Journal of Statistical Physics, Vol. 64, Nos. 1/2, 1991

Field-Induced Particle Pairing in an Ising System

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Received July 3, 1990; final February 20, 1991

We study the thermodynamic behavior of an Ising system on a Bethe lattice in which rearranging particles are "decorating" with their presence the bonds of the system, causing the local exchange coupling to depend on the decoration status. Such magnetic models have been proposed in efforts to understand the mechanisms responsible for the pairing of electrons in high-T_c superconductivity. In order to study in some detail this aspect, we focus on the question of conditions under which particle pairing occurs, and more specifically, on the role of an external magnetic field. We find a low-temperature region of the phase diagram where significant particle clustering occurs when the field is introduced.

KEY WORDS: Ising; Bethe lattice; bond decoration; pairing.

1. INTRODUCTION

The effort toward the theoretical understanding of high-T_c superconductivity (HTSC) has produced several proposed versions of the mechanisms responsible for the pairing of electrons.[1]

The thermodynamic phase diagrams of HTSC materials reveal that magnetic interactions play a prominent role.[2] An interesting model already studied to some extent[3,4] assumes a basic antiferromagnetic exchange interaction between any two neighboring lattice sites that changes to ferromagnetic when an impurity electron (or hole) is present there due to the interaction of the electronic spin with the adjacent Ising spins. It is argued that the pairing of impurity electrons (or holes) occurs due to the above assumptions. The need to understand in more concrete terms the

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0022-4715/91/0700-0385$06.50/0

conditions under which such pairing occurs or is destroyed serves as the basic motivation of the present work.

We study the thermodynamic behavior of an Ising system in which the exchange coupling depends on the status of decoration of the corresponding bonds. The bonds are decorated by the presence (or absence) of "particles" that are assumed to exist with a given concentration, freely rearranging their presence on the bonds of the system.[5]

A model Hamiltonian is thus introduced and a Bethe lattice of coordination $z=4$ is assumed. We therefore develop a formalism in Section 2 that allows us to calculate exactly the thermodynamic quantities of the system. Such a calculation is not possible in the case of real lattices, since the required thermodynamic quantities can be calculated only in the absence of applied magnetic field H.[6] On the other hand, H is an essential ingredient in our analysis, since, as we subsequently show, the presence of H induces particle clustering. Then, in Section 3 we study that behavior starting with a ground-state analysis, in order to reveal under what conditions the ground state will contain "particle" clustering in distinct pairs or larger multiplets that may behave as composite "particles." Finally, we explore the regions of the phase diagram where such clustering exists.

2. FORMALISM

We consider an Ising spin system on a Bethe lattice of coordination z with nearest neighbor interactions between the magnetic moments occupying the sites of the lattice. The Bethe lattice is decorated in such a way that each bond can either be occupied or unoccupied by a "particle." We consider the case where the "particles" have a concentration per bond c, i.e., they occupy a certain percentage ($100 \cdot c\%$, $c=0 \div 1$) of the bonds and are free to rearrange.

The exchange energy of these decorated bonds takes three values, depending both on the presence of a "particle" and on the sign of $(\sigma_i \sigma_j)$, with σ_i (± 1) and σ_j (± 1) being the spins of the magnetic moments that occupy the sites ij at the ends of the bond.

This system is described by a Hamiltonian

$$\mathscr{H} = \sum_{(i,j)} [J - J_0(1+\sigma_i\sigma_j)\, d_{ij}]\, \sigma_i\sigma_j - H\mu \sum_i \sigma_i \tag{1}$$

where the exchange coupling parameters J and J_0 are positive, the spin σ_i takes values ± 1, H is the applied magnetic field, and μ is the magnetic moment. The sum is taken over nearest neighboring sites (i, j) and d_{ij} is 1 or 0, depending on the presence or absence of a "particle" on the bond

between nearest neighboring sites i and j. In the absence of "particles" ($c=0$) this Hamiltonian describes a typical antiferromagnetic Ising system.

We introduce the decorated pair probabilities $P(\sigma, d, \sigma')$, where the spins refer to nearest neighboring sites, and d indicates the decoration status of the connecting bond. The knowledge of such pair probabilities allows for the calculation of all relevant thermodynamic quantities.

Since the coupling between neighboring spins is antiferromagnetic, the lattice splits into two sublattices. Thus, half of the lattice sites are labeled $\uparrow$ and the other half $\downarrow$. Consequently, the decorated pair probabilities can be expressed as

$$P(\sigma, d, \sigma') = (1/2)\, P_{\uparrow}(\sigma, d, \sigma') + (1/2)\, P_{\downarrow}(\sigma, d, \sigma') \tag{2}$$

where the $\uparrow(\downarrow)$ subscript indicates that the first site in the parentheses belongs to the $\uparrow(\downarrow)$ sublattice.

We observe that the single-site probability is given by

$$P_s(\sigma) = \sum_{d=0}^{1} \sum_{\sigma_i} P_s(\sigma, d, \sigma_i) \tag{3}$$

where s takes the label $\uparrow$ or $\downarrow$ for sublattice $\uparrow$ or $\downarrow$, respectively, and that

$$P_{\uparrow}(\sigma_i, d, \sigma_j) = P_{\downarrow}(\sigma_j, d, \sigma_i) \tag{4}$$

The concentration of the "particles" is expressed by

$$c = \sum_{\sigma_i} \sum_{\sigma_j} P(\sigma_i, 1, \sigma_j) = \sum_{\sigma_i} \sum_{\sigma_j} P_s(\sigma_i, 1, \sigma_j) \tag{5}$$

and the normalization condition is

$$\sum_{\sigma_i} \sum_{\sigma_j} \sum_{d=0}^{1} P_s(\sigma_i, d, \sigma_j) = 1 \tag{6}$$

with s denoting the label $\uparrow$ or $\downarrow$.

The probability $P_s(\sigma_0; d_1, \sigma_1; d_2, \sigma_2; \ldots; d_z, \sigma_z)$ of a given configuration of spins and bond decorations on a cluster consisting of a central site O belonging to the s sublattice and its z nearest neighboring sites can be expressed as

$$P_s(\sigma_0; d_1, \sigma_1; d_2, \sigma_2; \ldots; d_z, \sigma_z) = [P_s(\sigma_0)]^{1-z} \prod_{i=1}^{z} P_s(\sigma_0, d_i, \sigma_i) \tag{7}$$

due to the Bethe lattice topology.[7,8]

We introduce here the basic thermodynamic relations by properly extending Eggarter's[7] original idea:

$$\frac{P_s(\sigma_0; d_1, \sigma_1; d_2, \sigma_2; \ldots; d_z, \sigma_z)}{P_s(-\sigma_0; d_1, \sigma_1; d_2, \sigma_2; \ldots; d_z, \sigma_z)} = e^{\beta \Delta E} \tag{8}$$

where ΔE is the energy increase when the spin of the central site O is flipped from σ_0 to $-\sigma_0$.

The basic thermodynamic relation (8) can be expressed, utilizing Eqs. (3) and (7), in terms of the decorated pair probabilities introduced earlier in the form

$$\left(\frac{P_s(-\sigma)}{P_s(\sigma)}\right)^{z-1} \prod_{d=0}^{1} \left(\frac{P_s(\sigma, d, \sigma)}{P_s(-\sigma, d, \sigma)}\right)^{n_d} \left(\frac{P_s(\sigma, d, -\sigma)}{P_s(-\sigma, d, -\sigma)}\right)^{m_d}$$
$$= e^{2\beta H \mu \sigma} e^{-2\beta J(n_0 - m_0)\sigma} e^{\beta(J' - J)(n_1 - m_1)\sigma} \tag{8a}$$

where $J' = -(J - 2J_0)$. The subscript d in the exponents n_d and m_d indicates the decoration status (presence: $d=1$; absence: $d=0$) pertaining to bonds connecting the central site to those on the cluster perimeter, while the exponents n_d (m_d) themselves indicate the total number of sites on the cluster perimeter bearing spin 1 (-1) and the decoration status of the connecting bound d. It is obvious that $\sum_{d=0}^{1}(n_d + m_d) = z$.

All the decorated partial pair probabilities $P_s(\sigma, d, \sigma')$ can be determined by Eq. (8a) [which with the help of Eq. (4) gives six independent algebraic equations], along with the normalization conditions [Eqs. (5) and (6)].

The algebraic problem is formulated in terms of quantities ω and η, defined as follows:

$$\omega \equiv (1/4) \ln[P_\uparrow(\uparrow, d, \uparrow)/P_\uparrow(\downarrow, d, \downarrow)] \tag{9}$$

$$\eta \equiv (1/4) \ln[P_\uparrow(\uparrow, d, \downarrow)/P_\uparrow(\downarrow, d, \uparrow)] \tag{10}$$

Having obtained a solution for this system (the values of ω and η), we can obtain all the relevant thermodynamic quantities, which are expressed in terms of the pair probabilities as follows.

The mean energy per bond is given by

$$U = \frac{\langle \mathscr{H} \rangle}{N \text{ bonds}} = \sum_{(i,j)} P(\sigma_i, d_{ij}, \sigma_j)\{[J - J_0(1 + \sigma_i\sigma_j)\, d_{ij}]\, \sigma_i\sigma_j$$
$$- (1/2)\, H\mu(2/z)(\sigma_i + \sigma_j)\} \tag{11}$$

and in terms of the decorated partial pair probabilities

$$U = J(P_s(\uparrow 0\uparrow) + P_s(\downarrow 0\downarrow) - P_s(\uparrow 0\downarrow) - P_s(\downarrow 0\uparrow) - P_s(\uparrow 1\downarrow) - P_s(\downarrow 1\uparrow)) - J'(P_s(\uparrow 1\uparrow) + P_s(\downarrow 1\downarrow)) - HM \tag{12}$$

where M is the mean magnetization per bond, given by

$$M = (2/z)[P_s(\uparrow) - P_s(\downarrow)] \tag{13}$$

Another thermodynamic quantity of interest is the cluster formation probability $p_s(z')$, the probability to have a cluster of z' bonds with a

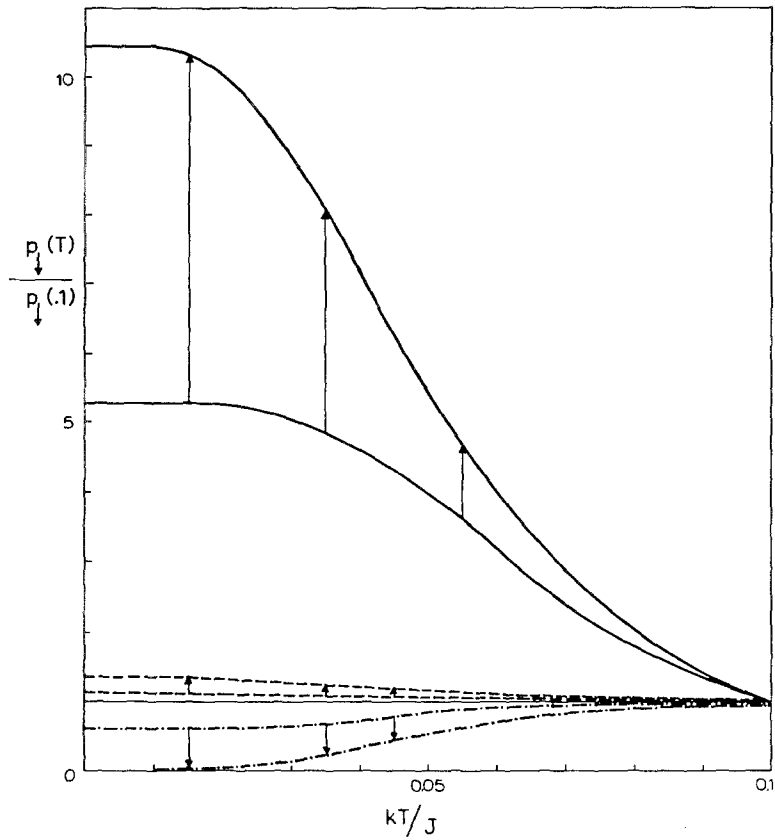

Fig. 1. $p_\downarrow(z';T)/p_\downarrow(z';0.1)$ vs. kT/J for the case of $J'/J = 1.1$, "particle" concentration $c = 0.1$, and two values of the magnetic field, $\mu H/J = 0$ and 0.05. (—) $z' = 4$, (– –) $z' = 1$, (– · –) $z' = 0$. The arrows indicate the direction toward which each curve is shifted by the introduction of the magnetic field.

"particle" and $z-z'$ bonds without a "particle" stemming from a central site that belongs to sublattice s ($\uparrow$ or $\downarrow$). This probability [using Eq. (7)] is given by

$$p_s(z';T)=\frac{z!}{z'!\,(z-z')!}\sum_{\sigma}[P_s(\sigma)]^{1-z}\left[\sum_{\sigma_i}P_s(\sigma,1,\sigma_i)\right]^{z'}\times\left[\sum_{\sigma_i}P_s(\sigma,0,\sigma_i)\right]^{z-z'} \tag{14}$$

Note that the $P_s(\sigma, d, \sigma')$ appearing on the right-hand side of Eq. (14) are temperature-dependent quantities.

3. CLUSTERING BEHAVIOR

The ground-state configurations of the system depend primarily on the relative strengths of J and J_0 [see Eq. (1)]. For small values of J_0 the

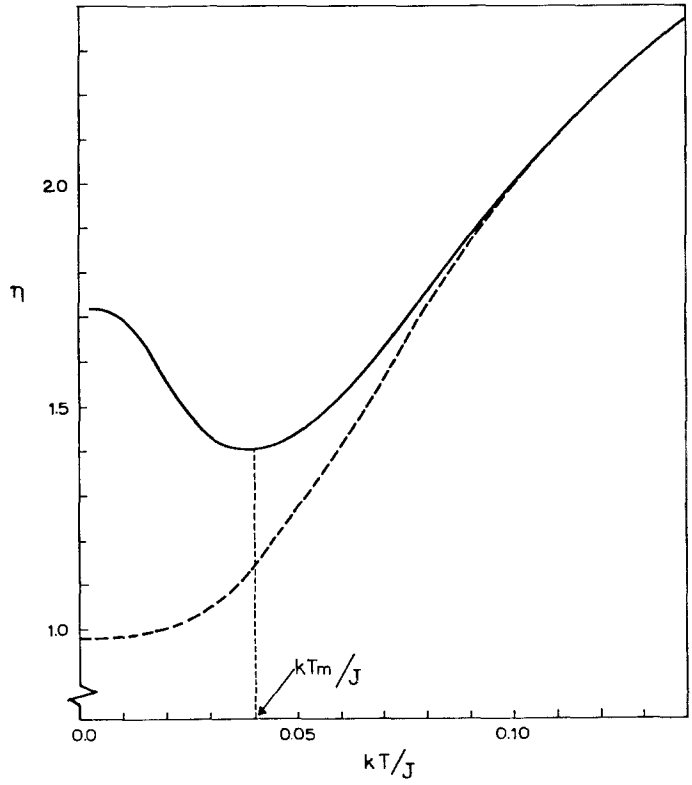

Fig. 2. η vs. kT/J for $J'/J=1.1$ and "particle" concentration $c=0.1$ at (—) $\mu H/J=0.05$ and (--) $H=0$. T_m is the temperature at which the $H=0$ curve exhibits a minimum.

system has a purely AF ground state at all "particle" concentrations, while beyond an appropriate value of J_0 ($J_0 > J$) the system prefers to flip a number of spins (depending on the concentration), forming a multiply degenerate ground state. In a Bethe lattice, in the absence of an external field H, the energy per bond of this ground state is

$$E(c) = -J'c - J(1-c) \tag{15}$$

and is multiply degeerate, because for every given distribution of the "particles" on the bonds there exists a state with energy $E(c)$. In the absence of H it is always possible to construct such a state corresponding

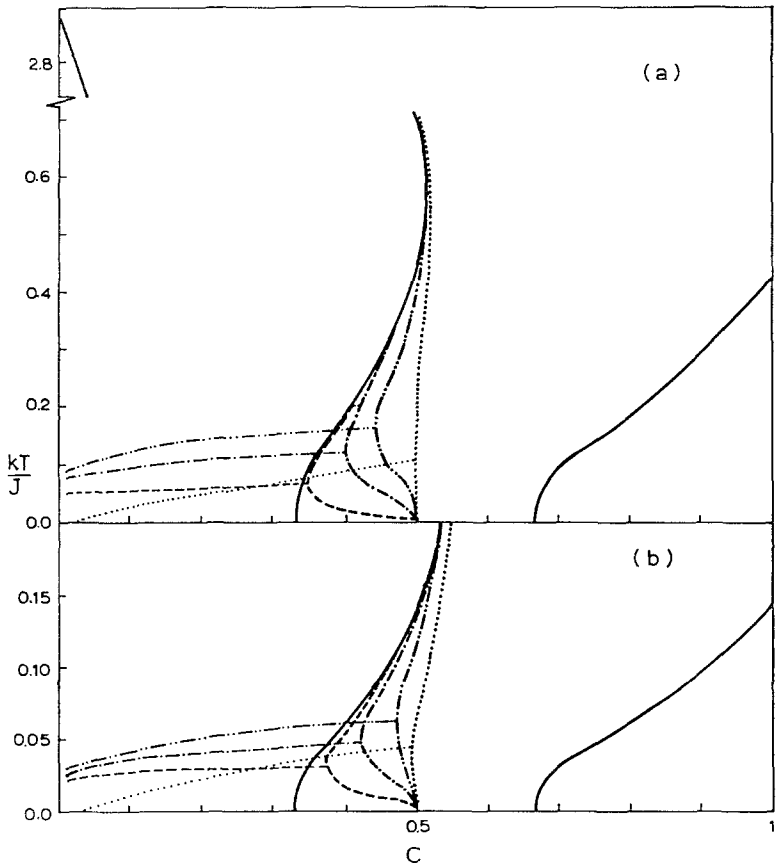

Fig. 3. Phase diagram (kT/J vs. c) for (a) $J'/J = 1.3$ at five values of $\mu H/J$: (—) 0, (– –) 0.02, (– · –) 0.1, (– · · –) 0.2, and (· · ·) 0.56, and (b) $J'/J = 1.1$ at five values of $\mu H/J$: (—) 0, (– –) 0.02, (– · –) 0.05, (– · · –) 0.1, and (· · ·) 0.18. The lighter curves present the corresponding T_m vs. c dependence.

to the given "particle" configuration, by properly arranging the spins, so that each bond is in its lowest energy corresponding to its decoration status.

Therefore, no clustering will occur unless such freedom of choice in ground-state spin orientation is restricted by introducing an external field H. Such introduction will make energetically favorable the configurations that contain "particle" z-plets (quadruplets for $z \doteq 4$) around flipped-up spins.

Indeed, in the low-temperature range the main effect induced by the magnetic field is the dramatic cluster formation we see in Fig. 1, where quadruplet ($z' = 4$) formation is favored, while the rest of the clusters are suppressed. In Fig. 1 the effect is shown in a plot of $p(z'; T)/p(z'; 0, 1)$ [see Eq. (14)] as a function of temperature T for the case of $J'/J = 1.1$, "particle" concentration $c = 0.1$, and $z' = 4$, 1, and 0. The value $kT/J = 0.1$ is an appropriate reference temperature to be explained below in relation to Fig. 2. For each z' case exhibited in Fig. 1, the $\mu H/J = 0$ and $\mu H/J = 0.05$ curves are presented. The arrows indicate the direction toward which each curve is shifted by the introduction of the field H.

A temperature T_m characteristic of the range where H-induced clustering is most pronounced can be defined from the temperature behavior of η [see Eq. (10)]. Figure 2 illustrates this behavior for the same values of parameters J'/J and c as in Fig. 1. While the values of η for zero and nonzero magnetic field practically coincide for temperatures kT/J

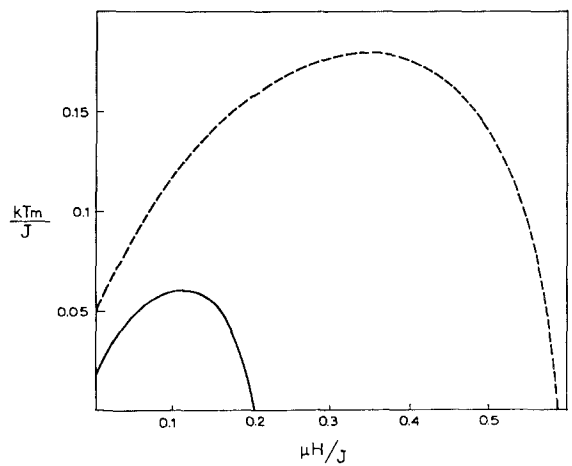

Fig. 4. kT_m/J vs. $\mu H/J$ at "particle" concentration $c = 0.34$ for (—) $J'/J = 1.1$ and (– –) $J'/J = 1.3$.

above 0.1, their behavior changes significantly as the temperature is lowered, with the nonzero-field curve of η exhibiting a minimum at kT_m/J.

At $H=0$ the T vs. c phase diagram of the system contains a paramagnetic (PM), an antiferromagnetic (AF), and a ferromagnetic (FM) state, while at nonzero fields only the PM and AF states are realized. The phase transitions from the AF to the PM state and from the FM to the PM state are of second order, and the phase boundary is shifted as a field is introduced, reflecting the shifting of the percolation threshold from $c=1/3$ to $c=1/2$ that effectively expands the AF region at low T. Figure 3 shows that phase diagram for various values of H with emphasis on the low-temperature part. Incorporated in the figure are the corresponding values of T_m, the temperature that marks the formation of clusters at low T.

Interestingly enough, T_m has little c dependence throughout the AF region, where T_m remains finite. Keeping this in mind, we show in Fig. 4 the clustering agent (H) dependence of T_m at a "particle" concentration $c=0.34$, which is slightly above the $H=0$ percolation threshold ($c=1/3$), for two values of J'/J. The area under the T_m vs. H curve contains (T, H) pairs for which the system is in a state of intense cluster formation. Increasing J'/J increases this area, as we see in Fig. 4.

ACKNOWLEDGMENTS

We wish to thank our colleagues Dr. Bela Mulder and Dr. Costas Krikos for very helpful discussions.

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