

Ground state of a dipole system in a plane rhombic lattice

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Numerical simulation is used to study the ground state of a system of magnetic or electric dipoles located at the sites of a plane rhombic lattice with an arbitrary rhombicity angle α . The energy density per particle is studied as a function of α for the microvortex, ferromagnetic, macrovortex, and antiferromagnetic states. It is shown that as α decreases from 90° , at least two orientation phase transitions occur, from a microvortex to a macrovortex structure and from the latter to an antiferromagnetic state with axis along the small diagonal of the rhombohedron. Of the various final configurations to which the dipole system of a hexagonal lattice ($\alpha = 60^\circ$) can relax from various initial states, only combinations of an even number of pairs of macroscopic vortex domains are observed. The ground state of a dipole system in a plane hexagonal lattice is shown to be a solitary macrovortex, and the ferromagnetic state is unstable with respect to long-wave fluctuations.

The ground state of a dipole lattice was first analyzed in Ref. 1 for dipoles described by an exact classical Hamiltonian which allows for both the long-range nature and the anisotropy of the dipole-dipole interaction:

$$\mathcal{H} = \frac{1}{2} \sum_{i,j} \left\{ \frac{\mathbf{d}_i \mathbf{d}_j}{r_{ij}^3} - \frac{3(\mathbf{d}_i \mathbf{r}_{ij})(\mathbf{d}_j \mathbf{r}_{ij})}{r_{ij}^5} \right\}, \quad (1)$$

where r_{ij} is the distance between the dipoles \mathbf{d}_i and \mathbf{d}_j . The ground state of a such a system in a three-dimensional cubic lattice was found to be antiferromagnetic with antiferromagnetic axis parallel to an edge of the cube.

This problem was analyzed in more detail both analytically and numerically in Ref. 2, where it was shown that for three-dimensional cubic and two-dimensional square lattice, the ground state of the dipole system has a periodic microvortex structure with period $2a$ along each coordinate axis (a is the lattice constant). The structure is continuously degenerate in the angular variables in the three-dimensional case and in the single (polar) angle in the two-dimensional case. Although the antiferromagnetic state found previously in Ref. 1 is a special case of a general microvortex structure, the lattice energy for the antiferromagnetic state need not be a minimum.

The problem of finding the ground and metastable states for dipole systems described by the Hamiltonian (1) differs markedly from the widely studied case of systems with short-range forces. These differences can be explained most clearly by considering the example of macroscopic inhomogeneities in a dipole system.

We will regard the \mathbf{d}_i as the magnetic moments of the atoms and add a short-range exchange term to (1). If we consider only inhomogeneities in the orientations of the \mathbf{d}_i which have a large-grain structure, we average over physically infinitesimal volumes $V \gg a^3$ and introduce the magnetization vector $\mathbf{M}(\mathbf{r})$, whose modulus is conserved and for which the classical Hamiltonian takes the form

$$\mathcal{H} = \int \left\{ -\frac{1}{2} \kappa (\nabla \mathbf{M})^2 + \frac{\mathbf{H}_m^2}{8\pi} \right\} d^3r. \quad (2)$$

Here $\kappa > 0$ is the exchange constant, and \mathbf{H}_m is a functional of \mathbf{M} which is determined by the magnetostatic equations with appropriate boundary conditions.

If we neglect the long-range magnetic dipole forces we see that $\mathbf{M}(\mathbf{r})$ is uniformly oriented in the ground state, so that the gradient term in (2) vanishes. In this case the magnitude of the magnetic dipole fields is a minimum in the ground state. The basic way to decrease these fields in a three-dimensional object is to minimize the average bulk magnetization, so that the object does not behave as a single giant dipole. The situation remains unchanged if the volume becomes infinite but the shape of the object remains the same, because the density of the fields \mathbf{H}_m depends only on the ratio of the three diameters of the object. If the average magnetization is to be decreased, the vectors $\mathbf{M}(\mathbf{r})$ must become inhomogeneously oriented, i.e., domain or vortex structures must form. Although a space charge field $\nabla \mathbf{M}$ will be produced, its contribution can be made negligible compared to the contribution from the surface charge on a uniformly magnetized object. The ground state must thus be inhomogeneous for a pure dipole-dipole interaction in three-dimensional objects. For systems with a short-range interaction (as opposed to dipole-dipole systems), the addition of a long-range force generally destabilizes a homogeneous ferromagnetic state but tends to stabilize inhomogeneous structures. In our case, however, the inhomogeneous ground state will be destabilized when a small positive exchange term is included in the dipole-dipole interaction, while other more homogeneous structures will be stabilized; the situation is thus in a sense opposite to what occurs for short-range systems. The above arguments become invalid for lattices that are infinite along only one or two coordinate axes, because the average density of the magnetic fields produced by the surface magnetic charges then vanishes. In this case (i.e., for one- or two-dimensional infinite systems), analytic methods can be developed which show^{3,4} that the ground state may be homogeneous and ferromagnetic.

The continuous medium approximation (2) cannot generally be used to analyze inhomogeneities in dipole-dipole

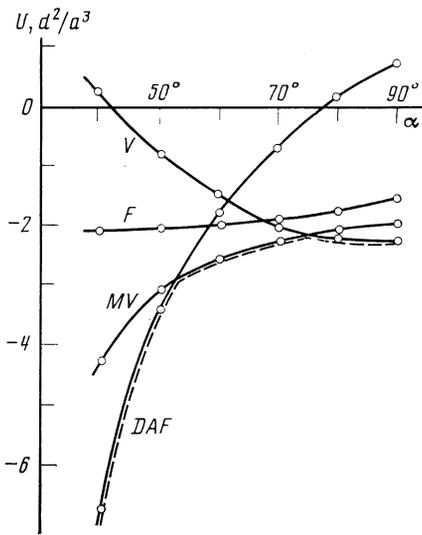


FIG. 1. Energy density per particle for different states of a dipole system as a function of the rhombicity angle α for a plane rhombic lattice: V , F , MV , and DAF are the vortex, ferromagnetic, macrovortex, and diagonal antiferromagnetic configurations, respectively. The circles on the curves show the energies, minimized with respect to the orientation of the dipole structure relative to the crystallographic axes. The dashed curve plots the ground-state energy as a function of α .

systems because it neglects the microscopic vortex structures which are actually present.² We will therefore return to the exact lattice Hamiltonian (1).

The structure of the ground state of a dipole system should be sensitive to the symmetry of the nearest-neighbor environment. We will study the effects of local symmetry on the ground state of a system of dipoles at the sites of a plane rhombic lattice with an arbitrary rhombicity angle α . Figure 2 below shows such lattices for the three angles $\alpha = \pi/2$ (square), $\alpha = \pi/3$ (hexagon), and $\alpha = \pi/6$. The samples used in the numerical simulations were taken to be disks with centers coinciding with the center of an elementary rhombic cell. The disks ranged from $10a$ to $40a$ in diameter and contained from 80 to 1500 dipole sites, depending on α . The energy density $U = \mathcal{H}/N(\alpha)$ per particle was calculated in units of d^2/a^3 .

In the first series of numerical experiments we calculated the energy as a function of α for four types of dipole structures: ferromagnetic, antiferromagnetic (along the rhombus diagonals), microvortex with period $2a$ (special cases of a vortex structure with antiferromagnetic vector parallel to the sides of the rhombus), and homogeneous vortex centered at the coordinate origin. For each structure we freely varied the degeneracy of the vortex configuration and the orientation of the ferromagnetic (or antiferromagnetic) axes relative to the crystallographic axes of the lattice. Figure 1 shows the results.

In accord with the results in Ref. 2, the microvortex structure V in Fig. 2 minimizes the energy of a system with $\alpha = \pi/2$; the antiferromagnetic structure in Ref. 1, antiferromagnetic axis along an edge of a square unit cell, is a special case. The antiferromagnetic structure with axis along the diagonal of the square cell has the highest energy of the

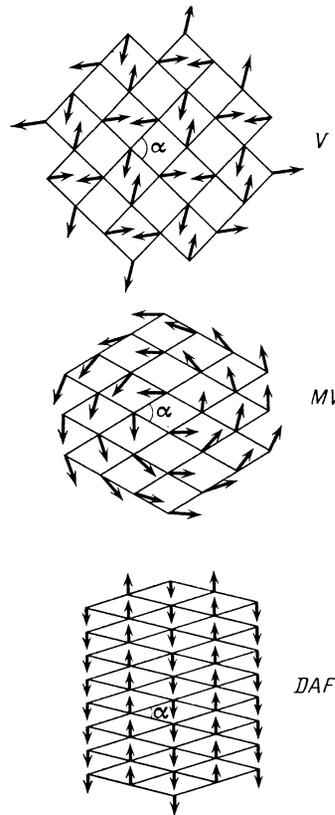


FIG. 2. Ground state configurations for plane rhombic dipole lattices: V vortex (microvortex); MV macrovortex; DAF , diagonal antiferromagnetic.

structures considered. As α decreases, the energy of the vortex configuration rises steadily while that of the diagonal antiferromagnetic (DAF) structure, with antiferromagnetic axis along the minor diagonal, drops monotonically. However, the macrovortex state MV (also shown in Fig. 2) becomes energetically favorable before the energy curves for the V and DAF states cross; indeed, the MV state has the lowest energy for α between $\alpha_2 \approx 75^\circ$ and $\alpha_1 \approx 50^\circ$. The DAF state is the ground state for $\alpha < \alpha_1$. Although the energy of the ferromagnetic state is higher than for the macrovortex state for all α , the difference decreases as the number of dipoles N increases.

Thus, at least two orientation phase transitions ($V \rightarrow MV \rightarrow DAF$) should occur as the lattice is deformed, i.e., as α decreases from 90° .

In the second series of numerical experiments we studied how the dipole orientations relax from different initial configurations to a ground or metastable final state. Similar studies were carried out for cubic and square lattices in Ref. 2, where the numerical method is described in detail. We chose to study a two-dimensional hexagonal dipole lattice ($\alpha = \pi/3$) in our work because the intermediate macrovortex phase is most sharply differentiated from the V and DAF phases for $\alpha \approx \pi/3$.

Table I shows the results of the numerical experiments. We see that as in the case of square lattices,² the dipoles tend to become oriented in the plane of the lattice—the effective

TABLE I. Final states of a disk-shaped hexagonal lattice ($N = 92$).

Initial configuration	Energy per particle d^2/a^3	Final configuration	Energy per particle d^2/a^3
Spatially random	0.2	Two vortex domains in the lattice plane	- 2.32
Diagonal antiferromagnetic	- 1.83		- 2.35
			- 2.37
Ferromagnetic (along major diagonal)	- 1.95	Four vortex domains	- 2.26
Microvortex with period $2a$	- 1.35	Ferromagnetic with two poles inside the disk	- 2.02
Ferromagnetic (along minor diagonal)	- 1.94	Solitary macrovortex	- 2.58
Solitary macrovortex	- 2.57		

dipole anisotropy of plane lattices is of the “easy plane” type.

We recall that the numerical method² used in the calculations is phenomenological and treats the relaxation of the dipole orientation to minimum energy at zero temperature. The system therefore stops at the first energy minimum that it encounters; in general, this minimum is only one of several possible metastable states. We note that the number of metastable states in plane lattices is much greater than for three-dimensional dipole systems because there are more barriers. By doing repeated simulations and comparing the final state energies, one can get a reasonably accurate idea of the structures that correspond to the ground state.

Table I shows that macrovortex structures were present in the final state for all structures that were able to reach a sufficiently deep energy minimum (energy $U \leq -2.26$ per particle) during relaxation from the initial state; however, two or four macrovortex domains rather than just one were present in the final state. The initially ferromagnetic structure with ferromagnetic axis along the minor diagonal was the only one which did not reach a deep energy minimum; instead, it relaxed to a metastable state of energy $U = -2.02$ which was quite far removed from the ground state energy $U = -2.58$. The configuration of this state is the discrete analog of a pair of “boojums,” i.e., point vortices on a surface. It is noteworthy that neither the microvortex nor the *DAF* states were metastable for the hexagonal lattice—because these states were specified, they relaxed to macrovortex structures. The specific solitary macrovortex in our numerical experiments was always of low energy, even initially, and remained a solitary macrovortex after the relaxation process (the final energy decreased only slightly, by

$\sim 0.01d^2/a^3$).

As anticipated, the ferromagnetic state differed from the ground state for a classical dipole-dipole spin system in a finite plane hexagonal lattice. Indeed, the ferromagnetic state was not even metastable—the dipole moments in this state were not oriented parallel to the local fields near the edge of the lattice, and the initial ferromagnetic configuration was therefore unstable with respect to long-wave fluctuations.

Our numerical simulations thus demonstrate that the ground state of a finite two-dimensional (disk-shaped) dipole lattice has a solitary macrovortex structure with energy $U = -2.58$. The closest metastable states into which relaxation occurs readily are the macroscopic two-vortex (vortex-antivortex pair, $U = -2.35$) and four-vortex states (two vortex-antivortex pairs, $U = -2.26$). Remarkably, we did not detect a single case in which the system itself relaxed to a state containing an odd number of macrovortices (including the ground state). Perhaps there is a topological constraint that requires the average circulation of the magnetic field in a system to remain zero if it is zero initially (this constraint could thus act as a “potential barrier”).

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