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Dipolar ground state of planar spins on triangular lattices

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An infinite triangular lattice of classical dipolar spins is usually considered to have a ferromagnetic ground state. We examine the validity of this statement for finite lattices and in the limit of large lattices. We find that the ground state of rectangular arrays is strongly dependent on size and aspect ratio. Three results emerge that are significant for understanding the ground state properties: (i) formation of domain walls is energetically favored for aspect ratios below a critical value; (ii) a vortex state is energetically favored in the thermodynamic limit of an infinite number of spins, but nevertheless such a configuration may not be observed even in very large lattices if the aspect ratio is large; (iii) finite range (R) approximations to actual dipole sums may give spurious results and the limit $R\rightarrow\infty$ depends on the way it is taken. For the usual, isotropic limit, the ferromagnetic state is linearly unstable and the domain wall energy is negative for any finite range cutoff.

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Electric or magnetic fields generated by point dipole sources have significant effects on polarizable materials. The effects can dominate in thin film and nanostructured elements. In one and two dimensions, long-range order of electric or magnetic polarizations in dipole lattices is possible[1] and it is particularly interesting in view of the very strong impact that lattice geometry can have on the nature of the long-range order.[2] Interest in these effects has been renewed by the ability to create arrays out of polarizable materials[3–5] with element sizes that can behave to a reasonable approximation as point dipole sources.

Whereas long-range ordering in infinite two-dimensional lattices has been examined in some detail for different rhombic lattices,[6,7] there is to date very little known about how exactly long-range order is affected by lattice size, shape, and dimension in the transition region between small and infinite lattices. We find that this is a nontrivial point for two-dimensional lattices, and note that many real systems of technological interest fall in the very large, yet noninfinite, category. Our results impact not only the nature of ordering in large, rectangular lattices, but also some inadequacies and failures in the use of an interaction cutoff for the dipolar interaction (see also Refs. 8 and 9).

In this manuscript we study a two-dimensional triangular lattice of classical planar spins with long-range dipolar coupling between spins. The nearest-neighbor distance between spins is taken as a unit length. The total dipolar energy is

$$E=\Omega\sum_{(ij)}\frac{1}{r_{ij}^3}\left[\vec{S}_i\cdot\vec{S}_j-3\frac{(\vec{S}_i\cdot\vec{r}_{ij})(\vec{S}_j\cdot\vec{r}_{ij})}{r_{ij}^2}\right], \qquad (1)$$

where (ij) is a couple of spins and r_{ij} is their distance. The energy can also be written in terms of an effective field $\vec{H}_i$ acting at a lattice site i as $E=-(\Omega/2)\Sigma_i\vec{S}_i\cdot\vec{H}_i$. Each $\vec{S}_i$ may represent either a single spin or the effective spin of a single-domain magnetic particle. It has been shown[10] that near-field corrections due to the finite size of magnetic particles can be accounted for with correction terms that do not alter the general qualitative features of the planar array interactions. The prefactor $\Omega=\frac{1}{2}g^2\mu_B^2S^2$ is positive and absorbs the modulus of the spin (so that $|\vec{S}_i|=1$). The prefactor can be set to $\Omega=1$, if there are no other terms in the energy.

The dipolar interaction between two spins $\vec{S}_1$ and $\vec{S}_2$ located at sites $\vec{r}_1$ and $\vec{r}_2$ is minimized by aligning them ferromagnetically along the line $\vec{r}_{12}=\vec{r}_1-\vec{r}_2$. A single chain of spins will, therefore, order ferromagnetically along the chain. For parallel chains of spins, the field $\vec{H}(d)$ generated by an infinite chain at a point some distance d away from the chain axis plays a special role because $\vec{H}(d)\equiv 0$ in the continuum approximation.[10] For a discrete lattice, $\vec{H}(d)$ does not vanish, but it decays exponentially[11,12] with the distance, with a sign depending on the precise discrete structure.

As a consequence of that,[1,2] geometry becomes especially important in two dimensions: the sign of $\vec{H}(d)$ depends on the lattice structure, and it is negative for a square lattice but positive for a triangular lattice.[10] Spin chains are ferromagnetically coupled in a triangular lattice and antiferromagnetically coupled in a square lattice.

This picture breaks down when the chains are finite in length. Consider a rectangular sample of sides L_x and L_y with aspect ratio $r=L_x/L_y\geqslant 1$. We shall show, using direct numerical evaluation of Eq. (1), that the energy of a domain wall parallel to the x axis scales with L_x and becomes negative for $r<r_c$, where the critical aspect ratio is $r_c\approx 4.8$. This implies that the domain wall formation is favored in rectangles with relatively small aspect ratios. Most significantly, increasing the size of the sample while keeping r fixed does not increase the number of domain walls. Whereas one might anticipate that the array shape can drive domain formation as it does in exchange coupled ferromagnets, the number of domains in a dipole ferromagnet is size independent. This feature is not found in exchange coupled ferromagnets. The difference is because the nonlocal dipole interaction in a dipole array produces both the magnetic anisotropy and the

magnetic coupling required for formation of a domain boundary wall. In the exchange coupled ferromagnet (FM), exchange interactions are usually negligible beyond nearest or next-nearest neighbors.

In the following we shall discuss these shape and size effects, and also show that vortex formation is energetically favored only for very large lattices when r is large. The appearance of vortices is a well-known fact, both in purely dipolar systems[13,14] and in dipole plus exchange systems,[15] but we are able to evaluate the vortex energy as a function of size and shape of the sample. Effects of local quadratic and quartic magnetic anisotropies are also discussed.

We begin by reviewing two results which are particularly enlightening as to why ferromagnetic lines and vortices are useful concepts for understanding ordering in two-dimensional dipolar lattices. Let us consider a closed curve Γ. If the spin is treated as a continuous field, we have $\vec{S}(\vec{r})$ at each point $\vec{r}$ of the curve. The first result is that, if $\vec{S}$ is tangent to Γ, the dipolar field $\vec{H}(P)$ generated in any point P not belonging to the curve vanishes.[16] This result shows that concentric circles in a vortex or circles belonging to neighboring vortices do not interact for continuous dipole sources. If the discrete lattice structure is considered, this is no more exact, but the interactions are weak, especially for nonconcentric circles, as it occurs in neighboring vortices.

The second result is that the field produced by all spins of a closed curve Γ in a point P belonging to the curve is tangent to the curve itself.[17] Therefore, the vortex is the spin configuration that minimizes the dipolar energy of a curve of spins, as the ferromagnetic configuration minimizes the dipolar energy of a straight line of spins.

Two conclusions follow. First, ferromagnetic lines or vortices are energetically favorable because in such configurations each spin is aligned along the dipolar field. Second, an interaction between (infinite) straight lines or vortex lines is weak (in a continuum approximation it is exactly zero) and exists only in discrete lattices. The type of alignment, therefore, depends not only on the size and shape of an array, but also on the local symmetry defining the geometry of the array.

Now let us consider a rectangular sample of sides L_x, L_y with $L_x \geqslant L_y$. Because of shape effects,[18] the ferromagnetic state is directed along the x axis. We create a domain wall along the x axis and form two equally large domains above and below it, with the magnetization pointing in $\pm\hat{x}$, respectively. In the inset to Fig. 1 we compare the energy of the two-domain state (E_2) with the single-domain (FM) state. Shown is the quantity $E_{dw}=(E_2-E_{FM})/L_x$, which is a function of the aspect ratio r only. The formation of a domain wall defining the two-domain state is energetically favored when $r<r_c\approx 4.8$. For larger r, the formation of the domain wall is energetically unfavorable. A distinguishing feature of the dipole lattice is that the energy of the domain wall per unit length depends on the aspect ratio only, not on the size of the sample. One does not see a proliferation of domains with increasing array size.

We now examine the energy of a vortex state in a rectangular sample. For the sake of simplicity, we consider an elliptic vortex, as defined in Ref. 19. This configuration is not

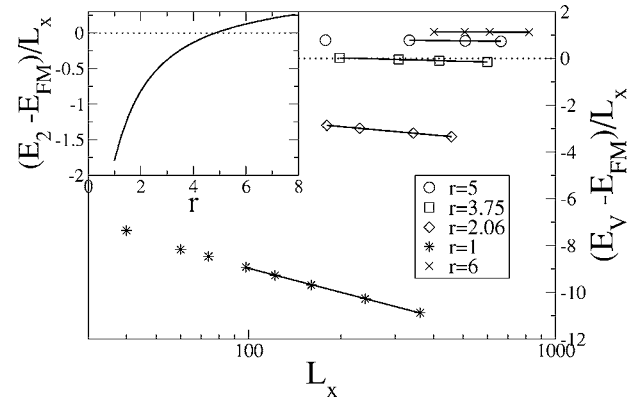

FIG. 1. Inset: the difference between the energy of the two-domain state, E_2, and the energy of the single-domain state, E_{FM}, per unit length L_x of a rectangular sample of sides L_x, L_y, as a function of the aspect ratio $r=L_x/L_y$. The plotted quantity is also called domain wall energy, E_{dw}. Main: energy of a vortex (E_V) as a function of the horizontal size L_x. Again, we scale with respect to E_{FM} and per unit length. Straight lines are fits to the equation $(E_V-E_{FM})/L_x=a(r)-b(r)\ln L_x$.

expected to be the "exact" ground state, because of corner effects. A rigorous treatment should allow for spin relaxation, which has been done in a few cases (see below). However, it is not feasible to do that for a large number of big samples of different aspect ratios. We are confident that our main results, Eq. (2) and Figs. 1 (main) and 2, are robust, because corner effects should be negligible in the limit of big sizes.

In Fig. 1 (main) we show the energy E_V of a vortex as a function of the size L_x, for different aspect ratios r. Unlike the domain wall energy, which depends only upon r, the quantity $(E_V-E_{FM})/L_x$ depends both on the shape and the size of the sample. We find that the vortex energy obeys the functional form

$$(E_V - E_{FM})/L_x = a(r) - b(r)\ln L_x, \tag{2}$$

with $a(r)$ and $b(r)$ plotted in Fig. 2. The first term $a(r)$ does not depend on L_x and displays an r dependence which

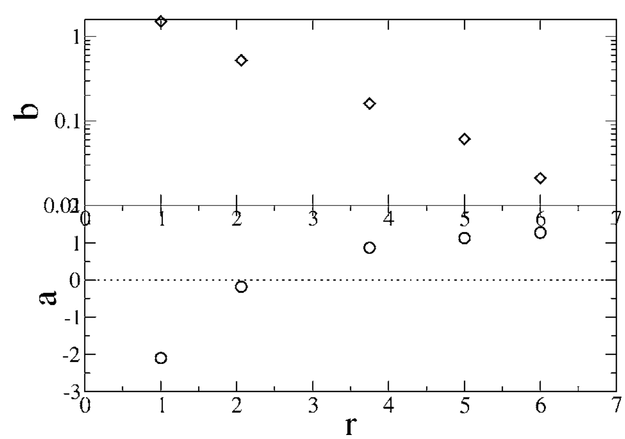

FIG. 2. Dependence of the parameters $a(r)$ (open circles) and $b(r)$ (open diamonds) on the aspect ratio r of a rectangular sample. Their meaning is illustrated in Fig. 1 (main).

strongly resembles $E_{dw}(r)$ (see the inset of Fig. 1). An average of the magnetization of the vortex in the upper $(y>0)$ and lower $(y<0)$ regions approximates a two-domain state, and $a(r)$ describes the interaction between these upper and lower parts of the vortex.

The second term, $-b(r)\ln L_x$, is always negative and drives vortex formation. Consider a two-domain ferromagnetic alignment as an initial condition on the array. The energy gain for deformation into a vortex increases as L_x is increased, but strongly decreases as r is increased. Therefore, provided that the size L_x is sufficiently large, the vortex state appears to have an energy lower than parallel aligned states for any aspect ratio. The size necessary for this depends on r.[20]

Our main study is based on the direct numerical evaluations of dipolar energy (1) for a number of fixed initial spin arrangements. This method allows us to determine the exact energies for specified configurations in very large lattices. In order to take into account the possibility of spin relaxation, in a few cases stable configurations have also been found using numerical methods that adjust local spin orientations in such a way as to minimize the total energy iteratively. The results are generally consistent with the main study: Vortex-like configurations appear for large enough arrays (large L_x), and can evolve into some type of domain structure that reduces magnetostatic energy near the array edges. For large values of the aspect ratio vortices do not form, but domains form in the proximity of the smallest sides because a FM state would have the local magnetization perpendicular to them, which is energetically unfavorable. These edge effects do not seem to penetrate the whole sample for large enough arrays. The actual configuration is determined by instabilities of parallel rectangular domains with respect to the formation of flux-closure domains with triangular shape. More general and precise conclusions would require a systematic simulation work[21] which is beyond the scope of this Rapid Communication.

We now turn to approximations involving the range R of the dipolar interaction. Truncation of dipole sums[9] by imposing finite range cutoffs for dipolar interactions is often used in numerical simulations in order to reduce computation times. This may be a severe approximation for dipole lattices regardless of the lattice size.

The stability of a ground state configuration can be examined by studying the frequencies of spin-wave excitations. It is widely accepted that, for an infinite range interaction, the ferromagnetic state on a triangular lattice is locally stable. In consequence, the linear spin-wave frequency spectrum is real over the entire Brillouin zone, and $\omega(q)\approx\sqrt{q}$ at small q. The nonanalyticity of $\omega(q)$ in $q=0$ is due to the long-range character of the interaction.

An estimate of the general behavior of spin-wave frequencies in parallel (FM) spin configuration under the finite range approximation can be made as follows. If the spin configuration is assumed to consist of infinite parallel lines it is easy to calculate the domain wall energy because interaction between lines decays exponentially, and we get $E_{dw}^{\infty}=0.2356$. This positive value means that creating a domain wall in an infinite system with infinite range interaction has a finite energy cost. Now let the range R be finite.

The spin-wave frequency has the following general form[22]: $\omega(\vec{q})=\sqrt{(A-B)(A+B)}$, where

$$A-B=\sum_i \frac{1}{r_i^3}[2+\cos(\vec{q}\cdot\vec{r}_i)], \tag{3}$$

$$A+B=D_{yy}(\vec{q})-D_{yy}(0), \tag{4}$$

with $D_{yy}(\vec{q})=\Sigma_i \frac{1}{r_i^3}(1-3y_i^2/r_i^2)\cos(\vec{q}\cdot\vec{r}_i)$.

The quantity $(A-B)$ is manifestly and strictly positive, while $(A+B)$ may take both signs, as we are going to argue. For infinite range interactions,[22] $D_{yy}(\vec{q})-D_{yy}(0)\approx cq$, with a positive prefactor c. For a finite range R and small q, we can expand the cosine in D_{yy} and replace the discrete summation on the angle $\theta[\vec{r}_i\equiv(r_i,\theta_i)]$ with an integral, getting

$$A+B\approx\frac{\pi}{8}\sum_r \frac{q^2}{r}(6\sin^2\phi-1), \tag{5}$$

where ϕ is the angle between the $\vec{q}$ and the x axis.

The above summation is limited by the range R of the interaction and it is valid for values of q small enough, $qR<1$. Equation (5) shows that $A+B$ is negative, therefore pointing out an instability, in the range $\sin^2\phi<\frac{1}{6}:|\phi|<\phi_c=24.1°$ and $|\pi-\phi|<\phi_c$ (see Ref. 23). It is worth noting that, with increasing R, ϕ_c keeps constant but the maximal value $q_M\approx 1/R$ at which $(A+B)<0$ decreases. The conclusion is that, for any finite value of the range R of dipolar interaction, there is a portion of the Brillouin zone where $\omega^2(\vec{q})<0$. This means that the ferromagnetic state is unstable for any finite R.

We have found numerically that the domain wall energy $E_{dw}(R)$, in the case of finite interaction range R, has *negative* values for any R. A limiting value exists of $E_{dw}(R\to\infty)=-0.3570$. This result means that the domain wall formation is energetically favored for any finite R, consistently with the spin-wave instability discussed before.

Note that there is an apparent inconsistency here. Above we stated that $E_{dw}^{\infty}>0$. How is it possible that $\lim_{R\to\infty}E_{dw}(R)=E_{dw}(\infty)<0$ and $E_{dw}^{\infty}>0$? The answer follows from our previous analysis: the domain wall energies $E_{dw}(\infty)$ and E_{dw}^{∞} differ because they correspond to different ways to take the thermodynamic limit. $E_{dw}(\infty)$ is evaluated assuming that each spin interacts with all spins within a circle of increasing radius R, which corresponds to a system of an aspect ratio of order 1. For this system (see the inset to Fig. 1) we find correctly a negative domain wall energy. On the other hand, evaluating E_{dw}^{∞} with the assumption that each spin interacts with an infinite number of other lines (i.e., a system with a very large aspect ratio), we find a positive domain wall energy. A quantitative understanding of the disagreement between $E_{dw}(\infty)$ and E_{dw}^{∞} is also possible.[24]

The tendency to form domain walls and vortices is very sensitive to the presence of local magnetic anisotropies. Our final considerations are for the effects of quadratic and quartic local anisotropies on spin configurations in a dipole lattice. The anisotropies are defined by

$$E^{ani} = -K_2 \sum_i \cos^2 \phi_i - K_4 \sum_i (\sin^4 \phi_i + \cos^4 \phi_i), \quad (6)$$

where ϕ_i is the angle formed by spin $\vec{S}_i$ with the x axis and K_2, $K_4 > 0$ so that both single-site anisotropies and shape anisotropy favor the x axis. We have evaluated[25] E^{ani} for a vortex configuration, with the result that

$$\frac{1}{L_x L_y}(E_V^{ani} - E_{FM}^{ani}) = K_2 \frac{r}{1+r} + K_4 \frac{r}{(1+r)^2} \quad (7)$$

which should be added to the vortex dipolar energy (per spin), $(E_V^{dip} - E_{FM}^{dip})/L_x L_y = \Omega\,[a(r) - b(r)\ln L_x]/L_y$. For $r \simeq 1$, the vortex state is favored for $L_x < \bar{c}(\Omega/K)$, with $K = \max\{K_2, K_4\}$ and $\bar{c} \approx 4/10$. For large r, a very small anisotropy is enough to favor the ferromagnetic state for any L_x.

As for future work, it would be interesting to perform more sophisticated analyses of the ground state (e.g., simulated annealing[21]), allowing for spin relaxation and an overcoming of energy barriers. The comprehension of temperature effects would be worth studying as well.

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[15] P.-O. Jubert and R. Allenspach, Phys. Rev. B **70**, 144402 (2004), and references therein. If the exchange is present, the core of the vortex is magnetized perpendicularly.

[16] This can be easily seen by rewriting $\vec{H}(P)$ in the form $H_{x,y}(P) = -\oint \nabla\left(\frac{\vec{r}\cdot\vec{\epsilon}_{x,y}}{r^3}\right)\cdot d\vec{\ell} \equiv 0$ where $d\vec{\ell} = d\ell \vec{S}$ is tangent to Γ and $\vec{\epsilon}_{x,y}$ are unit vectors.

[17] The proof is simple for a circle. For any spin tangent to the curve at the angle $\phi_0 + \phi$ there is another spin tangent in $\phi_0 - \phi$. An evaluation of the dipolar field in ϕ_0 shows immediately that it also is tangent to the circle.

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[19] Consider an ellipse concentric with the rectangle, with axes r_x and r_y parallel to the Cartesian axes and $r_x/r_y = r$. Now allow the size of the ellipse to vary while holding r constant. Each spin is intersected for some value of r_x: a vortex state is defined by a tangential alignment of the spin at its intersection with the ellipse.

[20] We have also tested, both numerically and analytically, the possibility of multivortex configurations, and we have found that increasing the number of vortices also increases the energy. See also the final discussion in Ref. 13, page 524.

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[23] It can be shown numerically that this result is exact, because lattice sites at any distance R are located on special symmetry points so that summing on them is equivalent to integrating on the full circle.

[24] The quantity $\Delta E_{dw}^{\infty} = E_{dw}^{\infty} - E_{dw}(\infty)$ can be evaluated analytically. It amounts to calculating the "complement" of $E_{dw}(R)$, i.e., to summing the dipolar coupling betweens sites i, j such that $r_{ij} > R$ and letting R going to infinity. We find $\Delta E_{dw}^{\infty} = \frac{16}{27}$, which matches very well with the numerical result $\Delta E_{dw}^{\infty} = 0.2356 + 0.357 = 0.5926$.

[25] We have calculated analytically the averages $\langle\cos^2\phi\rangle$, $\langle\cos^4\phi\rangle$,.., for a continuous field $\vec{S}(\vec{r})$ along an ellipse Γ, with $\vec{S}$ tangent to Γ.