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The randomly diluted site-bond, spin-1 Ising model on a honeycomb lattice

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Abstract. A new decoration method is presented which allows the quenched, randomly diluted site-bond, spin-1 Ising model on a regular lattice along a line in the plane of exchange interaction parameters versus temperature to be mapped onto a certain class of mixed-spin decorated-lattice problem. Approximate results for the quenched, randomly diluted site-bond, spin-1 Ising model on the honeycomb lattice are obtained through the use of the exact solution of the annealed model on the corresponding decorated lattice. The critical temperature and the magnetisation of the diluted system as functions of site and bond concentrations are calculated in detail.

1. Introduction

In recent years, much interest has been attracted to the thermodynamic properties of diluted magnetic systems. The random spin system can have two distinct kinds of thermodynamic behaviour [1]. In the first (quenched) case, the randomness is frozen in and does not change with temperature. In the second (annealed) case, the system is allowed to come into thermal equilibrium at each temperature. The annealed case is mathematically more tractable than the quenched case because it involves averaging the partition function rather than the free energy as in the quenched case. Several exact results have been obtained in the annealed limit [2–7], whereas no solution exists to date for the quenched problem.

More recently McGurn [8, 9] has proposed an exact mapping between the quenched, randomly diluted site (or site-bond), spin-$\frac{1}{2}$ Ising model defined on certain decorated lattices and the site (or site-bond) problem on the undecorated lattice. He uses this mapping together with the corresponding annealed limit solution on the decorated honeycomb lattice and obtains the first closed-form approximation to the thermodynamic properties over the entire temperature range for the quenched, randomly diluted site and site-bond, spin-$\frac{1}{2}$ Ising model on the honeycomb lattice. The critical temperature and the critical concentration obtained in this manner are found to agree well with perturbation theory results [10] in the low-dilution limit and the best known value [11], respectively. This method has also been successfully used to study the quenched, randomly diluted site-bond, spin-$\frac{1}{2}$ Ising model on the square lattice [12].

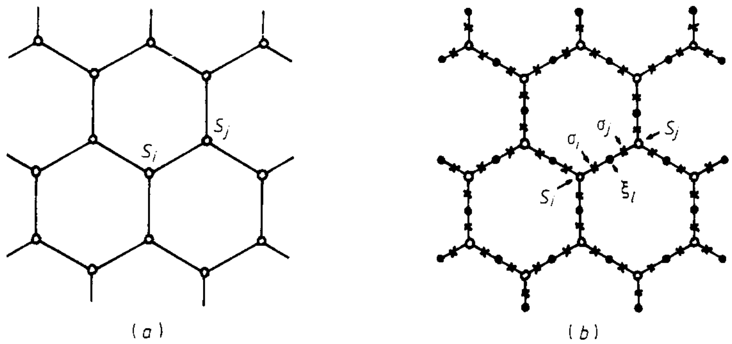

Figure 1. (*a*) Portion of the honeycomb lattice. (*b*) Portion of the decorated honeycomb lattice: ● sites occupied by decorated spins 1 (ξ); $\times$, sites occupied by spins $\frac{1}{2}$ (σ).

This technique, however, cannot be directly applied to systems of arbitrary spin value because the existence of the mapping between the two random systems mentioned above depends on the specific spin value. It is easily seen that no mapping exists if we replace spins $\frac{1}{2}$ in these two disorder Ising models by spins 1. It is for this reason that this technique has not yet been applied to the quenched, spin-1, random system.

The spin-1, isotropic, Blume–Emery–Griffiths (BEG) model in which the crystal-field interaction is absent is described by the Hamiltonian

$$-\beta H = \sum_{(i,j)} JS_iS_j + \sum_{(i,j)} KS_i^2S_j^2 \tag{1.1}$$

where $S_i = 0, \pm 1$; $\Sigma_{(i,j)}$ indicates summation over the nearest-neighbour pairs of sites. The exact solution of the transition temperature of the anisotropic BEG model on the honeycomb lattice under the restriction

$$\exp(K)\cosh(J) = 1 \tag{1.2}$$

has been obtained by Horiguchi [13] and Wu [14]. Kivelson *et al* [15] extend this model to when there is a complex magnetic field coupled to spins and Shankar [16] solves this model rigorously when the complex magnetic field takes some special values. The exact solution of the annealed, diluted-site, anisotropic BEG model on the honeycomb lattice under the same restriction has been found by Urumov [17].

The random-site-bond problem is another kind of disorder and has been studied in connection with the theory of polymer gelation [18]. In this paper we shall present a new decoration method to achieve an exact mapping of the quenched, randomly diluted site-bond isotropic BEG model on a regular lattice with the above restriction on the exchange interaction parameters versus temperature onto the quenched, randonly diluted site and bond, mixed-spin Ising model on the decorated lattice. Using this mapping and the annealed model solution of the corresponding decoration problem as an approximation to the quenched decorated mixed-spin system, we work out the thermodynamics of the quenched, randomly diluted site-bond, spin-1 Ising model on the honeycomb lattice.

2. Mapping

Figure 1(*a*) shows a two-dimensional honeycomb lattice in which a fraction of the bonds between sites and a fraction of the sites are randomly removed so that the concentrations of bonds and sites are p and x, respectively. The Hamiltonian of the quenched, randomly diluted site-bond, spin-1 Ising model which consists of bilinear and biquadratic exchange interaction terms is given by

$$-\beta H = \sum_{(i,j)} Jb_{ij}c_ic_jS_iS_j + \sum_{(i,j)} Kb_{ij}c_ic_jS_i^2S_j^2 \tag{2.1}$$

where b_{ij} ($= 0$ or 1) is the bond-occupancy operator, and c_i ($= 0$ or 1) is the site-occupancy operator. The bilinear ($J > 0$) and biquadratic (K) exchange interaction parameters are only between nearest-neighbour spins.

With the restriction of equation (1.2), the diluted site-bond Ising system of equation (2.1) can be mapped onto the decorated mixed-spin system shown in figure 1(b) in which the site disorder and the bond disorder are decoupled from one another.

In figure 1(b), the sites represented by open circles are diluted with a fraction of x being present while the sites represented by crosses and those represented by full circles are permanently occupied by the decorated spins $\frac{1}{2}$ (σ_i) and spins 1 (ξ_l), respectively. The bonds between neighbouring crosses and the full circles on these bonds are diluted with a fraction of p being present. The bonds between nearest-neighbour open circles and crosses are not diluted.

The Hamiltonian of the decorated system in figure 1(b) is then

$$-\beta H^{(\mathrm{d})} = \sum_{(i,j)} \{J'(c_iS_i\sigma_i + c_jS_j\sigma_j + \xi_l b_{ij}(\sigma_i + \sigma_j)] - \tfrac{1}{z}\delta(c_iS_i^2 + c_jS_j^2)\}. \tag{2.2}$$

Here $\Sigma_{(i,j)}$ is over nearest-neighbour pairs of spins on the disorder sublattice. σ_i and σ_j are the decoration spins on the bond between S_i and S_j. ξ_l is also the decoration spin but on the bond between σ_i and σ_j. $J'(>0)$ is the nearest-neighbour bilinear coupling parameter. δ is the crystal field of the random spin S_i in the decorated system. For simplicity the crystal field of the spins ξ_l is not considered here since these spins are not diluted. The occupation operators c_i and b_{ij} are the same as those in equation (2.1).

The mapping of the quenched limit partition function of the random system of equation (2.1) onto that of the decorated system of equation (2.2) can be carried out as follows.

Equation (2.2) can be rewritten as

$$-\beta H^{(\mathrm{d})} = \sum_{(i,j)} (-\beta H_{ij}^{(\mathrm{d})}) \tag{2.3}$$

where

$$-\beta H_{ij}^{(\mathrm{d})} = J'(c_iS_i\sigma_i + c_jS_j\sigma_j) + J'b_{ij}\xi_l(\sigma_i + \sigma_j) - \tfrac{1}{z}\delta(c_iS_i^2 + c_jS_j^2). \tag{2.4}$$

Then

$$Z^{(\mathrm{d})}(J', \delta) = \operatorname*{Tr}_{\{S_i\sigma_i\xi_l\}}[\exp(-\beta H^{(\mathrm{d})})] = \operatorname*{Tr}_{\{S_i\sigma_i\xi_l\}}\left(\prod_{(i,j)} \exp(-\beta H_{ij}^{(\mathrm{d})})\right) \tag{2.5}$$

is the partition function of the quenched, diluted, mixed-spin Ising model on the decorated lattice.

In order to calculate the partition function of (2.5) we shall first perform the trace over the decoration spins. A convenient way is to start from the calculation for one single decorated bond. For each bond between two neighbouring random sites in the decorated

Table 1. Configurations and the corresponding probabilities of occurrence.

(c_i, c_j, b_{ij})	Configuration	Probability of occurrence
(1, 1, 1)	(*a*) ○—×—●—×—○	x^2p
(1, 1, 0)	(*b*) ○—× ● ×—○	$x^2(1-p)$
(0, 1, 1)	(*c*) ○ ×—●—×—○	$x(1-x)p$
(0, 1, 0)	(*d*) ○ × ● ×—○	$x(1-x)(1-p)$
(0, 0, 1)	(*e*) ○ ×—●—× ○	$(1-x)^2p$
(0, 0, 0)	(*f*) ○ × ● × ○	$(1-x)^2(1-p)$

system there are six possible different bond configurations which are shown in table 1 for $-\beta H_{ij}^{(d)}$; their probabilities of occurrence are also listed.

We now determine the traces of the decoration spins σ_i, σ_j ξ_l in the factor exp $(-\beta H_{ij}^{(d)})$, referring to the bonds in table 1.

For case (*a*) in table 1, we have

$$\operatorname*{Tr}_{\sigma_i\sigma_j\xi_l}[\exp(-\beta H_{ij}^{(d)})] = 2\exp[-\tfrac{1}{3}\delta(S_i^2 + S_j^2)]\{[1 + 2\cosh(2J')]$$

$$\times \cosh[2J'(S_i + S_j)] + 3\cosh[J'(S_i - S_j)]\} \tag{2.6}$$

$$\equiv A\exp(JS_iS_j + KS_i^2S_j^2). \tag{2.7}$$

Here

$$A = 4[2 + \cosh(2J')] \tag{2.8}$$

$$\exp(2J) = \{3 + \cosh(2J')[1 + 2\cosh(2J')]\}[1 + 5\cosh(2J')]^{-1} \tag{2.9}$$

$$\exp(K) = \exp(J - \tfrac{2}{3}\delta)[1 + 5\cosh(2J')]\{2[2 + \cosh(2J')]\}^{-1} \tag{2.10}$$

$$\exp(-\delta)[\cosh(J')]^3 = 1. \tag{2.11}$$

From equations (2.9)–(2.11) it can be easily proved that J and K automatically satisfy the relation (1.2).

Also we have the following. For case (*b*),

$$\operatorname*{Tr}_{\sigma_i\sigma_j\xi_l}[\exp(-\beta H_{ij}^{(d)})] = 12. \tag{2.12}$$

For case (*c*),

$$\operatorname*{Tr}_{\sigma_i\sigma_j\xi_l}[\exp(-\beta H_{ij}^{(d)})] = 4[2 + \cosh(2J')]. \tag{2.13}$$

For case (*d*),

$$\operatorname*{Tr}_{\sigma_i\sigma_j\xi_l}[\exp(-\beta H_{ij}^{(d)})] = 12. \tag{2.14}$$

For case (*e*),

$$\operatorname*{Tr}_{\sigma_i\sigma_j\xi_l}[\exp(-\beta H_{ij}^{(d)})] = 4[2 + \cosh(2J')]. \tag{2.15}$$

For case (*f*),

$$\operatorname*{Tr}_{\sigma_i\sigma_j\xi_l}[\exp(-\beta H_{ij}^{(\mathrm{d})})] = 12. \tag{2.16}$$

In the above calculation of equations (2.12)–(2.14), we have used the relation (2.11).

According to the above calculation for all different types of bond configuration, the contributions from bonds where one or both of the neighbouring random sites are absent (or non-magnetic) only enter the partition function as multiplicative constants. When both random sites are present, a spin-dependent contribution of equation (2.7) is obtained.

Taking the traces of all the decoration spins in equation (2.5), we have

$$Z^{(\mathrm{d})}(J', \delta) = \{(4[2 + \cosh(2J')])^{p}12^{(1-p)}\}^{ZN/2}Z(J, K) \tag{2.17}$$

where N is the number of sites on the random sublattice, Z is the coordination number of the random sites and $Z(J, K)$ is the partition function of the Hamiltonian in equation (2.1). Hence the exact mapping between the partition function of the system in equation (2.1) onto the partition function of the system in equation (2.2) is obtained. It should be pointed out that this mapping is valid not only for honeycomb and decorated honeycomb lattices but also for any other two-dimensional regular lattice and its corresponding decorated lattice.

Using this mapping in conjunction with the annealed limit solution for the partition function of the system in equation (2.2) as we shall discuss in the following, we can obtain an approximation to the thermodynamics of the quenched, diluted site-bond, spin-1 Ising model on the honeycomb lattice.

3. Thermodynamics

The Hamiltonian of the annealed model on the decorated honeycomb lattice is given by

$$\begin{aligned}-\beta H_{\mathrm{an}}^{(\mathrm{d})} = \sum_{(i,j)} [&J'(c_iS_i\sigma_i + c_jS_j\sigma_j) + J'b_{ij}\xi_l(\sigma_i + \sigma_j) \\ &- \tfrac{1}{3}\delta(c_iS_i^2 + c_jS_j^2) + \tfrac{1}{3}\alpha(c_i + c_j) + b_{ij}\nu]\end{aligned} \tag{3.1}$$

where the last two terms are introduced to account for the numbers of the occupied sites and occupied bonds. The variables α and ν can be eliminated by using the following relations:

$$x = (1/N)\partial\{\ln[Z_{\mathrm{an}}^{(\mathrm{d})}(J', \delta, \alpha, \nu)]\}/\partial\alpha \tag{3.2}$$

$$p = (2/3N)\partial\{\ln[Z_{\mathrm{an}}^{(\mathrm{d})}(J', \delta, \alpha, \nu)]\}/\partial\nu. \tag{3.3}$$

Here

$$\begin{aligned}Z_{\mathrm{an}}^{(\mathrm{d})}(J', \delta, \alpha, \nu) = \operatorname*{Tr}_{\{(c_ib_{ij}\}}\Bigg[&\operatorname*{Tr}_{\{S_i\sigma_i\xi_l\}}\Bigg(\prod_{(ij)}\exp[J'(c_iS_i\sigma_i + c_jS_j\sigma_j) \\ &+ J'b_{ij}\xi_l(\sigma_i + \sigma_j) - \tfrac{1}{3}\delta(c_iS_i^2 + c_jS_j^2) \\ &+ \tfrac{1}{3}\alpha(c_i + c_j) + \nu b_{ij}]\Bigg)\Bigg]\end{aligned} \tag{3.4}$$

is the partition function of the Hamiltonian in equation (3.1).

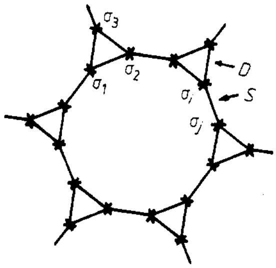

Figure 2. Portion of the Ising lattice for $Z_{\mathrm{pure}}(D, S)$ with the usual spins $\sigma = \pm 1$.

The partition function of (3.4) can be evaluated by taking the trace of c_i, b_{ij}, S_i and ξ_l as

$$Z_{\mathrm{an}}^{(\mathrm{d})}(J', \delta, \alpha, \nu) = B^N C^{3N/2} Z_{\mathrm{pure}}(D, S) \tag{3.5}$$

where $Z_{\mathrm{pure}}(D, S)$ is the partition function of the pure spin-$\frac{1}{2}$ Ising system on the lattice shown in figure 2 with couplings D and S as indicated.

The parameters in equation (3.5) are given by

$$B^4 = \{3 + \exp(\alpha)[1 + 2\exp(-\delta)\cosh(J')]\}^3 \times \{3 + \exp(\alpha)[1 + 2\exp(-\delta)\cosh(3J')]\} \tag{3.6}$$

$$\exp(4D) = \{3 + \exp(\alpha)[1 + 2\exp(-\delta)\cosh(3J')]\} \times \{3 + \exp(\alpha)[1 + 2\exp(-\delta)\cosh(J')]\}^{-1} \tag{3.7}$$

$$C^2 = 3[1 + \exp(\nu)]\{3 + \exp(\nu)[1 + 2\cosh(2J')]\} \tag{3.8}$$

$$\exp(2S) = \{3 + \exp(\nu)[1 + 2\cosh(2J')]\}/3[1 + \exp(\nu)]. \tag{3.9}$$

The concentrations x and p can be expressed as

$$x = \{32[\cosh(2J') - 1]\}^{-1}\{[1 + 3\varepsilon_1(D, S)][1 - \exp(-4D)][9\cosh(2J') - 3] + [3 - 3\varepsilon_1(D, S)][\exp(4D) - 1][\cosh(2J') + 5]\} \tag{3.10}$$

and

$$p = \{4[\cosh(2J') - 1]\}^{-1}\{3[1 - \varepsilon_2(D, S)][\exp(2S) - 1] + [1 + 2\cosh(2J')][1 + \varepsilon_2(D, S)][1 - \exp(-2S)]\} \tag{3.11}$$

where $\varepsilon_1(D, S)$ is the correlation function between the nearest-neighbour spins coupled by the D bond in figure 2 and $\varepsilon_2(D, S)$ is the correlation function between nearest-neighbour spins coupled by the S bond in the same system.

At the critical point for the system in figure 2, D and S in equations (3.10) and (3.11) should be replaced by the critical values D_{c} and S_{c}, respectively, and then x and p can be given in terms of the critical temperature of the decorated system.

We also have the following relationship:

$$\exp(2J_{\mathrm{c}}) = \{3 + \cosh(2J_{\mathrm{c}}')[1 + 2\cosh(2J_{\mathrm{c}}')]\}[1 + 5\cosh(2J_{\mathrm{c}}')]^{-1} \tag{3.12}$$

which relates the critical temperature of our system in (2.1) to that of the decorated system in (2.2). Thus, given a value for J_{c}, we can obtain J_{c}' by the use of equation (3.12) and hence x and p from equations (3.10) and (3.11) calculated for D_{c} and S_{c}.

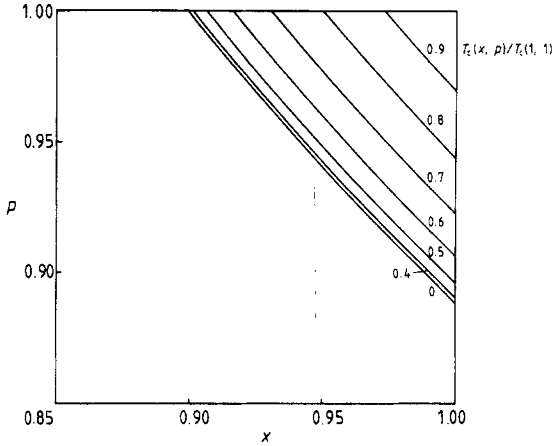

Figure 3. Contours of constant $T_c(x, p)/T_c(1, 1)$ in the plane of $x - p$ for the quenched, diluted site-bond, spin-1 Ising system on the honeycomb lattice (x is the site concentration, and p the bond concentration).

In figure 3 we have plotted the contours of constant $T_c(x, p)/T_c(1, 1)$ against x and p for the system in equation (2.1) by detailed numerical calculation. The contours reduce to the pure, diluted bond system results when $x = 1$, and the pure, diluted site system results when $p = 1$ respectively. The percolation value x_c is 0.8995 when $p = 1$ and the percolation value p_c is 0.888 when $x = 1$. The critical value of J is 1.317 when $x = p = 1$.

A comparison with the exact known results can be made here. When $x = p = 1$, our results reduce to the exact results obtained by Horiguchi [13] and Wu [14]. It should be noted that the results in the non-dilution limit obtained by Urumov [17] are not consistent with the exact results [13, 14]. For example, in the non-dilution limit the critical temperature in the absence of the crystal field used in [17] differs drastically from that of figure 3 in [13].

The magnetisation of the system in equation (2.1) for J is easily proved to be equal to that of the system in equation (2.2) for J', where J' is related to J by equation (2.9). We shall approximate this magnetisation by that of the annealed system in equation (3.1).

The magnetisation of the system in equation (3.1) is given by

$$M = \operatorname*{Tr}_{\{S_i \sigma_i \xi_l\}} \left[\operatorname*{Tr}_{\{c_i b_{ij}\}} \left(\sum_i [S_i \exp(-\beta H_{\text{an}}^{(\text{d})})][N Z_{\text{an}}^{(\text{d})}(J', \delta, \alpha, \nu)]^{-1} \right) \right]. \tag{3.13}$$

This can be calculated as

$$M = F\langle\sigma\rangle(D, S) + G\langle\sigma_1\sigma_2\sigma_3\rangle(D, S) \tag{3.14}$$

where

$$F = \{[1 - \exp(-4D)]/[\cosh(3J') - \cosh(J')]\}\tfrac{3}{4}[\sinh(3J') + \exp(4D)\sinh(J')] \tag{3.15}$$

$$G = \{[1 - \exp(-4D)]/[\cosh(3J') - \cosh(J')]\}\tfrac{1}{4}[\sinh(3J') - 3\exp(4D)\sinh(J')]. \tag{3.16}$$

Here D and S are as in equation (3.10). $\langle\sigma\rangle(D, S)$ is the magnetisation of the pure Ising system with the usual $\sigma = \pm 1$ spins in figure 2 and $\langle\sigma_1\sigma_2\sigma_3\rangle$ is the three-spin correlation function of the spins at the vertices of the triangle in the same system [9].

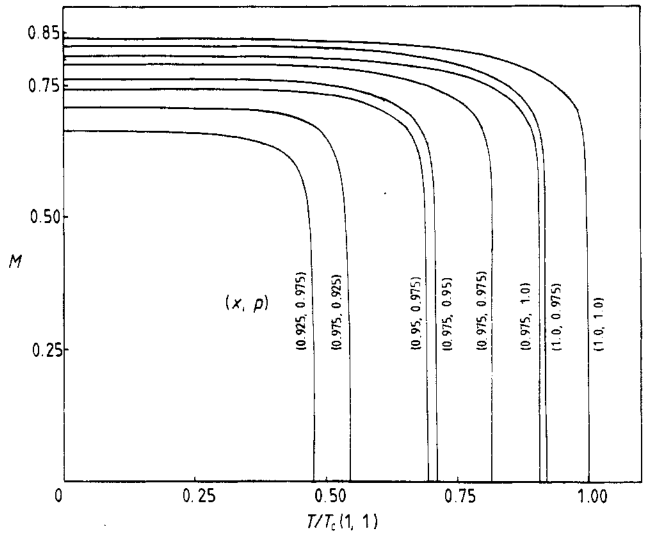

Figure 4. Magnetisation against $T/T_c(1, 1)$ for various values of x and p.

In figure 4, the magnetisation of the system in equation (2.1) in this approximation is plotted against $T/T_c(1, 1)$ for various values of x and p. In the vicinity of the transition point, the magnetisation vanishes rapidly. For temperatures lower than the transition temperature, the magnetisation decreases very slowly with increase in temperature. We note that in the low-temperature limit our results when $x = p = 1$ differ from those in [19]. We recognise that all the derivations of equations in [19] are rigorous but our results of detailed numerical calculation of equations derived in the same way as Urumov [19] are consistent with our non-dilution limit results calculated from equations (3.15) and (3.16). The magnetisation at zero temperature when $x = p = 1$ is 0.8395. We are sure that this value is more accurate than that in [19]. The critical exponents of the annealed solutions are different from those of the quenched system and the specific heat obtained in this manner near the transition point is not very good [8]. Hence we have not pursued these in this paper.

4. Conclusion

We have presented a new decoration method and obtained an exact mapping of the quenched, site-bond randomly diluted, spin-1 Ising model under certain restrictions on the exchange interaction parameters onto a class of decorated Ising systems.

We have used this mapping in conjunction with the annealed model solution of the decorated mixed-spin system to calculate approximately the critical temperature and magnetisation of the quenched, site-bond, spin-1 Ising system along a line in the plane of the exchange interaction parameters. All the results in the non-dilution limit reduce to the exact results. We expect our results to be quite good representations of the behaviour of the quenched, spin-1 Ising model in the above subspace.

Acknowledgment

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