Soliton and 2D Domains in Ultrathin Magnetic Films

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We show that many *two dimensional* domain patterns observed in Monte Carlo simulations can be obtained from the *many* soliton solutions of the imaginary time sine Gordon equation. This opens the door to analytic quantitative understanding of the micromagnetics in ultrathin films. [S0031-9007(97)02536-2]

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There has been much experimental interest recently in the magnetism of ultrathin films [1,2], partly motivated by the possible integration of the semiconductor microelectronics technology with magnetic elements [1] and possible device applications with the giant magnetoresistive (GMR) effect. From a fundamental physics viewpoint, these systems present opportunities for studying new phenomena that are beginning to be uncovered. The interaction energy between the spins at positions $\mathbf{R}$, $\mathbf{R}'$ is

$$H = 0.5 \sum_{ij=xyz,\mathbf{R}\mathbf{R}'} V_{ij}(\mathbf{R} - \mathbf{R}')S_i(\mathbf{R})S_j(\mathbf{R}'), \quad (1)$$

where $V = V_d + V_e + V_a$ is the sum of the dipolar energy $V_{dij}(\mathbf{R}) = g\nabla_i\nabla_j(1/|\mathbf{R}|)$; the exchange energy $V_e = -J\delta(\mathbf{R} = \mathbf{R}' + d)\delta_{ij}$; and the crystalline anisotropy energy V_a. Here d denotes the nearest neighbors. g and J are coupling constants. The form of the anisotropy energy depends on the material of interest. It can be uniaxial (e.g., $V_a = -K\sum_i S_{ix}^2$) or fourfold symmetric (e.g., $V_a = -K\sum_i [S_{ix}^2 - S_{iy}^2]^2/4$), with the easy or hard axis aligned along specific directions. The dipolar interaction often leads to the formation of domains. The pattern of the domains has recently received considerable interest under the context of the "self-assembled" systems where *electric* dipoles lead to the formation of domains in Langmuir films. Whereas the electric dipoles are always perpendicular to the film plane in that case, the magnetic dipoles can be parallel or perpendicular to the plane [2–6]. For discussions in this paper, we restrict our attention to those cases so that the spins lie in the plane of the film, the case of experimental interest in sensor type applications.

The domain pattern depends on the shape of the sample, which is especially important for small structures. The physics of the pattern of domains in small magnetic structures is the subject of the present paper. We have been studying the physics of spin reversals of different small structures [7], such as monolayer films with perpendicular [8] and fourfold in-plane [9] anisotropy, nanowires and particles [10], coupled films [11], and the shape of the nucleus [12]. This paper reports our findings that much of the domain patterns observed in the numerical simulations can be reproduced as the *analytic many soliton* solutions of the imaginary time sine-Gordon equations. This is illustrated by two examples in Figs. 1 and 2 where we show the simulation and analytic results side by side. These analytic results have the potential for greatly improving understanding quantitatively the domain structure and the switching process in small structures. Thus analytic calculations can be performed to predict trends as the system parameters are changed. These analytic results can be used as a starting point of a simulation, considerably shortening the simulation time; sometimes the simulations become entirely unnecessary. We now explain our results in detail.

Mathematically in the continuum approximation, the dipolar energy $E_d \approx \frac{1}{2}\int d\mathbf{R} \times d\mathbf{R}' S_i(\mathbf{R})S_j(\mathbf{R}')\nabla_i\nabla_j(1/|\mathbf{R} - \mathbf{R}'|)$ can be written in terms of the magnetic charges $\nabla \cdot \mathbf{S}$ after two integrations by parts and neglecting the boundary terms as $E_d \approx \frac{1}{2}\int d\mathbf{R}\, d\mathbf{R}'\nabla \cdot \mathbf{S}(\mathbf{R})\nabla \cdot \mathbf{S}(\mathbf{R}')\,(1/|\mathbf{R} - \mathbf{R}'|)$. Thus the dipolar energy is reduced if the "magnetic charges" are as small as possible. This is usually achieved when lines of dipoles form closed loops. The orientation of the spin is determined by its angle ϕ. For example, when the azimuth angle θ can be described as a vortex with $\phi = \theta - \pi/2$ the dipolar energy is minimized. When this type of global constraint is satisfied, the domain structure is usually determined by minimizing the exchange and the anisotropy energy; we obtain the equation

$$\nabla^2\phi - 0.5K \sin 4\phi/\overline{J} = 0. \quad (2)$$

Here $\overline{J} \approx zJ/4$ is the effective exchange. z is the number of nearest neighbors. It comes from converting the discrete model to the continuum approximation. The exactly soluble sine-Gordon equation $(\partial_x^2 - \partial_t^2)\phi - 0.5K \sin 4\phi/\overline{J} = 0$ is formally the same as the above Eq. (2) if we transform the y coordinate into the imaginary time *it*. In this way, we can generate a 90° domain wall "soliton" solution as $\phi = \tan^{-1}\exp[-\sqrt{2K/\overline{J}}\,x]$ where the angle ϕ changes by 90° as the wall is traversed and x changes sign. This solution is one dimensional and is well known [13].

Many soliton solutions are known but have never been exploited in the understanding of domain structures. A general two-soliton solution of the sine-Gordon equation has the form ([14])

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$$\phi = \tan^{-1}\left\{\frac{1-\frac{1-u_1u_2-\sqrt{(1-u_1^2)(1-u_2^2)}}{1-u_1u_2+\sqrt{(1-u_1^2)(1-u_2^2)}}\exp\left\{-\frac{x'-x_1'-u_1t'}{\sqrt{1-u_1^2}}-\frac{x'-x_2'-u_2t'}{\sqrt{1-u_2^2}}\right\}}{\exp\left[-\frac{x'-x_1'-u_1t'}{\sqrt{1-u_1^2}}\right]+\exp\left[-\frac{x'-x_2'-u_2t'}{\sqrt{1-u_2^2}}\right]}\right\}. \quad (3)$$

Here $x' = x\sqrt{2K/\bar{J}}, t' = t\sqrt{2K/\bar{J}}$. This solution has four arbitrary constants, u_1, u_2, x_1, and x_2. Using the transformation $u_1 = iv$, $u_2 = -iv$, $t' = i(y' - y_1'), x_1' = x_2'$, and choosing $x_1' = [\ln(1/v) - i\pi/2]/\gamma + x_0', y_1' = -i\pi/(2v\gamma) + y_0'$, we obtain the two-soliton solution in the form

$$\phi = \tan^{-1}\left(\sinh[\gamma v\sqrt{2K/\bar{J}}\,(y - y_0)] \times \{-v\,\sinh[\gamma\sqrt{2K/\bar{J}}\,(x - x_0)]\}\right), \quad (4)$$

where v is a parameter, $\gamma = 1/\sqrt{1 + v^2}$. This describes a closure domain. An example is shown in Fig. 1(B) for a triangular lattice of 3600 spins for $K = 0.2$ and $J = 2$. A closure domain can be viewed as the space-time trajectory of two solitons coming together and eventually moving apart. The parameter v describes the orientation of the domain wall. To fit into a sample of aspect ratio r, one expects $v = r$, as we have verified directly by numerical calculation. For a triangular lattice, the center of the defect (x_0, y_0) for the lowest energy configuration sits in the middle of the triangle. This type of domain wall is often observed in simulations in systems in zero external magnetic field. A typical finite temperature simulation result [11] is also shown in Fig. 1(A) for the same value of J and K and $g = 1$, obtained from cooling a high temperature configuration that starts off with all spins aligned in the x direction. To study the possible effect of the dipolar interaction and the accuracy of the analytic formula, we have numerically minimized the *total* energy of the system starting from the configuration given by the analytic formula and using a quasi-Newton algorithm for a system with 400 spins. We have explored different values of g less than 1 and find that the mean square difference between the initial and final azimuthal angles is less than 0.1 rad, out of a possible range of π. Thus the accuracy is 3%; the analytic formula is indeed a good approximation. With this analytic formula, it is much easier to investigate the physical properties of closure domains *quantitatively*. For example, we have investigated the size dependence of the energy difference between the closure domain and that with uniform magnetization along the x direction. The difference in energy divided by the effective coupling constants (g for the dipolar energy and $\sqrt{JK}$ for the sum of the exchange and the anisotropy energy) is shown in Fig. 3 below as a function of the sample size. For a rectangular sample of a triangular lattice with an aspect ratio of 0.866 and x dimension L_1, the dipolar

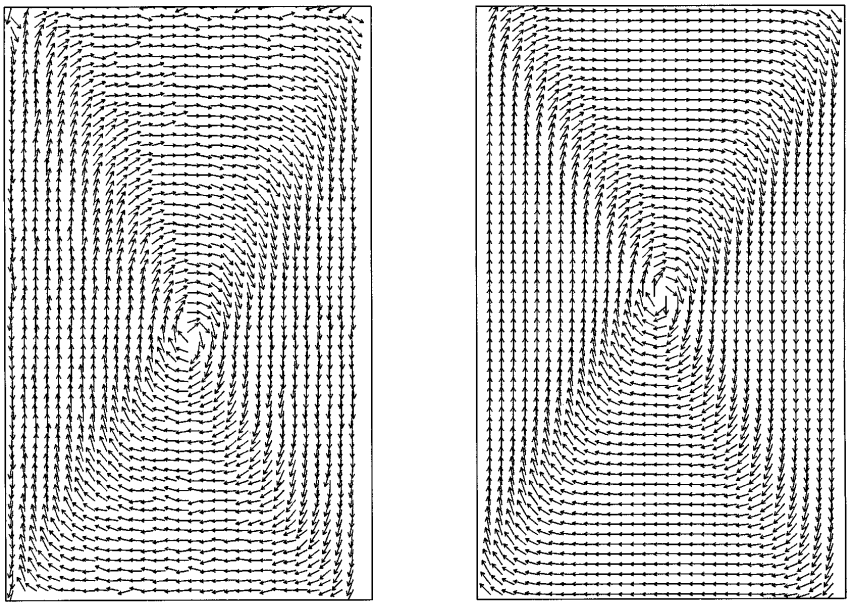

FIG. 1. Closure domain configuration for a rectangle from a two-soliton solution. The analytic results are in (B). The finite temperature Monte Carlo results observed in Ref. [11] are shown in (A). A triangular lattice can be viewed as a superposition of two rectangular lattices shifted by a unit translation vector with respect to each other. To save space, only half of the spins on one of the rectangular lattices were shown.

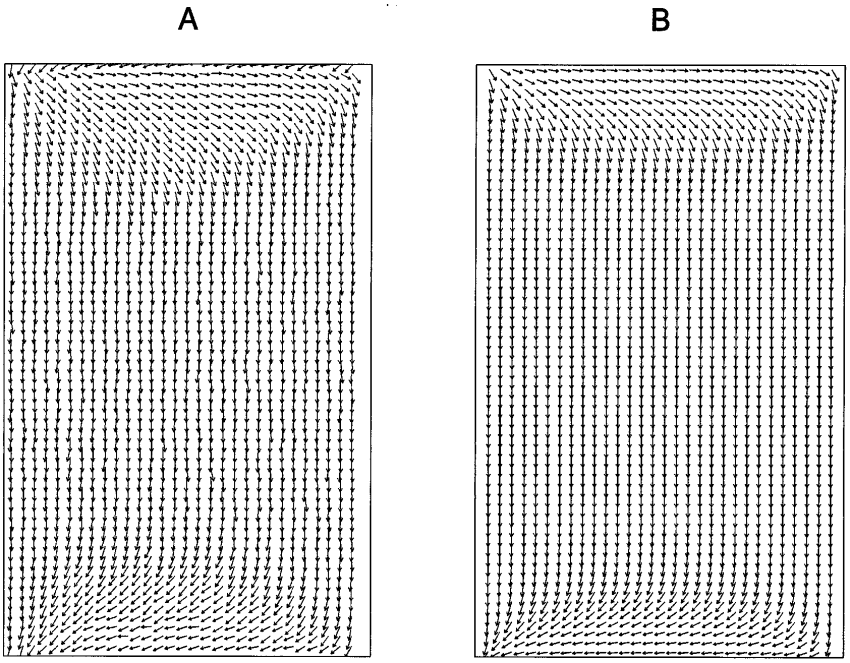

FIG. 2. Edge domain configuration for a rectangle from a two-soliton solution. The analytic results are in (B). The finite temperature Monte Carlo results observed in Ref. [11] for a two layer system are shown in (A). A triangular lattice can be viewed as a superposition of two rectangular lattices shifted by a unit translation vector with respect to each other. To save space, only half of the spins on one of the rectangular lattices were shown.

energy difference ΔE_p can be fitted by the formula $g(109.5 - 10.54L_1)$ with an error of less than 4%, whereas the sum of the anisotropy and exchange energy ΔE_w can be fitted by the formula $\sqrt{JK}\,(28.76 + 2.64L_1)$ with an error of less than 0.3%. The closure domain is lower in energy than the uniformly magnetized state when the sum of these two energies becomes negative. For a film of thickness d, we expect that approximately $g = g_0 d^2$, $J = J_0 d$, and $K = K_0 d$ where the subscript 0 refers to the bare coupling per spin. Thus the closure domain is lower in energy for sample sizes $L_1 > (109.5 + 2.876\sqrt{J_0K_0}/g_0 d)/(10.54 - 2.64\sqrt{J_0K_0}/g_0 d)$. This can only happen if the denominator is positive; i.e., $d > d_c = 0.25\sqrt{J_0K_0/g_0}$. As an example, consider bcc Fe where $g_0 \approx 0.254K$, $K_0 \approx 0.038K$, and $J_0 \approx 500K$. Thus the closure domain is lower in energy for thicknesses $d >$ 4.3 layers.

The solution (4) is, strictly speaking, applicable to infinite samples. The consideration of the domain patterns in small structures requires the imposition of finite boundary conditions. Solutions of Eq. (2) which satisfy these boundary conditions can be obtained starting from the ansatz suggested by Lamb [15] for the solution of the sine-Gordon equation. We seek solutions of Eq. (2) having the form $\phi(x, y) = \tan^{-1}[f(x')g(y')]$, where f and g are, in general, Jacobian elliptic functions defined by [16] $(f')^2 = \alpha f^4 + \beta f^2 - \gamma$ and $(g')^2 = -\gamma g^4 - (\beta - 1)g^2 + \alpha$ with α, β, and γ arbitrary constants, $x' = \sqrt{2K/J}\,x$, $y' = \sqrt{2K/J}\,y$. As an example, we consider configurations corresponding to edge domains with the boundary conditions that the spins point up (down) on the left (right) edge and horizontally on both the top and the bottom edge,

$$\phi = \tan^{-1}\left[A\,\mathrm{tn}(\Omega x', \lambda_f)\,\frac{\mathrm{cn}(\upsilon\sqrt{1 + k_g^2}\,y', k_{1g})}{\mathrm{dn}(\upsilon\sqrt{1 + k_g^2}y', k_{1g})} \right], \quad (5)$$

where $k_g^2 = [A^2\Omega^2(1 - A^2)]/[\Omega^2(1 - A^2) - 1]$, $k_{1g}^2 = A^2\Omega^2(1 - A^2)/[\Omega^2(1 - A^2) - 1]$, $\lambda_f^2 = [A^2 + \Omega^2(1 - A^2)^2]/[\Omega^2(1 - A^2)]$, and $\upsilon^2 = [\Omega^2(1 - A^2)^2 - 1]/[1 - A^2]$. The parameters A and Ω can be determined by requiring that the component of **S** normal to the surface boundary be zero so that the dipolar energy is minimized.

Figure 2(B) shows the edge domain pattern obtained by using Eq. (5) for a triangular lattice 3600 spins for $J = 2$ and $K = 0.2$. In Fig. 2(A) we show the Monte Carlo result [11] for a bilayer system for a triangular lattice of 3600 spins for the same value of J and K and $g = 1$. Similar domain patterns are also seen in the zero field remnant state for a system with a single layer [9].

To study the possible effect of the dipolar interaction and the accuracy of the analytic formula, we have numerically minimized the *total* energy of the system starting from the configuration given by the analytic formula and using a quasi-Newton algorithm for a system with 400 spins. When the dipolar interaction is too small, our algorithm recovers the minimum energy state of uniform magnetization. As long as the dipolar interaction is big enough, the minimum energy configuration from our algorithm is

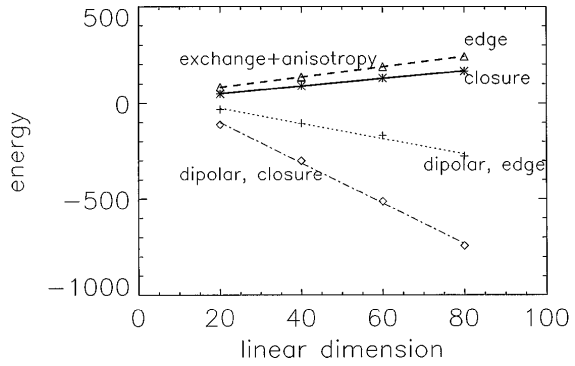

FIG. 3. The energy difference between the domain configuration and that with uniform magnetization as a function of the linear dimension of the sample. These energy differences are normalized by the coupling constants, as is described in the text.

essentially independent of the strength of the dipolar interaction. We obtain a state that resembles our analytic results. The mean square difference between the initial and final azimuthal angles is less than 10%. The analytic formula is indeed a good approximation, even though it is not as good as that for the closure domains. With this analytic formula, we have investigated the size dependence of the energy difference between the edge domain and that with uniform magnetization along the x direction. The results are shown in Fig. 3. For a rectangular sample of a triangular lattice with an aspect ratio of 0.866 and x dimension L_1, the dipolar energy difference ΔE_p can be fitted by the formula $g(52.87 - 3.97L_1)$ with an error of less than 5%, whereas the sum of the anisotropy and exchange energy ΔE_w can be fitted by the formula $\sqrt{JK}\,(10.46 + 1.9L_1)$ with an error of less than 1%. The edge domain is thus of lower energy when the sum of these two energies becomes negative. As expected, when compared with the closure domains, the dipolar energy gained is less while the cost in the anisotropy and exchange energy is comparable. For a film of thickness d, the edge domain is lower in energy for sample sizes $L_1 > (52.87 + 10.46\sqrt{J_0K_0}/g_0d)/(3.97 - 1.9\sqrt{J_0K_0}/g_0d)$. This can only happen if the denominator is positive; i.e., $d > d_{\rm ec} = 2\sqrt{J_0K_0}/g_0$. For bcc Fe, $d_{\rm ec} = 8.2$ layers.

In this paper we have discussed two examples of analytic solutions for domain patterns. Many possibilities remain to be explored. For example, consider

$$\phi = \tan^{-1}\left(\cos[\gamma v\sqrt{2K/J}\,(y - y_0)] \times \{v\,\sinh[\gamma\sqrt{2K/J}\,(x - x_0)]\}\right), \qquad (6)$$

where $\gamma = 1/\sqrt{1 - v^2}$. This solution can be considered the analytic continuation of the solution (4) with an imaginary v. When v is small, this solution describes two 90° domain walls separated by a distance $2\ln(2/v)\sqrt{J/2K}/\gamma$. As v is increased from zero, two separated 90° domain walls merge to become a 180° domain wall with vortices in between. This type of solution is not the lowest energy configuration in zero magnetic field but occurs as a rate limiting step in spin reversal processes at a *finite* magnetic field. Our solution provides for configurations that are local extrema of the exchange and anisotropy energy. The ordinary 180° domain wall in *zero* field, which consists of two 90° domain walls, is *not* a local extrema of the exchange and anisotropy energy. It is only stabilized by the magnetoelastic or dipolar energy [5,13].

In summary, we have provided examples of how the many soliton solutions can be used to understand the domain structures in ultrathin films. This opens the door to analytic quantitative understanding of the micromagnetics in these systems.

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