

# Incommensurate and aperiodic structures in frustrated antiferromagnets with hcp lattices

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We investigate magnetic states and phase transitions in anisotropic magnets with hexagonal close-packed (hcp) lattices. We show that the effects of frustration in these lattices lead to instability at the conical point: in place of the well-known  $120^\circ$  structure there appears an incommensurate structure which is continuously degenerate both with respect to the orientation of the wave vector in the basal plane and with respect to its magnitude (i.e., structures with inequivalent spirals). In antiferromagnets with the "easy plane" type of anisotropy, incommensurate configurations arise in the low-temperature region. In the presence of the "easy axis" type of anisotropy, at intermediate temperatures antiferromagnets can support incommensurate states with well-developed short-range order. As the temperature decreases, long-range order in the incommensurate structures arises only for small values of the anisotropy constant  $D$ ; if  $D$  is larger than a critical value, a frozen-in aperiodic structure forms in the low-temperature region. We also investigate the effects of additional interactions which lift the degeneracy of the structures in the ground state.

## 1. INTRODUCTION

At this time it is well known that the effect of frustration plays an important role in various magnetic systems. In particular, antiferromagnets with triangular lattices are typical examples of such frustrated spin systems, where the frustration manifests itself in many properties which differ from the corresponding unfrustrated systems. These differences are reflected above all in the rich variety of phases and phase transitions exhibited by such systems, along with their high frustration-induced sensitivity to various kinds of perturbing interactions. It is found that one effect of these perturbations is to make possible structures which originate with instabilities at high-symmetry points of the Brillouin zone in addition to the other structures which appear in these antiferromagnets.

In triangular antiferromagnets, which, in contrast to the usual systems, admit the existence of either Lifshits invariants which are linear in a derivative<sup>1</sup> or of competing exchange interactions,<sup>2</sup> such instabilities can arise because of the weak dipole forces. Just this situation is realized in the hexagonal magnet  $\text{RbFeCl}_3$  (Refs. 3,4), whose spectrum of excitations is degenerate at the conical point  $K$ ; in addition, this spectrum contains discontinuities<sup>5</sup> in one of the two intermediate states (i.e., in states with a twinned incommensurate structure).

Not long ago, interesting neutron and magnetic measurements<sup>6-8</sup> were carried out on compounds whose crystal lattices consist of two interpenetrating simple hexagonal lattices [i.e., antiferromagnets with hexagonal close-packed (hcp) lattices]. All of these compounds are characterized by strong antiferromagnetic interactions in the plane of the triangular lattice and weak exchange interactions between neighboring (different type) planes. In these compounds an instability at the conical point is also possible; however, the mechanism for producing it is different. As an example we note the hcp-like antiferromagnet  $\text{Cs}_2\text{Cr}_2\text{Br}_9$ , for which the

dispersion curves<sup>6</sup> near the symmetry point  $K$  have a clearly-expressed minimum; in contrast to the dipole mechanism, the frequency spectrum at the minimum points is continuously degenerate.

The topic of this paper is the investigation of possible spin structures in antiferromagnets with hcp lattices. We will investigate the stability of various structures as a function of the magnitude of the interplane interaction  $J'$  and the values of the single-ion anisotropy  $D$ . In simple hexagonal lattices with one type of layer,  $J'$  can stabilize the spin configuration,<sup>9</sup> while the "easy-axis" type of anisotropy leads to the appearance of two phase transitions as the temperature decreases; the first of these is connected with ordering of the longitudinal component of the spin, while the second is connected with ordering of its transverse component.<sup>10</sup> At the same time, in antiferromagnets with hcp lattices consisting of two types of layers, the noncollinear structures which form are found to be unstable against an arbitrarily small interplanar interaction  $J'$ . This circumstance is closely tied to the fact that the systems investigated here are frustrated not only in the plane but also in the third dimension; in this new direction the frustration is independent of the sign of  $J'$ . However, the presence of an easy-axis anisotropy in these frustrated systems does not lead to the appearance of structures with long-range order at intermediate temperatures: in place of these, structures form with well-developed short-range order. Also, structures with long-range order whose period is incommensurate with the lattice period only appear at low temperatures. For values of  $D$  above critical, modulated structures do not appear even in this low-temperature region: in this case, it is found that in almost all cases the state which appears has no particular period (i.e., the phase is aperiodic).

In what follows, rather than investigating these spin structures at  $T \neq 0$  with anisotropy included, we will first discuss the question of spin configurations in the ground state, described for hcp lattices by the Hamiltonian

$$\mathcal{H} = - \sum_{r,r'} J(\mathbf{r}-\mathbf{r}') \mathbf{S}_r \mathbf{S}_{r'} - \sum_{R,R'} J(\mathbf{R}-\mathbf{R}') \mathbf{S}_R \mathbf{S}_{R'} - J' \sum_{r,R} \mathbf{S}_r \mathbf{S}_R, \quad (1)$$

where  $\mathbf{S}_r$  and  $\mathbf{S}_R$  correspond to spins on alternate hexagonal lattices;  $J(\mathbf{r}-\mathbf{r}') = J_1$  for nearest-neighbor spins in the basal plane, and  $J(\mathbf{r}-\mathbf{r}') = J_2$  for the next-nearest neighbor spins [for the remaining cases,  $J(\mathbf{r}-\mathbf{r}') = 0$ ]. If  $J_1 < 0$ , but  $J' = 0$  and  $J_2 = 0$ , then the ground state of the system consists of three magnetic sublattices turned successively by  $120^\circ$  (the  $120^\circ$  structure). It is well known that this two-dimensional magnetic system [with spatial order parameter  $V = SO(3)$  where  $SO(3)$  is the three-dimensional rotation group] undergoes a phase transition at a temperature  $T_N = 0.33|J_1|$  (Ref. 11).

## 2. INSTABILITY AT HIGH-SYMMETRY POINTS; CONTINUOUS DEGENERACY

In this section we will discuss the possible spin structures for  $J' \neq 0$ . In the ground state (and also below the transition point to the paramagnetic phase) these structures can be determined by finding the minimum eigenvalue and eigenfunction of the Fourier components of the exchange interaction, i.e.,

$$A_{\alpha\beta}(\mathbf{Q}) = -(J_1(\mathbf{Q}) + J_2(\mathbf{Q})) \delta_{\alpha\beta} - J'(\mathbf{Q}) \delta_{\alpha+1\beta} - J'(-\mathbf{Q}) \delta_{\alpha\beta+1} \quad (2)$$

(the subscripts  $\alpha, \beta = 1, 2$  correspond to spins located at the nodes of the two different types of layers of the hcp lattices). Choosing the direction of the  $x$  axis along the elementary translation vector  $\mathbf{a} = a(1, 0, 0)$ , we find

$$\begin{aligned} J_1(\mathbf{Q}) &= J_1 [\cos Q_x + \cos(Q_x/2 + 3^{1/2} Q_y/2) + \cos(Q_x/2 - 3^{1/2} Q_y/2)], \\ J_2(\mathbf{Q}) &= J_2 [\cos 3^{1/2} Q_y + \cos(3Q_x/2 + 3^{1/2} Q_y/2) \\ &\quad + \cos(3Q_x/2 - 3^{1/2} Q_y/2)], \\ J'(\mathbf{Q}) &= J' \{ \exp(i3^{-1/2} Q_y) + \exp[-i(Q_x/2 + 3^{-1/2} Q_y/2)] \\ &\quad + \exp[i(Q_x/2 - 3^{-1/2} Q_y/2)] \} \cos(Q_x/2) \end{aligned} \quad (3)$$

(the lattice parameters  $a$  and  $c$  are set equal to unity). The eigenvalues  $\lambda_{\pm}(\mathbf{Q})$  and the eigenvector  $\mathbf{S}_{\pm}(\mathbf{Q})$  of the matrix (2) are represented in the following way:

$$\begin{aligned} \lambda_{\pm}(\mathbf{Q}) &= -J_1(\mathbf{Q}) - J_2(\mathbf{Q}) \pm |J'(\mathbf{Q})|, \\ \mathbf{S}_{\pm}(\mathbf{Q}) &= [\mathbf{S}_1(\mathbf{Q}) \pm e^{-i\varphi(\mathbf{Q})} \mathbf{S}_2(\mathbf{Q})] / 2^{1/2}, \end{aligned} \quad (4)$$

where  $\varphi(\mathbf{Q}) = \arg J'(\mathbf{Q})$ .

First, let the interaction between next nearest neighbors be  $J_2 = 0$ . Then from the condition that the function  $\lambda_{-}(\mathbf{Q})$  be a minimum with respect to  $\mathbf{Q}$  we obtain the equation for the equipotential curves:

$$\cos(Q_x/2) [\cos(Q_x/2) + \cos(3^{1/2} Q_y/2)] = (|j'|^2 - 1)/4, \quad Q_z = 0, \quad (5)$$

( $j' = J'/J_1$ ). From this it is clear that for  $j' = 0$ , then, as ought to be the case, we have a state with  $120^\circ$  structure which corresponds to any of the six equivalent points  $(\pm 4\pi/3, 0)$  and  $(\pm 2\pi/3, \pm 2\pi/3^{1/2})$ . For an arbitrarily small but nonzero  $j'$  these points, which are the symmetry

points  $K$ , are unstable: the smallest eigenvalue (independent of the sign of  $j'$ ) appears on a circle of radius  $2|j'|/3^{1/2}$  around each of these points, so that in this case there exists a spiral state which is infinitely degenerate relative to the orientation of the wave vector in the plane  $Q_x, Q_y$ . However, in the neighboring layers of the hcp lattice this spiral state is shifted in phase ( $\varphi \neq 0$ ). As  $|j'|$  increases the circles are transformed, and the state becomes degenerate not only with respect to the orientation of the modulation wave vector, but also with respect to its magnitude. For  $|j'| = 1$  the degeneracy curves determined by (5) have the form of triangles; the sides of each of these triangles lie along any three of the six straight lines:

$$Q_x = \pm\pi, \quad \pm Q_x \pm 3^{1/2} Q_y = 2\pi. \quad (6)$$

In this case, the vertices of the triangles are at the symmetry points  $M$ , corresponding to a structure with an antiparallel arrangement of the spins along one of the three equivalent directions in the basal plane. A further increase in  $|j'|$  transforms the degeneracy lines into curves whose form in the limit  $|j'| \rightarrow 3$  is again a set of circles. The centers of these circles, whose radii are  $[6(1 - |j'|^2/9)]^{1/2}$ , now lie at the  $\Gamma$  points of the Brillouin zone:  $(0, 0)$ ,  $(0, \pm 4\pi/3^{1/2})$ ,  $(\pm 2\pi, \pm 2\pi/3^{1/2})$ . For  $|j'| \geq 3$  these points correspond to uniform states on a triangular lattice. In Fig. 1a we show equipotential curves for various values of  $|j'|$ . These lines resemble the distribution of the effective exchange field for the intermediate nonuniform state, i.e., the state analogous to a type I superconductor, in  $\text{FeCO}_3$  (see Ref. 12); they also resemble the picture of force lines of a two-scale vortex structure in dipole systems.<sup>13</sup>

Inclusion of additional interactions in the basal plane leads to lifting of the continuous degeneracy along curve (5). Thus, even for small but nonzero values of  $J_2$  the wave vector of the spiral is fixed. In this case the eigenvalues  $\lambda_{\pm}$  in the neighborhood of the  $K$  point ( $|j'| \ll 1$ ) are given by the following expression:

$$\lambda_{\pm}(\mathbf{Q}_k + \mathbf{q}) = -^{3/2}|J_1| - 3J_2 \pm 3^{1/2}|J'|q/2 + ^{3/4}(3J_2 + |J_1|/2)q^2 + ^{1/16}(3^{1/2}|J_1| \pm 2|J'|/q_0)q_x(3q_y^2 - q_x^2). \quad (7)$$

Here  $\mathbf{Q} = \mathbf{Q}_k + \mathbf{q}$ , where  $\mathbf{Q}_k = (4\pi/3, 0, 0)$ ,  $q^2 = q_x^2 + q_y^2$ . Taking into account the cubic terms in  $\mathbf{q}$  in the expansion (7), the smallest eigenvalue  $\lambda_{-}(\mathbf{Q})$  is localized at the three equivalent points  $\mathbf{Q}_1$ , which are at a distance  $q_0 = 2|j'|[3^{1/2}(1 + 6J_2/|J_1|)]^{-1}$  from the point  $\mathbf{Q}_k$ . In Fig. 1b we show the equipotential lines  $\lambda_{-}(\mathbf{Q})$  near the point  $\mathbf{Q}_k$  for the case  $J_2 < 0$ . The minimum points are separated from each other by barriers whose maximum value is attained at the saddle points  $\mathbf{Q}_2$ . For  $J_2 > 0$  the positions of the characteristic points change places, i.e., where there were saddle points minimum points appear, and conversely where there were minimum points saddle points appear. In the limit  $J_2 = 0$  the coefficient of the cubic powers in  $\mathbf{q}$  for  $\lambda_{-}(\mathbf{Q})$  in (7) reduces to zero, so that the smallest eigenvalue appears on a circle, as it should.

## 3. EFFECT OF ANISOTROPY; SPIN STRUCTURES

In the presence of a single ion anisotropy energy  $E_a = -D\Sigma_i(S_i^z)^2$ , the ground state of the system depends significantly on the sign and magnitude of the anisotropy constant  $D$ . Thus, for  $D < 0$ , the spins are polarized in the

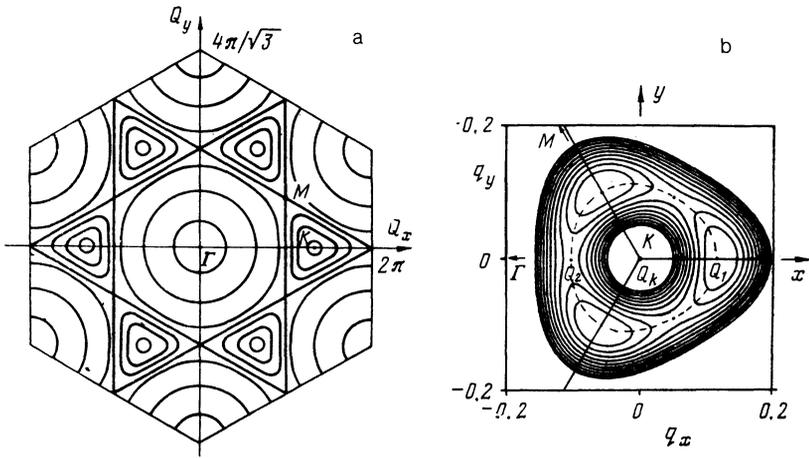


FIG. 1. a—Equipotential curves corresponding to the energy minimum for various values of  $J'$  ( $0 < |J'| < 3, J_2 = 0$ ); b — contours of  $\lambda_-(\mathbf{Q})$  in the neighborhood of the conical point for  $J_2 < 0 (|J_2| \ll |J_1|)$ .

basal plane and the structure which arises is described by a spatial dependence of the magnetic moment vector identical to that of the structures obtained in the previous section, i.e., its period is incommensurate with the lattice period. It is obvious that these structures correspond to states which lie near the points of transition to the paramagnetic phase ( $T \lesssim T_1$ ). In the other case, where  $D > 0$ , the spins lie in a vertical plane; because of the condition that the absolute value of the local magnetic moment be conserved, the ground state may differ strongly from the state which forms at  $T \lesssim T_1$ . As for structures which are close to collinear, this circumstance renders their existence with a modulation vector  $\mathbf{q}$  in the low-temperature region less likely.

In the limiting case of large values of  $D (> 0)$ , i.e., of Ising-like spins, the ground state has a degeneracy of  $2^R$ , where  $R = N^{1/2}$  (Ref. 14). Two of these degenerate states with energy per spin

$$E/N = -|J_1| - J' - D \quad (8)$$

( $J' > 0, J_2 = 0$ ) are shown in Figs. 2a, 2b. Conversely, in the region of small  $D (> 0)$  a long-period state becomes preferred, whose energy for  $|J'| \ll |J_1|$  is close to the energy of the three-sublattice structure. The latter can be found by minimizing the expression

$$\begin{aligned} \mathcal{H}/N = & \frac{1}{2} \sum_{\substack{\alpha, \beta: \\ m, n}} [ |J_1| \delta_{\alpha\beta} - \frac{1}{3} J' (\delta_{\alpha\beta-1} + \delta_{\alpha-1\beta}) ] \cos(\theta_\alpha^{(m)} - \theta_\beta^{(n)}) \\ & - \frac{1}{2} D \sum_{\alpha, m} \cos^2 \theta_\alpha^{(m)} - |J_1|, \quad (J_2 = 0), \end{aligned} \quad (9)$$

obtained from (1) by including the fact that the stable configurations are, as in the simple hexagonal lattices,<sup>9</sup> planar ( $m, n = 1, 2, 3$  are the indices of the magnetic sublattices, whose angle  $\theta$  is defined in the interval  $[0, 2\pi]$  in the vertical plane; the lower indices  $\alpha, \beta = 1, 2$ , as previously, label the types of layers in the hcp lattice). The planar configuration, which is degenerate with respect to the azimuthal angle, has the smallest (for  $\mathbf{Q} = \mathbf{Q}_k$ ) value of the energy if the angles of the sublattices are given in the following way:  $\theta_\alpha^{(1)} = -\theta_\alpha^{(2)} = \theta, \theta_\alpha^{(3)} = \pi$ ; the angle  $\theta$  measured from the  $c$ -axis is determined by the expressions

$$\cos \theta = \frac{3|J_1| - 2J'}{2(3|J_1| - D - 2J')}, \quad D \leq D_{II}; \quad (10)$$

$$\theta = 0, \quad D \geq D_{II}, \quad (11)$$

where  $D = 3/2|J_1| - J'$ . To the noncollinear structures there correspond the energies

$$E/N = -|J_1| - \frac{J' + D}{3} - \frac{(3|J_1| - 2J')^2}{6(3|J_1| - D - 2J')}; \quad D \leq D_{II} \quad (12)$$

and

$$E/N = -|J_1| - J'/3 - D, \quad D \geq D_{II}. \quad (13)$$

If  $D = 0$  in (10), then  $\theta = \pi/3$ ; consequently, the angle between any two sublattices equals  $2\pi/3$ . Thus we have a  $120^\circ$  structure (Fig. 2c), as we should, whose energy in (12) does not depend on the interplanar interaction  $J'$ , while its value

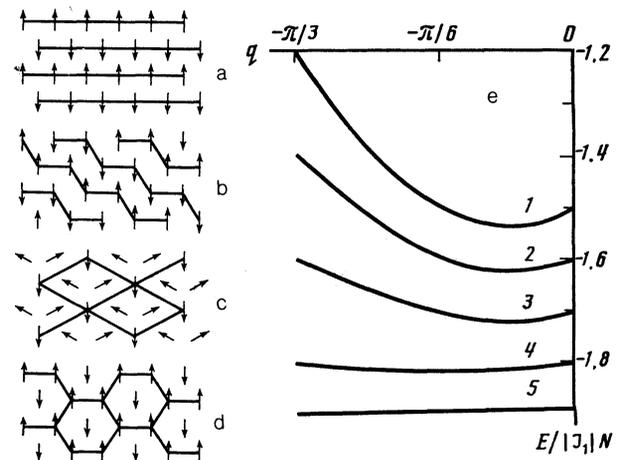


FIG. 2. a, b, c, d—Spin structures on a triangular lattice ( $J_1 < 0, J_2 = 0$ ): ground state for  $D > D_c, J' = 0$  (a, b) and  $D < 0, J' = 0$  (c); collinear structure  $\sqrt{3} \times \sqrt{3}$  (d); 3—dependence of the energy  $E$  on the modulation wave vector  $\mathbf{q} = \mathbf{Q} - \mathbf{Q}_k$  for various values of  $D (D > 0, \mathbf{Q}$  parallel to the translation vector  $\mathbf{a} = a(1, 0)$ ): 1— $D/|J_1| = 0$ ; 2— $D/|J_1| = 0.2$ ; 3— $D/|J_1| = 0.4$ ; 4— $D/|J_1| = 0.6$ ; 5— $D/|J_1| = 0.7$ .

$E/N = -3|J_1|/2$  coincides with the analogous expression for  $\lambda_-(\mathbf{Q}_k + \mathbf{q})$  from (7) for  $q = 0$  (and  $J_2 = 0$ ). As  $D$  increases the angle  $\theta$  decreases; for  $J' = 0$  and  $D \gg D_{11}$ , the state with the two interwoven sublattices in Fig. 2d has the same energy as the state shown in Figs. 2a, 2b. However, for  $J' > 0$  the state with noncollinear structure has higher energy (12) compared to the energy (8) of the degenerate states, if  $D$  exceeds a threshold value  $D_c$  (smaller than  $D_{11}$ ):

$$D_c = \frac{3}{2}(|J_1| - J') - (\frac{3}{2}J'|J_1|)^{1/2}, \quad J' \ll |J_1|. \quad (14)$$

Now let the wave vector  $\mathbf{Q}$  be unfixed. For  $D \lesssim D_c$ , the dependence of  $E$  on  $\mathbf{q} = \mathbf{Q} - \mathbf{Q}_k$  (Fig. 2d) has a minimum near the conical point  $K$  of the Brillouin zone, and conversely for  $D \gtrsim D_c$  the minimum of  $E(\mathbf{q})$  is realized at the symmetric  $M$  point [ $\mathbf{q} = (-\pi/3, 0)$ , i.e., the state in Fig. 2a].

Based on these results, we should expect the following picture of the spin ordering. In the region  $D < 0$ , when the easy-plane type of anisotropy is realized, the long-period structures which appear have the same form both at  $T = 0$  and below the transition point to the paramagnetic phase  $T_1$ . Therefore, in this case we should expect a unique phase transition with the appearance for  $T < T_1$  of a modulated structure in which the spins are polarized in the basal  $xy$  plane.

In the other region, where the easy-axis type of anisotropy is realized ( $D > 0$ ), the spin configurations are located in the vertical plane. Therefore two situations are possible here. The first is when  $0 < D < D_c$ . In this region of values of  $D$  the spins of the modulated structures are not collinear at  $T = 0$ . Therefore, these systems behave like systems where purely commensurate structures are realized<sup>10</sup>: as the temperature  $T$  decreases there should first appear correlations in the longitudinal components of the spin and only then, at lower temperatures, do correlations appear in the transverse components. Therefore, as the temperature decreases we should expect no more than two characteristic points at which a change occurs in the spin structure. In the second case ( $D > D_c$ , when only the longitudinal spin component is nonzero in the ground state, there also should exist two characteristic points. One of these points should be related to the development of correlations in structures with incommensurate period, while the other — in contrast to the first case ( $0 < D < D_c$ ) — is associated with the necessity for reconstruction of this structure, since it is different from the structures which occur at  $T = 0$  (Figs. 2a, 2b).

A numerical investigation of the magnetic state of the phases for various temperatures and values of the anisotropy (carried out using Monte Carlo methods) confirms the basic stages in the process of spin ordering mentioned above. Thus, in the presence of easy-plane anisotropy ( $D < 0$ ) there actually exists only a single phase transition at the point  $T_1$ . At this point the wave vector of the structure varies discontinuously from  $\mathbf{Q} = \mathbf{Q}_k$  to  $\mathbf{Q} = \mathbf{Q}_k + \mathbf{q}$ . The energy and other physical quantities also vary discontinuously, which is obviously connected with the sudden reconstruction of the structure from one period to another.

For the other sign of the anisotropy ( $D > 0$ ) the behavior of the system, as might be expected, is different for  $D < D_c$  and  $D > D_c$ . In Figs. 3a, 3b, and 3c, for the case  $D = 0.2|J_1|$ ,  $J' = 0.2|J_1|$ ,  $D_c = 0.65|J_1|$ , we display the Fourier spectrum of the total spin  $\mathbf{S}(\mathbf{Q})$  for  $\mathbf{Q}$  oriented along an elementary translation vector of the triangular lattice. As

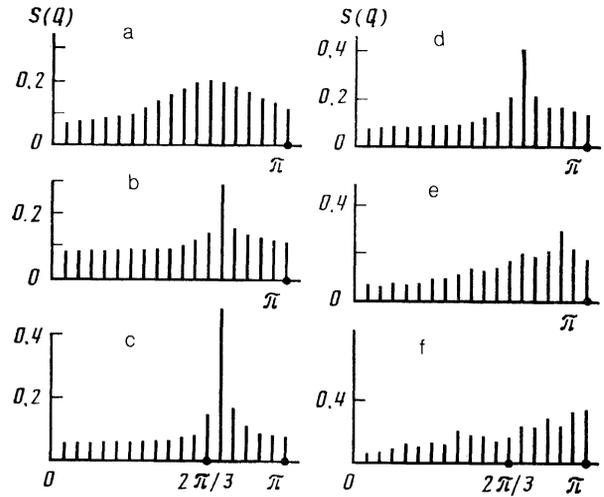


FIG. 3. Fourier spectrum of the magnitude of the vector  $\mathbf{S}(\mathbf{Q})$  for various values of the anisotropy  $D (> 0)$  and temperature  $T$  ( $J' = 0.2$ ;  $J_2 = 0$ ): a, b, c —  $D/|J_1| = 0.2$  and  $T = 0.4|J_1|$  (a),  $T = 0.3|J_1|$  (b),  $T = 0.2|J_1|$  (c); d, e, f —  $D/|J_1| = 1.2$  and  $T = 0.5|J_1|$  (d),  $T = 0.3|J_1|$  (e), and  $T = 0.04|J_1|$  (f).

the temperature decreases from the region where the spin is entirely paramagnetic, the first type of order to appear is short-range order in the various layers of the hcp lattice; this order is characterized by the wave vector  $\mathbf{Q}_k = (4\pi/3, 0, 0)$  [Fig. 3a; because of the condition  $S(\mathbf{Q}) = S(2\pi - \mathbf{Q})$  the value  $\mathbf{Q} = 2\pi/3$  corresponds to this point]. A further decrease in temperature leads to the appearance of a modulation vector  $\mathbf{q} = \mathbf{Q} - \mathbf{Q}_k$  in the basal plane (Fig. 3b), so that as a result short-range order is realized along all three spatial directions. Associated with the development of short-range correlations are anomalies (weakly expressed compared to the usual phase transitions) in the behavior of the heat capacity around the point  $T_1$ . Below this point, at first only the  $S^z$  components of the spin contribute to the magnitude of the peak in  $\mathbf{S}(\mathbf{Q})$  with  $\mathbf{Q} = \mathbf{Q}_k + \mathbf{q}$ ; however, after the temperature point  $T = T_2$  is reached, at which the heat capacity also has an anomaly, the magnitude of the peak in  $\mathbf{S}(\mathbf{Q})$  is also determined by the transverse spin components (Fig. 3c). At the point  $T = T_2$  long-range order appears, in this case not only for the spin components but also for the so-called chiral vector  $\mathbf{k}$ , which is given by the relation<sup>15</sup>

$$\mathbf{k} = 2 \cdot 3^{-1/2} \{ [S_m S_n] + [S_n S_l] + [S_l S_m] \}, \quad (15)$$

taking into account normalization of its modulus to unity; here  $m, n$ , and  $l$  are respectively the vertices of an elementary triangle in the layer when the latter is circled in the counterclockwise direction.

For  $D > 0.65|J_1|$ , the transverse components are not ordered at any temperature. Furthermore, there is no long-range order in the longitudinal components down to zero temperature. In this case the critical value is  $D_c = 0.652|J_1|$  (Figs. 3d, 3e, 3f). In the intermediate temperature region this spectrum (Fig. 3d) is similar to the corresponding spectrum for  $0 < D \lesssim D_c$  (Fig. 3b). However, below the characteristic point  $T = T_2$  its form becomes even more complex and irregular as the temperature decreases (Fig. 3e, 3f). These variations in  $\mathbf{S}(\mathbf{Q})$  reflect the necessity of reconstructing

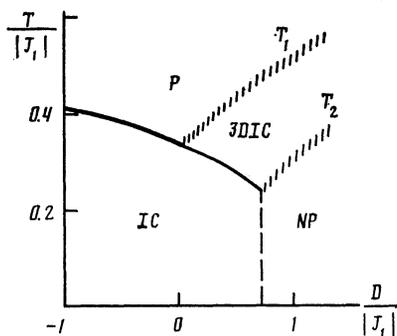


FIG. 4. Phase diagram in the  $TD$  plane for  $J' = 0.2$  ( $J_2 = 0$ );  $IC$ —incommensurate phase,  $NP$ —aperiodic phase,  $3DIC$ —incommensurate state with  $3D$  short-range order,  $P$ —paramagnetic phase.

tion in the system from a state where the absolute value of the local magnetic moment is not conserved to a state where, in contrast, it should be conserved as  $T \rightarrow 0$ . At the same time, numerical calculations show that such variations in an Ising-like system take place very slowly: as  $T$  decreases the spins are frozen in and the ground state becomes difficult to reach. Therefore as a result the state of the system is characterized by an aperiodic structure. Fig. 4 shows the phase diagram for various values of  $D$  and  $T$ ; at  $D = 0$  the transition point to an ordered state is close to the value  $T_N = 0.33|J_1|$  for a two-dimensional Heisenberg system.<sup>11</sup>

The additional interaction  $J_2$  stabilizes the magnetic structures, which is reflected in the spin ordering at higher temperatures. However, the qualitative phase diagram for the most part remains the same as for  $J_2 = 0$ . In particular, as previously, there exists a characteristic temperature  $T_2$  below which the spins freeze in for sufficiently large  $D$ , forming an aperiodic structure.

#### 4. CONCLUSION

In this paper, we have investigated the magnetic states which occur in antiferromagnets with hcp lattices. We have shown that in such lattices, which are frustrated not only in the basal plane but also in the third direction, the ground state is degenerate on a closed contour in  $(Q_x, Q_y)$  space. As a function of the interplanar interaction  $J'$  the wave vector of the states in isotropic magnets—states with inequivalent spirals—can lie either near the  $K$  symmetry point ( $|J'/J_1| \ll 1$ ) or near the  $\Gamma$  point ( $3 - |J'/J_1| \ll 1$ ) of the magnetic Brillouin zone. In this case, in contrast to materials with a simple hexagonal lattice where instability at the con-

ical point  $K$  is possible because of dipole interactions, the instability of these systems is due to its frustration in the third direction. The frustration which appears in this direction is independent of the sign of  $J'$ ; therefore the modulation wave vector is also independent of the sign of  $J'$ . Including the exchange interactions between the next-nearest neighbor spins lifts the continuous degeneracy of the structures, so that as a result the wave vector of the modes becomes fixed.

In easy-plane magnets below the transition point to the paramagnetic phase, the spiral (incommensurate) state is realized in all temperature regions; the transition itself between the two phases is a first-order transition.

In easy-axis magnets, because of the conservation of the magnitude of the spin at each node of the lattice in the ground state, an incommensurate structure is possible only for small values of  $D$ . As the temperature falls, anomalies in the behavior of the specific heat arise at two characteristic points. Below the first point there exists an intermediate-temperature incommensurate phase with well-developed short-range order, while at the second point  $T_2$  we have either an incommensurate phase with long-range order when  $D \lesssim D_c$  (in this case,  $T_2$  is a second-order transition point) or an aperiodic frozen-in phase for  $D > D_c$ .

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