Effect of impurities on the phase-transition temperature in a two-dimensional Ising lattice with nearest-neighbor and non-nearest-neighbor interaction

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The effect of impurities on the phase transition in a two-dimensional Ising lattice is studied taking into account the interaction of some of the non-nearest neighbors. It is assumed that the impurities are positioned only on atomic bonds linking nearest sites and that they alter the exchange interaction between these sites. The exact dependence of the phase-transition temperature on the impurity concentration is obtained by the method proposed previously by Lushnikov. The cases when the impurity completely disrupts the interaction between the nearest neighbors and when the impurity reverses the sign of this interaction are discussed in detail.

INTRODUCTION

Only a small number of exactly soluble problems concerned with phase transitions in systems undergoing ordering are known at the present time. It is therefore interesting to study the effect of different parameters on the phase-transition temperature in the framework of a model that permits a rigorous treatment and quantitative analysis. We have analyzed the dependence of the phase-transition temperature on the concentration of specific impurities in a planar Ising lattice with nearest- and non-nearest-neighbor interaction. The model taken, which is known as the Union Jack, is described in Sec. 1. The thermodynamics of such a model has been analyzed by Vaks, Larkin, and Ovchinnikov[1]. A generalization of the results of[1] to the case of a lattice with interestitial impurities is carried out by Lushnikov's method[2], which makes it possible to establish certain isomorphism relations between the lattice with impurities and the original system. In Sec. 2, the concentration dependence of the phase-transition temperature in the case when the impurity completely destroys the exchange interaction between nearest neighbors is considered in detail. The phase-transition curves are found to be substantially different for different signs and magnitudes of the exchange interaction of non-nearest neighbors. If the interaction of the non-nearest neighbors has the character of an antiferromagnetic interaction, the temperature of the phase transitions can turn out to be a nonunique function of the concentration, and in a broad range of concentrations the possibility appears that three different phase states of the system can exist. The content of Sec. 3 is devoted to the special case in which the impurity changes the sign of the interaction between nearest neighbors. In this case also, the most possibilities, in the sense of the number of different phases, appear when the interaction between non-nearest neighbors is antiferromagnetic.

1. FORMULATION OF THE MODEL AND DERIVATION OF THE BASIC EQUATIONS

We shall consider a complex planar Ising lattice (Fig. 1), consisting of sites (atoms) of two types: atoms of the first type interact only with their nearest neighbors in a square lattice, which are atoms of the other type (J_1 is the exchange energy of this interaction); atoms of the second type interact, in addition, with their next-nearest neighbors, i.e., with atoms also of the second type (J_2 is the exchange energy of this interaction). A lattice with such interaction is often called a

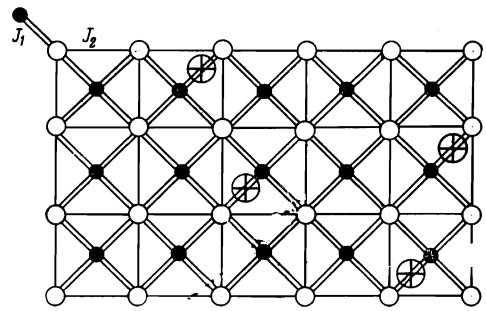

FIG. 1

Union Jack. The thermodynamics of the phase transition in this lattice was first studied by Vaks, Larkin, and Ovchinnikov[1].

We shall consider a phase transition in such a lattice, with interestitial impurities affecting the magnitude of the exchange interaction between neighboring sites. It is assumed that the impurities can be positioned only on the atomic bonds linking nearest lattice sites, and that they change the magnitude (and also, possibly, the sign) of the exchange interaction energy J_1. We assume that the impurities are in thermodynamic equilibrium with the lattice. In such a case, using the method proposed earlier by Lushnikov[2], we can obtain the exact dependence of the phase-transition temperature on the impurity concentration for any relationship between the quantities J_1 and J_2, for all possible changes of the exchange energy J_1, and for all concentrations.

We write the free energy of the lattice under consideration, with no impurities, in the following form:

$$F(T)=\Phi(x, y), \tag{1}$$

where $x = \tanh(J_1/T)$, $y = \tanh(J_2/T)$ and the function $\Phi(x, y)$ is given in[1]. In[2] it was shown that the partition function of a lattice with impurities can be expressed in terms of the partition function of the lattice without impurities. We note that the impurities affect only the exchange energy J_1, and therefore all the transformations in the Lushnikov scheme leave the y-dependence of the function $\Phi(x, y)$ unchanged. As a result of these transformations, it is easy to obtain the following expression for the free energy F_c of the lattice with impurities in terms of the free energy of the same system without impurities:

$$\frac{1}{NT}F_c=\frac{1}{NT}\Phi\left(\frac{1-\eta}{1+\eta}, y\right)-\frac{1}{2}\ln\eta+c\ln\xi+(1-c)\ln(1-\xi) - c\frac{J}{T}-(1-c)\frac{J_1}{T}, \tag{2}$$

where N is the number of atomic bonds between nearest neighbors in the lattice, c is the concentration of impurities, and

$$\eta=(1-\xi)\exp(-J_1/T)+\xi\exp(-J/T), \tag{3}$$

where J is the new exchange interaction energy between atoms of the first and second type, due to the presence of an impurity between them. We define the impurity concentration c as the ratio of the number of impurities to N. The quantity ξ is found from the condition $\partial(T^{-1}F_c)/\partial\xi = 0$. Substituting the expression (2) into the latter condition and eliminating ξ by means of (3), we obtain the fundamental equation used and discussed in this paper:

$$\left[\frac{1}{NT}\frac{\partial}{\partial\eta}\Phi\left(\frac{1-\eta}{1+\eta},y\right)-\frac{1}{2\eta}\right]\left[\eta-\exp\left(-\frac{2J_1}{T}\right)\right]\left[\exp\left(-\frac{2J}{T}\right)-\eta\right]$$
$$+c\left[\exp\left(-\frac{2J}{T}\right)-\eta\right]-(1-c)\left[\eta-\exp\left(-\frac{2J_1}{T}\right)\right]=0. \tag{4}$$

It follows from this expression that the thermodynamic quantities of the lattice with impurities, considered as functions of the variables $(1-\eta)/(1+\eta)$ and y, have the same singularities as the corresponding quantities for the ideal lattice, considered as functions of the variables x and y. One can convince oneself that the logarithmic terms appearing in (2) introduce no additional singularities into F_c for $c \neq 0$ and $c \neq 1$.

Thus, to find the dependence of the phase-transition temperature T_c on the concentration c we must solve Eq. (4) jointly with the equations in[1] that give the singular points of the function $\Phi(x, y)$. In our case, the latter equations are either

$$\frac{4\eta^2}{(1-\eta^2)^2}=\frac{(1+y)^2}{2-(1+y)^2}, \tag{5}$$

or

$$\frac{4\eta^2}{(1-\eta^2)^2}=\frac{(1+y)^2}{2y^2-(1+y)^2}, \tag{6}$$

The algebraic equations (5) and (6) determine two branches of the dependence $y = y(\eta)$, for which the variable ranges over the intervals $-1 \le y \le \sqrt{2}-1$ and $-1 \le y \le 1-\sqrt{2}$ $(0 \le \eta \le \infty)$ respectively.

The scheme for finding the dependence $T_c = T_c(c)$ is as follows. We substitute the expression $y = y(\eta)$ found from (5) or (6) into (4) and find $\eta_c = \eta(T, c)$ at the phase-transition point. After this, the expression $y = y(\eta_c)$ determines the dependence of interest—the concentration dependence of the phase-transition temperature. In order to realize this procedure, it is convenient to introduce the following function of the variable η:

$$\varphi(\eta)\equiv\frac{\partial}{\partial\eta}\Phi\left(\frac{1-\eta}{1+\eta},y\right)\Big|_{y=y(\eta)}-\frac{1}{2\eta}. \tag{7}$$

For the first branch of the dependence $y = y(\eta)$, we obtain

$$y=y_1(\eta)\equiv-1+2\sqrt{2}\eta/(1+\eta^2), \tag{8}$$

and, at the same time, the function $\varphi(\eta)$ should be taken in the form

$$\varphi=\varphi_1(\eta)\equiv\frac{1+\eta^2}{4\eta(1-\eta^2)}\left\{1-\frac{2}{\pi}\frac{\sqrt{2}\eta}{1+\eta^2-\sqrt{2}\eta}\left[\frac{2\sqrt{2}\eta-1-\eta^2}{2\sqrt{2}\eta+1+\eta^2}\right]^{1/2}\right.$$
$$\left.\times\arccos\frac{(1-\eta^2)^2}{4\eta^2}\right\}-\frac{1}{2\eta}. \tag{9}$$

For the second branch of the dependence $y = y(\eta)$ we have

$$y=y_2(\eta)\equiv-(1+2\sqrt{2}\eta/(1+\eta^2))^{-1}, \tag{10}$$

and the function $\varphi(\eta)$ is defined by the expression

$$\varphi=\varphi_2(\eta)\equiv\frac{1+\eta^2}{4\eta(1-\eta^2)}\left\{1-\frac{2}{\pi}\frac{\sqrt{2}\eta}{1+\eta^2-\sqrt{2}\eta}\left[\frac{2\sqrt{2}\eta+1+\eta^2}{2\sqrt{2}\eta-1-\eta^2}\right]^{1/2}\right.$$
$$\left.\times\arccos\frac{(1-\eta^2)^2}{4\eta^2}\right\}-\frac{1}{2\eta}. \tag{11}$$

We note that the relations (9) and (11) specify completely-defined analytic functions of the variable η, in which

$$\sqrt{1-z}\arccos z=\sqrt{z-1}\ln(z+\sqrt{z^2-1})$$

holds for values $z > 1$.

Inasmuch as the function $\varphi(\eta)$ appearing in the formulation of Eq. (4) has been found in explicit form, the difficulties of the subsequent analysis lie only in the cumbersome nature of the corresponding transcendental equations. It is clear that the concrete form of the dependence $T_c = T_c(c)$ is determined by the values of the parameters of the problem (the quantities J_1, J_2, and J); therefore, we shall consider the most interesting and physically intelligible cases individually.

2. CASE OF COMPLETE BREAKING OF THE BOND BETWEEN NEAREST NEIGHBORS

We shall consider first the simplest and physically most transparent case, in which the impurity completely breaks the bond between nearest atoms. Complete rupture of the bond corresponds to $J = 0$, and, when (7) is taken into account, Eq. (4) takes the form

$$\varphi(\eta)\left[\eta-\exp\left(-\frac{2J_1}{T}\right)\right](1-\eta)+c(1-\eta)-(1-c)\left[\eta-\exp\left(-\frac{2J_1}{T}\right)\right]. \tag{12}$$

To classify the results arising from the analysis of Eq. (12), it is convenient to introduce the dimensionless parameter $\alpha = |J_1/J_2|$, which can vary in the range $0 \le \alpha \le \infty$. The limiting values of α correspond to ordinary square Ising lattices with exchange interaction equal either to J_2 (for $\alpha = 0$, $J_2 \neq 0$) or to J_1 (for $\alpha = \infty$, $J_1 \neq 0$). We note that a concentration $c = 1$ in the case of complete rupture of the bonds, irrespective of the magnitude of J_1, transforms the system considered into an ordinary square lattice with exchange interaction J_2 between nearest neighbors.

We shall assume for definiteness that $J_1 > 0$. If $J_2 > 0$, the ground state of the system without impurities corresponds both to ferromagnetic ordering of the atoms of the second type, coupled by interaction energy J_2 (F-state) and to ferromagnetic ordering of the whole lattice (FF-state). In this case, Eq. (12) has a solution for all concentrations, if $\varphi = \varphi_1(\eta)$ and $0 \le \eta \le 1$. The dependence of the phase-transition temperature T_c on the impurity concentration c is elementary to obtain using (8) and can be represented schematically by the graphs shown in Fig. 2, in which T_0 is the phase-transition temperature for $c = 0$. The curve $\alpha = \infty$ corresponds to the case of a simple square lattice with interaction, of magnitude J_1, between nearest neighbors only. The presence, noted by Lushnikov[2], of the critical concentration $c = 0.5$ is characteristic for this curve. For impurity concentrations greater than this value, a phase transition is not observed in the simple Ising lattice. The inclusion of any (even arbitrarily small) interaction J_2 ($J_2 > 0$) leads to the disappearance of the critical concentration on the phase-transition curve. This is a completely intelligible result, since,

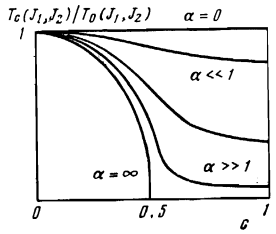

FIG. 2

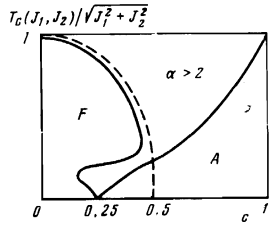

FIG. 3

besides the interaction between nearest neighbors, an interaction of the ferromagnetic type appears between next-nearest neighbors, which is not destroyed by the impurities. With decrease of α, the concentration dependence of the phase-transition temperature becomes weaker, and in the limit $\alpha = 0$ the phase-transition temperature does not depend on the concentration. The latter fact is completely natural, since for $J_1 = 0$ the impurities do not influence the state of the system.

If $J_2 < 0$, then for $\alpha > 1$ the ground state of the system without impurities is, as before, the FF-state, while for $\alpha < 1$ it corresponds to antiferromagnetic ordering of the atoms of the second type, defined by the interaction J_2 (A-state). In the case $\alpha > 1$ Eq. (12) has a solution for all concentrations, both for $\varphi = \varphi_1(\eta)$ and for $\varphi = \varphi_2(\eta)$, where $0 \le \eta \le 1$, but in the case $\alpha < 1$ a solution of (12) is possible only for $\varphi = \varphi_2(\eta)$ for $0 \le \eta \le 1$. The dependence of the phase-transition temperature on the concentration in the case $\alpha > 2$ is shown in Fig. 3. The dashed curve corresponds to the case $J_2 = 0$ and coincides with the curve $\alpha = \infty$ in Fig. 2. The solid curve separates the region of existence of the ordered phase from the region of existence of the disordered phase. The region of ferromagnetic-type states of the system is indicated by the letter F, and the region of ordering of the antiferromagnetic type by the letter A. It is found that, for $J_2 < 0$ and $\alpha > 1$, the phase-equilibrium curves at $T = 0°K$ necessarily pass through the point $c = c_k = 0.25$. This critical concentration separates the ranges or existence of the F and A ground states and is a singular point for a lattice of the type considered, with impurities. At $c = c_k$, a rearrangement of the ground state of the system under consideration occurs (we have an F-state for $c < c_k$ and an A-state for $c > c_k$).

The following physical explanation can be given for the appearance of the above-mentioned critical concentration for $J_2 < 0$ and $|J_2| < J_1$. At $T = 0°K$, the state of the system is determined entirely by energy relationships, and it is therefore necessary to trace the distribution of impurities taking only energetic considerations into account. For $c = 0$ and $\alpha > 1$, the ground FF-state existing in the system is "unfavorable" with respect to the interaction of the non-nearest neighbors, since $J_2 < 0$. Therefore, the impurities added to the system ($c \neq 0$) will gather into complexes, "blocking" sites of the second type. In fact, if four impurities surround an atom of the second type, it is favorable for the atom to flip its "spin", creating local antiferromagnetic order. The energy is then reduced by an amount $8|J_2|$. For a low concentration ($c \ll 1$) the impurities will gather principally into isolated clusters, each consisting of four impurities, and the energy is lowered by $2J_2$ for each impurity in the clusters. However, it turns out that the formation of complexes in which the impurities are densely arranged along closed lines separating regions of FF-states with oppositely oriented total spins corresponds to the same energy lowering per impurity. A narrow region of antiferromagnetic order appears along the boundary line itself. In proportion with the increase in the impurity concentration, the total area of local antiferromagnetic order increases and the number of neighborhoods of ferromagnetically ordered regions with opposite spins increases. As a result, at a certain concentration c_k the network of antiferromagnetic order covers the whole lattice and the total spin of the system becomes equal to zero. This process should proceed in the same way for any $J_2 < 0$ and $\alpha > 1$, and therefore the quantity c_k depends neither on J_2 nor on α and is a geometrical characteristic of the original lattice. It is found that $c_k = 0.25$.

The behavior of the left branch of the phase-equilibrium curve in Fig. 3 for $T \neq 0$ can be understood by considering the example $|J_2| \ll J_1$ ($\alpha \gg 1$). For $kT \gg |J_2|$, the phase-transition curve will differ little from the curve $\alpha = \infty$. A sharp change in the behavior of this curve can set in only when $kT \sim |J_2|$, and for $kT \ll J_2$ the considerations that determine the structure of the ground state become important and the curve should pass through the point $c = c_k$, $T = 0$. The temperature $kT \sim |J_2|$ can be compared with the disorder temperature introduced by Stephenson[3] for the lattice of the model assumed. Near this temperature, the short-range order in the system should change.

We note that for all $\alpha > 2$ there is a range of concentration values $c > c_k$ for which the system is characterized by three phase-transition temperatures, separating the regions of the A-phase, the disordered phase, the F-phase, and the disordered phase again.

Figure 4a shows the phase-equilibrium curves for the cases $\alpha = 2$ (the dashed line) and $1.102 < \alpha < 2$ (the solid line). For $\alpha = 2$ a single phase-transition temperature corresponds to each concentration, and for $\alpha < 2$ there appears a range of concentrations to the left of the point c_k ($c < c_k$) in which the system experiences three phase transitions (the F-phase, the disordered phase, the A-phase, the disordered phase).

For $\alpha = 1.102$, the range of concentrations that permit three phase transitions expands down to $c = 0$ and the phase-equilibrium curve takes the form of the solid curve in Fig. 4b. The dashed curve in Fig. 4b corresponds to values of α in the range $1 < \alpha < 1.102$. As the parameter α approaches unity, the temperature region of existence of the F-phase decreases, and for $\alpha = 1$ it degenerates into the isolated point $c = 0$, $T = 0$. This is connected with the fact that the value $\alpha = 1$ for $J_2 < 0$ corresponds to a completely compensated impurity-free lattice of the type considered, in which an ordered ferromagnetic-type state cannot exist for

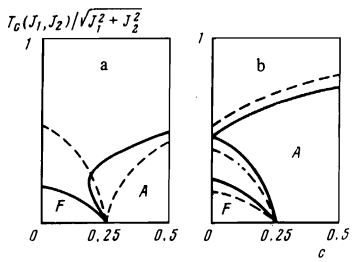

FIG. 4

$T \neq 0$ (cf.[1]). As regards the A-phase, however, in the case $\alpha < 1.02$ there is for this a region of existence for any concentration. Finally, for $\alpha < 1$ the system can be found only in two phases: in the A-phase and the disordered phase. The phase-transition curve in this case is analogous to the upper dashed line in Fig. 4b. For $\alpha = 0$ the phase-transition temperature ceases to depend on the impurity concentration.

We turn now to the case $J_1 < 0$. We note that if we simultaneously replace J_1 by $-J_1$ and η by $1/\eta$ in Fig. (12), its form is unchanged. Consequently, the analysis of the solutions of Eq. (12) carried out above is also applicable in the present case. It is necessary only to keep in mind that $1 \leq \eta \leq \infty$. Since the functions $y = y_1(\eta)$ and $y = y_2(\eta)$ given by the formulas (8) and (10) are also unchanged by the above replacement, both the classification of the solutions of Eq. (12) by means of the parameter α, and the form of the phase-equilibrium curves shown in Figs. 2–4 are conserved.

It is necessary only to make a few remarks concerning the ground state of the system. If $J_2 > 0$, the ground state of the system without impurities corresponds to an F-state of the atoms of the second type and to antiferromagnetic order of the atoms of the whole lattice (an FA-ground state). The presence of impurities in the system does not affect the F-order of the atoms of the second type at $T = 0°K$, but destroys the FA-order of the system as a whole. A nonzero total spin M appears, which increases with increasing impurity concentration, reaching its greatest value when $c = 1$. The point $c = 1$ corresponds to a simple square lattice with interaction $J_2 > 0$ between nearest neighbors. Thus, the presence of impurities in the system makes possible a continuous transition from a state with $M = 0$ ($c = 0$) to a state with $M \neq 0$ ($c \neq 0$) at $T = 0°K$.

If $J_2 < 0$, then, for $\alpha > 1$, the ground state of the system without impurities is, as before, an F-state for the atoms of the second type and an FA-state of the whole lattice, and for $\alpha < 1$ it corresponds to an A ground state of the atoms of the second type. The existence of the critical concentration $c_k = 0.25$ for $\alpha > 1$ can be explained by the same arguments as were presented in the case $J_1 > 0$, these being applied, however, only with respect to the atoms of the second type.

3. THE IMPURITY CHANGES THE SIGN OF THE EXCHANGE INTERACTION

We turn now to the case when the impurity reverses the sign of the interaction J_1 between nearest atoms, without changing its magnitude. The new exchange energy is $J = -J_1$, and, when (7) is taken into account, Eq. (4) takes the form

$$\varphi(\eta)\left[\eta-\exp\left(-\frac{2J_1}{T}\right)\right]\left[\exp\left(\frac{2J_1}{T}\right)-\eta\right]+c\left[\exp\left(\frac{2J_1}{T}\right)-\eta\right] -(1-c)\left[\eta-\exp\left(-\frac{2J_1}{T}\right)\right]=0. \tag{13}$$

If $T_0(J_1, J_2)$ is the phase-transition temperature in the lattice without impurities, then, as shown in[1], the relation $T_0(J_1, J_2) = T_0(-J_1, J_2)$ holds. It is easy to see that, in the case we are considering, the relation

$$T_c(J_1, J_2) = T_{1-c}(\pm J_1, J_2), \tag{14}$$

is fulfilled, where $T_c(J_1, J_2)$ is the transition temperature in the lattice with impurities.

The symmetry described by the relation (14) permits us to perform the analysis for only one sign of J_1. We shall assume, for definiteness, that $J_1 > 0$. If $J_2 > 0$, Eq. (13) has a solution for all concentrations for $\varphi = \varphi_1(\eta)$ and $0 \leq \eta \leq \infty$. The dependence of the phase-transition temperature $T_c(J_1, J_2)$ on the impurity concentration c in this case is shown in Fig. 5. The curves terminating at the points c_0 and $1 - c_0$ on the abscissa correspond to the case $\alpha = \infty$ (a simple square lattice with exchange interaction J_1 between nearest neighbors only). Characteristic of this curve is the presence, noted by Lushnikov[2], of two critical concentrations: $c_1 = c_0 = (2 - \sqrt{2})/4$ and $c_2 = 1 - c_0$, between which a phase transition is not observed. When any arbitrarily small interaction J_2 ($J_2 > 0$) is switched on, the critical concentrations on the phase-transition curve disappear. This result can be understood on the basis of the following arguments. As already noted, if $J_2 > 0$ the ground state of the system without impurities corresponds to F-ordering of the atoms of the second type and FF-ordering of the whole lattice. For $c = 0$, the system possesses a nonzero total spin M. The presence of impurities reversing the sign of J_1 "flips" some of the spins of the atoms of the first type, as a result of which the total spin M is decreased. But since the impurities do not affect the F-ordering of the atoms of the second type, there appears the possibility of a continuous transition from a state $M = 0$ with $c = 0$ to a state $M = 0$ with $c = 1$. Thus, the interaction of non-nearest neighbors stabilizes the ferromagnetic-type ordering of the whole lattice in the ground state, for any impurity concentration.

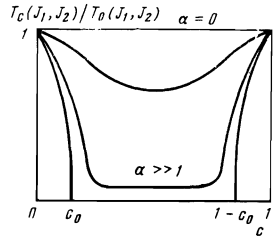

FIG. 5

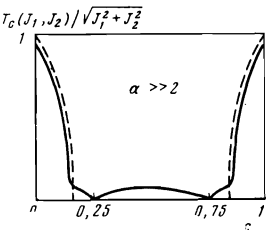

FIG. 6

With decrease of α, the concentration dependence of the phase-transition temperature becomes weaker, and in the limit $\alpha = 0$ the phase-transition temperature does not depend on the concentration.

The ground state of the system without impurities for the case $J_2 < 0$ has already been discussed. If $\alpha > 1$, Eq. (13) has a solution for all concentrations, both for $\varphi = \varphi_1(\eta)$ and for $\varphi = \varphi_2(\eta)$, with $0 \leq \eta \leq \infty$, while if $\alpha < 1$ solutions are possible only for $\varphi = \varphi_2(\eta)$ and $0 \leq \eta \leq \infty$. The concentration dependence of the phase-transition temperature in the case $\alpha \gg 2$ is shown in Fig. 6. The dashed curve corresponds to the case $J_2 = 0$. The solid curve separates the region of existence of the ordered phase from the region of existence of the disordered phase. It is found that, for $J_2 < 0$ and $\alpha > 1$, the phase-equilibrium curves necessarily pass through the points $c = c_{k1} = 0.25$ and $c = c_{k2} = 0.75$ for $T = 0$. We note that, in accordance with (14), the critical points are positioned symmetrically about $c = 0.5$. The critical concentrations c_{k1} and c_{k2} separate the ranges of existence of the F and A ground states and are singular points for the lattice with impurities being studied. For $c = c_{k1}$ and $c = c_{k2}$, a rearrangement of the ground state of the

system occurs (we have an F-state for $c < c_{k1}$ and $c > c_{k2}$, and an A-state for $c_{k1} < c < c_{k2}$).

The explanation of the appearance of the critical concentrations c_{k1} and c_{k2} in the case $J_2 < 0$, $\alpha > 1$ is analogous to the explanation of the appearance of the critical concentration in the case of complete rupture of the bonds (cf. Sec. 2). The sharp bend in the phase diagram in Fig. 6 for $\alpha \gg 2$ in the low-temperature region can also be understood on the basis of the same arguments that were used to explain the behavior of the phase-equilibrium curve in Fig. 3 for the case of complete rupture of the bonds.

As regards the phase-equilibrium curves for $\alpha \leq 2$, in the concentration range $0 < c < 0.5$ they can be described schematically by the graphs in Fig. 4. The dashed line in Fig. 4a again corresponds to the case $\alpha = 2$, and for $1.102 < \alpha < 2$ we can make use of the solid line in Fig. 4a. For $\alpha < 2$ concentration ranges $c < c_{k1}$ and $c > c_{k2}$ (increasing with decrease of α) appear in which the system can be found in three phase states (the F-phase, the disordered phase, the A-phase, and the disordered phase again). For $\alpha = 1.102$ the ranges of the concentrations that permit three phase transitions cover the intervals $0 \leq c \leq 0.25$ and $0.75 \leq c \leq 1$, and the phase-equilibrium curve takes the form of the solid line in Fig. 4b. The dashed line in Fig. 4b corresponds to a value of α in the range $1 < \alpha < 1.102$. As the parameter α approaches unity, the temperature range of existence of the F-phase decreases, and for $\alpha = 1$ it degenerates into the isolated points $c = 0$, $T = 0$ and $c = 1$, $T = 0$. At the same time, the A-phase for $\alpha < 1.112$ can exist for any impurity concentration. If $\alpha < 1$, the system can be found only in two phases: in the A-phase and in the disordered phase. The phase-transition curve in this case is analogous to the upper dashed line in Fig. 4b. For $\alpha = 0$ the phase-transition temperature does not depend on the impurity concentration.

CONCLUSION

We have analyzed the dependence of the phase-transition temperature on the impurity concentration in the two simplest cases: when the impurity breaks the bond between nearest neighbors ($J = 0$) and when it changes the sign of the interaction ($J = -J_1$). In principle, it is not difficult to construct the corresponding graphs for other values of J, since for this it is sufficient to analyze Eq. (4) with other values of the parameters. However, we shall confine ourselves to just a few qualitative remarks, some of which are obvious after the investigations described above.

First of all, and we see this as the main result, the ground state of the system is an ordered state for all concentrations. We draw special attention to this fact, because, in a number of papers devoted to the effect of impurities on the phase transition in a simple Ising lattice with interaction between nearest neighbors only[2,4,5], it was concluded that, in a certain range of concentrations, the ground state of the system is a disordered state. Such behavior of a simple lattice at $T = 0°K$ is connected with the fact that, in the indicated concentration range at low temperatures, the impurities form clusters that do not interact with each other and behave like particles of an ideal gas. The inclusion of interaction between non-nearest neighbors makes the ground state ordered.

Furthermore, it is always possible to find values of the parameters of the problem such that more than one phase-transition temperature exists in a wide range of concentrations. Finally, if $J_2 < 0$, the ground state is characterized by the existence of critical points separating ferromagnetic-type and antiferromagnetic-type states at $T = 0°K$.

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Note added in proof (April 24, 1974). In the recently published article by Kasai and Syozi [6], the dependence of the phase-transition temperature on the impurity concentration in a two-dimensional Ising lattice, equivalent to a certain specific Union Jack lattice in which the impurities change the sign of the exchange interaction between nearest neighbors, was analyzed. In this model, the critical concentration separating the regions of ferromagnetic and antiferromagnetic order at $T = 0$ are absent. The physical situation that arises is similar to the one that we discuss in connection with Fig. 5.

[1] V. G. Vaks, A. I. Larkin, and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. 49, 1180 (1965) [Sov. Phys.-JETP 22, 820 (1966)].
[2] A. A. Lushnikov, Zh. Eksp. Teor. Fiz. 56, 215 (1969) [Sov. Phys.-JETP 29, 120 (1969)].
[3] J. Stephenson, Phys. Rev. B1, 4405 (1970).
[4] I. Syozi and S. Miyazima, Progr. Theor. Phys. 36, 1083 (1966); Y. Kasai, A. Miyazima, and I. Syozi, Progr. Theor. Phys. 42, 1 (1969).
[5] A. M. Kosevich and V. A. Shklovskiĭ, Zh. Eksp. Teor. Fiz. 60, 1086 (1971) [Sov. Phys.-JETP 33, 588 (1971)].
[6] Y. Kasai and I. Syozi, Progr. Theor. Phys. 50, 1428 (1973).

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