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QUENCHED BOND-DILUTE ISING FERROMAGNET IN SQUARE LATTICE: THERMODYNAMICAL PROPERTIES

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ABSTRACT

Within an effective field framework which improves the Molecular Field Approximation, we calculate the phase diagram, magnetization, specific heat and susceptibility associated with the quenched bond-dilute Ising ferromagnet in square lattice. The results are qualitatively (and within certain extent quantitatively) satisfactory; in particular the effects, on the specific heat and susceptibility, of the (eventually) coexisting finite and infinite clusters are exhibited.

I - INTRODUCTION

During recent years much effort has been dedicated to quenched (and annealed) bond-dilute magnetic systems. Because of its relative simplicity the square lattice spin - $\frac{1}{2}$ Ising ferromagnetic is of course one of the most intensively studied. Nevertheless, even its (exact) phase diagram is still unknown (excepting the terminal critical points and derivatives; see, for example, Ref. [1,2] and references therein for details on the available approaches). The situation is even worse in what concerns the thermodynamical properties. Some approximate calculations of the specific heat [3,4] and spontaneous magnetization[2] are already available, but to the best of our knowledge no attempts have been published concerning the magnetic susceptibility.

Recently Honmura and Kaneyoshi[5] have introduced, for the spin - $\frac{1}{2}$ pure Ising model, a new type of effective field approximation (based in the use of a convenient differential operator into the first Callen spin correlation identity[6]) which, within a mathematically simple framework, substantially improves the standard Molecular Field Approximation (MFA) results (this point will be exhibited herein and is extensively commented in Ref.[2]). This approach shares with the MFA a great versatility and has already been applied to a variety of interesting situations such as pure sytems[7], site-random[8] and bond-random [2,9] magnets including spin-glass[10] and amorphous[11,12] systems, transverse Ising model[13] and surface problems[14]. Most of these works have been devoted to the analysis of the phase diagram and the spontaneous magnetization; the specific heat (and eventually the short range order parameter) has been focused in pure isotropic [5], pure anisotropic [15] and bond-dilute isotropic [9] systems; the zero field isothermal magnetic susceptibility has been focused only once [15] (pure anisotropic system).

In the present work we study the quenched bond-dilute spin - $\frac{1}{2}$ Ising ferromagnet in square lattice, and calculate the most relevant thermodynamical quantities (phase diagram, spontaneous magnetization, short range order parameter, specific heat and zero field magnetic susceptibility) within an unified approximation framework; in particular the present approach for the specific heat is different (and more satisfactory in the sense that it decouples the bond concentration from the lattice coordination number) from that appearing in Ref. [9]. By following along the lines of Ref. [15] we treat the magnetic susceptibility by two slightly different procedures (more or less adapted to the low and high temperature regions).

II - MODEL AND FORMALISM

II.1 - Spontaneous magnetization

Let us consider the Hamiltonian

$$\mathcal{H} = - \sum_{<i,j>} J_{ij}\sigma_i\sigma_j \qquad (\sigma_i, \sigma_j = \pm 1) \tag{1}$$

where <i,j> run over all the couples of nearest-neighbouring sites of a square lattice, and J_{ij} is a random variable associated with the following probability distribution law:

$$P(J_{ij}) = (1-p)\delta(J_{ij}) + p\delta(J_{ij}-J) \qquad (0\leq p\leq 1; J>0) \tag{2}$$

The starting point for the thermal treatment of the present Ising system is the following first Callen identity[6]:

$$\langle\sigma_i\rangle = \langle\tanh\beta\sum_j J_{ij}\ \sigma_j\rangle \qquad (\beta\equiv 1/k_B T) \tag{3}$$

where <...> denotes the canonical <u>thermal</u> average for a given configuration of the $\{J_{ij}\}$ and j runs over the 4 nearest-neighbours of site i. By following Ref. [5] we introduce now the differential operator $D \equiv \partial/\partial x$ into Eq. (3) and obtain

$$\langle\sigma_i\rangle = \langle e^{\beta D\sum_j J_{ij}\sigma_j}\rangle \tanh x\Big|_{x=0}$$

$$= \langle\prod_j(\cosh \beta J_{ij}D + \sigma_j \sinh \beta J_{ij}D)\ \rangle \tanh x\Big|_{x=0} \tag{4}$$

The performance of the <u>configurational</u> average (noted $\langle\ldots\rangle_J$) yields

$$\langle\langle\sigma_i\rangle\rangle_J = \langle\langle\prod_j(\cosh \beta J_{ij}D + \sigma_j\sinh \beta J_{ij}D)\rangle\rangle_J \tanh x\Big|_{x=0} \tag{5}$$

This equation is untractable as it holds, therefore we shall decouple[2] next-nearest-neighbour spin correlations; Eq. (5) becomes

$$\langle\langle\sigma_i\rangle\rangle_J \equiv m = \left\{\left[p\cosh\frac{D}{t}+(1-p)\right] + m\,p\sinh\frac{D}{t}\right\}^4 \tanh x\Big|_{x=0}$$

$$= Am + Bm^3 \qquad (6)$$

where $t \equiv k_B T/J$ and

$$A \equiv \frac{p^4}{2}\left(\tanh\frac{4}{t} + 2\tanh\frac{2}{t}\right) + 3p^3(1-p)\left(\tanh\frac{3}{t} + \tanh\frac{1}{t}\right)$$

$$+ 6p^2(1-p)^2\tanh\frac{2}{t} + 4p(1-p)^3\tanh\frac{1}{t} \qquad (7)$$

$$B \equiv \frac{p^4}{2}\left(\tanh\frac{4}{t} - 2\tanh\frac{2}{t}\right)$$

$$+ p^3(1-p)\left(\tanh\frac{3}{t} - 3\tanh\frac{1}{t}\right) \qquad (8)$$

Eq. (6) admits two solutions, namely the paramagnetic one ($m \equiv 0$) and the ferromagnetic one

$$m = \left(\frac{1-A}{B}\right)^{\frac{1}{2}} \qquad \text{(see Fig. 1)} \qquad (9)$$

The critical line is given by $A = 1$ (see Fig. 2) and its terminal points are $t_c(p=1) \simeq 3.0898$ and $p_c \simeq 0.4284$ ($t_c^{exact} \simeq 2.2692$ [16] and $p_c^{exact} = 1/2$ [17]; $t_c^{MFA} = 4$ and $p_c^{MFA} = 0$).

II.2 - Short range order parameter and specific heat

The internal energy $\langle\langle E\rangle\rangle_J$ per site is given by

$$\langle\langle E\rangle\rangle_J = -\frac{1}{2}\langle\langle \sum_k J_{ik}\sigma_i\sigma_k\rangle\rangle_J \tag{10}$$

where <i,k> are nearest-neighbours. By using the two-site Callen identity[6] we rewrite this equation as follows:

$$\langle\langle E\rangle\rangle_J = -\frac{1}{2}\langle\langle \sum_k J_{ik}\sigma_k \, e^{\beta D\sum_j J_{ij}\sigma_j}\rangle\rangle_J \tanh x\Big|_{x=0}$$

$$= -\frac{1}{2\beta D}\frac{\partial}{\partial\eta}\langle\langle e^{\beta D\eta\sum_j J_{ij}\sigma_j}\rangle\rangle_J\Big|_{\eta=1} \tanh x\Big|_{x=0}$$

$$\simeq -\frac{1}{2\beta D}\frac{\partial}{\partial\eta}\prod_j\langle\langle e^{\beta D\eta J_{ij}\sigma_j}\rangle\rangle_J\Big|_{\eta=1} \tanh x\Big|_{x=0} \tag{11}$$

where we have introduced the D-operator and decoupled[2] the next-nearest-neighbour spin correlations. By performing the derivative with respect to η and applying the D-operator we obtain

$$\langle\langle E\rangle\rangle_J = -2Jp\tau \tag{12}$$

where the short range order parameter $\tau \equiv \langle\langle\sigma_i\sigma_k\rangle\rangle_J$ is given by

$$\tau = v_0 + 3v_2 m^2 + v_4 m^4 \tag{13}$$

with

$$v_0 = \frac{1}{8} p^3 \left(\tanh \frac{4}{t} + 2\tanh \frac{2}{t}\right) + \frac{3}{4} p^2(1-p) \times$$

$$\times \left(\tanh \frac{3}{t} + \tanh \frac{1}{t}\right) + \frac{3}{2} p(1-p)^2 \tanh \frac{2}{t}$$

$$+ (1-p)^3 \tanh \frac{1}{t} \tag{14}$$

$$v_2 = \frac{1}{4} p^3 \tanh \frac{4}{t} + \frac{1}{4} p^2(1-p) \left(3\tanh \frac{3}{t} - \tanh \frac{1}{t}\right)$$

$$+ \frac{1}{2} p(1-p)^2 \tanh \frac{2}{t} \tag{15}$$

and

$$v_4 = \frac{1}{8} p^3 \left(\tanh \frac{4}{t} - 2\tanh \frac{2}{t}\right) \tag{16}$$

The thermal behaviour of τ is depicted in Fig. 1. The specific heat per site is given by

$$C = \frac{\partial \langle\langle E \rangle\rangle_J}{\partial T} = - 2k_B p \frac{\partial \tau}{\partial t} \tag{17}$$

and its thermal behaviour is shown in Fig. 3 for selected values of p. As it is usual in effective-field theories the well known logarithmic (at least for p=1) singularity is not recovered; nevertheless an improvement is obtained with respect to the MFA results, as a paramagnetic tail (proportional to $1/T^2$) is present. In spite of the fact that the singularity which appears is of an incorrect type, an essential phenomenon is clearly exhibited; we refer to the fact that, for $p_c<p<1$, two different contributions to the specific heat are present (the singular one coming from the unique infinite cluster, and the regular one coming from the isolated finite clusters), whereas, for $o<p<p_c$, the singularity disappears and the specific heat is due exclusively to the finite clusters (see also Ref. [3] and [4] where indications in the same sense are presented).

II.3 - Susceptibility

Let us now add to the Hamiltonian (1) the term $-g\mu_B H\sum_i \sigma_i$ ($g \equiv$ Landé factor; $\mu_B \equiv$ Bohr magneton; $H \equiv$ external magnetic field); consequently identity (4) is generalized into

$$\langle\sigma_i\rangle = \langle\prod_j(\cosh \beta J_{ij}D + \sigma_j \sinh \beta J_{ij}D)\rangle \tanh(x + \beta g\mu_B H)\Big|_{x=0} \tag{18}$$

The zero field isothermal magnetic susceptibility per site χ_o is given by

$$\chi_o = \frac{g^2\mu_B{}^2}{J}\chi \tag{19}$$

where

$$\chi \equiv \frac{\partial m}{\partial h}\Big|_{h=0} \tag{20}$$

and $h \equiv g\mu_B H/J$.

By taking on both sides of Eq. (18) the configurational average and derivating with respect to h at the point $h=0$ we obtain

$$\chi = \frac{1}{t} \langle\langle \prod_j (\cosh \beta D J_{ij} + \sigma_j \sinh \beta D J_{ij}) \rangle\rangle \operatorname{sech}^2 x \Big|_{x=0}$$

$$+ \frac{\partial}{\partial h} \langle\langle \prod_j \cosh \beta D J_{ij} + \sigma_j \sinh \beta D J_{ij} \rangle\rangle \Big|_{h=0} \tanh x \Big|_{x=0} \qquad (21)$$

By decoupling now [15] the next-nearest-neighbour spin correlations we straightforwardly obtain our _first_ approximation for the susceptibility:

$$\chi_I = \frac{\ell \operatorname{sech}^2 x \Big|_{x=0}}{t \left(1 - \frac{\partial}{\partial m} \ell \tanh x \Big|_{x=0}\right)} \qquad (22)$$

where

$$\ell \equiv \left[(1-p) + p\left(\cosh \frac{D}{t} + m \sinh \frac{D}{t}\right) \right]^4 \qquad (23)$$

By evaluating Eq. (22) we finally arrive to

$$\chi_I = \frac{F}{t(1 - A - 3Bm^2)} \qquad (24)$$

where A, B and m are repectively given by Eqs. (7), (8) and (9) and where

$$F = \Big[\frac{1}{8} p^4 \left(\operatorname{sech}^2 \frac{4}{t} + 4\operatorname{sech}^2 \frac{2}{t} + 3\right) + p^3(1-p)\left(\operatorname{sech}^2 \frac{3}{t} + 3\operatorname{sech}^2 \frac{1}{t}\right) + 3p^2(1-p)^2\left(\operatorname{sech}^2 \frac{2}{t} + 1\right) + 4p(1-p)^3 \operatorname{sech}^2 \frac{1}{t} + (1-p)^4 \Big]$$

$$+ 6m^2 \left[\frac{1}{8} p^4\left(\operatorname{sech}^2 \frac{4}{t} - 1\right) + \frac{1}{2} p^3(1-p)\left(\operatorname{sech}^2 \frac{3}{t}\right.\right.$$

$$\left.\left. - \operatorname{sech}^2 \frac{1}{t}\right) + \frac{1}{2} p^2(1-p)^2\left(\operatorname{sech}^2 \frac{2}{t} - 1\right)\right]$$

$$+ \frac{1}{8} m^4 \left[\operatorname{sech}^2 \frac{4}{t} - 4\operatorname{sech}^2 \frac{2}{t} + 3\right] \qquad (25)$$

The temperature dependence of χ^I shown in Fig. 4 for selected values of p; remark that, in the limit $t \to \infty$, $\chi \sim 1/t$. The low temperature region is an extremely interesting one. We observe that only for p = 1, χ vanishes in the limit $t \to 0$ as only in this case no finite clusters of spins exist; for $p_c<p<1$, χ diverges twice, one at the critical point (infinite cluster contribution) and another one at t = 0 (finite clusters contribution), in other words, we observe the coexistence of a Curie-Weiss-type law with a Curie-type one; finally for $p<p_c$ only the t = 0 divergence remains. Although these effects were expected, this is the first time as far as we know, that they are exhibited.

Let us now focuse another type of approximation which will yield our <u>second</u> proposal for the reduced susceptibility denoted by χ_{II}.

Both single-site (Eq. (3)) and two-site Callen identity[6] can be generalized[18] into

$$\langle f'\sigma_i\rangle = \langle f'\tanh \beta\left[\sum_j J_{ij}\sigma_j + g\mu_B H\right]\rangle \qquad (26)$$

where f' denotes an arbitrary spin function not including the i-th spin. Now, let us take f' as follows:

$$f' = f\left\{1 + \tanh\left[\beta \sum_j J_{ij}\sigma_j\right] \tanh(\beta g\mu_B H)\right\} \qquad (27)$$

with another arbitrary spin function f which also does not include the i-th spin. Then equation (26) may be rewritten as

$$\langle\sigma_i\rangle + \langle\sigma_i \prod_j e^{\beta J_{ij}\sigma_j D}\rangle \tanh x\Big|_{x=0} \tanh \beta g\mu_B H$$

$$= \langle\prod_j e^{\beta J_{ij}\sigma_j D}\rangle \tanh x\Big|_{x=0} + \tanh \beta g\mu_B H \qquad (28)$$

where we introduced the differential operator D and we choosed f = 1.

By decoupling the nearest-neighbour spin term, and by further decoupling the next-nearest-neighbour spin correlations, equation (28) can be rewritten as

$$\langle\sigma_i\rangle + \langle\sigma_i\rangle\langle\prod_j e^{\beta J_{ij}\sigma_j D}\rangle \tanh x\Big|_{x=0} \tanh \beta g\mu_B H$$

$$= \prod_j \langle e^{\beta J_{ij}\sigma_j D}\rangle \tanh x\Big|_{x=0} + \tanh \beta g\mu_B H \qquad (29)$$

By taking on both sides of eq. (29) the configurational average and derivating with repect to h($h \equiv g\mu_B H/J$) at the point h = 0 we obtain the following approximate zero field reduced susceptibility:

$$\chi^{II} = \frac{1 - m^2}{t(1 - A - 3Bm^2)} \qquad (30)$$

We remark that the present denominator coincides with that of Eq. (24); consequently χ^{I} and χ^{II} diverge at one and the same critical point. The temperature dependence of χ^{II} is illustrated in Fig. 4 for selected values of p; we remark that in the high temperature region χ^{I} is a better approximation than χ^{II}, whereas at low temperature χ^{II} tends to be better than χ^{I}.

III - CONCLUSION

We discuss the quenched bond-diluted spin - $\frac{1}{2}$ Ising ferromagnet in square lattice. Within an effective field unified framework which extends the one recently introduced by Honmura and Kaneyoshi[5], we calculate the most relevant thermodynamical quantities, namely the phase diagram in the (bond) concentration-temperature space, spontaneous magnetization, short range order parameter, specific heat and zero field isothermal magnetic susceptibility. The latter has been computes within two slightly different approaches which extend those appearing in Ref.[15]: they are expected to provide approximations which fit better the unknown exact results in the low and high temperature regions. Interesting effects (see Fig. 3 and 4) come up in the thermal behaviours of both specific heat and susceptibility due to the eventual coexistence, in the system, of an infinite cluster with finite ones (whose respective weighs depend on the bond concentration).

The present framework shares with the Mean Field Approximation the fact that the critical exponents are classical

(Landau-type); on the other hand substantial improvements are exhibited in several senses which can be of qualitative (paramagnetic tail in the specific heat, non vanishing bond percolation critical probability) or even quantitative (numerical value of the pure case critical temperature) nature. Furthermore let us conclude by saying that the present theory, with no mathematical complexities, can be suitable for analyzing complex Ising systems.

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CAPTION FOR FIGURES

FIG. 1 - Thermal dependence of the reduced spontaneous magnetization (continuous lines) and square root of the short range order parameter (dashed lines) for typical values of the bond concentration p.

FIG. 2 - Critical temperature as a function of bond concentration ((P) and (F) respectively denote para- and ferromagnetic phases)

FIG. 3 - Thermal dependence of the specific heat per site for typical values of the bond concentration p.

FIG. 4 - Thermal dependence of the reduced inverse magnetic susceptibility (continuous: χ_I^{-1}; dashed: χ_{II}^{-1}; dot-dashed: unknown χ_{exact}^{-1} (indicative)) for typical values of the bond concentration p.

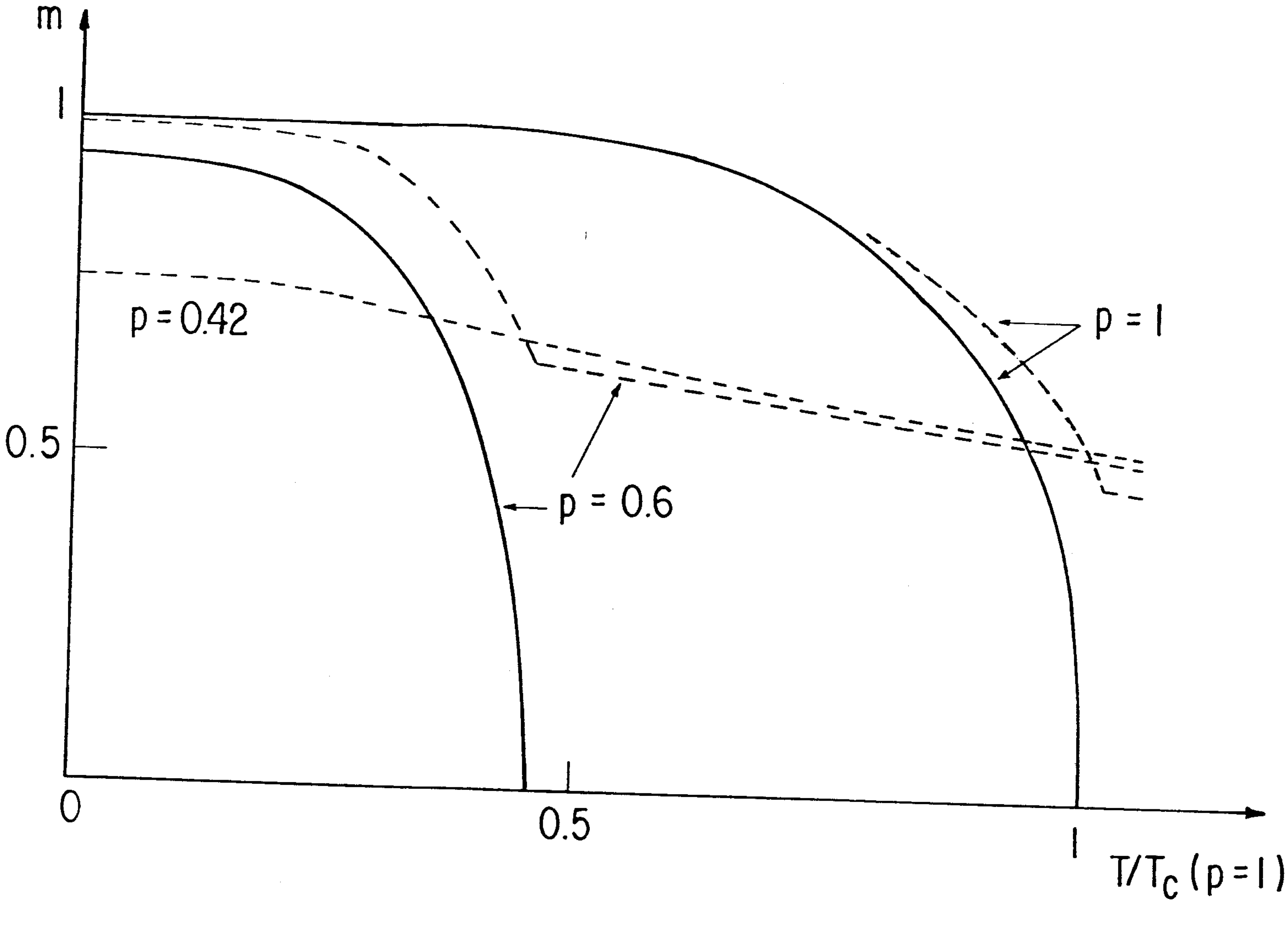

FIG.1

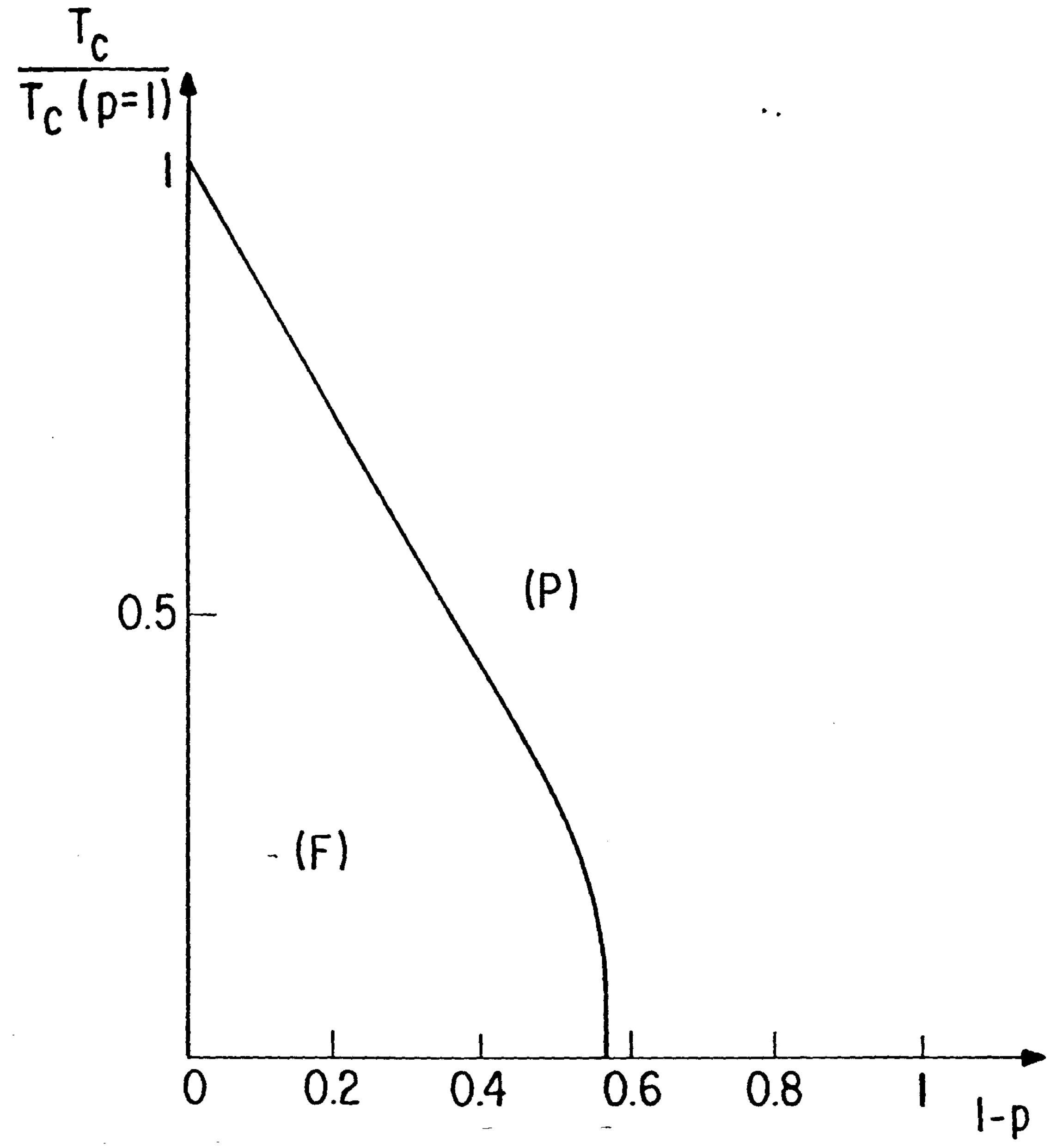

FIG. 2

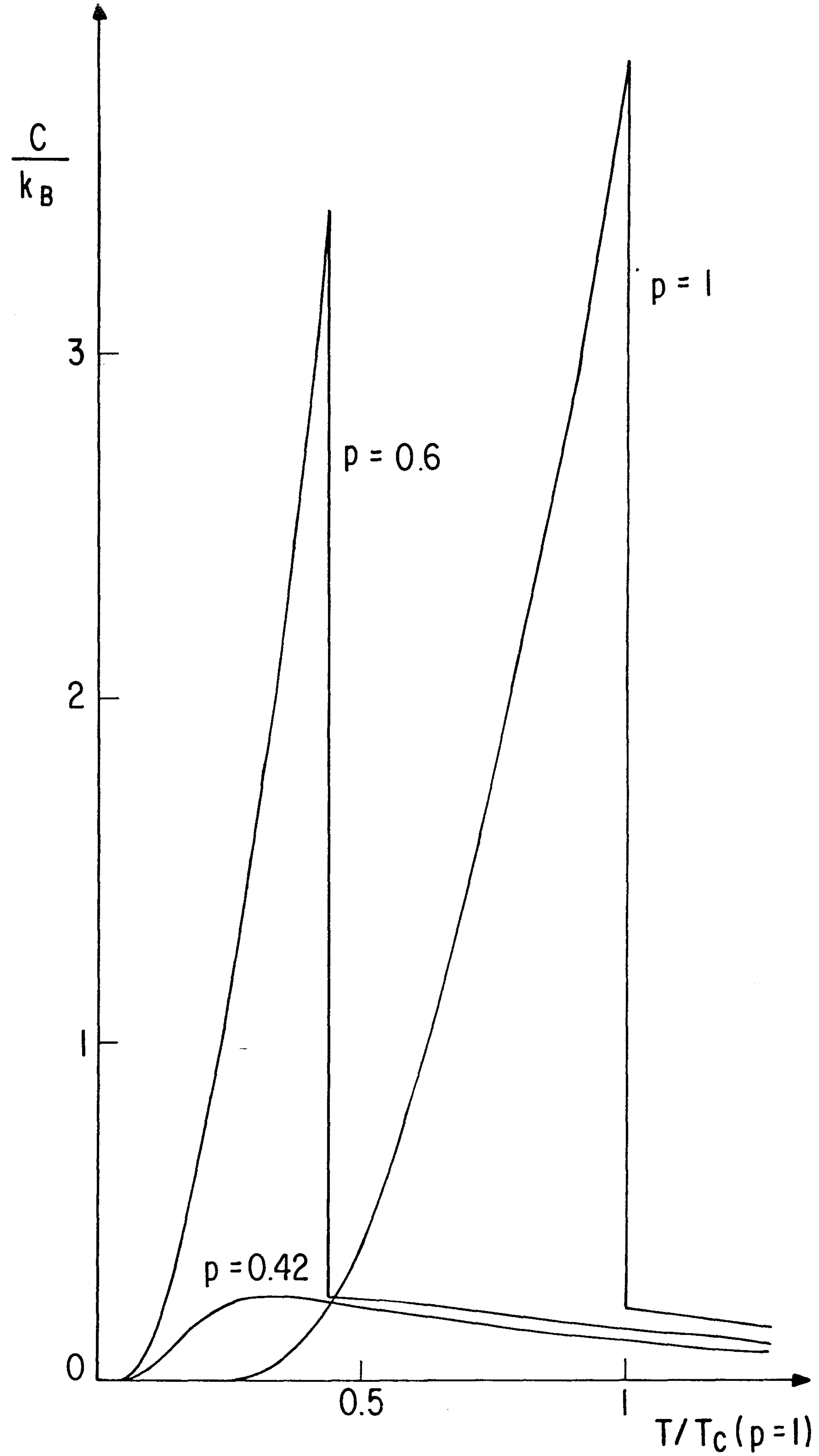

FIG. 3

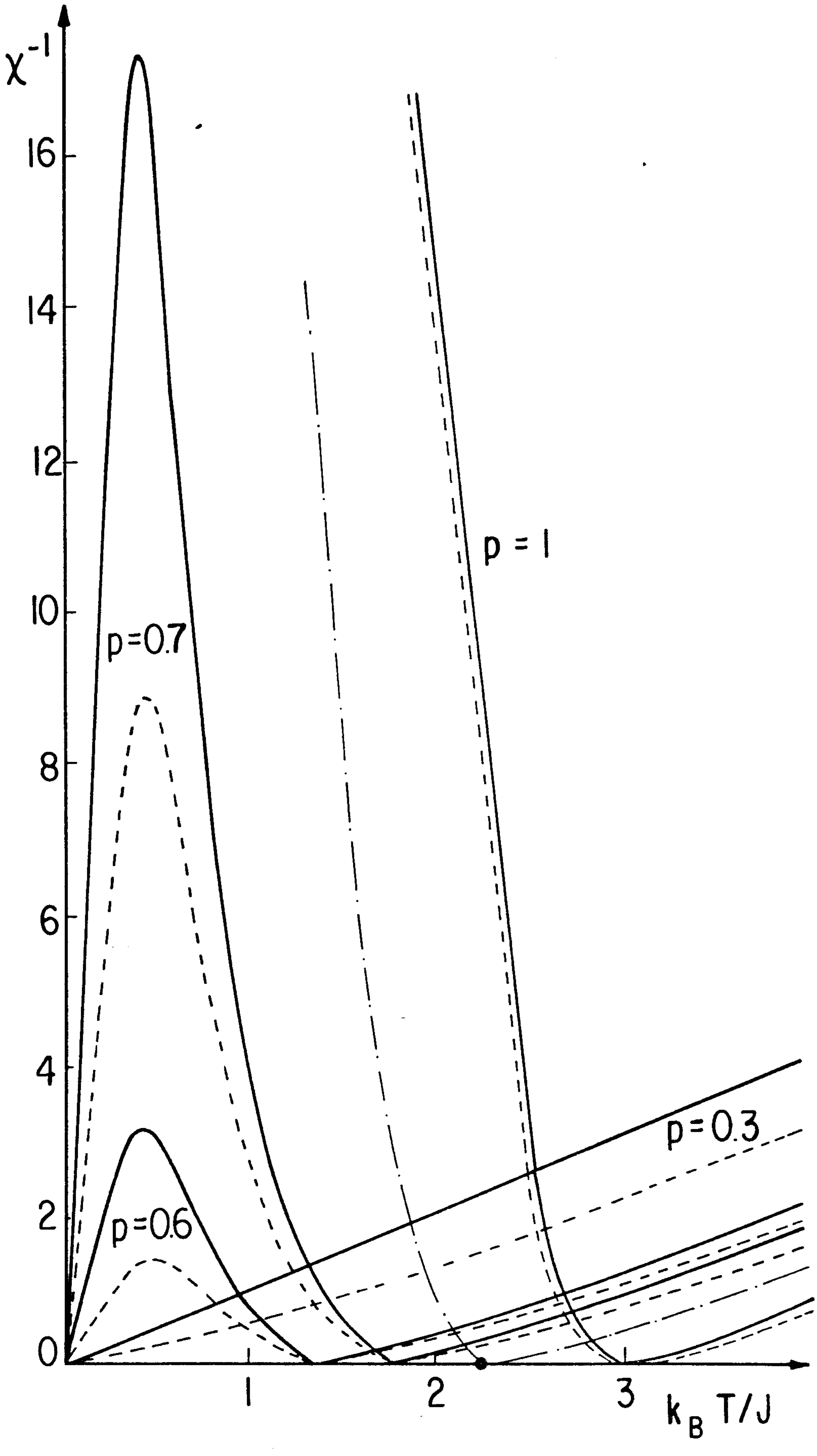

FIG. 4