PHASE TRANSITIONS AND SPONTANEOUS MAGNETIZATION IN AN ISING LATTICE CONTAINING IMPURITIES

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The phase transitions and the spontaneous magnetization of a three-dimensional ferromagnetic Ising lattice containing interstitial impurities, which change the magnitude and sign of the exchange integral between neighboring lattice sites, are considered. It is assumed that the impurities are in thermodynamic equilibrium with the lattice. If the presence of the impurity changes the sign of the exchange integral, then under certain conditions in such a system two or even three temperatures may exist at which there is a phase transition of the ferromagnetic–paramagnetic or antiferromagnetic–paramagnetic type.

INTRODUCTION

THE low-temperature behavior of the spontaneous magnetic moment of a ferromagnetic Ising lattice containing interstitial impurities, which change the magnitude and sign of the exchange integral between neighboring lattice sites, was investigated in an article by one of the authors.[1] It was found that in order to investigate the low-temperature properties of such a system it is convenient to use the model proposed by Lushnikov,[2] for which one can obtain the exact expression which relates the free energy of the Ising lattice containing impurities to the free energy of the corresponding ideal lattice. One of the conclusions of article[1] consists in the fact that a small concentration of impurities, which change the sign of the exchange integral between neighboring lattice sites and strongly decrease its absolute magnitude, leads to a sharply nonmonotonic dependence of the spontaneous moment of a ferromagnetic lattice on the temperature. The physical reason for this property is that at sufficiently low temperatures the impurities form clusters, leading to the appearance of regions with their magnetization opposite to the nominal magnetization.

For a larger concentration of such impurities a nonunique dependence of the (paramagnetic–ferromagnetic) phase-transition temperature on the impurity concentration appears, as was shown in the article by Kasai, Miyazima, and Syozi[3] for the example of a square lattice. Because of this the system under consideration may possess two phase transition points (the lowest temperature phase and the high temperature phase are paramagnetic, but the intermediate phase is ferromagnetic). This conclusion is in agreement with the more general results of Fisher[4] for a model with so-called "mobile impurities" (impurities which are in thermodynamic equilibrium with the lattice).

In the present article it is shown that in a three-dimensional ferromagnetic Ising lattice containing interstitial impurities, which change the sign of the exchange integral between nearest-neighbor lattice sites (we shall call such impurities antiferromagnetic), the appearance of three phase transition points is possible. In this connection the lowest temperature phase is antiferromagnetic. The ferromagnetic phase corresponds to a finite temperature interval separating the region of the paramagnetic phase from the antiferromagnetic state. Finally, the high-temperature phase is, of course, a paramagnetic phase. In connection with the derivation of the basic result of the present work, the physical reasons which lead to the existence of several phase transition points in the given model are discussed in detail.

1. THE RELATION BETWEEN SHORT-RANGE AND LONG-RANGE ORDERING IN LUSHNIKOV'S MODEL

Let us consider an Ising lattice containing impurities, which are introduced between two neighboring lattice sites and change the exchange interaction between them. We shall assume that the impurities are in thermodynamic equilibrium with the lattice, i.e., their distribution is determined by the minimum of the free energy of the lattice with impurities. As far as we know this model was first studied in detail by Lushnikov.[2]

Since each impurity changes only a single bond between the sites, it is convenient to formulate the problem of interest to us in terms of the bonds between sites. If the neighboring sites are in identical spin states, then we shall call their bond positive. We shall call the bond negative if the neighboring sites have oppositely directed spins.

Let ν denote the concentration of negative bonds (the ratio of the number of negative bonds to the total number of bonds in the lattice). For an ideal lattice the quantity ν is a measure of the short-range order and simply defines the energy E of the lattice per bond: $E = -J(1 - 2\nu)$, where J denotes the exchange integral of the ideal lattice.

In a perfect lattice ν is a quite definite function of the temperature: $\nu = \nu(y^2)$ where $y = e^{-\beta J}$ and $\beta = 1/T$. Since the spontaneous magnetic moment of a perfect lattice, which is the parameter of long-range order, is also a single-valued function of y^2 ($M = M(y^2)$), then the relation between the parameters of short-range and long-range order in a perfect lattice is trivial.

For a lattice containing impurities, the relation between the corresponding quantities is not so simple. However, we shall show that the concentration ν_c of negative bonds in a lattice containing impurities is related to the temperature and impurity concentration by means of a simple relation $\nu_c = \nu(\eta)$, where η is a parameter which is determined from the appropriate equation in article[2]. The proof will be based on the fact that the quantity E_c (the energy of the lattice containing impurities, calculated per bond) may be obtained in two ways. On the one hand it may be expressed in terms of the concentration $\nu(\eta)$ of negative bonds in a perfect lattice by its standard calculation according to the formula

$$E_c = -\frac{d}{d\beta}[\beta F_c],$$

where F_c is the free energy of the lattice with impurities, calculated per bond. On the other hand, by means of simple considerations it may also be related to the concentration of negative bonds, ν_c. By equating the obtained expressions and carrying out simple algebraic transformations, we actually obtain $\nu_c = \nu(\eta)$.

Thus, we first derive an expression for the energy E_c of the lattice containing impurities. As shown in[2] the free energy F_c of the lattice with impurities is related to the free energy $F = F(y^2)$ of a perfect lattice by the following equation:

$$\beta F_c = \beta F(\eta) - \frac{1}{2}\ln\frac{1}{\eta} + c\ln\xi + (1-c)\ln(1-\xi) - c\beta J_1 - (1-c)\beta J, \quad (1)$$

where J_1 is the new exchange integral, associated with the presence of the interstitial impurity, and the quantity $\eta \equiv (1-\xi)y^2 + \xi v^2$ is determined from the equation

$$-\frac{c}{\eta - y^2} + \frac{1-c}{v^2-\eta} + \frac{\nu(\eta)}{\eta} = 0. \quad (2)$$

as was proved in[1]. Here c denotes the impurity concentration (the ratio of the number of impurities to the total number of bonds in the lattice), and $v^2 \equiv \exp(-2\beta J_1)$. As indicated in[1], the quantity ξ which appears in the fundamental formulas (1) and (2) is the concentration of impurities on positive bonds, i.e., the ratio of the number of impurities located on positive bonds to the total number of positive bonds in the lattice. The following expression for the energy of a lattice containing impurities follows from Eq. (1) with Eq. (2) taken into consideration:

$$E_c = 2\eta^{-1}\nu(\eta)\{J(1-\xi)y^2 + J_1\xi v^2\} - cJ_1 - (1-c)J. \quad (3)$$

Now let us obtain an expression for E_c by another method, using the physical meaning of the quantity ξ. It is obvious that one can write the lattice energy E_c in the form

$$E_c = -(1-\nu_c)\{\xi J_1 + (1-\xi)J\} + \nu_c\{\zeta J_1 + (1-\zeta)J\},$$

where ζ denotes the concentration of impurities on negative bonds, i.e., the ratio of the number of impurities located on negative bonds to the total number of negative bonds. Taking it into consideration that ν_c is the concentration of negative bonds in the lattice with impurities, we write $c = \zeta\nu_c + \xi(1-\nu_c)$. Then we have the following simple expression for the energy E_c:

$$E_c = cJ_1 + (1-c)J - 2(1-\nu_c)\{\xi J_1 + (1-\xi)J\}, \quad (4)$$

Type of lattice	γ	η_0	c_0	c_k	$1-c_0$
Square	4	$\sqrt{2}-1$	0.146	0.5	0.854
Honeycomb	3	$2-\sqrt{3}$	0.115	0.352	0.885
Diamond	4	0.437	0.22	0.590	0.78
Simple cubic	6	0.641	0.322	0.757	0.678
Body-centered cubic	8	0.727	0.366	0.828	0.634

Note. The values of the parameters η_0 and c_0 are taken from [3], the values of c_k are taken from [5].

where ξ is found from Eq. (2) as has already been noted. Equating relations (3) and (4) and using expression (2), one can show that

$$\nu_c = 1 - \frac{c}{\xi} + \frac{v^2\nu(\eta)}{\eta}.$$

Finally, having rewritten (2) in the form

$$\frac{c}{\xi} = 1 + \frac{(v^2-\eta)\nu(\eta)}{\eta},$$

we finally have $\nu_c = \nu(\eta)$.

Since it was shown in[1] that the spontaneous magnetization is a single-valued function of η, namely, $M_c = M(\eta)$, then the relation $\nu_c = \nu(\eta)$ obtained by us establishes the connection between the parameters of short-range and long-range spin ordering in a lattice with impurities.[1)]

It was shown in[2] that the thermodynamical quantities of an Ising lattice with impurities, regarded as functions of the parameter η, have the same singularities as the corresponding quantities for a perfect lattice, regarded as functions of y^2. The phase transition in the lattice with impurities take place at $\eta = \eta_0 = \exp(-2J/T_0)$, where T_0 is the Curie temperature of the perfect lattice. It is very important to note that η_0 is a number which is characteristic of the type of lattice being considered (see the table). But in a perfect lattice $\nu(\eta_0) = c_0$, where c_0 denotes the concentration of negative bonds at the phase transition point; c_0, just like η_0, is a number which has a specific value for a given type of lattice (see the table). Since we have proved that $\nu_c = \nu(\eta)$, then from the above discussion it follows that: if a phase transition occurs in the lattice with impurities at a certain temperature T_λ, then the concentration of negative bonds at the point $T = T_\lambda$ is the same as at the phase transition point of the original perfect lattice. In other words, the nature of the short-range spin ordering at the phase transition point for the lattice containing impurities, which is determined by the concentration ν_c of negative bonds, only depends on the type of lattice (square, cubic, etc.), but does not depend on the impurity concentration c or on the value of the new exchange integral J_1. However, the temperature of the phase transition naturally depends on both c and J_1. And what is more, the kind of phase transition is changed in the lattice with impurities (it becomes a third-order transition[2]).

The formulated result for the model under consideration provides a specific example of Fisher's remark[6] with regard to the fact that the behavior of a substance

[1)] We note that in [3] the quantity ϵ, which is the average value of the spin-spin correlator between nearest neighbors, is chosen as a measure of the short-range order. The quantity ϵ is related to ν in a simple manner: $\epsilon = 1-2\nu$.

near its critical point is primarily determined by the statistical properties of the system, i.e., not by the interaction forces in the system (its energy), but by the extent of its ordering (the entropy of the system).

2. CLASSIFICATION OF THE ORDERED STATES IN A FERROMAGNETIC LATTICE CONTAINING ANTIFERROMAGNETIC IMPURITIES

In what follows we shall confine our attention to an investigation of Ising spin lattices which also permit antiferromagnetic ordering in addition to ferromagnetic ordering. As is well known (see, for example,[7]), this is the case for those lattices in which one can divide the lattice sites into two classes α and β such that all of the nearest neighbors of a site belonging to class α are sites of class β, and vice versa. The simplest examples of such lattices are the square, simple cubic, and body-centered cubic lattices.

In order to be definite we shall assume $J > 0$ and $J_1 < 0$. For $c = 0$ Eq. (2) for the determination of the quantity η has the natural solution $\eta = y^2$, leading to the trivial result $F_c = F(y^2)$. For $c = 0$ the lattice under consideration is ferromagnetic with its Curie point T_0 determined from the condition $y^2 = \eta_0$.

For $c = 1$ the solution to Eq. (2) is given by $\eta = v^2$ and correspondingly $F_c = F(v^2)$, where upon a change of the temperature T in the interval $(0, \infty)$ the quantity $v^2 \equiv \exp(-2\beta J_1)$ varies over the interval $(\infty, 1)$. For $c = 1$ the lattice being analyzed is antiferromagnetic with an exchange integral J_1 and a Neél point determined from the condition $v^2 = 1/\eta_0$.

As will be clear from the following, the classification of the different states of the investigated system is essentially based on the properties of the function $\nu = \nu(x)$; therefore it is helpful to consider its behavior over the entire range of variation of the independent variable x, i.e., over the interval $(0 < x < \infty)$. A schematic graph of the function $\nu(x)$, an analytic expression for which can only be obtained for the two-dimensional lattice, is shown in Fig. 1. Its continuity and monotonic increase are the characteristic features of this graph. In the interval $0 < x < 1$ the function $\nu(x)$ determines the concentration of negative bonds in the ferromagnetic Ising lattice. At the point $x = \eta_0$, corresponding to the Curie temperature, $\nu(\eta_0) = c_0$, and the graph of the function has a vertical tangent. This is related to the fact that the heat capacity of an Ising lattice tends to infinity at the Curie point. In the interval $1 < x < \infty$ the same function determines the concentration of negative bonds in the antiferromagnetic Ising lattice. For $x = 1/\eta_0$, corresponding to the Neél temperature, $\nu(1/\eta_0) = 1 - c_0$, and the graph of the function again has a vertical tangent. For $x = 1$ (this corresponds to an infinitely high temperature) the number of negative bonds in the lattice is equal to the number of positive bonds and $\nu(1) = 1/2$.

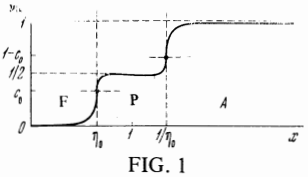

FIG. 1

By virtue of the monotonic nature of the function $\nu(x)$ we may conclude that a long-range ferromagnetic ordering exists in the lattice for $\nu < c_0$, and a long-range antiferromagnetic ordering exists for $\nu > 1 - c_0$. If the concentration of negative bonds is found in the interval $c_0 < \nu < 1 - c_0$, then the lattice is found in a paramagnetic state.

Now let us return to the statement which was proved in the preceding section, enabling us to find the concentration of negative bonds in the lattice containing impurities, namely, the formula $\nu_c = \nu(\eta)$. The possibility of such a classification of the states in a lattice containing impurities follows from the single-valued correspondence between the concentration of negative bonds and the long-range order in the lattice, and also from the properties of the function $\nu(\eta)$.

If $0 < \nu_c < 1/2$ (this is possible only for $0 < \eta < 1$), then one can call the states of the system ferromagnetic-like (FLS). However if $1/2 < \nu_c < 1$ (which can be realized only for $1 < \eta < \infty$), then it is natural to call the corresponding states antiferromagnetic-like (ALS). In the FLS region a transition may occur between the ferromagnetic and paramagnetic phases of the system, and in the ALS region a transition may occur between the antiferromagnetic and the paramagnetic phases. Having set $\eta = 1$ and $\nu(1) = 1/2$ in Eq. (2), one can obtain the dependence of the concentration c on that temperature T, which separates the FLS and ALS regions. On the (c, T) plane the indicated temperature corresponds to points on a certain curve (we shall call it the limiting curve). From Eq. (2) one obtains the following equation for the limiting curve:

$$c[1 - \operatorname{th} \beta J_1 / \operatorname{th} \beta J] = 1. \tag{5}$$

We recall that $\beta = 1/T$, $J > 0$, and $J_1 < 0$.

An interesting property of the limiting curve is the fact that for given values of J and J_1 this curve does not depend on the type or dimension of the lattice under consideration. The schematic form of the graph of the limiting curve is depicted on Fig. 2, where $c_1 = [1 + |J_1|/J]^{-1}$. We now note that the following limiting behavior of the function ν_c follows from Eq. (2): for $T = 0$ and any impurity concentration $\nu_c|_{T=0} = c$. But since FLS exist for $\nu_c < 1/2$, and ALS exist for $\nu_c > 1/2$, then a natural division of the states into FLS and ALS occurs on the $T = 0$ axis in Fig. 2: all of the points in the (c, T) plane lying to the left of the limiting curve describe FLS, and all of the points to the right of the limiting curve are ALS. Let us perform a comparative analysis of Fig. 1 and Fig. 2. Since $\nu_c|_{T=0} = c$, then the states of the lattice for $T = 0$ and $c > 1/2$ are ALS. If the ratio $J/|J_1|$ of the exchange integrals is such that $c_1 > 1 - c_0$, then for $1 - c_0 < c < c_1$ the vertical straight line $c = \text{const}$ certainly intersects the

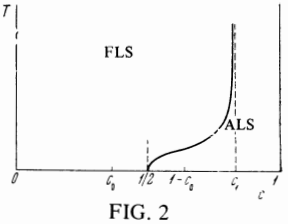

FIG. 2

limiting curve, and therefore the theoretical possibility of the existence of phase transitions (ferromagnetic–paramagnetic and paramagnetic–antiferromagnetic) arises in the range of concentrations $1 - c_0 < c < c_1$. The conditions for realizing this possibility will be considered below.

3. SPONTANEOUS MAGNETIZATION OF A LATTICE CONTAINING IMPURITIES

On the basis of exact results for the planar square Ising lattice, the low-temperature behavior of the spontaneous magnetization was analyzed in article[1] for the case of a small impurity concentration ($c \ll 1$). Using the results of this analysis and also the qualitative considerations discussed in[1], one can easily predict the low-temperature behavior of the magnetization of a three-dimensional ferromagnetic lattice for $c \ll 1$.

Let us start with the case $J_1 = 0$, when the impurity in its interstitial position completely breaks the coupling between the neighboring spins. A reduction of the magnetic moment of the ferromagnetic lattice containing impurities as $T \to 0$ in comparison with its nominal value in this case can be achieved only in the following manner. Certain groups of spins arise, bounded by closed surfaces which pass through the interstitial positions at which the impurities are located, and consequently there is a simultaneous breaking of the bonds with the remaining part of the lattice. The smallest group of this type is an individual spin, which has all of its bonds with its nearest neighbors broken. For small impurity concentrations the formation of precisely such groups is most probable.

Since the accumulation of impurities surrounding a single spin can only occur in a random fashion (for $J_1 = 0$ it is not energetically favored), then the number of such clusters for small concentrations ($c \ll 1$) is proportional to c^γ, where γ denotes the number of nearest neighbors.

In the case $J_1 < 0$ but $|J_1| \ll J$ the mechanism for the reduction of the magnetic moment as $T \to 0$ is completely different. In this case the formation of an individual cluster in which the impurities completely surround a single reversed spin is energetically favored. However, the distribution of the individual clusters remains a random distribution (their amalgamation is not energetically favored); therefore for small impurity concentrations ($c \ll 1$) the number of such clusters will be proportional to the first power of the concentration.

In order to quantitively verify these conclusions we shall carry out a calculation of the spontaneous magnetization of a three-dimensional lattice with the aid of an approximate method, namely, the Bethe-Peierls method. As is well known,[8] this method gives good results for low temperatures.

In the Bethe-Peierls method the internal energy of a perfect Ising lattice may be written in the following form:[8]

$$E(\eta) = -J\{2\sigma(\eta) - 2M(\eta) + 1\}, \quad \eta = y^2 \equiv e^{-2\beta J}, \tag{6}$$

where the quantities σ and M, which are the parameters, respectively, of short-range and long-range ordering, are found from the relations

$$\sigma(\eta) = \frac{2z^2}{(1+z\eta)(1+z^x)} - 1, \quad M(\eta) = \frac{z^x - 1}{z^x + 1}, \tag{7}$$

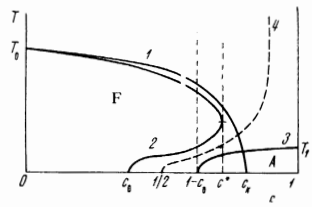

FIG. 3

in which $x \equiv \gamma/(\gamma - 1)$ (γ denotes the number of nearest neighbors in the lattice), and the quantity z is found from the equation

$$\left(\frac{\eta + z}{1 + z\eta}\right)^{\gamma - 1} = z. \tag{8}$$

Using the relation cited earlier between the internal energy and the concentration of negative bonds in an Ising lattice, $E(\eta) = J\{2\nu(\eta) - 1\}$, and comparing this with Eq. (6), we obtain

$$\nu(\eta) = M(\eta) - \sigma(\eta). \tag{9}$$

Let us substitute expression (9) into Eq. (2) and find its solution as $T \to 0$ in the case $|J_1| \ll J$. It is easy to verify that for $c \ll 1$ the solution of interest to us possesses the property $\eta \ll 1$. Then the expansion $\nu(\eta) = 2\eta^\gamma + 0(\eta^{2\gamma - 2})$ is valid, where 0(x) indicates a quantity of the order of x for $x \ll 1$. The corresponding expansion of the parameter $M(\eta)$ has the form

$$M(\eta) = -\{1 - 2\eta^\gamma - O(\eta^{2\gamma - 2})\}.$$

Then in the case of the complete rupture of the bonds ($J_1 = 0$), by repeating the corresponding arguments of article[1], one can show that the low-temperature expansion of the relative change Δm in the magnetic moment, calculated per spin, will be given by

$$\Delta m = -2c^\gamma\{1 + ae^{-2\beta J}\}, \tag{10}$$

where a is a constant which depends only on c.

Thus, for $T \to 0$ and $c \ll 1$ we actually have the estimate $|\Delta m| \sim c^\gamma$ for the relative decrease of the spontaneous moment.

In the case $J_1 < 0$ and $|J_1| \ll J$ in similar fashion one can show that

$$\Delta m = -c\{1 + be^{-2\beta|J_1|}\},$$

where b is again a certain constant which only depends on c. Thus, the assertion formulated above about the linear dependence of Δm on c has been proved for $J_1 < 0$ and $|J_1| \ll J$.

4. PHASE TRANSITIONS IN A FERROMAGNETIC LATTICE CONTAINING ANTIFERROMAGNETIC IMPURITIES

In the recently published article[3] a quantitative analysis was made of the dependence of the phase transition temperature on the impurity concentration for the case of a planar square Ising lattice. It was shown that for $J_1 < 0$ and $|J_1| < J$ the phase transition temperature is a double-valued function of the concentration and has the form of curve 2 in Fig. 3. As $J_1 \to 0$ the graph of this function approaches a monotonically decreasing curve of type 1 on Fig. 3, and for $J_1 = 0$ it terminates at the point $c = c_k$ on the concentration axis. However, for

all plane lattices known to us $c_k < 1/2$, i.e., the end point of the curve lies to the left of the limiting curve. An analysis of the situation in three-dimensional Ising lattices indicates (see the table) that the latter assertion does not hold for them. As will be clear from the following, this is associated with the appearance of new physical phenomena which are characteristic for three-dimensional lattices, these phenomena being impossible in principle in planar lattices.

Let us analyze the curves of the phase transition in a three-dimensional ferromagnetic Ising lattice containing antiferromagnetic impurities in the case when $c_k > 1 - c_0$ and $c_1 > 1 - c_0$. We recall that c_k determines the point of intersection of the phase transition curve with the concentration axis in the case of a lattice with impurities which completely rupture the bonds between nearest neighbors ($J_1 = 0$). This curve is obtained from Eq. (2) for $J_1 = 0$. An elementary analysis shows that it is a monotonically decreasing curve, passing through the point $c_k = \eta_0 + (1 - \eta_0)c_0$ for $T = 0$. We note that whereas the quantities c_0 and c_k for the three-dimensional lattice can be obtained only by some kind of numerical method, the quantity c_1 is determined by the exact analytic expression $c_1 = [1 + |J_1|/J]^{-1}$.

One can cite convincing physical arguments which indicate that, for $J_1 < 0$, $|J_1| < J$, and $c > c_0$, the dependence of the paramagnetic-ferromagnetic transition temperature on the concentration should be described by a double-valued function, and a characteristic loop of the type exhibited by curve 2 on Fig. 3 appears on the corresponding graph of $T_\lambda = T_\lambda(c)$. These considerations are especially clear for $|J_1| \ll J$. It is obvious that in this case for $T \gg |J_1|$ the phase transition curve will practically coincide with curve 1 on Fig. 3 (with the curve for $J_1 = 0$). In addition, for sufficiently small values of the ratio $|J_1|/J \ll 1$, this agreement will hold almost up to $c = c_k$.

The points describing the ferromagnetic state of the substance must be located below and to the left of the phase transition curve on the (c, T) plane. On the other hand, for $T = 0$ the concentration of negative bonds in the lattice coincides with the concentration of impurities, $\nu_c = c$, as we have already indicated. Since $c_k > c_0$, it follows that in virtue of what has been stated above all of the states to the right of c_0 (up to the point $c = 1 - c_0$) on the concentration axis ($T = 0$) are paramagnetic.

In order for a paramagnetic state to exist on the $T = 0$ axis, and for a ferromagnetic state to exist somewhat below curve 2 (near it $T \gg |J_1|$), it is necessary that a paramagnetic-ferromagnetic phase transition occur at temperatures $T \lesssim |J_1|$. In other words, the phase transition curve 2 must actually have the form of a loop of the type depicted on Fig. 3. Since this curve certainly passes through the point $c = c_0$, $T = 0$, in order to prove this assertion it is sufficient to show that a bulge exists in curve 2 having a vertical tangent at $c = c^* > c_0$. We shall present a rigorous proof of the existence of this loop somewhat later, but right now let us turn to the analysis of the antiferromagnetic states of the lattice under consideration.

First of all we note that for $c > 1/2$ one can assume as a starting point an antiferromagnetic Ising lattice with an exchange integral J_1 ($J_1 < 0$), and the remaining impurity bonds in the lattice, with an exchange integral J ($J > 0$), are considered as defect imperfections with a concentration $1 - c$.

It is obvious that the Neél temperature T_1 for a lattice with $c = 1$ will have an order of magnitude $T_1 \sim |J_1| \sim T_0|J_1|/J$. From symmetry considerations it is obvious (one can prove this by a rigorous analysis of the initial equations) that for $T = 0$ the antiferromagnetic ordering encompasses the interval $1 - c_0 < c < 1$ and vanishes at the point $c = 1 - c_0$. The curve of the antiferromagnetic-paramagnetic phase transition is schematically represented by curve 3 on Fig. 3; it is monotonic and single-valued. Using as an example the case $|J_1| \ll J$ it is easy to understand why the mechanism which leads to the appearance of the loop on curve 2 cannot influence the monotonic behavior of curve 3. In fact, the characteristic temperature for the formation of clusters of defect bonds of the type discussed in Sec. 3 is of the order of the quantity $J \gg |J_1| \sim T_1$, i.e., clearly above the Neél temperature. Therefore the formation of such clusters cannot influence the behavior of the system in the temperature range $T < T_1$.

From the point of view of the possibility of different phase transitions, the most interesting situation is that in which

$$c_0 < 1/2 < 1 - c_0 < c^* < c_k. \tag{11}$$

Upon fulfillment of conditions (11) and for $|J_1| < J$ the entire range of possible impurity concentrations c splits up into the following regions:

1) $0 < c < c_0$. In this region at low temperatures the system is found in a ferromagnetic ordered state and the Curie temperature is of the order of the quantity T_0;

2) $c_0 < c < 1 - c_0$. For these concentrations, two phase transitions are possible. The lowest temperature phase is the paramagnetic phase. With an increase of the temperature, the transition into the ferromagnetic phase occurs for $T \lesssim |J_1|$. With a further increase of the temperature, the system again experiences a transition from the ferromagnetic state into the paramagnetic state (the transition temperature is given by the upper part of loop 2 in Fig. 3);

3) $1 - c_0 < c < c^*$. In this range of concentrations three phase transitions are possible, separating the regions corresponding to antiferromagnetic, paramagnetic, and ferromagnetic states of the substance. The antiferromagnetic phase exists at very low temperatures (its region of existence lies below curve 3). The paramagnetic phase occurs at higher temperatures. Above it (in temperature) there is a finite temperature interval in which the ferromagnetic phase exists. And, finally, the paramagnetic phase again occurs at temperatures lying above curve 2.

4) $c^* < c < 1$. In this range the system is found in the antiferromagnetic state at low temperatures, and the Neél temperature is of the order of magnitude of T_1.

If the inequalities (11) are replaced by other inequalities, then the classification of the states in different ranges of the concentration can be carried out in analogous fashion.

Finally, it is perhaps worth mentioning that the behavior of the heat capacity C(c, T) and of the spontaneous magnetic moment $M_c(T)$ over the entire range of temperatures and concentrations for the three-dimen-

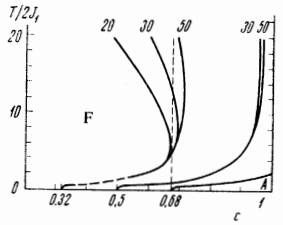

FIG. 4

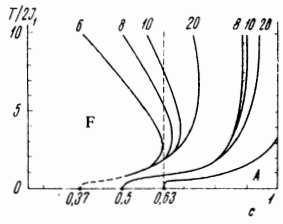

FIG. 5

sional case can be investigated with the aid of the Bethe-Peierls method discussed above. We note that the application of the method of the molecular field in its simplest version (the Bragg-Williams method, see[8]) does not even qualitatively give the result established above about the double-valued nature of the curve $T_\lambda(c)$, and accordingly the existence of two or three points in temperature at which there is a phase transition. This is related to the fact that in the Bragg-Williams method the parameter of short-range order vanishes at the phase transition point, that is, $\nu_c(\eta_0) = 1/2$. Then for $c > c_0$ the lower branch of the curve $T_\lambda(c)$ coincides with the axis of abscissas and the ALS and FLS regions overlap, which is impossible in principle in view of the presence of the limiting curve.

Finally, let us return to the proof that in a three-dimensional Ising lattice the case when $c^* > 1 - c_0$ can actually be realized. As already mentioned, in order to construct the quantitative dependence of the phase transition temperature on the impurity concentration it is sufficient to know two numbers that characterize the type of lattice being considered, namely, the numerical values of the parameters η_0 and c_0. We have taken these numbers from article[3] and they are cited in the accompanying table. With the aid of machine calculations of Eq. (2) we plotted curves showing the dependence of the phase transition temperature on the impurity concentration for two types of lattices—simple cubic (see Fig. 4) and body-centered cubic (Fig. 5) and for different values of the ratio $n = J/|J_1|$ (the values of n are written above each curve). The left-hand group of curves in each Figure represents the dependences of the Curie temperatures on the impurity concentration in the FLS region; the middle group of curves represents the family of the corresponding limiting curves. Finally, in the lower right-hand corner is shown the curve of the antiferromagnetic-paramagnetic transition for $n = \infty$ (the analogous curves for finite values of n will end at the same points on the coordinate axes, but will pass somewhat above the curve shown).

From an investigation of the cited curves it follows that in the simple cubic lattice for $n > 25$ the corresponding loop on the phase transition curve has a bulge for which $c^* > 1 - c_0$. In the body-centered lattice (where the number of nearest neighbors is larger) this same result is attained for smaller values of n, namely, for $n > 6$. Thus, in principle impurities can exist such that a sufficient concentration of them will lead to the result that the situation analyzed above is realized in the system.

In conclusion we note that upon reversing the signs of the exchange integrals ($J < 0$, $J_1 > 0$) the curves shown in Figs. 3, 4, and 5 undergo mirror reflection, corresponding to the substitution $c \to 1 - c$. Therefore everything discussed above can be attributed to an antiferromagnetic Ising lattice containing ferromagnetic impurities.

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116