Ground state in systems with dipole interaction

P. I. Belobrov, R. S. Gekht, and V. A. Ignatchenko

Physics Institute, Siberian Division, USSR Academy of Sciences
(Submitted 6 July 1982)
Zh. Eksp. Teor. Fiz. **84**, 1097–1108 (March 1983)

A solution is obtained for the problem of determining the configuration of the ground state of a system of magnetic or electric dipoles located at the sites of a simple cubic lattice. It is shown that the ground state consists of four sublattices and has continuous degeneracy with respect to two parameters. In two-dimensional systems a continuous degeneracy in one parameter remains, while in one-dimensional systems the degeneracy is completely lifted. The ground-state configuration has a vortical structure with point group D_2 for electric dipoles and D_{2h} for the magnetic moments; a particular case of a vortex structure is the previously obtained [J. M. Lattinger and L. Tisza, Phys. Rev. **70**, 954 (1946); **72**, 257 (1947)] antiferromagnetic state of such a system. Numerical experiments performed by the molecular-dynamics method have confirmed the analytic results concerning the ground-state configuration and made it possible to establish the laws governing the formation of the ground state in finite samples and to observe the formation of a periodic vortex structure from an initial nonperiodic configuration.

PACS numbers: 41.10. – j

INTRODUCTION

Lattinger and Tisza developed in their classic paper[1] the principles of investigation of the ground state of a system with dipole interaction, and deduced that the magnetic moments located at the sites of a simple cubic lattice of an infinite three-dimensional crystal are antiferromagnetically ordered. Although their paper left open many questions (the degree to which the solution obtained is general, the character of the degeneracy of the ground state, the influence of the shape and size of the sample, and others), this problem, to our knowledge, did subsequently not received due attention. The apparent reason is that in most physical systems the dipole interaction is a small perturbation against the background of the stronger interaction that imposes the corresponding ordering on the system. Thus, in magnetically ordered crystals the ground state of the spin system is determined by exchange interaction, and the role of the magnetodipole interaction reduces to stimulation of the formation of the domain structure, to renormalization of the magnetic-resonance frequency, and to other effects that are extremely important but do not influence the character of the magnetic ordering.

Recently, however, systems for which the dipole interaction is decisive have attracted considerable interest. These are the nuclear magnetic moments at infralow spin temperatures (see, e.g., the review[2]), small ferromagnetic particles in a nonmagnetic matrix,[3,4] molecular and liquid crystals consisting of molecules with constant dipole moment,[5] rare-earth ionic compounds having a predominantly dipole-dipole interaction,[6] and others. The need has therefore arisen to return to a more detailed analysis of a ground state described by a dipole-dipole Hamiltonian.

The present paper is devoted to an investigation of the ground state of systems with pure dipole interaction between the particles in a simple cubic lattice. In Sec. 1 we separate, by analyzing the singularities of the spectra and of the eigenvectors of the dipole-dipole interaction matrix, the minimum number (equal to four) of dipole sublattices for which a configuration corresponding to the energy minimum was found. The obtained structure has a vortical character and is degenerate with respect to two parameters.

In Sec. 2 we study various causes of partial or total lifting of the spatial degeneracy of the dipole-sublattice orientations. Methods of investigating the ground state of finite systems are considered in Sec. 3, in which different system configurations are investigated on the basis of the distribution function of the angles between the orientations of the dipoles in neighboring sites. In Sec. 4 are given the results of a numerical experiment carried out by the molecular-dynamics method. The main results are discussed in the Conclusion.

1. STRUCTURE OF GROUND STATE

We consider a system of particles with dipole moment $\mathbf{P}$ at the sites of a simple cubic lattice, described by the Hamiltonian

$$\mathscr{H}=\frac{1}{2}\sum_{i,j}\left[\frac{\mathbf{P}_i\mathbf{P}_j}{r_{ij}^3}-\frac{3(\mathbf{P}_i\mathbf{r}_{ij})(\mathbf{P}_j\mathbf{r}_{ij})}{r_{ij}^5}\right], \tag{1}$$

where r_{ij} is the distance between the moments located at the sites i and j. We shall seek the ground state, just as in Ref. 1, in the class of ordered configurations that are invariant to translations of the form $2al_1\mathbf{i}+2al_2\mathbf{j}+2al_3\mathbf{k}$; a is the lattice constant, l_j are arbitrary integers, and $\mathbf{i}, \mathbf{j}, \mathbf{k}$ are unit vectors collinear with the crystallographic axes.

Following Ref. 1, the Hamiltonian $\mathscr{H}$ of the dipole interaction can be reduced to the form

$$\mathscr{H}=-\frac{N}{16}\sum_{\mathbf{v},\boldsymbol{\mu}}\sum_{\alpha}P_{\mathbf{v}}{}^{\alpha}F_{\mathbf{v}\boldsymbol{\mu}}^{\alpha\alpha}P_{\boldsymbol{\mu}}{}^{\alpha}, \tag{2}$$

where N is the number of dipole moments in the sample, $\mathbf{v}=(\nu_1,\nu_2,\nu_3)$ and $\boldsymbol{\mu}=(\mu_1,\mu_2,\mu_3)$ are the numbers of the unit-cell sites, $\alpha=(x,y,z)$, $\mathbf{F}_{\mathbf{v}\boldsymbol{\mu}}^{\alpha\alpha}$ is the lattice sum of the dipole-interaction tensor. The configuration of the dipoles in

 0038-5646/83/030636-07$04.00

the ground state was found in Ref. 1, after diagonalizing the quadratic form (2), as a superposition of basic configurations corresponding to the maximum eigenvalue of the metric F^{α}_{μ}. An arbitrary configuration **P** of the ground state, for a unit cell of eight dipoles located successively at the sites (0, 0, 0), (1, 0, 0), (1, 1, 0), (0, 1, 0), (1, 1, 1), (0, 1, 1), (0, 0,1), (1, 0, 1), is then represented in the form

$$\frac{1}{P_0}\begin{pmatrix}\mathbf{P}_1\\ \mathbf{P}_2\\ \mathbf{P}_3\\ \mathbf{P}_4\\ \mathbf{P}_5\\ \mathbf{P}_6\\ \mathbf{P}_7\\ \mathbf{P}_8\end{pmatrix}=a\begin{pmatrix}1\\ 1\\ -1\\ -1\\ 1\\ 1\\ -1\\ -1\end{pmatrix}\mathbf{i}+b\begin{pmatrix}1\\ -1\\ -1\\ 1\\ 1\\ -1\\ -1\\ 1\end{pmatrix}\mathbf{j}+c\begin{pmatrix}1\\ -1\\ 1\\ -1\\ 1\\ -1\\ 1\\ -1\end{pmatrix}\mathbf{k},$$

where P_0 is the modulus of the dipole moment of the particle, and a, b, and c are the expansion coefficients. It can be seen from the right-hand side of this expression that at all values of a, b, and c the last four components of the matrix-columns corresponding to the directions of the dipoles on the upper face of the unit cell duplicate the first four components, which determine the dipole orientations on the lower face, and the dipoles have the same direction in those sites which are arranged along the principal diagonals of the unit cell ($\mathbf{P}_1$ and $\mathbf{P}_5$, $\mathbf{P}_2$, and $\mathbf{P}_6$, etc.). Consequently, for an arbitrary configuration of the ground state, only the orientations of four dipole moments are independent.

In contrast to Ref. 1, we introduce four sublattices that make it possible to decrease the dimensionality of the basis and carry out a complete analysis of the general solution. Assume that the dipole sublattices are sequentially arranged on the lower face of the unit cell in the sites (0, 0, 0), (1, 0, 0), (1, 1, 0), (0, 1, 0). The energy U of the dipole interaction, normalized to one particle, is given for a simple cubic lattice with four dipole sublattices for a spherical sample by[7]

$$U=-\frac{1}{8}\sum_{k,n=1}^{4}\sum_{\alpha}q_{kn}{}^{\alpha}P_k{}^{\alpha}P_n{}^{\alpha}, \tag{3}$$

where $\mathbf{P}_k$ is the sublattice dipole moment normalized to one particle; k and n are the indices of the dipole sublattices. The matrix $q_{kn}{}^{z}$ is of the form

$$q^{z}_{kn}=\begin{pmatrix}0 & -q & 2q & -q\\ -q & 0 & -q & 2q\\ 2q & -q & 0 & -q\\ -q & 2q & -q & 0\end{pmatrix}. \tag{4}$$

The two other matrices $q_{kn}{}^{x}$ and $q_{kn}{}^{y}$ are obtained by respective permutations of two rows and two columns, the second and third for $q_{kn}{}^{x}$ and the third and fourth for $q_{kn}{}^{y}$. The elements of the symmetric matrix (4) can be expressed in terms of the elements of the matrix $F^{\alpha\alpha}_{\nu\mu}$, and the value $q = 1.336a^{-3}$ is determined by the lattice sums calculated in Ref. 1 for an infinite sample. The matrices $q_{kn}{}^{x}$, $q_{kn}{}^{y}$, $q_{kn}{}^{z}$ have identical eigenvalues:

$$\lambda_1=4q,\quad \lambda_2=\lambda_3=-2q,\quad \lambda_4=0. \tag{5}$$

Since the determinant of the matrices q^{α}_{ik} is zero, the direction of the dipole moment of one of the sublattices can be specified arbitrarily, and the directions of the other three sublattices are expressed in terms of the direction of this arbitrary sublattice. The state with minimum energy for each of the basis configurations will be realized for the maximum eigenvalue $\lambda_1 = 4q$. We seek the ground state in only this basis. The sublattice moments Pk expressed in terms of the corresponding eigenvalues of the matrices q^{α}_{kn} take then the form

$$\frac{1}{P_0}\begin{pmatrix}\mathbf{P}_1\\ \mathbf{P}_2\\ \mathbf{P}_3\\ \mathbf{P}_4\end{pmatrix}=a\begin{pmatrix}1\\ 1\\ -1\\ -1\end{pmatrix}\mathbf{i}+b\begin{pmatrix}1\\ -1\\ -1\\ 1\end{pmatrix}\mathbf{j}+c\begin{pmatrix}1\\ -1\\ 1\\ -1\end{pmatrix}\mathbf{k}, \tag{6}$$

where a, b, and c are the expansion coefficients and are connected by the condition $a^2 + b^2 + c^2 = 1$ that the modulus of the moment be constant. Taking the condition $\mathbf{P}_k{}^2 = P_0{}^2$ into account, we change to a spherical coordinate system

$$\mathbf{P}_k=P_0(\sin\theta_k\cos\varphi_k,\ \sin\theta_k\sin\varphi_k,\ \cos\theta_k).$$

From the energy-minimum condition $\partial U/\partial\theta_i = 0$, $\partial U/\partial\varphi_i = 0$ we obtain from (3)

$$\begin{gathered}Q_i{}^{x}\cos\theta_i\cos\varphi_i+Q_i{}^{y}\cos\theta_i\sin\varphi_i-Q_i{}^{z}\sin\theta_i=0,\\ \sin\theta_i(Q_i{}^{y}\cos\varphi_i-Q_i{}^{x}\sin\varphi_i)=0,\end{gathered} \tag{7}$$

where

$$Q_i{}^{x}=\sum_{k=1}^{4}q_{ik}{}^{x}\sin\theta_k\cos\varphi_k,\qquad Q_i{}^{y}=\sum_{k=1}^{4}q_{ik}{}^{y}\sin\theta_k\sin\varphi_k,$$

$$Q_i{}^{z}=\sum_{k=1}^{4}q_{ik}{}^{z}\cos\theta_k. \tag{8}$$

The general nontrivial solution of the system (7) is of the form

$$\begin{gathered}\theta_1=\theta_3=\psi,\quad \theta_2=\theta_4=\pi-\psi,\\ \varphi_1=\pi-\chi,\quad \varphi_2=\pi+\chi,\quad \varphi_3=-\chi,\quad \varphi_4=\chi,\end{gathered} \tag{9}$$

where ψ and χ are arbitrary angles, because $\det q^{\alpha}_{kn} = 0$. Expressing the coefficients a, b, and c in (6) in terms of ψ and χ, we can represent the projections of the dipole moments P_g at the sites of the cubic lattice with coordinates $g = (h, k, l)$ in the form

$$\begin{gathered}P^{x}_{hkl}=(-1)^{k+l}P_0\sin\psi\cos\chi,\quad P^{y}_{hkl}=(-1)^{h+l}P_0\sin\psi\sin\chi,\\ P^{z}_{hkl}=(-1)^{h+k}P_0\cos\psi.\end{gathered} \tag{10}$$

Expression (10) determines the ground state of the Hamiltonian (1). After substituting the values (10) for the angles of the sublattices in expression (3) we find that the minimum of the energy does not depend on the angles ψ and χ, and it value per particle is

$$U_{min}=-2qP_0{}^2. \tag{11}$$

The substantially different dipole structures corresponding to one and the same energy (11) of the ground state (10) are exhausted when the degeneracy parameters ψ and χ vary in the intervals $0\leqslant\psi\leqslant\pi/2$ and $0\leqslant\chi\leqslant\pi/4$. In the ground state the direction of the field **H** for the magnetic moment and **E** for the electric ones coincides naturally with direction of the

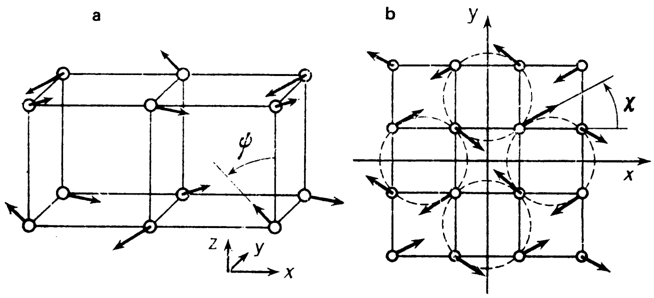

FIG. 1. Vortex configuration of ground state of dipole systems: a—in space, b—projection on xy plane. The vortex lines are shown dashed; ψ and χ are the continuous-degeneracy parameters.

dipoles in each sublattice and is determined in the following manner:

$$\mathbf{E}_k=4q\mathbf{P}_k, \tag{12}$$

i.e., U can now be represented in terms of the field $\mathbf{E}_k$ acting on the dipole moment of the sublattice $dU = -\mathbf{E}_k d\,\mathbf{P}_k$, and again obtain (11).

The arrangement of the dipole moments at the unit-cell sites is illustrated in Figs. 1a and 1b. The dipole moments located at the vertices of the principal diagonals of the cube are mutually parallel. The dipole moments in the mutually perpendicular planes xy and xz are directed along the tangent to some closed line or vortex. The circulation of the field along this line differs from zero. Figure 1b shows the structure of one layer for the values $\psi = \pi/2$ and $\chi = \pi/3$, on which the vortex lines are shown dashed. In a layer shifted by the lattice constant relative to the one shown, the orientations of the moments in the direction of the vortex lines are reversed. In the general case ($\psi \neq \pi/2$) the vortex structure is three-dimensional, and continuous degeneracy with respect to the two variables ψ and χ manifests itself in the fact that it is possible to vary smoothly the orientations of the dipole moments by satisfying the conditions (10). Despite the substantial distortion of the shapes of the vortices and of the change of the structure, the system energy remains constant and equal to $-2qP_0^2$. In three cases, 1) $\psi = \pi/2, \chi + 0$; 2) $\psi = \pi/2, \chi = \pi/2$; 3) $\psi = 0$, the vortex structure is antiferromagnetic.

In the particular case $\chi = \pi/2$ all the moments lie in the xy plane, i.e., we have a state of "fanfold structure" type, constituting a state made up of two antiferromagnetic sublattices with arbitrary angle (equal to 2χ in this case) between their antiferromagnetism vectors.[7]

The vectors in the right-hand side of (6) are representations of the point group D_2. The ground state of the Hamiltonian (1) has therefore for the electric dipole moments the point group D_2, while for the magnetic moments, as axial vectors, the ground state has the point group D_{2h}. The dipole interaction in a simple cubic lattice consequently lowers the symmetry to rhombic.

An interesting fact is the absence of dipole-dipole anisotropy in an infinite cubic crystal at a matched rotation of all four sublattices, with the symmetry D_2 (D_{2h}) preserved. It is just to this rotation that an arbitrary continuous change of the angles ψ and χ corresponds. Dipole anisotropy sets in if one considers not the ground state (for example, the well-known presence of dipole-dipole anisotropy in ferromagnetic ordering of dipole moments). For low-dimensional and finite crystals, the degeneracy in ψ and χ is lifted and magnetic anisotropy sets in also in the ground state.

2. PARTIAL LIFTING OF THE DEGENERACY

When finding the ground state of finite systems and when lowering their dimensionality, one can expect lifting of the degeneracy. We consider a cluster structure of eight dipoles placed in the vertices of a cube. Substituting the solution (10) in the Hamiltonian (1), we express the cluster energy per particles in terms of the variables ψ and χ:

$$\frac{U}{P_0^2/a^3} = -2+\frac{\sqrt{2}}{4}\cos^2\psi+\left[A+B\sin^2\left(\chi-\frac{\pi}{4}\right)\right]\sin^2\psi + C\sin 2\psi\sin\left(\chi-\frac{\pi}{4}\right), \tag{13}$$

where

$$A=\frac{1}{2}\left(\frac{\sqrt{2}}{8}+\frac{\sqrt{3}}{9}\right),\quad B=\frac{3\sqrt{2}}{8}-\frac{\sqrt{3}}{9},\quad C=\frac{1}{2}\left(\frac{\sqrt{6}}{9}-\frac{3}{4}\right).$$

We obtain the ground state of the cluster from the condition that the energy (13) be a minimum with respect to ψ and χ. From the equations obtained it follows that the configuration of the ground state will depend on the arbitrary angle χ, defined in the entire interval from 0 to 2π. We choose χ to be the independent variable; then ψ is connected with χ by the relation:

$$\operatorname{ctg}\psi=\sqrt{2}\sin\left(\chi-\pi/4\right). \tag{14}$$

Substituting (14) in (13) we find that the energy per particle is equal to $U = -1.82P_0^2/a^3$, which is much higher than the energy $U = -2.68P_0^2/a^3$ in an infinite sample. It can be seen from (14) that the polar angle ψ lies in the interval $35° \lesssim \psi \lesssim 145°$. Since ψ cannot be equal to zero or π, the antiferromagnetic state is not a state with minimum energy, although its value $U = -1.63P_0^2/a^3$ is close to the energy of the degenerate structure. However, addition of one face with four dipoles to the cube (say along the z axis) makes the antiferromagnetic state (the dipole moments are aligned parallel along the z axis, or antiparallel and make a checkerboard on the xy plane) energetically most favored. For an infinite rectangle with a base on one face of the unit cell, the energy of the ground state with antiferromagnetic arrangement of the moments is $U = -2.2P_0^2/a^3$.

If a sphere degenerates into a disk with one layer of dipoles, then substituting (10) in the Hamiltonian (1) we find, after calculating the lattice sums, that the energy is independent of the angle χ and is given by

$$\frac{U}{P_0^2/a^3} = -1.82-0.51\sin^2\psi. \tag{15}$$

Expression (15) has a minimum value $U = -2.33P_0^2/a^3$ at $\psi = \pi/2$, i.e., the dipole moments lie in the plane of the disk, forming the structure shown in Fig. 2b with arbitrary value of the angle χ.

The substitution of the general solution of the three-

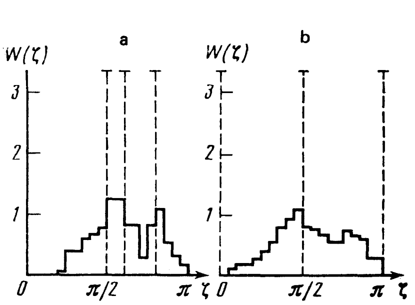

FIG. 2. Histograms of the distribution functions of the angles between the directions of the nearest dipoles: a—vortical configuration of ground state; b—vortical final structure after relaxation from a helicoidal initial configuration. The dashed lines shown the $W(\zeta)$ for the initial states.

dimensional problem (10) in the dipole Hamiltonian and the subsequent minimization with respect to the parameters ψ and χ can be regarded as a simple method of obtaining the ground state for the concrete cases of lowering the sample dimensionality. The results obtained by this method agree, naturally, with the expressions obtained by minimizing the dipole energy with respect to all the angles θ_k and φ_k of the dipole sublattices.

The cases considered above show thus that with decreasing dimensionality of space and with decreasing number of particles in the system with the dipole Hamiltonian (1) the energy of the ground state, normalized to one particle, increases. At the same time, partial lifting of the degeneracy takes place, i.e., continuous degeneracy with respect to two variables turns in the planar case into degeneracy with respect to only one variable, and in the one-dimensional case the degeneracy is completely lifted. A special case is a three-dimensional cubic cluster in which degeneracy with respect to one parameter remained. It is naturally of interest to consider the change of the energy, of the configuration, and of the degeneracy of the ground state on going from a cubic cluster to a simple cubic lattice; this will be done after analyzing the methods for investigating finite systems.

3. METHOD OF NUMERICAL INVESTIGATION OF THE GROUND STATE OF FINITE SYSTEMS

The limiting cases considered in the preceding section give grounds for hoping that definite regularities exist in samples of finite dimensions. This pertains to establishment of a stable configuration of dipole moment on the boundary of a sample, and to the character of the lifting of the degeneracy on going from a cubic crystal to an infinite sample. We shall use the circumstance that a state with minimum energy corresponds to an arrangement of the moments such that the local field at a site coincides with the direction of the dipole moments; this remains naturally valid for samples of any shape and with any arrangement of the dipole moments in space.

The equation that makes it possible to find such a configuration is the Landau-Lifshitz equation

$$\partial \mathbf{m}_i/\partial t = -\gamma [\mathbf{m}_i \times \mathbf{H}_i^d] - \xi\gamma [\mathbf{m}_i \times [\mathbf{m}_i \times \mathbf{H}_i^d]], \qquad (16)$$

where γ is the gyromagnetic ration, $\mathbf{H}_i^d = -M^{-1}\partial\mathscr{H}/\partial\mathbf{m}_i$ is the dipole field of the ith particle, and ξ is the relaxation parameter. Since in the determination of the ground state interest attaches only to the projection of the dipole moment on the local field at the corresponding site, we can leave out of the right-hand side of (16) the first term, which describes the precession of the moment around the local field $\mathbf{H}_i^d$. Taking this circumstance into account and changing to a spherical coordinate system, we obtain equations for the angles θ_i and φ_i:

$$\frac{d\theta_i}{dt} = \xi\gamma (H_i^{d,x} \cos\theta_i \cos\varphi_i + H_i^{d,y} \cos\theta_i \sin\varphi_i - H_i^{d,z} \sin\theta_i),$$
$$\frac{d\varphi_i}{dt} = \xi\gamma (H_i^{d,y} \cos\varphi_i - H_i^{d,x} \sin\varphi_i) \operatorname{cosec}\theta_i. \qquad (17)$$

The different characters of the relaxation of the electric and magnetic dipole moments notwithstanding, the final state of the relaxation process is determined by equating the right sides of Eqs. (17) to zero. The resultant system of equations (17) contains all the metastable configurations as well as the ground state. The method of finding the lowest minimum consists of going through all the solutions of the equations and comparing them with one another. To search through all the metastable states it is necessary to specify different initial configurations and to carry out the relaxation process in accord with Eqs. (17), and choose the structure with the deepest minimum.

To describe the different structures and distinguish one from the other, we introduce the distribution function $W(\zeta)$ of the angles between the orientations of the dipoles in neighboring sites, with $\cos\zeta = \cos\theta_{ij} = \mathbf{P}_i\mathbf{P}_j/P_0^2$. Obviously, a regular vortex structure of the ground state 10 is characterized, for nearest dipole separated by a distance a, by only three different angles ζ_1, ζ_2, ζ_3, for which we have

$$\cos\zeta_1 = \frac{\mathbf{P}_{hkl}\mathbf{P}_{h+1kl}}{P_0^2} = \sin^2\psi\cos 2\chi - \cos^2\psi,$$
$$\cos\zeta_2 = \frac{\mathbf{P}_{hkl}\mathbf{P}_{hk+1l}}{P_0^2} = -\sin^2\psi\cos 2\chi - \cos^2\psi, \qquad (18)$$
$$\cos\zeta_3 = \frac{\mathbf{P}_{hkl}\mathbf{P}_{hkl+1}}{P_0^2} = \cos 2\psi.$$

Since the values of ζ_1, ζ_2, and ζ_3 are encountered for the regular structure (10) with equal probability, the distribution function $W(\zeta)$ normalized to unity can be represented for such a configuration in the form

$$W(\zeta) = {}^1/_3 \sum_{i=1}^{3} \delta(\cos\zeta - \cos\zeta_i), \qquad \sum_{i=1}^{3} \cos\zeta_i = -1. \qquad (19)$$

The values of $\cos\zeta_i$ determine uniquely the type of structure of the degenerate state. The parameters χ and ψ, the change of which does not change the energy of the ground state, are connected with ζ_i in accordance with (18) in the following manner:

$$\cos 2\chi = (\cos\zeta_1 - \cos\zeta_2)/(1 - \cos\zeta_3), \qquad \psi = \zeta_3/2. \qquad (20)$$

In the general case of a vortex structure, the distribution function $W(\zeta)$ differs from zero at three points ζ_i at which

$$g(\zeta_i) = \int_{\zeta_i - \varepsilon}^{\zeta_i + \varepsilon} W(\zeta) \sin\zeta \, d\zeta = {}^1/_3, \qquad (21)$$

where $\epsilon \to 0$. In those cases, however, when the degeneracy parameters satisfy the condition $\cot \psi = \sin\chi$, the two points ζ_2 and ζ_3 coalesce into one, and consequently $g(\zeta_i)$ differs from zero only at two points, with $g(\zeta_2) = 2g(\zeta_1)$. For a "fanfold structure" corresponding to a state with two antiferromagnetic sublattices, $W(\zeta)$ has two values that are symmetrical about $\zeta = \pi/2$, and one at the point $\zeta = \pi$. For an antiferromagnetic structure with the filaments directed along an arbitrary axis, the nonzero values of $W(\zeta)$ are at the points $\zeta_i = 0$ and $\zeta_i = \pi$, with $g(0) = 1/3$, $g(\pi) = 2/3$.

For a finite number of particles and as a result of the destruction of the vortex (10), smearing of the distribution function $W(\zeta)$ should take place on the boundary. In the case of strong smearing of $W(\zeta)$ it is convenient to identify the vortex structure by the function $W_2(\xi)$ of the distribtuion of the angles between the dipole orientations at sites separated by a distance 2a. For the ground state of an infinite sample $W_2(\zeta)$ differs from zero only at the point $\zeta = 0$.

4. RESULTS OF NUMERICAL EXPERIMENT

The main questions faced in the computer experiment were the investigation of the energy, configuration, and degeneracy of the ground state on going from a cubic cluster to a spherical sample of a simple cubic lattice. Besides the influence of the finite dimensions and of the shapes of the samples, we investigated the configurations and energies of metastable states that have no translational symmetry with respect to orientations of dipoles with period 2a.

The dipole-moment configurations with minimum energy were determined by the method of molecular dynamics, using the system of relaxation equations (17). In Table I is given the ground-state energy per particle for lattice clusters inscribed in a sphere. The dipole moments were located at the sites of a simple cubic lattice, the origin was chosen at the center of the sphere, and the coordinate system was oriented along the crystallographic axes. The system energy and the local fields were calculated by summing the paired dipole-dipole interactions over all the lattice sites, and no conditions whatever were imposed on the sample boundary (free boundary). The final configuration was taken to be a structure satisfying the local-minimum condition.

TABLE I. Ground-state energy of lattice clusters inscribed in a sphere.

Number of dipoles in sample	Energy per particle in units of P_0^2/a^3	Total dipole moment of cluster per particle, in units of P_0	Number of coordination sphere
8	−1.82	$3.1\cdot10^{-4}$	1
32	−1.95	$4\cdot10^{-5}$	2
56	−2.12	$1.2\cdot10^{-4}$	3
88	−2.2	$3.7\cdot10^{-2}$	4
304	−2.44	$1\cdot10^{-4}$	9
968	−2.58	$2.6\cdot10^{-5}$	19
∞	−2.68	0	

The orientations of the dipoles of a cubic cluster of eight particles relaxed to the ground state (10) independently of the initial configurations, which were chosen regular as well as random. No metastable configurations were observed, the energies of all the states coincided and were equal to $-1.82P_0^2/a^3$ (see Table I and Sec. 2), and all the final configurations were degenerate with respect to one variable and satisfied the conditions (14). We note that in the final configuration the orientations of dipoles located at the sites of the principal diagonal of the cube coincided.

Subsequent minimization with respect to the coordination spheres has shown that the appearance of degeneracy in the second variable [the lifting of condition (14)] appears in practice already in the transition from $N = 56$ to $N = 88$, i.e., in a sample with four coordination spheres. This corre-

TABLE II. Final states of spherical sample ($N = 304$) for different initial states.

Initial configuration	Energy in units of P_0^2/a^3	Final configuration	Energy in units of P_0^2/a^3	Type of finite state
Cylindrical*	−1.96	cylindrical mixed: anti-	−1.99	metastable
Anticylindrical	−2.28	cylindrical + vortical	−2.33	?
Radial	3.88	two domains with vortical structure	−2.33	metastable
Helicoidal with period 4a	−2.21	vortical $\chi=40°$, $\psi=75°$	−2.43	ground
Ferromagnetic	0	vortical $\chi=30°$, $\psi=70°$	−2.41	»
Antiferromagnetic	−2.38	antiferromagnetic	−2.44	»
Fanfold $\chi=30°$, $\psi=90°$	−2.37	fanfold $\chi=30°$, $\psi=90°$	−2.44	»
Random	−0.03	fanfold $\chi=36°$, $\psi=74°$	−2.42	ground

*For the definition of the configuration see the text.

sponds physically to the fact that the configuration of the ground state of the final sample can be broken up into an internal volume, where the orientations of the dipoles correspond to configurations of an infinite three-dimensional lattice (degeneracy in two parameters), and on the boundary surface, where the orientations of the dipoles recall the distribution of vortices in an infinite two-dimensional sample (degeneracy in one variable in the plane of a disk). The transition region from the inner volume to the boundary is blurred and contains from two to three coordination spheres. Since the directions of the dipoles and the fields coincide in the ground state, the corresponding surface and volume distributions of the local fields are formed already in a cluster with four coordination spheres.

A histogram of the distribution function $W(\zeta)$ for a vortex configuration of the ground state of the dipole Hamiltonian shown in Fig. 2a. The dashed histogram in this figure shows the values of $W(\zeta_i)$ for the initial vortex structure ($\psi = 45°, \chi = 30°$). The smearing of the distribution function $W(\zeta)$ is due to the restructuring of the orientation of the dipoles in the transition region and on the boundary.

The numerical experiment revealed several metastable states, on which we shall dwell in greater detail. In the initial configuration the dipole moments located in the xy plane perpendicular to the radius vector joining the z axis with the given site. For a cylindrical configuration the dipoles are parallel in planes perpendicular to the z axis, and for the anticylindrical—in the opposite direction. In these configurations the orientation of the dipole moments forms a system of parallel and antiparallel coaxial vortices. Since in both cases the field directions at the sites coincided with orientations of the dipoles inside the sphere, the change in energy upon minimization (Table II) is connected only with the reorientation of the dipoles on the boundary. In addition to the coaxial vortices, notice must be taken of the existence of a high density of local vortices (or diameter a) in the anticylindrical structure; this explains the low energy of this state.

In the radial initial configurations all the moments were oriented along the radius-vector of the corresponding sites. The high energy of this state is due to the fact that in each site the field and the dipole are oppositely directed. The relaxation from the radial initial configuration into the final one has lead to division of the sphere into two regions with almost vortical structure in each. The regions are separated by a plane passing through the center and directed perpendicular to one of the crystallographic axes. In the nearest planes, where the lattice sites are located, the vortex directions are parallel. The barrier connected with transition of this configuration into the ground state is due to the appearance of stability of the separating plane.

The orientations of the dipoles in the initial helicoidal configuration were specified in the following manner:

$$P_{hkl}^{x}=P_0\cos(\pi l/2), \quad P_{hkl}^{y}=P_0\sin(\pi l/2), \quad P_{hkl}=0.$$

It can be seen from these expressions that the period of the initial state was equal to 4a along the z axis. Minimization of this configuration led to a ground state having a vortical structure with period $2a$ inside the sphere. Figure 2b shows a histogram of the final distribution function $W(\zeta)$, from

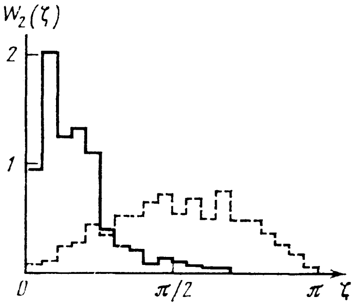

FIG. 3. Histograms of the distribution functions $W_2(\zeta)$ of the angles between the orientations of dipoles separated by a distance $2a$. The dashed and solid histograms show respectively $W_2(\zeta)$ for the initial random configuration and for the final vortial structure.

which it can be found in accord with Eqs. (20) that $\psi \approx 75°$ and $\chi \approx 40°$ (see Table II). It must be noted that relaxation from a ferromagnetic state with period a and from random nonperiodic initial configuration (Fig. 3) also led to a vortex structure with period $2a$. If partial configurations of the ground state (antiferromagnetic and fanfold) were specified, they did not change in the process of minimization inside the sphere (see Table II). The difference between the energies of their initial and final configurations is due to alignment of the directions of the boundary dipoles.

The numerical experiments confirm fully the analytic results of Secs. 1 and 2. The main regularity in the formation of the ground state in finite samples is the appearance of vortical configurations.

CONCLUSION

We investigated equilibrium configurations of magnetic or electric dipoles placed at the sites of a simple cubic lattice.

Analytic solutions for an infinite three-dimensional crystal or along corresponding directions of a low-dimensional crystal were sought, as in Ref 1, in the class of solutions having translational symmetry with period $2a$. It was shown that the general solution in this class is the solution (10), consisting of four sublattices whose dipole moments for a vortex structure (see Fig. 1) that is degenerate in two parameters. The antiferromagnetic state obtained in Ref. 1 is a particular case of this vortex structure (corresponding to a two-sublattice model), not different in energy from the other vortex-structure configurations.

We also investigated analytically the simplest low-dimensional crystals and finite clusters of 8 and 12 particles. By low-dimensional crystal is meant here a disk of infinite diameter and one layer thick (two-dimensional crystal) or a rectangle of infinite length with base $a \times a$ ("one-dimensional" crystal). The solution was sought in the class of four-sublattice vortex structures of the type (10), having a period $2a$ along the axes corresponding to the infinite dimension of the crystal. For a two-dimensional crystal, the degeneracy is lifted with respect to one parameter—the axis of the magnetic dipoles lies in the plane of the disk ($\psi = \pi/2$); a vortex structure with arbitrary value of the angle χ is preserved in the plane. For the one-dimensional crystal the degeneracy in

χ is lifted: The dipole moments lie along the axis of the one-dimensional crystal, forming an antiferromagnetic structure.

Corresponding to the minimum energy for a finite cluster (a unit cell consisting of eight particles) is a configuration in which χ and ψ are uniquely interconnected. Thus, not all vortex structures that are possible in an infinite crystal can be realized in such a cluster; in particular, the constraint (14) forbids formation of an antiferromagnetic structure. However, the addition of one face with four dipoles to the cube (cluster $a\times a\times 2a$) leads to a situation in which antiferromagnetic ordering becomes convenient.

We performed also a numerical experiment by the molecular-dynamics method for finite systems of 8 to 88, 304, and 968 particles (see Table I), located at the sites of a simple cubic lattice inscribed in a sphere of the appropriate diameter. We specified some initial configuration of the dipoles and the system relaxed to a minimum (to one of the minima). By specifying different initial configurations and calculating the energy of each final configuration, it was possible to classify with sufficient probability the final configurations as belonging to the ground or to one of the metastable states. The numerical experiment had two aims in mind.

First, as indicated above, the obtained analytic solution (10) is general in a class of structures that are periodic with a period $2a$. It is natural to ask whether some solutions that do not satisfy this condition exist. Second, it was of interest to trace the influence of the finite nature of the system on the character of the ground-state configurations.

The numerical experiments have shown that the final states whose energy is close to the global minimum always have a sufficiently clearly pronounced period 2a, regardless of their initial state (stochastic initial structure, structures with period a, 4a, etc.) This is evidence of the stability of the obtained ground state. In one case (radially symmetric initial state) this law was violated, but only on one plane (of the type of a disclination plane or a domain wall) that divides the sphere in half; in each hemisphere the solution had a clearly pronounced period $2a$. Metastable states, however, did not satisfy this condition. All the investigated excited states, structures with macroscopic inhomogeneities, and metastable configurations always had an energy higher than the energy of the vortex lattice. Consequently, within the framework of the numerical experiment the ground state of the dipole system on a simple cubic lattice is stable to long-wave fluctuations of the degeneracy parameters.

As for the influence of the surface, it manifested itself in formation of a "skin layer" one or two lattice constants thick, in which the character of the configurations of the dipoles, remaining vortical, differed substantially from the configuration in the remaining volume of the sphere, where the configuration of the ground state was always close to the periodic vortex structure (10) typical of an infinite sample. Such a limited influence of the surface is due to the fact that the vortex structure, closing the magnetic (electric) fluxes in small volumes, leads to a strong screening of the dipole interaction, so that the latter lose to a considerable degree their long-range properties.

Thus, both the analytic calculations and the numerical experiment show that the ground state of a system of dipoles corresponds to configurations with largest possible number of vortices (closed force lines and field intensity) arranged with a minimum possible period.

The authors thank M. Sh. Erukhimov, A. I. Kruglik, and V. I. Ponomarev for useful discussions.

[1]J. M. Lattinger and L. Tisza, Phys. Rev. **70**, 954 (1946); 72, 257 (1947).
[2]V. G. Pakazan'ev, G. V. Skrotskii, and L. I. Yakub, Usp. Fiz. Nauk **116**, 485 (1975) [Sov. Phys. Usp. **18**, 583 (1975)].
[3]A. V. Gavrilova, Yu. D. Tyapkin, and M. P. Usikov, Dokl. Akad. Nauk SSSR **176**, 1052 (1967) (Sov. Phys. Dokl. **11**, 970 (1967)].
[4]I. A. Favorskiĭ, Fiz. Tverd. Tela (Leningrad) **22**, 2222 (1980) [Sov. Phys. Solid State **22**, 1296 (1980)].
[5]L. M. Blinov, Usp. Fiz. Nauk **114**, 65 (1974) [*sic*].
[6]E. Lagendijk, H. W. J. Blöte, and W. J. Huiskamp, Physica **61**, 220 (1972).
[7]R. S. Gekht, V. A. Ignatchenko, Izv. AN SSR ser.fiz. **44**, 1362 (1980); Fiz. Nizk. Temp. **7**, 1176 (1981) [Sov. J. Low Temp. Phys. **7**, 571 (1981)].

Translated by J. G. Adashko