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EFFECT OF MAGNETIC IMPURITIES ON THE PHASE TRANSITION TEMPERATURE IN A TWO-DIMENSIONAL ISING LATTICE

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Let us consider a square Ising lattice with annealed bond impurities. The impurities affect the magnitude or the magnitude and the sign of the exchange interaction J_o between neighbouring spins in the lattice. The value of the new interaction due to the impurities is denoted by J. The exact dependence of the phase transition temperature on the impurity concentration in this model has been obtained by Lushnikov (1969) in the case of temperature - independent interaction J.

Recently the author (Grozdev 1984, 1988) discussed in detail the opposite case of a temperature - dependent interaction J(T) in two forms:

$$J(T) = \frac{1}{2} kT \ln I_o(\alpha J_o/kT) \tag{1}$$

and

$$J(T) = \frac{1}{2} kT \ln\left[\sinh(\alpha J_o/kT)/(\alpha J_o/kT)\right], \tag{2}$$

where I_o is the modified Bessel function of order zero, T is the absolute temperature, k is the Boltzman constant and α is an arbitrary (but finite) factor. The first form (1) arises naturally in a decorated lattice model of a mixed system of Ising and classical planar spins (Falk 1980). The second form (2) arises in an analogous model of a mixed system of Ising and three dimensional classical vector spins (dos Santos et al. 1986).

In this Letter we consider another form of the temperature-dependent interaction due to the annealed bond impurities in the square Ising lattice,

$$J(T) = \frac{1}{2} kT \ln \frac{\sinh\left[(2s + 1)\alpha J_o/kT\right]}{(2s + 1)\sinh(\alpha J_o/kT)}, \tag{3}$$

which arises in the Ising model decorated with higher Ising spins of magnitude s (Yamada 1969, Gonçalves and Horiguchi 1984). Because the expression under the logarithm sign in equation (3)

$$g_s(x) = \sinh\left[(2s + 1)x\right] / \left[(2s + 1)\sinh x\right] \qquad (4)$$

is an even function of x and $g_s(x) \geq 1$ for all $x = \alpha J_0/kT$ and s = 1/2, 1, 3/2, ..., only two different physical situations may be considered: (i) when the ideal lattice is ferromagnetic ($J_0 > 0$) and the impurity changes the magnitude but not the sign of J_0; (ii) when the ideal lattice is antiferromagnetic ($J_0 < 0$) and the impurities introduce a positive interaction in the lattice.

Using the Lushnikov method (1969) (for details see Grozdev 1984) it is easy to obtain the basic equations, which give the exact dependence of the phase transition temperature T_c on the impurity concentration C (defined as ratio of the number of impurities to the number of bonds) in both the cases. In the first case (i) we have

$$\frac{\sqrt{2}}{4} - \frac{C}{\sqrt{2} - 1 - \exp(-2x/\alpha)} + \frac{1 - C}{1/g_s(x) - \sqrt{2} + 1} = 0. \qquad (5)$$

In the second case (ii) we need two equations to describe the dependence of T_c on C,

$$\frac{\sqrt{2}}{4} - \frac{C}{\sqrt{2} + 1 - \exp(2|x/\alpha|)} + \frac{1 - C}{1/g_s(x) - \sqrt{2} - 1} = 0 \qquad (6a)$$

for small concentrations (antiferromagnetic lattice at C = 0) and

$$\frac{\sqrt{2}}{4} - \frac{C}{\sqrt{2} - 1 - \exp(2|x/\alpha|)} + \frac{1 - C}{1/g_s(x) - \sqrt{2} + 1} = 0 \qquad (6b)$$

for large concentrations (ferromagnetic lattice at C = 1).

Equations (6a) and (6b) must be solved together in order to obtain results for all concentrations.

Because of the transcendental nature of the basic equations (5) and (6), we must turn to numerical calculations. For the case (i) ($J_0 > 0$ and $J(T) > 0$) we have solved equation (5) at s = 1/2 and α = 2, 3 and 4 in order to reveal α-dependence of the solution. For s = 1/2 the higher Ising spin reduces to the ordinary Ising spin and instead the expressions (3) and (4) we have

$$J(T) = \frac{1}{2} kT \ln \cosh(\alpha J_0/kT) \qquad (7)$$

and

$$g_{1/2}(x) = \cosh x, \qquad (8)$$

as in ordinary decorated Ising lattices (Syozi 1972). The results are plotted in the form kT_c/J_0 against C in figure 1 (solid curves). For comparison with the case of constant interaction due to impurities ($J_0 > 0$ and $J = \beta J_0$, where β = constant) the corresponding Lushnikov curves are also plotted (dashed curves). The values of β are chosen to give at C = 1 the same T_c as in the case under consideration: $\beta = 0.57$ for $\alpha = 2$, $\beta = 0.86$ for $\alpha = 3$ and $\beta = 1.15$ for $\alpha = 4$. It can be seen in figure 1 that the solid curves resemble the appropriate dashed curves. Indeed the curves are concave downwards for small α and $\beta < 1$ and upwards for large α and $\beta > 1$. Evidently, there is a boundary value of α at which the solid curves change their behaviour. The corresponding boundary value for the dashed curves is $\beta = 1$. Using this value of β, we estimate the boundary value of α as about 3.47. With increasing α up to 3.47 and β up to 1 the concentration dependence of the phase transition temperature in both cases becomes weaker (for $\beta = 1$ there is no concentration dependence of T_c in the Lushnikov case) but with further increasing of α and β this dependence becomes again stronger. The ground state of the system with impurities is ferromagnetic in both cases. Each curve in figure 1 separates the region of existence of the ferromagnetic phase from the region of

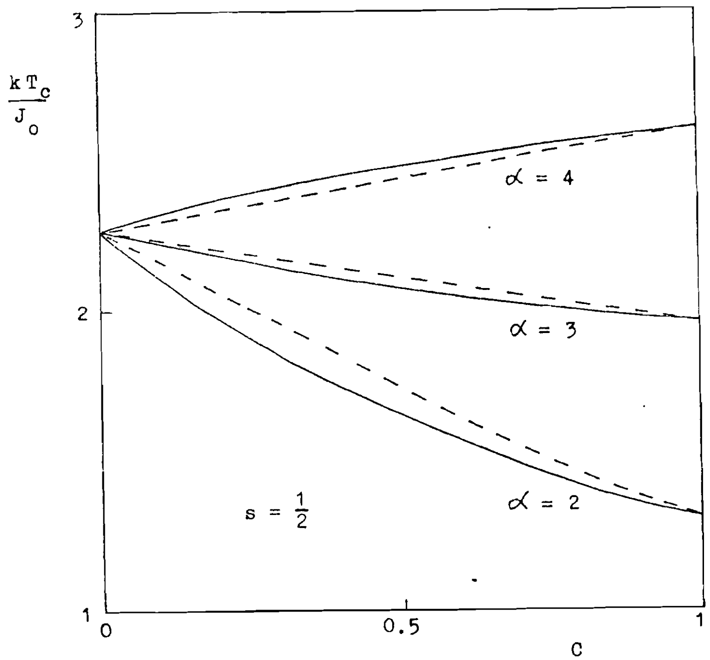


Figure 1. The phase transition temperature T_c as a function of impurity concentration C in a ferromagnetic ($J_o > 0$) square Ising lattice. The solid and dashed curves show the results for the cases $J(T) = \frac{1}{2}$ kT ln cosh$(\alpha J_o/kT)$ with α = 2, 3, 4 and $J = \beta J_o$ with β = 0.57, 0.86, 1.15, respectively.

existence of the disordered phase. But the ferromagnetic regions under the solid curves are reduced for $\alpha < 3.47$ and broadened for $\alpha > 3.47$ in comparison to the corresponding ferromagnetic regions under the dashed curves. As was pointed out by Grozdev (1984)(see also Grozdev 1988), this effect is a direct consequence of the temperature - dependent character of the exchange interaction J(T).

Qualitatively the same picture as in figure 1 we obtain by numerical investigations of equation (5) in the cases s = 1 at α = 1, 2 and 3, s = 3/2 at α = 0.5, 1 and 2, etc. In order to demonstrate the s - dependence of the solution of equation (5), we show in figure 2 the T_c versus C curves for given α (= 2) and s = 1/2, 1 and 3/2.

We turn now to the case (ii) ($J_o < 0$ and $J(T) > 0$) for which one can expect an interesting phase diagram on account of the competition between negative and positive interactions in the model with impurities. Equations (6a) and (6b) can be solved numerically at each value of α and s but for illustration we consider here only the cases s = 1/2 (solid curve in figure 3) and s = 3/2 (dashed curve in figure 3) at given α (= 2). The dash-dotted curve in the same figure gives the result of Lushnikov (1969) for the case when the impurity reverses the sign of the interaction J_o without changing its magnitude ($J_o < 0$ and $J = - J_o$). The solid curve in figure 3 also represents schematically the behaviour of the phase transition temperature on the impurity concentration in the cases of J(T) in the form (1) (Grozdev 1984) and (2) (Grozdev 1988) with $\alpha = 2$.

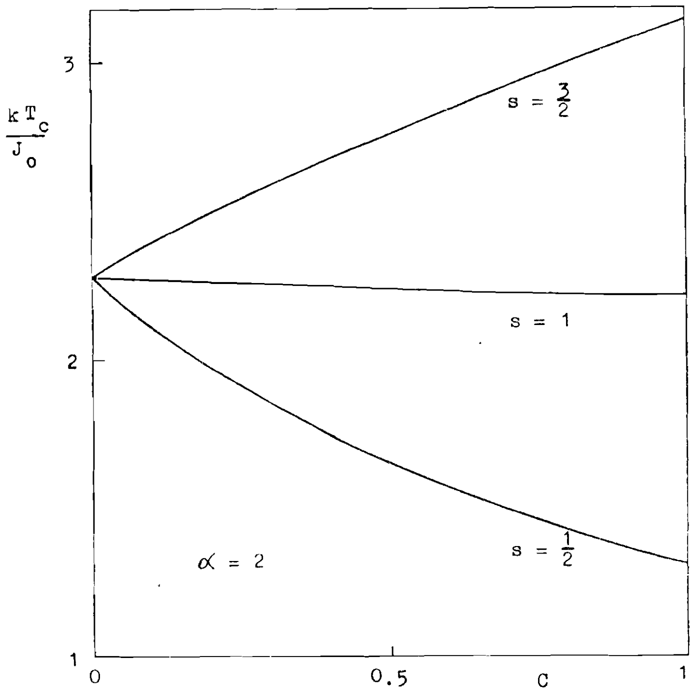
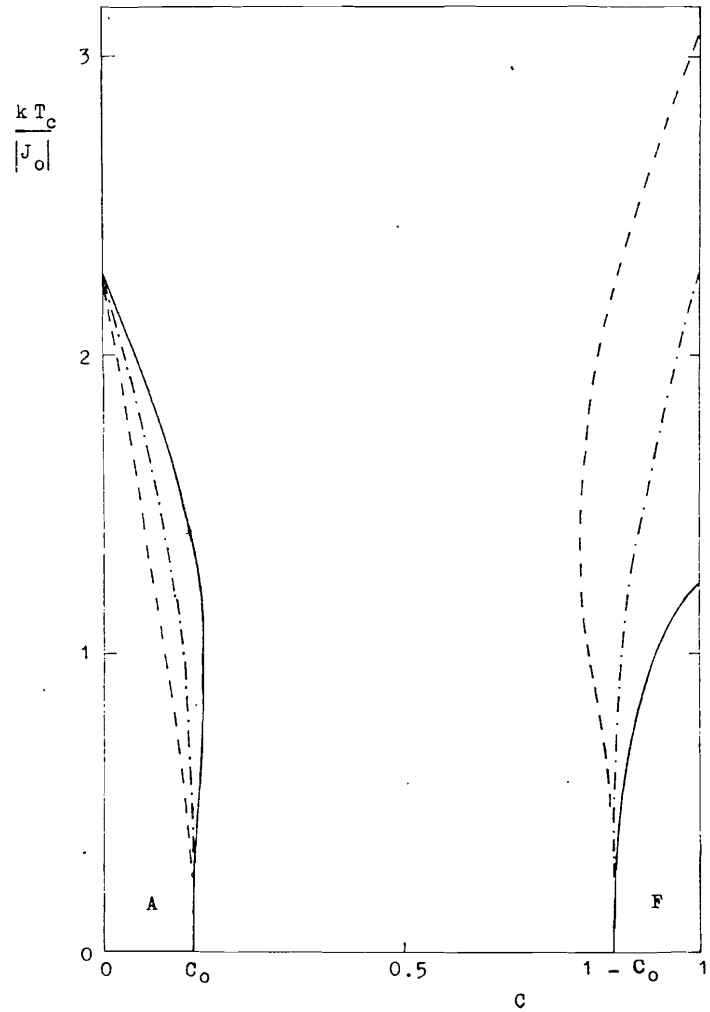


Figure 2. The phase transition temperature T_c as a function of impurity concentration C in a ferromagnetic ($J_o > 0$) square Ising lattice. The curves show the results for the case of J(T) in the form (3) with s = 1/2, 1, 3/2 and α = 2.

Figure 3. The phase transition temperature T_c as a function of impurity concentration C in an antiferromagnetic ($J_o < 0$) square Ising lattice. The solid and dashed curves show the results for the case of J(T) in the form (3) with α = 2, s = 1/2 and 3/2, respectively. The dash-dotted curve represents the Lushnikov result for the case $J = -J_o$. Here the ferro- and antiferromagnetic regions are abbreviated as F and A, respectively.

All curves in figure 3 separate the region of existence of the ordered phase (the antiferromagnetic one under their left-hand branches and the ferromagnetic one under their right-hand branches) from the region of existence of the disordered phase. The critical concentrations $C_1 = C_0 =$



$(2-\sqrt{2})/4$ and $C_2 = 1 - C_0$ are common for all curves. There is no phase transition for $C_1 < C < C_2$ in Lushnikov's case of temperature-independent interaction due to the impurities. But re-entrant phenomena can be observed from the phase diagrams in the case of temperature - dependent interaction due to the impurities. Indeed, there appears an interval of concentrations to the right of the point $C_1 = C_0$ in the case $s = 1/2$ and $\alpha = 2$ (the solid curve in figure 3) and an interval of concentrations to the left of the point $C_2 = 1 - C_0$ in the case $s = 3/2$ and $\alpha = 2$ (the dashed curve in figure 3) for which two phase transitions are possible. Another consequence of the temperature - dependent character of J(T) is the reduction of the ferromagnetic (antiferromagnetic) region and the broadening of the antiferromagnetic (ferromagnetic) region under the solid (dashed) curve in comparison to the corresponding regions under Lushnikov's curve in figure 3.

One can explain the existence of two kinds of phase diagrams (at given α and different s) by the s-dependence of the effective interaction (3). Indeed, it is easy to show that the normalized effective interaction $J(T)/\alpha J_0$ is equal to s at T = 0 and smoothly decreases to its asymptotic value of zero with increasing T. Thus the effective interaction due to the impurities is ferromagnetically stronger for higher s not only at low temperatures but also in an intermediate temperature region where the re-entrant phenomena arise. In Yamada's model, an analogous effect is according to the increasing freedom of decoration spin variables (Horiguchi and Gonçalves 1983). But

it must be remarked that a phase diagram at given s can be changed from one kind to another by appropriate choosing of α.

It is interesting to point that our results are compatible with the results of Kasai et al. (1969) obtained for the generalized version of the so-called "exclusive double bond model". Of course, the "annealed" disorder is not normally found in real mixed magnets (Stinchcombe 1983). But recently De' Bell (1980) has adapted successfully an annealed bond-decorated Ising model as a simplest qualitative model of real amorphous antiferromagnets which show re-entrant phenomena as described above. Finally, we believe after Rapaport (1972) that our exact results are very close to those for the corresponding more realistic quenched model.

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Гроздев К.И. E17-88-812

Влияние магнитных примесей на температуру фазового перехода в двумерной модели Изинга

Найдена точная зависимость температуры фазового перехода от концентрации подвижных примесей внедрения в двумерной модели Изинга. При наличии примеси между ближайшими спинами идеальной решетки обменное взаимодействие всегда положительно и зависит от температуры так же, как в случае декорированной модели смешанных систем изинговских спинов и изинговских спинов величиной s. Обсуждены особенности фазовых диаграмм системы с примесями в обоих случаях ферро- и антиферромагнитной идеальной решетки.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Effect of Magnetic Impurities on the Phase Transition Temperature in a Two-Dimensional Ising Lattice

A two-dimensional Ising model with annealed bond impurities is studied exactly. The exchange interaction between spins due to impurities is taken to be temperature-dependent and positive as in a decorated model of a mixed system of Ising spins and higher Ising spins of magnitude s. The peculiarities of the phase diagrams of the system with impurities are discussed in both cases of ferro- and antiferromagnetic ideal lattices.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

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