

## Fluctuation and elastic properties of domain walls in two-dimensional dipolar systems

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We discuss the fluctuation of domain walls in two-dimensional systems interacting with short-range exchange, anisotropy, and long-range dipolar interactions. The elastic energy of different domain walls are calculated. Some of the domain-wall distortion modes are soft in the long-wavelength limit. The competition of the stabilizing long-range dipolar interaction and low-dimensional fluctuation suggests the possibility of a finite-temperature roughening of an array of one-dimensional walls in the film.

### I. INTRODUCTION

There has been much interest recently in two-dimensional (2D) dipole systems from two different areas; the ultrathin magnetic films and self-assembled Langmuir monolayers with electric dipoles.<sup>1</sup> The magnetic work is partly motivated by the possible integration of the semiconductor microelectronics technology with magnetic elements.<sup>2</sup> This is stimulated by the success in the growth of magnetic films on top of semiconductor surfaces such as GaAs. Much effort was devoted in characterizing the fundamental physics of magnetic films from 1 to 100 layers.<sup>3</sup> Depending on material parameters, the magnetization can lie parallel or perpendicular to the film. New physics occurs because of the competition between the stabilizing *long-range* dipole interaction and the *low dimensionality* fluctuation effects.<sup>4</sup> In this paper we examine the finite-temperature fluctuation of the domain walls. These effects are important in understanding domain formation, hysteresis, and relaxation phenomena in the films.<sup>5</sup> Whereas in three-dimensional situations, domain walls are flat, recent experimental results<sup>6-8</sup> indicate that walls in ultrathin films are not flat.

A magnetic domain wall is an interface between a spin-up region and a spin-down region. The statistical mechanics of interfaces have been actively studied over the last ten years.<sup>9</sup> The movement of an interface at low driving force proceeds not with the whole interface marching forward in unison but with part of the interface moving forward one at a time. This involves distorting the interface and thus the elastic energy and the roughness of the interface is an important consideration. The mobility of the interface in the presence of external pinning potentials is often discussed in terms of a roughening transition. At low temperatures, the free energy of steps is finite. The movement of domain walls is activated in character and depends on the driving force in an exponential manner. The interfaces become rough and mobile if the temperature is higher than the roughening temperature. The free energy of steps becomes zero; the nature of the growth of domains becomes different. The growth rate of the domain depends linearly on the driving force in the low force regime. 2D interface in 3D systems roughens at a finite temperature.<sup>10</sup> 1D interfaces in

2D systems are always rough at any finite temperature. These studies assume that the interaction potential is short ranged.

For magnetic domain walls, because of the long-range nature of the dipolar force, the physics of the fluctuation is different from ordinary walls. The fluctuation of a physical quantity depends on the energy cost of distortion for that quantity. The long-range dipolar potential can increase the energy of distortion and reduce the thermal fluctuation. An example of this suppression of fluctuation is provided for by the question of the existence of long-range magnetic order. For 2D systems, the fluctuation of the magnetization is of the order of  $\int d^2q kT/\omega_q$  where  $\omega_q$  is the energy of the magnetic excitations at wave vector  $q$ . When the spins interact only with nearest-neighbor exchange,  $\omega_q \propto q^2$ ; the fluctuation is infinite and there is no long-range order.<sup>4</sup> When the long-range dipolar interaction is included,  $\omega_q \propto q$  for some spin arrangements. The fluctuation becomes finite and long-range order is restored.<sup>11,12</sup>

For magnetic domain walls, the physics of its low-dimensional fluctuation is more subtle than the physics of the low-dimensional fluctuation of spins. We are interested in the mean-squared fluctuation of the position of the wall,  $\langle(\delta r)^2\rangle$ , which is proportional to  $\int d^{d-1}q kT/E_q$ , where  $E_q$  is the elastic energy of distortion for the walls at wave vector  $q$ ;  $d$  is the spatial dimension. The behavior of  $E_q$  is more complex than the behavior of the spin excitation energy  $\omega_q$ . In the absence of external pinning potentials, this elastic energy can assume different forms for different spin arrangements. For a two-dimensional wall in a 3D system, the elastic energy is proportional to  $q$ . The mean-squared fluctuation of the position of the wall becomes finite. A 2D magnetic domain wall in 3D bulk systems is never rough at any temperature. For 2D systems,  $E_q$  can be negative, proportional to  $q$ ,  $q^2$  or  $q^2 \ln(q)$ . With external pinning potentials, it is constant at small  $q$  at zero temperature. At finite temperatures, the constant can become zero and the interface then is said to become rough. We find that a single wall in an  $n$ -layer system still roughens at any finite temperature even when the dipolar interaction is included. For spins oriented along the  $y$  axis separated by an *array* of Néel walls running perpendicular to the  $x$  axis a

distance  $d$  apart, the walls are flat for length scales less than  $d$ . There exist a temperature  $T_R$  above which the walls become rough.  $T_R \approx 8\pi^2 g_0^2 \mu_B^2 n^2 a / d$  as the pinning strength approaches zero. Here  $a$  is the lattice constant;  $\mu_B$ , the Bohr magneton;  $g_0$ , the  $g$  factor.

We also investigate the elastic behavior  $E_q$  of magnetic domain walls for different spin arrangements in ultrathin films. *In particular, we find that Bloch walls perpendicular to the  $x$  axis separating domains with spins along the  $z$  axis are unstable against distortion.* We now discuss our results in detail.

## II. ELASTIC ENERGY

The finite-temperature statistical mechanics and dynamics of domain walls are often discussed in terms of a phenomenological model consisting of the elastic energy  $E_e$  to deform the wall and a pinning potential  $E_p$  that is due to the intrinsic periodic structure of the crystal lattice. For a deformation of wave vector  $q$  described by the displacement  $\delta r_q$ , the elastic energy is often assumed to be proportional to the strain squared, i.e.,  $E_e = A \sum_q q^2 |\delta r_q|^2$  for some constant  $A$ . The pinning potential is assumed to have the form  $\sum_G B_G \sum_j \cos(G \cdot r_j)$ , where  $G$  is the reciprocal-lattice vector of the lattice. In the case of impurity pinning,  $G$  is no longer a discrete variable. Also, different probability distributions for  $B_G$  can be assumed.

We first discuss the domain-wall elastic energy. For magnetic domain walls in bulk materials, in the long-wavelength limit the elastic energy is not proportional to  $q^2$  but, because of the long-range nature of the dipolar forces, is instead proportional  $|q|$  in 3D.<sup>13</sup> In 2D, for magnetization in the plane, it is proportional to  $q^2 \ln(q)$  for a single 1D wall and to  $q/d$  for arrays of 1D domain walls separated by distances  $d$ . We explain how this result is obtained.

Depending on how the spins are rotated from one domain to another, there are different kinds of domain walls. For a Bloch (Néel) wall, the orientation of the spins in the middle of the wall is parallel (perpendicular) to the wall. The helicity (up or down) of the spins in the middle of the wall is another characterization. We call the plane of the film the  $xy$  plane and first consider the calculation for the elastic energy for spins oriented along the  $y$  axis separated by Néel walls running perpendicular to the  $x$  axis of identical "helicity." A Néel wall of width  $w$  located at position  $c$  is characterized by specifying the spin orientations at position  $\mathbf{r}$  by the angles  $\theta = \pi/2, \phi = f(x - c)$  where  $f$  is continuous function that is equal to 0 at  $x = -\infty$  and  $\pi$  at  $x = \infty$ ; changing between the asymptotic values over a range  $w$  around  $c$ . For example, when only the exchange and anisotropy is present,  $f = \pi(1 - \tanh[(x - c)/w])/2$ .  $f$  assumes more complicated forms when the dipolar interaction is included.<sup>5,14</sup> The interaction energy between the spins can be written as

$$E = 0.5 \sum_{ij=xyz, RR'} V_{ij}(R - R') S_i(R) S_j(R'),$$

where  $V = V_d + V_e + V_a$  is the sum of the dipolar energy

$$V_{dij}(R) = (\delta_{ij}/R^3 - 3R_i R_j/R^5) g^2 \mu_B^2;$$

the exchange energy  $V_e = -J\delta(|R - R'| = a)\delta_{ij}$ ; and the anisotropy energy  $V_a = -K\delta(R = R')\delta_{iz}\delta_{jz}$ . Here  $a$  are nearest-neighbor distances. The elastic energy is given by the domain-wall energy change as its position  $c$  is changed by  $\delta c_k = c_0(\cos(k \cdot r))$ . The details of this is discussed in Appendix A. In calculating this change, one ends up with the derivative of  $f$ , which behaves like a  $\delta$  function in the limit that the wave vector is less than the inverse domain-wall width. We get

$$\delta E = 0.5 \sum_{RR'} V_{yy}(R - R') S_0^2 [\delta c(R) - \delta c(R')]^2. \quad (1)$$

The prime on the summation indicates that we sum over those  $R, R'$  only at the  $(d - 1)$ -dimensional undistorted wall position. Because of the factor  $\delta c(R) - \delta c(R')$  the anisotropy term does not enter into the  $V$  of the above equation. At long wavelengths, the dominant contribution to  $\delta E$  comes from the dipolar term, to which we turn our attention.

In 2D the  $R$  can only lie in the  $xy$  plane, the dipolar interaction coupling  $S_z$  is different from that coupling the  $x$  and the  $y$  components. For a general spin orientation the dipolar energy is

$$E_d = 0.5 \sum_{ij=xy, RR'} V_{dij} S_i(R) S_j(R') - (V_{dxx} + V_{dyy}) S_z(R) S_z(R'). \quad (2)$$

In terms of the Fourier transform  $S_q = \sum_R \exp(iq \cdot R) S_R / \sqrt{N}$ , and

$$D_{ij}(q) = \sum_R [\cos(q \cdot R) - 1] V_{dij}(R); \quad (3)$$

Eq. (1) can be rewritten as

$$\delta E = 0.5 \sum_q D_{yy}(q) S_0^2 \delta c_q^2. \quad (4)$$

For Bloch walls perpendicular to the  $x$  axis separating spins along the  $z$  axis, the energy change is similar except that  $D_{yy}$  in the Eq. (4) is replaced by  $-D_{xx} - D_{yy}$ . This corresponds to the second term on the right-hand side of (2) and is negative. The dipolar contribution dominates over the positive contribution due to the exchange term in the long-wavelength limit and indicates an instability of straight walls. We think this instability reflects the physics that the system wants to form domains in *all* possible directions. The final result of this instability requires a careful analysis of the nonlinear terms and is beyond the scope of the present paper. Examples of the end result of this instability may be the very interesting domain shapes observed for the electric dipoles in lipid monolayers.<sup>1</sup> For 2D walls in 3D systems, no such soft mode exists.

Because  $V_d$  is essentially the second derivative of the Coulomb  $1/r$  potential,  $D$  in Eq. (3) is identical in form to the dynamical matrix  $D$  of the Wigner crystal in two dimensions and can be summed with the Ewald sum technique.<sup>15,16</sup> This is recapitulated in detail in Appendix B. Applying this to the wall energy of an array of 1D walls, we obtain

$$D_{ij} = g^2 \mu_B^2 \left[ \sum_R [1 - \cos(q \cdot R)] [4\epsilon^2 R_j R_i \phi_3(\epsilon R^2) - 2\delta_{ij} \epsilon \phi_1(\epsilon R^2)] \sqrt{a_c \epsilon / \pi} \right. \\ \left. + \sqrt{\pi / a_c} \epsilon \sum_G \{ (q_i + G_i)(q_j + G_j) \phi_1[(q + G)^2 / 4\epsilon] - G_i G_j \phi_1(G^2 / 4\epsilon) \} \right].$$

Here  $\phi_1(x) = \sqrt{\pi/x} \operatorname{Erfc}(\sqrt{x})$ ;  $\phi_3(x) = \exp(-x)(1 + 1.5/x)/z + 0.75\phi_1(z)/z^2$ .  $\epsilon$  is an arbitrary cutoff parameter usually chosen to be  $\sqrt{\pi/ad}$  so that the rates of convergence of the  $R$  and the  $G$  sum are comparable.  $R = ia\hat{x} + jd\hat{y}$  for integer  $i$  and  $j$  are the positions of the spins on the walls,  $G$  are the corresponding reciprocal-lattice vector. The sum over  $R$  and  $G$  are rapidly convergent. In the long-wavelength limit  $D_{ij} \rightarrow 2\pi g^2 \mu_B^2 q_i q_j / (qd)$ . The elastic behavior can be different for different types and structures of walls. For an array of Néel walls at distances  $d$  apart separating spins along the  $y$  axis the relevant matrix element is  $D_{yy} \rightarrow 2\pi g^2 \mu_B^2 q_y^2 / (qd)$ . The maximum  $q$  in the  $x$  direction is  $q_0 = \pi/d$ . For  $q_y \gg q_0$ ,  $q_y \approx q$ ,  $D_{yy} \propto q_y$ . For  $q_y < q_0$ ,  $q_y$  cannot be approximated by  $q$ ,  $D_{yy} \propto q_y^2/q$ . Thus the walls are quite stiff for  $q_y > q_0$ , it becomes softer at smaller  $q$ . This "anomalous"  $q$  dependence corresponds to the plasmon dispersion in the Wigner crystal language and to the Higgs phenomena in the language of high-energy physics.

The numerical results for the elastic behavior of domain walls under different spin arrangement and wave-vector directions are illustrated in Fig. 1. In Fig. 1 the two curves in the middle corresponds to elastic energies of 2D Bloch walls in 3D systems when the wave vector is parallel and perpendicular to the direction of the dipole  $p$  in the middle of the wall. They correspond to the "longitudinal" and the "transverse" branch, respectively. At small wave vectors, the longitudinal (transverse) elastic energy is proportional to  $q$  ( $q^2$ ).

The Ewald sum technique can also be applied to calculate the elastic energy of an isolated 1D wall in 2D magnets, we get the result

$$D_{ij}(q) = g^2 \mu_B^2 \sum_G \{ (G + q)_i (G + q)_j E_1[(q + G)^2 / 4\epsilon] - G_i G_j E_1(G^2 / 4\epsilon) \} / a \\ + \sum_R [1 - \cos(q \cdot R)] [4\epsilon^2 R_j R_i \phi_3(\epsilon R^2) - 2\delta_{ij} \epsilon \phi_1(\epsilon R^2)] \sqrt{a_c \epsilon / \pi}.$$

Here  $E_1(x) = \int_x^\infty ds \exp(-s)/s$  is the airy function. In the small- $q$  limit,  $E_1(q) \rightarrow \ln(q)$ , the elastic energy is proportional to  $q^2 \ln(q)$ . This is stiffer than the ordinary elasticity.

The elastic behavior of the 1D walls is also illustrated in Fig. 1. The top (bottom) curve corresponds to a 1D Néel (Bloch) wall separating magnetization parallel (perpendicular) to the plane. The lower curve is negative, as

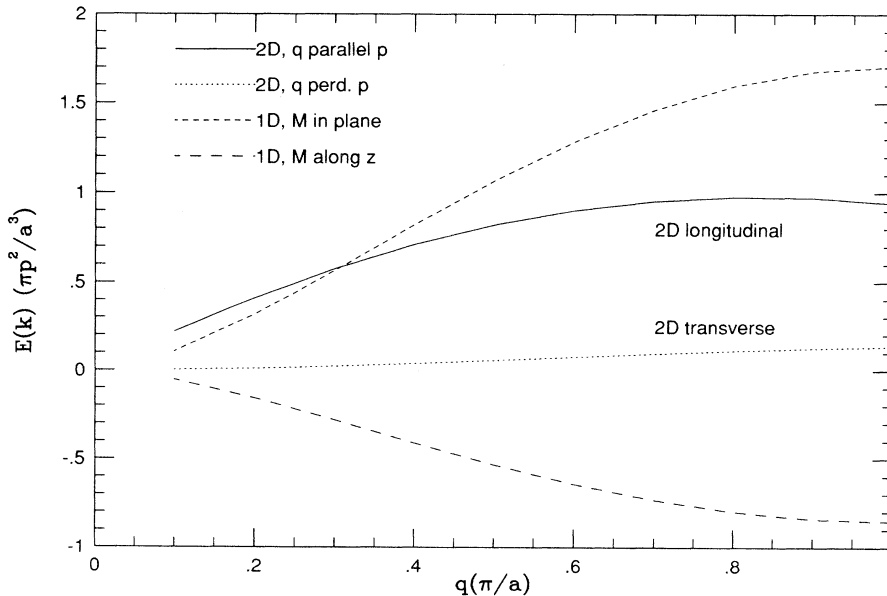


FIG. 1. Dipolar contribution to the bending energy of domain walls for 2D Bloch walls and 1D walls.  $p$  is the dipole moment  $g\mu_B$ .  $a$  is the lattice constant.

is discussed above. We next turn our attention to the effect of the elastic energy on thermal fluctuations in the presence of external pinning potentials.

### III. STATISTICAL MECHANICS

In this section we discuss the finite-temperature properties of an elastic interface in the presence of an external pinning potential. The total energy of the system is

$$E = \sum_q D_{yy}(z) |\delta c_q|^2 - \lambda \sum_R \cos(2\pi \delta c_R).$$

It consists of the elastic energy and a periodic pinning term which comes from the discreteness of the lattice. This pinning term represents a simpler example of more complicated pinning problems such as those due to external impurities.

In the limit of small  $\delta c_q$ , one can expand the pinning potential and obtain an approximate energy of the system as

$$E_q = -\lambda N + \sum_q [D_{yy}(q) + \Delta] |\delta c_q|^2 + O(\delta c^3),$$

where, at zero temperature,  $\Delta \approx \lambda 2\pi^2$ . The pinning potential thus provides for a gap which reduces the fluctuation of the walls to finite values. At finite temperatures, approximating the cosine term in  $E$  by a cumulant expansion,<sup>17</sup> the average pinning potential provides for an effective gap  $\Delta \approx 2\pi^2 \lambda \exp(\langle -2\pi^2 (\delta r)^2 \rangle)$ .  $\Delta$  becomes zero if the average self-consistent  $\langle (\delta r)^2 \rangle$  exhibits infinite fluctuation. A key signature for a finite-temperature roughening transition comes from the finite-temperature fluctuation  $\langle (\delta r)^2 \rangle$  of the interface in the absence of the pinning potential. If  $\langle (\delta r)^2 \rangle$  is logarithmically divergent in the absence of the pinning potential, then  $\Delta$  becomes zero at a finite temperature and a roughening transition is possible. This can be seen from the above by a self-consistent argument as follows. When the divergence is logarithmic,  $D_{yy} \propto q^{d-1}$  at small  $q$ ; in the presence of a gap  $\Delta$ ,

$$\langle (\delta r)^2 \rangle = kT \sum_q 1/E_q = T\alpha \ln(D_{yy}(1/a)/\Delta)$$

for some constant  $\alpha$ . Substituting this into the expression for  $\delta$ , we obtain a self-consistent gap equation  $\Delta = 2\pi^2 \lambda (D_{yy}(1/a)/\Delta)^{-2\pi^2 \alpha T}$ . Collecting terms, we get

$$\Delta = [2\pi^2 \lambda D_{yy}(1/a)^{-2\pi^2 \alpha T}]^{1/(1-2\pi^2 \alpha T)}.$$

A finite gap exists only if  $T < T_R = 1/(2\pi^2 \alpha)$ . This provides for an estimate of the roughening temperature. If the dependence is less than logarithmic a gap is possible at *all* temperature. On the other hand, if the divergence is more than logarithmic, no gap is possible at any finite temperature.

For ordinary 2D interfaces, the elastic energy is proportional to  $q^2$ .  $\langle (\delta r)^2 \rangle \propto \int d^2 q / q^2$  is indeed logarithmically divergent. When the elastic energy is proportional to  $q$ ,  $\langle (\delta r)^2 \rangle \propto \int d^2 q / q$  is not divergent. Because of the increased stiffness, a two-dimensional wall in bulk materials never roughens. On the other hand, for an ar-

ray of walls in 1D,  $\langle (\delta r)^2 \rangle \propto \int dq / q$  is logarithmically divergent again, indicating a roughening transition. This self-consistent way of looking at the fluctuation represents one approach to the problem.

To obtain a deeper appreciation of the problem we shall explore a different approach of focusing on the finite-temperature partition function of the interface with the energy  $E$ . The quantity of interest is the partition function

$$Z = \exp(-\beta F) = \int \prod_q d\delta r_q \exp(-E(\delta r)/kT).$$

For ordinary 2D interfaces, the partition function for the roughening problem is related to that for the 2D Coulomb gas.<sup>10</sup> From this physical properties of the roughening transition were deduced. We shall focus on the long-wavelength limit and shall neglect the exchange contribution which is proportional to  $q^2$ . For practical quantitative calculations of finite-temperature physical properties, the exchange contribution can be important. In this paper, we shall focus on demonstrating the possibility of a roughening transition. In 2D the partition function for the arrays of 1D dipolar domain walls is

$$Z = \int \prod_q d\delta c_q \exp(-\beta D_{yy}(q) |\delta c_q|^2) \times \exp\left[\beta \lambda \sum_R \cos(2\pi \delta c_R)\right].$$

Following by now familiar steps, we expand the second exponential as a power series in  $\lambda$  as

$$Z = \int \prod_q d\delta c_q \sum_n \left[\beta \lambda \sum_R \cos(2\pi \delta c_R)\right]^n \times \exp(-\beta D_{yy}(q) |\delta c_q|^2) / n!.$$

Performing the Gaussian integration over  $\delta c_q$ ,<sup>10</sup>  $Z$  becomes the partition function of a collection of 1D Coulomb gas:

$$Z = \exp(-\beta F_0) \times \sum_{m, \{\epsilon_j\}} (\beta \lambda)^{2m} \exp\left[-\sum_{ij} \epsilon_i \epsilon_j V(ij)\right] / m!.$$

Here

$$V(R) = 2d^2 \int d\mathbf{q} [1 - \cos(\mathbf{q} \cdot \mathbf{R})] / ((2\pi)^3 \mu_B^2 g^2 q_y).$$

For  $R_y < d$ ,

$$V(R) = V_0(R) \approx \delta(x) \ln(y) d / ((2\pi)^2 \mu_B^2 g^2).$$

For  $R_y \gg d$ ,  $V(R) \propto |R_y|$ . The Coulomb gas on different chains are decoupled. The 1D Coulomb gas with logarithmic interaction has been studied in the context of the Kondo problem.<sup>18</sup> Renormalization-group equations were derived for the coupling constants  $\lambda$  and  $T/g$ . These equations are derived by performing a scaling transformation and demanding that the form of the partition function remain the same after the coupling constants are renormalized. They are equally applicable here until the length scale reaches  $d$ . In the limit  $\lambda \rightarrow 0$  qualitatively different scaling behavior for the coupling con-

stants occurs depending on whether the temperature is above or below the roughening temperature  $T_R = 8n^2\pi^2\mu_B^2g^2(1+2\beta\lambda)/d$  for an  $n$ -layer system. Low  $T$  in the original system corresponds to a high temperature in the Coulomb fluid, it becomes metallic and the effective coupling  $T/g$  scales to zero. High  $T$  in the original system corresponds to a low temperature in the Coulomb fluid, opposite charges form bound pairs. It remains insulating and the effective coupling  $T/g$  scales to infinity. The position correlation function  $\langle(\delta r_q)^2\rangle$  can also be calculated in the Coulomb gas mapping. Below (above) roughening it is finite (infinite) as  $q \rightarrow 0$ , corresponding to the presence (absence) of a gap.

The limit by  $d$  is analogous to finite-size systems which does not exhibit a genuine mathematical singularity. Yet we expect qualitative changes in growth behavior as  $T_R$  is crossed.

To get a feel for the magnitude of the  $T_R$ , note that  $2\pi(\mu_B g)^2 \approx 10$  K. Thus  $T_R \approx n^2 100$  K ( $a_0/d$ ). Thus the transition seems experimentally accessible.

For a single 1D wall, the elastic energy is proportional to  $q^2 \ln(q)$ . It is stiffer than ordinary situations. Nevertheless, the wall still roughens at any finite temperatures, consistent with the  $d \rightarrow \infty$  limit of the above result.

In conclusion, we have investigated finite-temperature fluctuation of magnetic domain walls in ultrathin magnetic films and explore the interesting physics that results from the competition of the long-range potential and low-dimensional fluctuations. While previous experimental work indicates that domain walls exhibit large fluctuation in 2D, further systematic studies on samples with well characterized parameters is necessary to confront theory with experiment. It is quite likely that the electron wave function is of the order of six monolayers<sup>19</sup> so that experimental systems less than six monolayers can be modeled by an effective single layer spin with some effective local moments. In this paper we have performed explicit calculations on 2D and 3D systems. Similar calculations can also be carried out for films of finite thickness. For an  $n$ -layer system, because the exchange  $J$  is much larger than the dipolar interaction constant  $g$ , we expect the spins on different layers to line up so long as  $n \leq J/g$ . The system can then be modeled as a 2D system with the effective dipolar coupling between different columns of spins at different  $xy$  positions multiplied by  $n$ . The possible effects of long-range potentials on the roughening and pinning transition have been discussed previously,<sup>20-22</sup> but with elasticity that is appropriate only for 3D systems.

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## APPENDIX A

In this appendix we consider the elasticity of flat domain walls. This calculation is not as trivial as one would think because there are second derivatives of different quantities and there is a cancellation so that the energy change is zero in the zero wave-vector limit when the whole wall is rigidly transported. Thus Goldstone's theorem is obeyed.

We first consider a Bloch domain wall along the  $y$  direction with spins pointing up and down along the  $z$  axis on opposite sides of the wall. For this case  $\phi = \pi/2$ . The polar angle  $\theta$  of a spin at site  $r$  is thus given by  $\theta(r) = f[x - c(r)]$ .  $f$  is continuous function that is 0 and  $-\pi$  at  $x = \pm\infty$ , changing between the asymptotic values over a range  $w$  around  $c$ . For example, when only the exchange and anisotropy is present,  $f = \pi\{1 - \tanh[(x - c)/w]\}/2$ .  $f$  assumes more complicated forms when the dipolar interaction is included. We consider the domain-wall energy changed as  $c$  is changed by  $\delta c = c_0 \cos(ky)$ . We focus on the dipolar contribution, the other contribution is easy to deal with. The dipolar energy from  $V_{dij}$  can be written as a sum of two contributions. The first term is  $E_a = \sum \cos(\theta_i - \theta_j)/r_{ij}^3$ . The second term is  $E_b = -3 \sum \sin\theta_i \sin\theta_j y_{ij}^2/r_{ij}^5$ . Since

$$\sin\theta_i \sin\theta_j = 0.5[\cos(\theta_i - \theta_j) - \cos(\theta_i + \theta_j)],$$

$E_b = E_1 - E_2$  where  $E_{1,2} = 1.5 \int y^2 \cos(\theta_i \pm \theta_j)/r^5$ . We assume the continuum limit and approximate the sum over  $i$  and  $j$  by integrals.

To calculate the energy change as  $c$  is changed, we expand these energies as a power series in  $\delta c$  and get

$$\begin{aligned} \delta c^2 \partial_c^2 \cos(\theta_i + \theta_j) &= -\cos(\theta_i + \theta_j)(\delta c_i \partial_c \theta_i + \delta c_j \partial_c \theta_j) \\ &\quad - \sin(\theta_i + \theta_j)(\delta c^2 \partial_c^2 \theta_i + \delta c^2 \partial_c^2 \theta_j). \end{aligned} \quad (\text{A1})$$

Similarly

$$\begin{aligned} -\delta c^2 \partial_c^2 \cos(\theta_i - \theta_j) &= \cos(\theta_i - \theta_j)(\delta c_i \partial_c \theta_i - \delta c_j \partial_c \theta_j)^2 \\ &\quad + \sin(\theta_i - \theta_j)(\delta c_i^2 \partial_c^2 \theta_i - \delta c_j^2 \partial_c^2 \theta_j). \end{aligned}$$

There is a cancellation between the first and the second term on the right-hand side. To see this, we transform the second term by an integration by parts:

$$\begin{aligned} \int y^2 \sin(\theta_i + \theta_j) \delta c^2 \partial_c^2 \theta_i / r^5 &= - \int \partial_{xi} [y^2 \delta c^2 \sin(\theta_i + \theta_j) / r^5] \partial_{xi} \theta_i \\ &= \int [5xy^2 \delta c^2 \sin(\theta_i + \theta_j) / r^7] \partial_{xi} \theta_i - y^2 2\delta c_i (\partial_x \delta c_i) \\ &\quad \times \sin(\theta_i + \theta_j) / r^5 [\partial_{xi} \theta_i - y^2 \delta c_i^2 \cos(\theta_i + \theta_j) / r^5] (\partial_{xi} \theta_i)^2. \end{aligned}$$

Thus

$$\begin{aligned} \int y^2 \sin(\theta_i + \theta_j) [\delta c_i^2 \partial_c^2 \theta_i + \delta c_j^2 \partial_c^2 \theta_j] / r^5 &= \int [5xy^2 \sin(\theta_i + \theta_j) / r^7] [\delta c_i^2 \partial_{xi} \theta_i + \delta c_j^2 \partial_{xj} \theta_j] \\ &\quad - y^2 2 [\delta c_i (\partial_x \delta c_i) \partial_{xi} \theta_i + \delta c_j (\partial_x \delta c_j) \partial_{xj} \theta_j] \sin(\theta_i + \theta_j) / r^5 \\ &\quad - y^2 \cos(\theta_i + \theta_j) / r^5 [\delta c_i^2 (\partial_{xi} \theta_i)^2 + \delta c_j^2 (\partial_{xj} \theta_j)^2]. \end{aligned}$$

Similarly

$$\begin{aligned} - \int y^2 \sin(\theta_i - \theta_j) [\delta c_i^2 \partial_c^2 \theta_i - \delta c_j^2 \partial_c^2 \theta_j] / r^5 &= \int [-5xy^2 \sin(\theta_i - \theta_j) / r^7] [\delta c_i^2 \partial_{xi} \theta_i - \delta c_j^2 \partial_{xj} \theta_j] \\ &\quad - y^2 2 [\delta c_i (\partial_x \delta c_i) \partial_{xi} \theta_i - \delta c_j (\partial_x \delta c_j) \partial_{xj} \theta_j] \sin(\theta_i - \theta_j) / r^5 \\ &\quad + y^2 \cos(\theta_i - \theta_j) / r^5 [\delta c_i^2 (\partial_{xi} \theta_i)^2 + \delta c_j^2 (\partial_{xj} \theta_j)^2]. \end{aligned}$$

Collecting terms, we get

$$\begin{aligned} E_b / 1.5 &= \int (2/2)(y^2 / r^5) [-\cos(\theta_i - \theta_j) - \cos(\theta_i + \theta_j)] \delta c_i \partial_{xi} \theta_i \delta c_j \partial_{xj} \theta_j + O(\partial \delta c) \\ &\quad - 5xy^2 / 2r^7 [\sin(\theta_i + \theta_j) [\delta c_i^2 \partial_{xi} \theta_i - \delta c_j^2 \partial_{xj} \theta_j] + \sin(\theta_i - \theta_j) [\delta c_i^2 \partial_{xi} \theta_i - \delta c_j^2 \partial_{xj} \theta_j]]. \end{aligned}$$

There is a cancellation of the terms involving the cos factor so that now these factors occur only when products of both  $\partial_x \theta_i$  and  $\partial_x \theta_j$  occur. Those terms involving  $O(\partial_x \delta c)$  is zero because  $\delta c$  is only a function of  $y$ . Thus they are not explicitly displayed above.

When the form of  $\delta c$  is incorporated and the sum over  $i, j$  is carried out, the first two terms of  $E_b$  depend on  $k$  but the last two does not. The last two cancel one the first two terms in the limit  $k=0$ . This cancellation can be seen directly from Eq. (A1) with a slightly different integration by parts. When all the  $\delta c$  are the same, the second term of Eq. (A1) is then

$$\begin{aligned} \int y^2 \sin(\theta_i + \theta_j) [\partial_i^2 \theta_i + \partial_j^2 \theta_j] / r^5 \\ = \int y^2 / r^5 \sin(\theta_i + \theta_j) [\partial_i + \partial_j]^2 (\theta_i + \theta_j). \end{aligned}$$

When we integrate by parts once, we obtain terms differentiating the sin function and  $y_{ij}^2 / r_{ij}^5$ . This second class of terms is zero because it changes sign under the interchange of  $i$  and  $j$ . Thus the second term of (A1) thus becomes

$$\int [-y^2 \cos(\theta_i + \theta_j) / r^5 [(\partial_{xi} \theta_i) + (\partial_{xj} \theta_j)]^2].$$

This term completely cancels the first term of (A1). The cancellation can also be seen by explicit calculation. For example for spin in the wall in the  $xy$  plane one has, for  $c=0$ ,

$$\begin{aligned} \int [5xy^2 \sin(\theta_i + \theta_j) / r^7] \delta c_i^2 \partial_{xi} \theta_i \\ = \int d^2 r_j 5x_j y_j^2 \sin(\pi/2 + \theta_j) / r^7 \delta c_i^2 \\ = -2 \int dy_j \int_0^\infty dx_j 5x_j y_j^2 \sin(\pi/2) / r^7 \delta c_i^2 \\ = -2 \int dy_j y_j^2 / r^3 \delta c_i^2. \end{aligned}$$

This just cancels out the other term.

In a similar manner, we get

$$\begin{aligned} 2E_a &= \int \cos(\theta_i - \theta_j) \delta c_i \partial_{xi} \theta_i \delta c_j \partial_{xj} \theta_j / r^3 + O(\partial \delta c) \\ &\quad + 3x / 2r^5 [\sin(\theta_i - \theta_j) [\delta c_i^2 \partial_{xi} \theta_i - \delta c_j^2 \partial_{xj} \theta_j]]. \end{aligned}$$

Just as for  $E_b$ , the first term of  $E_a$  is a function of  $k$  but the second is not. These two terms cancel each other in the zero  $k$  limit.

The terms of the order of  $\sin(\theta_i + \theta_j) \approx \sin(2\theta_i) \approx 0$  for  $\theta=0, \pi/2$ . For domains with spin along the  $z$  axis separated by walls with spins along the  $y$  axis.  $E_b=0$ ,

$$E = \int (\delta c_i - \delta c_j)^2 \partial_{xi} \theta_i \partial_{xj} \theta_j / y^3.$$

$\partial_x \theta$  is like a  $\delta$  function localized at the domain walls. In the limit that the wave vector is less than  $w$ , the detail form of  $f$  is not important, the result is Eq. (2) and below is obtained.

A similar calculation can be carried out for a Néel wall with all spins in the  $xy$  plane. We have  $\theta=\pi/2, \phi=f[(x-c(r))]$ . For the dipolar energy, the first term is  $E_a = \sum \cos(\phi_i - \phi_j) / r_{ij}^3$ . The second term is

$$E_b = -3 \sum [\sin \phi_i \sin \phi_j y_{ij}^2 + \cos \phi_i \cos \phi_j x_{ij}^2] / r_{ij}^5,$$

$\sin \phi_i \sin \phi_j = 0.5 [\cos(\phi_i - \phi_j) - \cos(\phi_i + \phi_j)]$ . Thus  $E_b = E_1 - E_2$ , where  $E_{1,2} = 1.5 \int -(\pm y^2 + x^2) \cos(\phi_i \pm \phi_j) / r^5$ . Now expand as a power series in  $c$ . Going through the same manipulation as before, we found that

$$\begin{aligned} \int (y^2 - x^2) \sin(\phi_i + \phi_j) \delta c_i^2 \partial_c^2 \phi_i / r^5 &= \int \{ [5x(y^2 - x^2) + 2xr^2] \delta c_i^2 \sin(\phi_i + \phi_j) / r^7 \} \partial_{xi} \phi_i - y^2 2 \delta c_i (\partial_x \delta c_i) \\ &\quad \times \sin(\phi_i + \phi_j) / r^5 [\partial_{xi} \phi_i - (y^2 - x^2) \delta c_i^2 \cos(\phi_i + \phi_j) / r^5] (\partial_{xi} \phi_i)^2. \end{aligned}$$

Collecting terms, we get

$$\begin{aligned} E_b/1.5 = & \int (2/2)/r^5 [-(y^2-x^2) \cos(\phi_i + \phi_j) + (y^2+x^2) \cos(\phi_i - \phi_j)] \delta c_i \partial_{x_i} \phi_i \delta c_j \partial_x \phi_j + O(\partial \delta c) \\ & - [5x(y^2-x^2) - 2xr^2]/2r^7 \sin(\phi_i + \phi_j) [\delta c_i^2 \partial_{x_i} \phi_i - \delta c_j^2 \partial_{x_j} \phi_j] \\ & + [5x(y^2+x^2) + 2xr^2]/2r^7 \sin(\phi_i - \phi_j) [\delta c_i^2 \partial_{x_i} \phi_i - \delta c_j^2 \partial_{x_j} \phi_j]. \end{aligned}$$

In a similar manner, we get

$$\begin{aligned} 2E_a = & \int \cos(\phi_i - \phi_j) \delta c_i \partial_{x_i} \phi_i \delta c_j \partial_{x_j} \phi_j / r^3 + O(\partial \delta c) \\ & + 3x/2r^5 [\sin(\phi_i - \phi_j) [\delta c_i^2 \partial_{x_i} \phi_i - \delta c_j^2 \partial_{x_j} \phi_j]]. \end{aligned}$$

For the special cases:  $\phi = 0$  at the wall. The only  $q$ -dependent term is

$$E_b/1.5 = - \int 2y^2/r^5 \delta c_i \delta c_j.$$

From this Eq. (2) is obtained.

For the case of the electric dipoles in lipid monolayers, sometimes one is dealing with a mixture of two different dipole densities but aligned in the same direction. If we focus on the order parameter consisting of the difference in dipole densities, it is still possible to apply the above results. A negative dependence of  $q^2 \ln(q)$  was obtained for the distortion of a line in the case.<sup>23</sup> This reference also quotes results for an array of lines, which we think is incorrect.

## APPENDIX B

Below, we give a derivation of the Ewald sum for the dipolar interaction for the elasticity of the domain walls. The dipolar interaction is the second derivative of the  $1/r$  Coulomb potential:  $V_{dij} = g^2 \mu_B^2 \partial_i \partial_j 1/R_{ij}$ . We thus first focus on sums of the form

$$S(x, d, n) = \sum_R \frac{1}{|x + R|^n}.$$

The space dimension is denoted by  $d$  and the lattice vectors by  $R$ ;  $x$  is the  $d$ -dimensional vector separating the two charges. We will first use the following identity:

$$\frac{1}{x} = \frac{1}{(x^2)^{(1/2)}} = \frac{1}{\Gamma(1/2)} \int_0^\infty e^{-tx^2} t^{-1/2} dt,$$

from which, after  $p$  differentiations with respect to  $x^2$ , one gets

$$\frac{1}{(x^2)^{(p+1/2)}} = \frac{1}{\Gamma(p+1/2)} \int_0^\infty e^{-tx^2} t^{(p-1/2)} dt$$

or after substituting  $2p+1$  by  $n$ :

$$\frac{1}{x^n} = \frac{1}{\Gamma(n/2)} \int_0^\infty e^{-tx^2} t^{(n/2-1)} dt.$$

We can then write the sum  $S(x, d, n)$  as follows:

$$\sum_R \frac{1}{|x + R|^n} = \sum_R \frac{1}{\Gamma(n/2)} \int_0^\infty e^{-t|x+R|^2} t^{(n/2-1)} dt. \quad (B1)$$

Now we can see that if the integral is taken from some nonzero number  $\epsilon$  infinity, then the summation over  $R$  is very rapidly convergent. The rest of the integral, considered as a function of  $x$ , is slowly convergent and therefore its Fourier transform would be rapidly convergent. We will use the Poisson's summation formula which transforms sums on the real lattice to sums on the reciprocal lattice:

$$\sum_R f(R+x) = \frac{1}{a_c} \sum_G \hat{f}(G) e^{iG \cdot x} \nabla f. \quad (B2)$$

Here  $a_c$  is the area of the unit cell,  $G$ 's are the reciprocal-lattice vectors to  $R$ 's, and  $\hat{f}$  is the Fourier transform of the function  $f$  defined by

$$\hat{f}(k) = \int d^d r e^{-ikr} f(r).$$

So, after breaking up the integral into two parts, and applying the above summation formula to the slowly convergent part, we have

$$\begin{aligned} \sum_R \frac{1}{|x + R|^n} = & \frac{1}{\Gamma(n/2)} \epsilon^{n/2} \phi_{n/2-1}(\epsilon|x+R|^2) \\ & + \frac{1}{a_c} \sum_G e^{iGx} \hat{f}(G), \end{aligned} \quad (B3)$$

where  $\phi_n(z) = \int_1^\infty dt t^n \exp(-zt)$ ,

$$\begin{aligned} \hat{f}(G) = & \frac{1}{\Gamma(n/2)} \int d^d r e^{-iGr} \int_0^\epsilon e^{-tr^2} t^{(n/2-1)} dt \\ = & \frac{1}{\Gamma(n/2)} \int_0^\epsilon e^{-G^2/4t} (\pi/t)^{(d/2)} t^{(n/2-1)} dt \\ = & \frac{\pi^{(d/2)}}{\Gamma(n/2)} \left[ \frac{G^2}{4} \right]^{(n-d)/2} \Gamma \left[ \frac{d-n}{2}, \frac{G^2}{4\epsilon} \right]. \end{aligned} \quad (B4)$$

$\Gamma(x) = \int_0^\infty t^x e^{-t} dt$ . The rapidly convergent part can also be expressed as a  $\Gamma$  function. Finally, the Ewald sum can be written in the following form:

$$\sum_R \frac{1}{|x + R|^n} = \frac{1}{\Gamma(n/2)} \left\{ \sum_R \frac{\Gamma(n/2, \epsilon|x+R|^2)}{|x+R|^n} + \frac{\pi^{(d/2)}}{a_c} \sum_G \left[ \frac{G^2}{4} \right]^{(n-d)/2} \Gamma \left[ \frac{d-n}{2}, \frac{G^2}{4\epsilon} \right] e^{iGx} \right\}. \quad (B5)$$

For  $d=2$  and  $n=1$ ; the  $\Gamma$  function is reduced to a complementary error function  $\text{erfc}(x) = 2 \int_x^\infty \exp(-t^2) dt / \sqrt{\pi}$  and the sum  $S$  becomes:

$$\sum_R \frac{1}{|x+R|} - \frac{1}{a_c} \int d^2r \frac{1}{|x+r|} = \sum_R \frac{\text{Erfc}(\epsilon|x+R|)}{|x+R|} + \frac{\pi}{a_c} \sum_G' \left[ \frac{2}{G} \right] \text{Erfc} \left[ \frac{G}{2\epsilon} \right] e^{iGx} - \frac{2}{a_c} \frac{\sqrt{\pi}}{\epsilon}. \quad (\text{B6})$$

Differentiating this twice with respect to  $x$  and setting  $x$  to zero afterwards, the result in Eq. (1) is obtained. In a similar manner, the result in Eq. (2) corresponds to  $d = 1$  and  $n = 1$ .

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- <sup>1</sup>For some recent references, see, for example, H. M. McConnell, *Annual Review of Physical Chemistry*, edited by H. L. Strauss, G. T. Babcock, and S. R. Leone (Annual Review, Palo Alto, 1991), p. 171; M. M. Hurley and Sherwin J. Singer, *Phys. Rev. B* **46**, 5783 (1992); J. Hautman *et al.*, *J. Chem. Soc. Faraday Trans.* **87**, 2031 (1991).
- <sup>2</sup>G. Prinz, *Science* **1092**, 250 (1990).
- <sup>3</sup>B. Heinrich and J. F. Cochran, *Adv. Phys.* **42**, 524 (1993).
- <sup>4</sup>N. D. Mermin and H. Wagner, *Phys. Rev. Lett.* **17**, 1133 (1966).
- <sup>5</sup>See, for example, A. Hubert, *Theorie der Domanewande in Geordnetn Medien* (Springer-Verlag, New York, 1974).
- <sup>6</sup>A. Berger, U. Linke, and H. P. Oepen, *Phys. Rev. Lett.* **68**, 839 (1992).
- <sup>7</sup>J. Pommier, P. Meyer, G. Penissard, J. Ferre, P. Bruno, and D. Renard, *Phys. Rev. Lett.* **65**, 2054 (1990).
- <sup>8</sup>P. Bruno *et al.*, *J. Appl. Phys.* **68**, 5759 (1990).
- <sup>9</sup>G. Forgacs, R. Lipowsky, and Th. M. Nieuwenhuizen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic, New York, 1993).
- <sup>10</sup>S. T. Chui and J. D. Weeks, *Phys. Rev. B* **14**, 4978 (1976); *Phys. Rev. Lett.* **40**, 733 (1978).
- <sup>11</sup>Y. Yafet, J. Kwo, and E. M. Gyorgy, *Phys. Rev. B* **33**, 6519 (1986).
- <sup>12</sup>R. P. Erickson, *Phys. Rev. B* **46**, 14 194 (1992).
- <sup>13</sup>*Magnetic Domain Walls in Bubbled Materials*, edited by A. P. Malozemoff and Slonczeski (Academic, New York, 1979).
- <sup>14</sup>R. Kirchner and W. Doering, *J. Appl. Phys.* **39**, 855 (1968).
- <sup>15</sup>L. Bonsall and A. Maraduddin, *Phys. Rev. B* **15**, 1959 (1977).
- <sup>16</sup>J. Ziman, *Principles of Solid State Physics* (Cambridge University Press, Cambridge, England, 1965).
- <sup>17</sup>T. M. Hakim, H. R. Glyde, and S. T. Chui, *Phys. Rev. B* **37**, 974 (1988).
- <sup>18</sup>K. D. Schotte, *Z. Phys.* **230**, 99 (1970); See also, P. W. Anderson, *Basic Notions of Condensed Matter Physics* (Benjamin, New York, 1984).
- <sup>19</sup>R. F. Willis *et al.*, *Phys. Rev. B* **49**, 3962 (1994).
- <sup>20</sup>J. P. Bouchaud and A. Georges, *Phys. Rev. Lett.* **68**, 3908 (1992).
- <sup>21</sup>S. T. Chui, *Phys. Rev. B* **28**, 178 (1983), App. D.
- <sup>22</sup>J. Lajzerowicz, *Ferroelectrics* **24**, 179 (1980).
- <sup>23</sup>H. M. McConnell, *J. Phys. Chem.* **96**, 3167 (1992).