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EFFECT OF ANNEALED BOND 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 which affect the magnitude (and possibly the sign) of the exchange interaction J_0 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 the model has been obtained by Lushnikov [1] in the case of temperature-independent interaction J. Recently the author [2] discussed in detail the opposite case of a temperature-dependent interaction

$$J(T) = \frac{1}{2} kT \ln I_0(\alpha J_0/kT), \tag{1}$$

which arises naturally in a "decorated lattice" model of a mixed system of Ising and classical planar spins [3]. In (1) I_0 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.

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

$$J(T) = \frac{1}{2} kT \ln[\mathrm{sh}(\alpha J_0/kT)/(\alpha J_0/kT)], \tag{2}$$

which arises in a decorated Ising model with three dimensional classical vector spins [4]. Because the function sh x/x in (2) is an even function of x and sh x/x ≥ 1 for all $x = \alpha J_0/kT$, only two different physical situations may be considered: (i) when the lattice without impurities 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 a method of Lushnikov [1] (for details see [2]) 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 the ratio of the number of impurities to the number of bonds) in both the cases. In the first case (i) we have

$$\frac{\sqrt{2}}{4} - \frac{C}{\sqrt{2} - 1 - \exp(-2J_0/kT)} + \frac{1 - C}{(\alpha J_0/kT)\,\mathrm{sh}(\alpha J_0/kT) - \sqrt{2} + 1} = 0 \quad (3)$$

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

$$\frac{\sqrt{2}}{4} - \frac{C}{\sqrt{2} + 1 - \exp(2|J_0|/kT)} + \frac{1 - C}{(\alpha J_0/kT)/\mathrm{sh}(\alpha J_0/kT) - \sqrt{2} - 1} = 0 \quad (4)$$

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

$$\frac{\sqrt{2}}{4} - \frac{C}{\sqrt{2} - 1 - \exp(2|J_0|/kT)} + \frac{1 - C}{(\alpha J_0/kT)/\mathrm{sh}(\alpha J_0/kT) - \sqrt{2} + 1} = 0 \quad (5)$$

for large concentrations (ferromagnetic lattice at C = 1). Of course, eqs. (4) and (5) must be solved together to obtain results for all concentrations.

The difficulties of the subsequent analysis lie only in the transcendental nature of the basic equations and we must turn to numerical calculations. For case (i) we have solved (3) numerically at three different values of α (= 2, 4 and 6). The results are plotted in the form kT_c/J_0 against C in Fig. 1 (solid curves). For comparison with the case of temperature-dependent interaction J(T) in the form (1), the corresponding curves from[2] are also plotted (dashed curves). The gro-

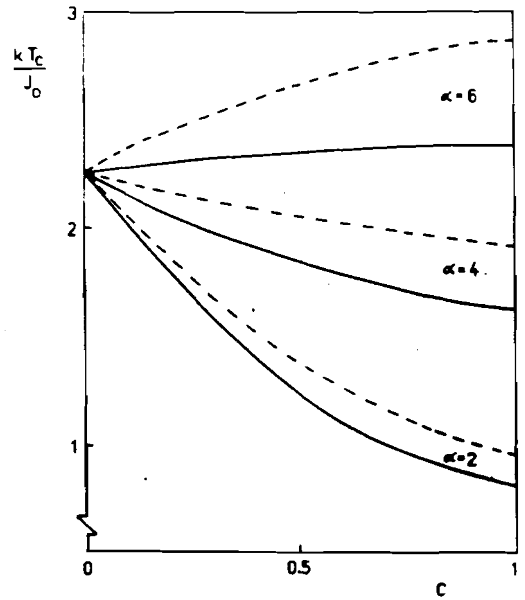

Fig. 1. Phase transition temperature T_c as a function of impurity concentration C in a ferromagnetic ($J_0 > 0$) square Ising lattice. The solid and dashed curves show the results for the cases $J = \frac{1}{2}kT\ln[\mathrm{sh}(\alpha J_0/kT)/(\alpha J_0/kT)]$ *and* $J = \frac{1}{2}kT\ln I_0(\alpha J_0/kT)$ *(with α=2,4, and 6) respectively.*

und state of the system with impurities is ferromagnetic in both cases. The curves in Fig. 1 separate the region of existence of the ferromagnetic phase from the region of existence of the disordered phase. It can be seen in Fig. 1 that the solid curves resemble the appropriate dashed curves. Indeed the curves are concave downwards for small α and upwards for large α. We estimate the boundary value of α as about 5.66 for the solid curves and as about 4.76 for the dashed cerves. A further discussion in connection with Lushnikov's curves[1] can be obtained in[2] and easy adapted to the case under consideration.

For case (ii) one can expect an interesting phase diagram on account of the competition between negative and positive interactions in the lattice with impurities. Eqs. (4) and (5) can be solved numerically at each value of α but for illustration we consider only the case α=2 (solid curve in Fig.2). The dash-dotted curve in the same figure represents Lushnikov's result[1] for the case with the impurity reverses the sign of the interaction J_0 without changing its magnitude ($J_0 < 0$ and $J = -J_0$). For comparison with the case of J(T) in the form (1) the corresponding curve from[2] is also plotted (dashed curve). All curves in Fig. 2 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

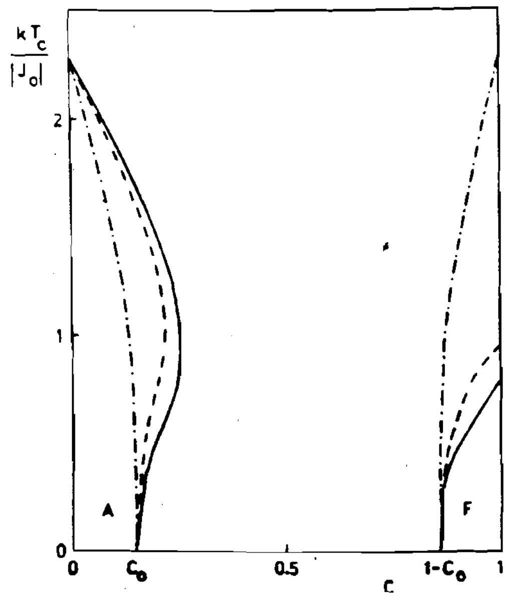

Fig. 2. Phase transition temperature T_c as a function of impurity concentration C in an antiferromagnetic ($J_0 < 0$) square Ising lattice. The solid, dashed and dash-dotted curves show the results for the cases $J = \frac{1}{2}kT \times \ln[\mathrm{sh}(2J_0/kT)/(2J_0/kT)]$, $J = \frac{1}{2}kT\ln I_0(2J_0/kT)$ *, and* $J = -J_0$*, respectively. Here ferro- and antiferromagnetic regions are abbreviated as F and A, respectively.*

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 in both cases of temperature-dependent interaction due to the impurities there appears a range of concentrations to the right of the point $C_1 = C_0$ for which the system experiences two phase transitions. As was pointed in [2], another consequence of the temperature-dependent character of J(T) is the strong reduction of the ferromagnetic region and the broadening of the antiferromagnetic region under both the solid and dashed curves in Fig. 2 in comparison to the corresponding regions under Lushnikov's curve. This effect is more expressed in the case under consideration.

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Гроздев К.И. E17-88-251

Влияние подвижных примесей внедрения 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 также, как в случае декорированной модели смешанных систем изинговских спинов и трехмерных классических векторных спинов. 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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Grozdev K.I. E17-88-251

Effect of Annealed Bond 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 mixing system of Ising spins and three dimensional classical vector spins. The peculiarities of the phase diagrams of the system with impurities are discussed in both cases of ferro- and antiferromagnetic ideal lattices.

The invesigation has been performed at the Laboratory of Computing Tecnhiques and Automation, JINR.

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