization inside a DW. Two states with opposite chirality are equivalent in energy (we will not consider magnets without inversion center where this is not true). In the quantum case there is generally a nonzero transition amplitude mixing the two states and lifting the degeneracy;[3–5] under favorable circumstances this tunnel splitting can be detected with a resonant technique of some kind. In antiferromagnets (AF) tunneling is more favorable than in ferromagnets, both in the case of fine particles[6] and domain walls.[4]

In this paper we show that in the simplest model of mesoscopic AF with half-integer spin S of magnetic ions topological effects forbid chirality tunneling for a DW with an odd number $n_\perp$ of spins in its cross section. We further show that in the presence of even weak external magnetic field this strict ''selection rule'' is relaxed, which leads to the appearance of two different values of tunnel splitting in any half-integer S sample with weakly fluctuating $n_\perp$. For any S, the tunneling amplitude is shown to be an oscillating function of the field with the period $\delta H \propto \sqrt{JK}/n_\perp$, where J and K are, respectively, the exchange and anisotropy constants.

II. MODEL

Consider a thin quasi-one-dimensional stripe of two-sublattice weakly anisotropic antiferromagnet, which we for the sake of simplicity treat as a system of $n_\perp$ AF chains of spin-S magnetic atoms, coupled with the same exchange constant $J>0$ for any neighboring spins. We assume that magnetic atoms form a perfect crystal structure on a bipartite lattice, as shown in Fig. 1; note that $n_\perp$ can be odd or even without introducing any frustration. We assume a rhombic anisotropy of the form

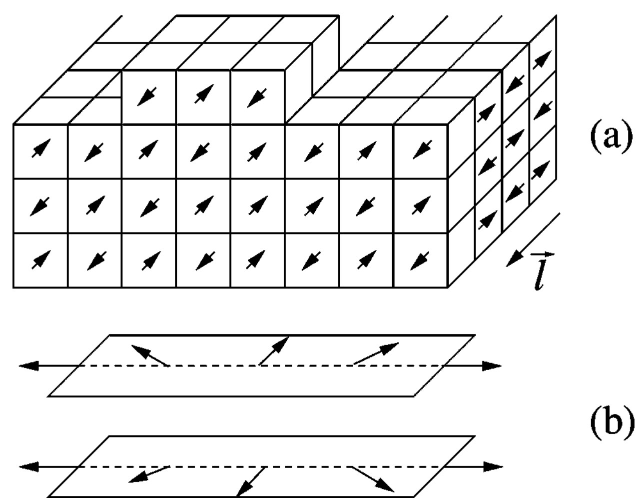

FIG. 1. (a) a schematic picture of the cross section of antiferromagnetic mesoscopic stripe; (b) two domain walls with opposite chiralities.

$$w_a = \sum_i [K_1 (S_i^Z)^2 + K_2 (S_i^Y)^2], \tag{1}$$

where i labels lattice sites and $K_{1,2} \ll J$ are the anisotropy constants, $K_1 > K_2 > 0$, so that Z is the hard axis and X is the easy axis in the easy plane XY.

Due to the quasi-1D structure, one can assume that the sublattice magnetization depends only on the space coordinate x along the wire (note that X and x axes do not need to coincide). Using the standard technique,[7] one can obtain the effective Euclidean action of AF in continuum approximation, which has the form of a well-known $O(3)$ nonlinear σ model

$$\mathcal{A}_E = \frac{1}{4} n_\perp \hbar S W + i 2\pi n_\perp S \hbar (Q + Q'_H), \tag{2}$$

$$W[\boldsymbol{l}] = \int d^2x \left\{ (\partial_\alpha \boldsymbol{l})(\partial_\alpha \boldsymbol{l}) + \frac{1}{\Delta^2}[(1+\rho) l_Z^2 + l_Y^2] + \tilde{w}_a \right\},$$

$$Q = \frac{1}{4\pi} \int d^2x \, \boldsymbol{l} \cdot (\partial_1 \boldsymbol{l} \times \partial_2 \boldsymbol{l}),$$

$$Q'_H = \frac{\gamma}{4\pi c} \int d^2x \, \boldsymbol{H} \cdot (\boldsymbol{l} \times \partial_2 \boldsymbol{l}).$$

Here $\boldsymbol{l}$ is the unit Néel vector, $(x_1, x_2) = (x, c\tau)$ is the Euclidean plane, $c = JSaZ_c/\hbar$ is the limiting velocity of spin waves, Z_c is the lattice coordination number, a is the lattice constant, $\Delta = a(JZ_c/4K_2)^{1/2} \gg a$ is the characteristic DW thickness, $\rho = K_1/K_2 - 1$ is the rhombicity parameter, $\gamma = g\mu_B/\hbar$ is the gyromagnetic ratio, g denotes the Landé factor, and μ_B is the Bohr magneton. The quantity $\tilde{w}_a(\boldsymbol{l}) = (\gamma/c)^2 (\boldsymbol{H} \cdot \boldsymbol{l})^2$ describes effective renormalization of the anisotropy induced by the field. In Eq. (2), the term proportional to Q is the so-called topological term originating from the sum of Berry phases[8] of individual spins, Q being the homotopical (Pontryagin) index of mapping of the (x_1, x_2) plane onto the sphere $\boldsymbol{l}^2 = 1$, and Q'_H is the contribution from magnetic field.

A static DW solution $\boldsymbol{l}_0(x)$ corresponds to the rotation of vector $\boldsymbol{l}$ in the easy plane XY:

$$l_{0X} = \sigma' \tanh(x/\Delta), \quad l_{0Y} = \sigma/\cosh(x/\Delta), \quad l_{0Z} = 0, \tag{3}$$

where $\sigma, \sigma' = \pm 1$. The quantity σ' is the ''topological charge'' of the DW, and the chirality σ determines the sign of $\boldsymbol{l}$ projection onto the ''intermediate'' axis Y. Two states with $\sigma = \pm 1$ are equivalent in energy; change of σ describes reorientation of the macroscopic number of spins $N_{\mathrm{DW}} \sim \Delta/a \gg 1$, typically $N_{\mathrm{DW}} \sim 70$–100.

III. CHIRALITY TUNNELING IN ABSENCE OF MAGNETIC FIELD

Let us consider first the case $\boldsymbol{H} = 0$. Tunneling between the DW states with opposite chiralities can be studied using the instanton formalism. Since the tunneling here occurs between two *inhomogeneous* states, the corresponding instantons are non-one-dimensional (space and time). The structure of instanton solution $\boldsymbol{l}_{\mathrm{inst}}(x, \tau)$ is shown in Fig. 2; it has the following asymptotic behavior:

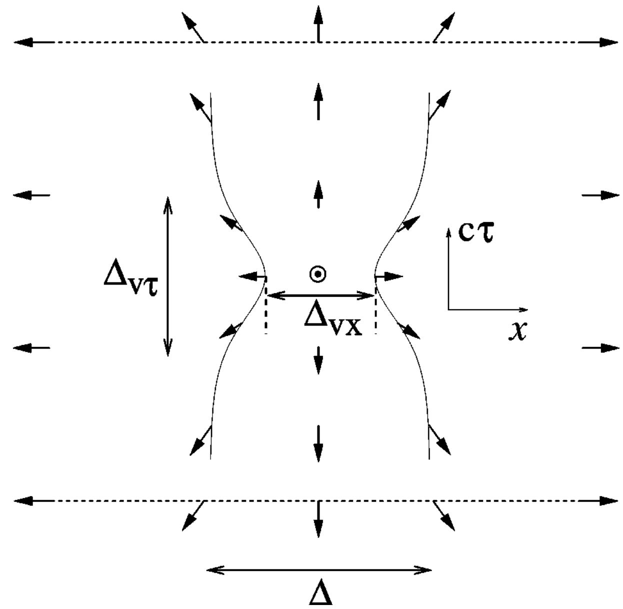

FIG. 2. The structure of instanton connecting two DW states with opposite chiralities. Arrows denote projections of vector $\boldsymbol{l}$ on the easy plane; on the thin solid line vector $\boldsymbol{l}$ forms an angle of about 45° with the easy axis.

$$l_X \to \pm \sigma', \; x \to \pm\infty, \quad l_Y \to \mp \sigma, \; x = 0, \; \tau \to \pm\infty,$$

$$l_Z \to p = \pm 1, \; x \to 0, \; \tau \to 0, \tag{4}$$

note the appearance of another topological charge $p = \pm 1$. Along any closed path in the Euclidean plane going around (but far from) the instanton center vector $\boldsymbol{l}$ rotates by the angle $2\pi\nu$ in the easy plane XY, where $\nu = \sigma\sigma' = \pm 1$. Thus, the instanton configuration has the properties of an *out-of-plane magnetic vortex* (i.e., with $l_Z \neq 0$ in the center) and is characterized by two topological charges:[9] vorticity ν and polarization p. The instanton solution satisfies the equations

$$\nabla^2 \theta + \sin\theta \cos\theta [(\rho + \cos^2 \varphi)/\Delta^2 - (\nabla \varphi)^2] = 0,$$

$$\nabla \cdot (\sin^2 \theta \nabla \varphi) - (1/\Delta^2) \sin^2 \theta \sin \varphi \cos \varphi = 0, \tag{5}$$

where we have introduced angular variables as $l_X + i l_Y = \sin\theta e^{i\varphi}$, $l_Z = \cos\theta$, and $\nabla = (\partial_1, \partial_2)$ denotes the Euclidean gradient.

We are not able to find the exact solution of Eqs. (5), but the tunneling amplitude can be estimated from approximate arguments. One can observe that, in contrast to the same problem for ferromagnet,[10] Eqs. (5), as well as their solutions, are *real*. Thus in the absence of magnetic field the real part of $\mathcal{A}_E$ is given by $n_\perp SW/4$, and the imaginary part is determined solely by the topological term (note that Q is a total derivative and does not contribute to the equations of motion). Then constructing the instanton solution can be viewed as minimization of W; it should be remarked that W formally coincides with the energy of a vertical Bloch line in a 2D DW, which is rather well studied.[11]

Another observation is that in AF in the absence of magnetic field the translational DW motion in real space and its internal degree of freedom (chirality) are uncoupled, in contrast to ferromagnets;[4] for $\boldsymbol{H}\neq 0$ this coupling appears but becomes important only in strong fields $H\sim H_c=(4Z_cS^2JK_1)^{1/2}/\gamma$.[12] Thus for weak fields one can consider the tunneling assuming a fixed position of the DW in the real space. For uniform boundary conditions at infinity the quantity Q determining $\mathrm{Im}\,\mathcal{A}_E$ can take only integer values, but in our case $Q=-p\nu/2=\pm\frac{1}{2}$ is half-integer, which is typical for out-of-plane vortices.[9] For the given σ' there are two instanton solutions with the same vorticity ν and opposite polarizations p which equally contribute to $\mathrm{Re}\,\mathcal{A}_E$ but have different signs of $\mathrm{Im}\,\mathcal{A}_E$. Using the standard instanton technique,[13] one obtains for the tunnel splitting

$$\Gamma=C\hbar\omega_l(n_\perp\widetilde{W}S/4)^{1/2}e^{-n_\perp\widetilde{W}S/4}|\cos\Phi|, \tag{6}$$

where $\widetilde{W}=W[\boldsymbol{l}_{\mathrm{inst}}(x,\tau)]-W[\boldsymbol{l}_0(x)]$ is the difference of the real part of Euclidean action calculated on the instanton solution and on a static DW without instanton, $\omega_l=(c/\Delta)\sqrt{\rho}$ is the frequency of the out-of-plane magnon localized at the DW (''attempt frequency''), the square root in the preexponent comes from the zero mode of the istanton motion along the imaginary time axis (recall that the position in real space is fixed), C is a numerical constant accumulating the effect of fluctuations around the instanton (except the zero mode), and, finally, Φ is the phase determined by the p-dependent part of $\mathrm{Im}\,\mathcal{A}_E$. In the simplest model with $\boldsymbol{H}=0$ considered so far $\Phi=\pi n_\perp S$ due to the presense of the topological term, and thus *the tunneling amplitude vanishes when S is half-integer and $n_\perp$ is odd,* the effect which was missed in Ref. 4 as well as in our earlier work.[3] Thus the tunneling is forbidden for roughly one-half of DW's in half-integer S AF, somewhat similarly to the case of half-integer S nanoparticles with uncompensated total spin.[14] In the present case, however, the effect is more subtle: we consider the system consisting of an *even* number of spins, and the total spin is not necessarily half-integer when S is half-integer; thus the effect cannot be explained on the basis of the Kramers theorem without using additional assumptions (e.g., one may speculate[17] that a domain wall in the spin-S chain has an ''internal'' spin which is just S).

Below we will see that in presence of magnetic field the situation is different: both integer and half-integer $n_\perp$ contribute, but with different tunneling rates. To calculate the real part of the Euclidean action $\widetilde{W}$, one can observe that the problem has three different length scales: the DW thickness Δ, the vortex core size in spatial direction Δ_{vx}, and the characteristic size of the core in the imaginary time direction $\Delta_{v\tau}$. For strong easy-plane-type anisotropy, $\rho\gg 1$, the vortex core is nearly axially symmetric: up to distances $r\ll\Delta$ the anisotropy in the easy plane can be neglected, and the solution in the core reduces to the well-known case of a usual vortex in an easy-plane magnet,[15] with $\theta=\theta_0(\xi)$, $\varphi=\nu\chi$, $\nu=\pm 1$,

$$d^2\theta_0/d\xi^2+(1-\nu^2/\xi^2)\sin\theta_0\cos\theta_0=0. \tag{7}$$

Here (r,χ) are the polar coordinates in (x_1,x_2) plane, $r=(x_1^2+x_2^2)^{1/2}$, $\chi=\arctan(x_2/x_1)$, and $\xi=r\sqrt{\rho}/\Delta$. Thus $\Delta_{vx}=\Delta_{v\tau}=\Delta/\sqrt{\rho}\ll\Delta$, i.e., the core is isotropic and much smaller than the DW thickness. In the opposite ''almost easy-axis'' case $\rho\ll 1$ the core is strongly asymmetric: its spatial size $\Delta_{vx}=\Delta$, but the imaginary time size $\Delta_{v\tau}=\Delta/\sqrt{\rho}$ is much larger.[16]

On the other hand, for $r\gg\Delta_{vx},\Delta_{v\tau}$, i.e., far outside the core, one can put $\theta\simeq\pi/2$, which reduces the system (5) to the 2D elliptic sine-Gordon equation,

$$\boldsymbol{\nabla}^2\varphi=(1/2\Delta^2)\sin 2\varphi. \tag{8}$$

In the large rhombicity limit $\rho\gg 1$ within a wide range of r (for $\Delta/\sqrt{\rho}\ll r\ll\Delta$) the solutions (7) and (8) can be regarded as coinciding, and the integrand in $\widetilde{W}$ is proportional to $1/r^2$. Then, one may divide the integration domain into two parts: $r<R$ and $r>R$, where R is an arbitrary point in between $\Delta/\sqrt{\rho}$ and Δ. For $r<R$ the solution (7) may be used, yielding[15] $\widetilde{W}_{r<R}=2\pi\ln(\zeta R\sqrt{\rho}/\Delta)$ with the numerical factor $\zeta\simeq 4.2$. For $r>R$, one can use a trial function which has correct asymptotic behavior and approximately satisfies Eq. (8):

$$\tan\varphi=\tanh[(x_2\sqrt{\rho})/(\Delta_{vx}^{-1}\Delta^2)]/\sinh(x_1/\Delta),$$
$$\cos\theta=[\cosh(x_1/\Delta_{vx})\cosh(x_2\sqrt{\rho}/\Delta)]^{-1}, \tag{9}$$

and evaluate $\widetilde{W}$ numerically, which for $\rho\gg 1$ (in this case $\Delta_{vx}=\Delta/\sqrt{\rho}$) gives $\widetilde{W}_{r>R}=2\pi\ln(\zeta'\Delta/R)$ with $\zeta'\simeq 0.525$. Summing up the two contributions, we obtain

$$\widetilde{W}\simeq 2\pi\ln(2.2\sqrt{\rho}),\quad \rho\gg 1. \tag{10}$$

In the weak rhombicity limit $\rho\ll 1$ the trial function (9), with $\Delta_{vx}=\Delta$, can be used for the entire (x_1,x_2) plane, yielding the result

$$\widetilde{W}\simeq 8\rho^{1/2},\quad \rho\ll 1, \tag{11}$$

which coincides with one obtained earlier in the effective Lagrangian approach.[3,17,4] Thus, our approach works both in weak and strong rhombicity limits, and can be used for variational calculation in the whole range of ρ (this study will be reported elsewhere). Only for extremely small rhombicities $\rho\ll 4/(n_\perp S)^2$, i.e., very close to the easy-axis regime, Eq. (11) breaks down; the low-energy spectrum coincides with that of the free rotator, which yields the tunnel splitting $\Gamma\sim(\hbar c/2\Delta n_\perp S)$.[17]

Comparing the results for tunneling in the AF domain wall with those for ferromagnets,[4,5] one can see that for a ferromagnetic DW the tunneling exponent contains an additional large factor Δ/a; also, for ferromagnet $\widetilde{W}\propto\sqrt{\rho}$ at large ρ while for AF $\widetilde{W}(\rho)$ grows much slower.

IV. EFFECT OF MAGNETIC FIELD

Consider now the behavior of the imaginary part of the Euclidean action when a weak external magnetic field $\boldsymbol{H}$ is applied to the system (we ignore here the field-induced anisotropy $\widetilde{w}_a$ because its effect is rather trivial). One can see that the mixed product in Q'_H significantly differs from zero only in the vortex core, and thus for large rhombicity $\rho\gg 1$ the isotropic vortex solution (7) may be used to estimate it. After integration we obtain

$$Q_H' \approx p\lambda(H_X/H_c), \tag{12}$$

where $H_c=(4Z_cS^2JK_1)^{1/2}/\gamma$ denotes the magnitude of field for which the field-induced anisotropy becomes equal to the easy-plane one, H_X is the field component along the easy axis, $\lambda=\int_0^\infty d\xi\{\frac{1}{2}\sin 2\theta_0+\xi(d\theta_0/d\xi)\}$ is a numerical constant, $\lambda\approx 3.83$. This results in the following expression for the phase factor Φ in Eq. (6):

$$\Phi \mapsto \Phi_H=\pi n_\perp S[1+(\lambda H_X/2H_c)]. \tag{13}$$

Thus *the tunneling amplitude oscillates as a function of the field with the orientation-dependent period*

$$\delta H=(2H_c/n_\perp S\lambda). \tag{14}$$

This period can be rather small: assuming $S=\frac{5}{2}$ and a typical $H_c\sim 100$ kOe, one gets $\delta H\sim 2$ kOe–20 Oe for $n_\perp=10–10^3$. A similar oscillating behavior was predicted earlier for tunneling in small ferromagnetic[18] and antiferromagnetic[19,20] particles, with the difference that in the AF case instead of the field $H_c\propto\sqrt{JK_1}$ in Eq. (14) a much stronger exchange field $H_e\propto J$ would be present; thus *the period of oscillations is much smaller in DW's than in fine particles.* For half-integer S magnetic field lifts the degeneracy of two odd-$n_\perp$ DW states with opposite chirality, allowing tunneling between them.

Another consequence of the above result is that for half-integer S in the presence of the field there are two different values of the tunnel splitting for even and odd $n_\perp$, which means that in any mesoscopic sample with weakly fluctuating cross section there should be *two different resonance peaks which exchange their positions in a quickly oscillating manner when the field increases, with the period given by Eq. (14)*; this beautiful *experimentally observable* effect was overlooked in previous studies. It is worthwhile to remark that the same effect should be also present in half-integer S AF nanoparticles with uncompensated spins considered first by Loss and co-workers[14] and also studied later in Refs. 21, provided that there is some weak interaction (magnetic field or the Dzyaloshinskii-Moriya interaction[22]) contributing to the phase factor Φ and shifting it from a multiple of $\pi/2$.

We would like to finish with a word of caution: in the presence of field the problem of chirality tunneling is actually more complicated then one can guess from the simple arguments presented above. The point is that the field contribution Q_H', unlike Q, is *not* a total derivative and thus yields an *imaginary* perturbation to the equations of motion, causing nontrivial changes in the instanton structure and in the spectrum of fluctuations in the presence of the instanton which eventually contributes to the phase Φ.[20] However, using the perturbation theory in $\boldsymbol{H}$, one can show that corrections from the change of instanton structure contribute to $\widetilde{W}$ as $(H/H_c)^2$ and to Φ as $n_\perp(H/H_c)^3$. Indeed, the Euclidean action has the form $\mathcal{A}_E^{(H)}[\boldsymbol{l}]=\mathcal{A}_E^{(0)}[\boldsymbol{l}]+i(\boldsymbol{H}\cdot\boldsymbol{F}[\boldsymbol{l}])$, so that the instanton solution in the presence of the field is $\boldsymbol{l}_{\rm inst}(H)=\boldsymbol{l}_{\rm inst}(0)+\Delta\boldsymbol{l}$, where the real part of the correction $\Delta\boldsymbol{l}$ contains only *even* powers of $\boldsymbol{h}\equiv\boldsymbol{H}/H_c$, while Im $\Delta\boldsymbol{l}$ contains only *odd* powers of $\boldsymbol{h}$ (one can show that H_c is the only scale arising in the problem[23]). Thus, the instanton action is $\mathcal{A}_E^{(H)}[\boldsymbol{l}_{\rm inst}(H)]=\mathcal{A}_E^{(H)}[\boldsymbol{l}_{\rm inst}(0)]+\Delta\mathcal{A}_E$, where $\Delta\mathcal{A}_E=i\boldsymbol{H}\cdot(\delta\boldsymbol{F}/\delta l_i)\Delta l_i+(\delta^2\mathcal{A}_E^{(H)}/\delta l_i\delta l_j)\Delta l_i\Delta l_j+\ldots$, and the leading terms in Re $\Delta\mathcal{A}_E$ and in Im $\Delta\mathcal{A}_E$ are of the second and of the third order in $\boldsymbol{h}$, respectively. There is also a contribution to Φ from the fluctuation determinant which does not contain $n_\perp$ (cf. Ref. 20). One can see that all those corrections, though quantitatively important, cannot change our main result (14) for the *period* of oscillations, as far as $n_\perp\gg 1$ (in practice $n_\perp\gtrsim 10$ is sufficient).

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