Phase diagrams for the disordered Ising model with second-neighbor interactions

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The phase diagrams of the disordered Ising lattice with simple quadratic (SQ) symmetry and second-neighbor interaction are investigated by using an effective-field theory with correlations. The calculations are based on the δ-function distributions for the exchange integrals. It is found that phase diagrams exhibit some peculiar behavior. In particular, a type of reentrant phenomenon is predicted.

I. INTRODUCTION

The magnetic properties of structurally disordered ferromagnets have been intensively studied during the last 20 years. The quenched disorder is usually represented by the appropriate probability distribution for the exchange integrals. The most often used distribution is a bimodal Handrich-Kaneyoshi (H-K) function[1-4] although the Gaussian distribution[5,6] has also been applied for calculations of magnetic properties.

The above investigations have been carried out by means of an effective-field theory with correlations (EFTC) applied for the one-site cluster model[1,3,6] and for two-site clusters[2,4] as well. The obtained results are mostly concerned with the phase diagrams and with such interesting phenomenon as "reentrant magnetism."

However, all those papers, dealing with fluctuations of the exchange integral, were restricted to the nearest-neighbor (NN) approximation. This limitation may lead to some inconsistency of the theory in the region of strong structural fluctuations. To make this statement more clear, let us note that the magnetic exchange fluctuations originate from the structural disorder of the system. Thus, the primary reason for the exchange fluctuations are the fluctuations of interatomic distances. Those structural fluctuations are quenched and they reflect a degree of amorphization of the system. As a result of amorphization, the coordination zones become diffused and for sufficiently great disorder they may overlap each other. In other words, some of the atoms which originate from the second zone, as a result of amorphization, may be shifted in the region of the first zone and therefore cannot be excluded from our consideration. In such a situation the effective number of atoms in the neighborhood of a given lattice site varies with the change of the degree of disorder, and the effective strength of magnetic bonds also becomes different. Thus, we see that the restriction of the theory to the first coordination zone (NN approximation) may be unsatisfactory for the region of strong structural fluctuations.

To improve on the theoretical description, in the first step we propose to include into calculations the interaction with the next-nearest-neighbor (NNN) coordination zone, while both zones, the first and the second, can fluctuate independently. Such interaction with the second coordination sphere has already been considered in dilute alloys.[7,8] The results obtained there show that improvement can be important and it may lead to the considerable changes in phase diagrams, critical concentrations, and so on.

In the present paper, using the integral operator method[3,6] based on the exact Callen identity,[9] we shall study the influence of the second coordination zone and its fluctuations on the phase transition of the disordered Ising ferromagnet with simple quadratic (SQ) structure.

In Sec. II the outline of the theory is given. In the frame of EFTC the expression for Curie temperature in NNN approximation and with fluctuations has been derived. The standard one-site model has been used for calculations and the probability function was assumed in the form of H-K distribution.

In Sec. III the numerical results are illustrated in the figures and a detailed discussion is presented.

II. THEORY

The Ising Hamiltonian is assumed in the form

$$\mathcal{H}=-\frac{1}{2}\sum_{i,j}J_{ij}\mu_i\mu_j,\quad \mu_i=\pm 1\ , \tag{1}$$

where J_{ij} are the uncorrelated random exchange integrals.

For this Hamiltonian we will make use of the Callen identity,[9] which can be written as

$$\langle\langle \mu_i \rangle\rangle_r=\langle\langle \tanh(\beta\sum_{j\epsilon i}J_{ij}\mu_j)\rangle\rangle_r\ ;\quad \beta=1/kT\ , \tag{2}$$

where, by $\langle\langle \cdots \rangle\rangle_r$ we will denote a double average, thermal $\langle \cdots \rangle$, and over configurations $\langle \cdots \rangle_r$.

With the help of the integral operator method[3,6] the Callen identity can be transformed approximately as

$$m=\int_{-\infty}^{+\infty}d\omega\tanh(\beta\omega)\frac{1}{2\pi}\int_{-\infty}^{+\infty}dt\,e^{i\omega t}[\langle\cos(tJ_{ij})\rangle_r-im\langle\sin(tJ_{ij})\rangle_r]^z[\langle\cos(tJ_{ij'})\rangle_r-im\langle\sin(tJ_{ij'})\rangle_r]^{z'}\ , \tag{3}$$

where the self-consistency condition has been assumed, namely

$$\langle\langle \mu_i \rangle\rangle_r = \langle\langle \mu_j \rangle\rangle_r = \langle\langle \mu_{j'} \rangle\rangle_r \equiv m \ . \tag{4}$$

In Eq. (3) by z and z' we denote the numbers of NN and NNN, respectively, whereas J_{ij} and $J_{ij'}$ are the exchange integrals for the first and second coordination sphere.

It is necessary to point out that in derivation of Eq. (3) the following standard approximations have been made: First, the configurational averaging for spins and for exchange integrals have been taken independently of each other. Second, the multispin correlations and the structural correlations for different exchange integrals have been decoupled. The above approximations are typical for the EFTC.[1,3,6] As usual, in this theory the correlations for different spins are not considered, however the autocorrelations are taken into account and they markedly improve the results in comparison with the classical molecular-field approximation. For only the first coordination zone taken into account, this method would be of the same accuracy as the first Matsudaira approximation.[10] However, one has to stress that in this work the autocorrelations of spins are taken into account both for the first and second coordination zones [see Eq. (3)], which extends the standard formulation of the EFTC.

To calculate the average values on the right-hand side of Eq. (3) we will make use of the H-K distribution for the exchange integrals, extended for the first and second coordination zones:

$$p(J_{ij},J_{ij'}) = \tfrac{1}{2}\{\delta[J_{ij}-(J+\Delta)]+\delta[J_{ij}-(J-\Delta)]\} \times \tfrac{1}{2}\{\delta[J_{ij'}-(J'+\Delta')]+\delta[J_{ij'}-(J'-\Delta')]\} \ , \tag{5}$$

where

$$J_{ij} = J+\Delta_{ij} \ , \quad J_{ij'} = J'+\Delta_{ij'} \ , \tag{6}$$

and

$$\Delta = \sqrt{\langle(\Delta_{ij})^2\rangle_r} \ , \quad \Delta' = \sqrt{\langle(\Delta_{ij'})^2\rangle_r} \ . \tag{7}$$

Here, J and J' are the mean values of the exchange integrals and Δ, Δ' are the standard deviations for the first and second spheres, respectively.

With the help of distribution (5) the configurational mean values in Eq. (3) can be calculated in the following form:

$$\begin{aligned} &\langle\cos(tJ_{ij})\rangle_r = \cos(tJ)\cos(t\Delta) \ , \\ &\langle\cos(tJ_{ij'}\rangle_r = \cos(tJ')\cos(t\Delta') \ , \\ &\langle\sin(tJ_{ij})\rangle_r = \sin(tJ)\cos(t\Delta) \ , \\ &\langle\sin(tJ_{ij'}\rangle_r = \sin(tJ')\cos(t\Delta') \ . \end{aligned} \tag{8}$$

Further calculations can be performed for the particular crystallographic structure defined by z and z' numbers. We will deal with the SQ lattice, where $z=4$ and $z'=4$, then, Eq. (3) for magnetization can be written in the form

$$m = \int_{-\infty}^{+\infty} d\omega \tanh(\beta\omega) \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, e^{i\omega t} \sum_{\substack{n=1 \\ (\text{odd})}}^{7} C_n m^n \ , \tag{9}$$

where C_n coefficients are built from trigonometric functions of J, J', Δ, Δ', and t—a variable of integration. The integration on the right-hand side of Eq. (9) is not difficult to perform although rather time-consuming, however, if we are interested in Curie temperature, only one term has to be calculated:

$$1 = \int_{-\infty}^{+\infty} d\omega \tanh(\beta_C\omega) \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, e^{i\omega t} C_1 \ , \quad \beta_C = \frac{1}{kT_C} \ . \tag{10}$$

By performing this integration, the equation for Curie temperature can be written in the final form:

$$1 = \frac{1}{2^{12}} \sum_{n=1}^{10} \sum_{m=1}^{13} T_{n,m} [\tanh\beta_C(\alpha_n+\beta_m) + \tanh\beta_C(\alpha_n-\beta_m)] \ , \tag{11}$$

where the matrix elements α_n, β_m, and $T_{n,m}$ are listed in the Appendix.

Equation (11) is used for numerical calculations of phase diagrams for SQ lattice, with fluctuations of the first and second coordination spheres taken into account. The results of calculations and the discussion will be presented in the next section.

III. THE NUMERICAL RESULTS AND THE DISCUSSION

The numerical results for phase diagrams have been obtained for a given set of parameters J'/J, Δ/J, and Δ'/J. In Fig. 1 the kT_C/J dependency vs J'/J for various parameters Δ/J has been shown, whereas the condition $\Delta'/J=0$ has been assumed. This figure illustrates the influence of the interaction with the second coordination zone on the transition temperature of the SQ ferromagnet, whereas fluctuations are present at the first zone only.

The curve for $\Delta/J=0$ describes a special case without any fluctuations (the ideal crystal with NNN interaction) and it can be related to the similar result described in Ref. 8. We see that for negative J' values a strong reentrant magnetism is observed for $\Delta/J=0$. With increase of Δ/J parameter the reentrant magnetism generally decreases and the area of ferromagnetic region is also reduced. However, the end of a given phase diagram (the point where the phase curve approaches the horizontal axis J'/J) shifts along that axis in a rather complicated way.

Starting with Δ/J from zero and increasing it through the region $0 \le \Delta/J < 0.5$ the end of the phase diagram moves from $J'/J=0$ to $J'/J=-0.5$. Then, for $\Delta/J=0.5$ we obtained a jump of J'/J to the value -0.25, and next, increasing Δ/J ($0.5 \le \Delta/J \le \frac{2}{3}$) the end of the phase diagram moves from -0.25 to $-\frac{1}{3}$, respectively. Further, if $\frac{2}{3} \le \Delta/J \le 1$, the end of the phase curve travels gradually from $J'/J=-\frac{1}{3}$ to $J'/J=0$. As a re-

sult of those changes, the reentrant magnetism occurs rapidly when the value $\Delta/J=0.5$ is passed.

It is seen from Fig. 1 that for $\Delta/J \geq 1.1216$ the ferromagnetic state can occur only for positive values of J'/J. In the region $1.1216 \leq \Delta/J < 1.4154$ a type of reentrant magnetism is predicted, namely, for very low temperatures the narrow ferromagnetic state is observed first, then the sample passes a transition temperature and becomes paramagnetic and, further, with increase of temperature the reentrant magnetism occurs again. This behavior is a consequence of the S shape of phase curves in the above region of Δ/J parameter.

For $1.4154 \leq \Delta/J < 1.7763$ the reentrant magnetism does not occur. At $\Delta/J=1.7763$ the phase diagram is broken into two curves, each of them demonstrating a weak reentrant magnetism again. This feature is illustrated for $\Delta/J=1.8$ where a gap between both pieces of the curves is seen. In this gap a paramagnetic state is present only.

Further increase of Δ/J towards the value 2.2195 leads to complete vanishing of the reentrant magnetism. One can see that for such strong fluctuations the ferromagnetic region is reduced for very small temperatures only. Above $\Delta/J=3$ the ferromagnetic state cannot be found.

The above features have been confirmed in Fig. 2, where J'/J is assumed to be a parameter and Δ/J can be changed continuously on the axis. Figure 2, like Fig. 1, was obtained for $\Delta'/J=0$. The curve for $J'/J=0$ reproduces the result already known for a SQ lattice with NN interactions (e.g., see Ref. 3). If the J'/J parameter increases infinitesimally from zero value, then the end of the phase curve jumps from $\Delta/J=1$ to $\Delta/J=2$ (e.g., see curve $\Delta/J=0.05$ in Fig. 2). As a result of that jump, a narrow ferromagnetic state occurs for very low temperatures in the $1<\Delta/J<2$ region, if only $J'/J \gtrsim 0$. If we compare the curves for $J'/J=0$, 0.05, 0.2, and 0.5 in Fig.

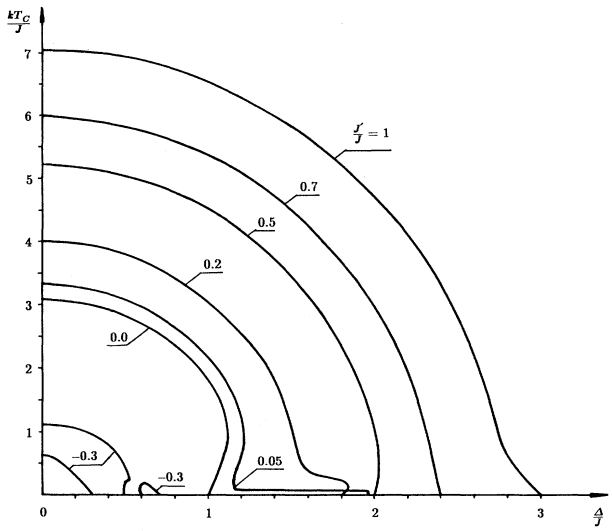

FIG. 2. Phase diagrams kT_C/J vs fluctuation of the first coordination zone Δ/J, plotted for several values of NNN interaction J'/J. The Δ'/J value is equal to zero.

2, we see that for successive curves the reentrant magnetism at intermediate temperatures gradually vanishes, but at the same time the new reentrant magnetism arises from the low-temperature region.

In general, the ferromagnetic range spreads up in Fig. 2 if the J'/J parameter is increased. On the other hand, for negative values of J'/J the ferromagnetic range becomes small and is restricted by several phase curves for the same parameter J'/J. It is illustrated in Fig. 2 for $J'/J=-0.3$ where two ferromagnetic areas are marked out by three phase boundaries.

Let us note that results identical with those presented in Figs. 1 and 2 can be obtained, if we assume that the second coordination zone can fluctuate ($\Delta'>0$), whereas for the first sphere we will put $\Delta=0$. It is a consequence

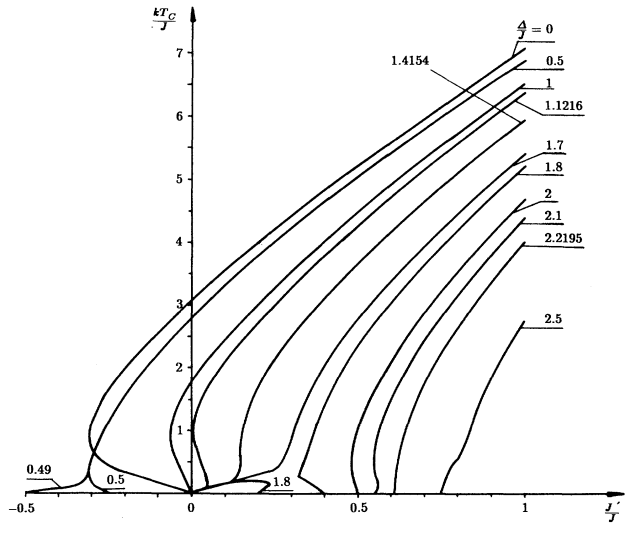

FIG. 1. Phase diagrams kT_C/J vs NNN interaction J'/J, plotted for several fluctuation parameters Δ/J. The Δ'/J value is equal to zero.

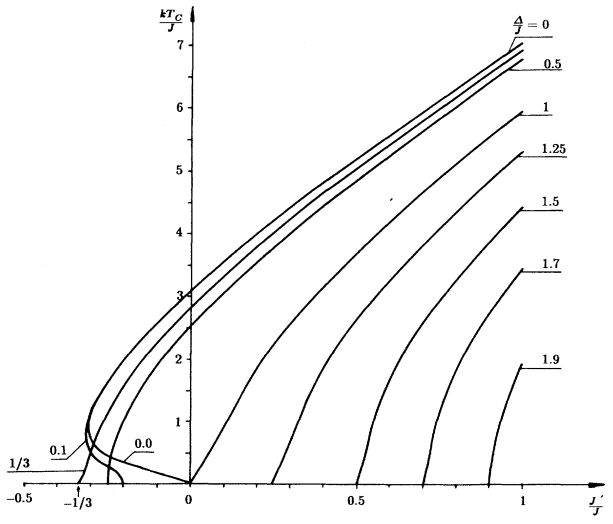

FIG. 3. Same as in Fig. 1, but for $\Delta'=\Delta$.

of the symmetrical property of Eq. (11) if the following parameters are interchanged; $\Delta \rightleftarrows \Delta'$ and (or) $J \rightleftarrows J'$. This property follows directly from the special symmetry of the SQ lattice ($z=z'$).

In Fig. 3 the phase diagrams are presented for the case when the exchange integrals for both coordination zones can fluctuate with the same magnitude: $\Delta/J=\Delta'/J$. This figure can be then compared with corresponding Fig. 1. The curve for $\Delta/J=0$ is identical for both Fig. 3 and Fig. 1 and illustrates the behavior of the phase transition in the absence of structural fluctuations. In the initial range of fluctuations, when $0 \leq \Delta/J \leq \frac{1}{3}$, the end of phase curve ($kT_C/J=0$) moves along the interval $\langle 0; -\frac{1}{3} \rangle$, and as a consequence, the reentrant magnetism vanishes. For $\frac{1}{3} \leq \Delta/J \leq 1$ the discussed phase point moves back to the value $J'/J=0$, so that for $\Delta/J=\Delta'/J=1$ the ferromagnetic phase can be expected only for positive values of J'/J. If the fluctuation parameter Δ/J is further increased, then the whole diagram is shifted to the positive direction along the J'/J axis. No reentrant magnetism is observed during this process and the general character of phase diagrams, when compared with Fig. 1, is much less complicated Thus, one can conclude that in the presence of fluctuations at both zones ($\Delta=\Delta'$), the phase curves are more stable vs Δ, in contrast to the case when only one sphere is disordered.

The above conclusion has been confirmed in Fig. 4. This figure corresponds to Fig. 2 but has been obtained for $\Delta=\Delta'$. It is seen from Fig. 4 that for $J'/J \geq 0$ the phase diagrams have a regular shape, and do not show any reentrant magnetism when presented in ($\Delta=\Delta'; kT_C/J$) coordinate system. The reentrant magnetism can be expected only for $J'/J<0$, provided the Δ/J parameter is sufficiently small. The example illustrated in Fig. 4 (curve $J'/J=-0.3$) shows that the range of the ferromagnetic state is then restricted by two phase boundaries.

Two other curves are of particular interest in Fig. 4.

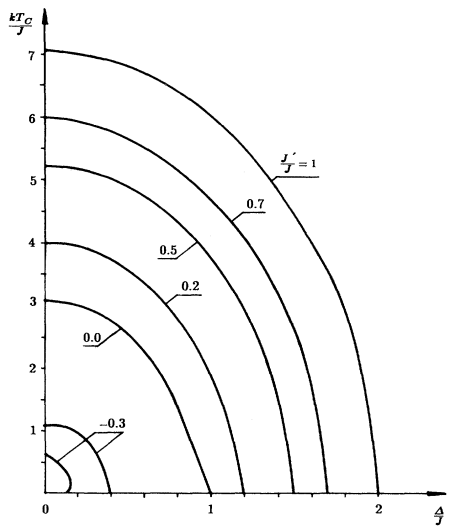

FIG. 4. Same as in Fig. 2, but for $\Delta'=\Delta$.

The first one, for $J'/J=0$, represents the interaction with the second coordination sphere via fluctuations ($\Delta=\Delta'$) only. The second one, for $J'/J=1$, describes the case when the interaction with NNN is equivalent to the interaction with the first sphere. In such a case, the SQ lattice with NNN interaction, becomes equivalent to a bcc ferromagnet with $z=8$ in NN approximation. This special case follows directly from the symmetry ($z=z'$) of SQ lattice.

Comparing Figs. 2 and 4 we see that the largest value of Δ/J, below which the ferromagnetic state can be expected, depends on the fluctuations of the second zone. This value is equal to 3 for $\Delta'=0$ (Fig. 2), and decreases to $\Delta/J=2$, when both fluctuations are present ($\Delta=\Delta'$ in Fig. 4). Above those two values only a paramagnetic phase can be found in corresponding figures.

IV. CONCLUSIONS

We have determined the complete phase diagrams of the disordered square Ising lattice with fluctuating nearest-neighbor and next-nearest-neighbor interactions obeying a bimodal Handrich-Kaneyoshi distribution. The calculations have been carried out by means of the effective field theory with correlations. The main conclusion of our study is that the influence of the second coordination zone on the magnetic properties may be very important. This influence takes place not only in the case of absence of the structural fluctuations, but also for their presence, as well.

When only one sphere is disordered, the behavior of the phase diagrams, for a given Δ/J parameter, is determined by the relative strength of interaction J'/J with the next sphere (Figs. 1 and 2). Especially in the region $1.1216 \leq \Delta/J < 1.4154$ we found a different type of reentrant phenomenon.

When structural fluctuations are present for both zones, they may result in vanishing of the reentrant magnetism phenomenon, even if the mean interaction with the second zone is small (e.g., compare curves for $J'/J=0$ in Figs. 2 and 4).

The diffraction experiments performed for various amorphous materials show that the first coordination zone is much less diffused than the second one. However, the second zone is usually very diffused and sometimes it even may be difficult to identify its position in the diffraction picture. This fact confirms our assumption that the atoms from the first and second zones may be partly mixed with each other and therefore both zones can contribute to the magnetism.

The results obtained here are encouraging for further investigations of structurally quenched ferromagnets with more complex lattices, when NNN interactions are taken into account.

ACKNOWLEDGMENT

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APPENDIX

The matrix elements α_n, β_m, and $T_{n,m}$ are of the following form:

$\alpha_1=4J+4J'$
$\alpha_2=4J+2J'$
$\alpha_3=4J-2J'$
$\alpha_4=4J$
$\alpha_5=2J+4J'$
$\alpha_6=2J-4J'$
$\alpha_7=2J+2J'$
$\alpha_8=2J$
$\alpha_9=4J'$
$\alpha_{10}=2J'$

$\beta_1=4\Delta+4\Delta'$
$\beta_2=4\Delta-4\Delta'$
$\beta_3=4\Delta+2\Delta'$
$\beta_4=4\Delta-2\Delta'$
$\beta_5=4\Delta$
$\beta_6=2\Delta+4\Delta'$
$\beta_7=2\Delta-4\Delta'$
$\beta_8=2\Delta+2\Delta'$
$\beta_9=2\Delta-2\Delta'$
$\beta_{10}=2\Delta$
$\beta_{11}=4\Delta'$
$\beta_{12}=2\Delta'$
$\beta_{13}=0$

$T_{1,1}=1$
$T_{1,2}=1$
$T_{1,3}=4$
$T_{1,4}=4$
$T_{1,5}=6$
$T_{1,6}=4$
$T_{1,7}=4$
$T_{1,8}=16$
$T_{1,9}=16$
$T_{1,10}=24$
$T_{1,11}=6$
$T_{1,12}=24$
$T_{1,13}=18$

(for $m=1,2,\ldots,13$)
$T_{2,m}=3T_{1,m}$
$T_{3,m}=T_{1,m}$
$T_{4,m}=3T_{1,m}$
$T_{5,m}=3T_{1,m}$
$T_{6,m}=-T_{1,m}$
$T_{7,m}=8T_{1,m}$
$T_{8,m}=6T_{1,m}$
$T_{9,m}=3T_{1,m}$
$T_{10,m}=6T_{1,m}$

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