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LETTER TO THE EDITOR

The dilute spin-one Ising model on a honeycomb lattice

Viktor Urumov
Institut za Fizika, Univerzitet 'Kiril i Metodij', p. fah 162, Skopje 91001, Yugoslavia

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Abstract. Given some restriction on the interaction parameters, the critical temperature for the spin-one Ising model on a honeycomb lattice described with the Blume–Emery–Griffiths Hamiltonian with random non-magnetic impurities in equilibrium (annealed site-disorder case) is obtained exactly.

The study of various Ising models is a subject with a long history (Domb 1973). The free energy and the logarithmic singularity of the specific heat for the two-dimensional Ising model on a square lattice were found by Onsager (1944), the first derivation for the magnetisation was published by Yang (1952) and exact results for the correlations and the susceptibility were discussed by McCoy and Wu (1973). Another problem of interest and practical importance is the behaviour of random systems in which some of the constituent atoms of the physical system are foreign to the host lattice, thus acting as impurities and introducing constitutional disorder. Two different types of model are encountered: the quenched case and the annealed case. In the former more natural case, the impurities are frozen in their random positions, while in the latter they are free to move and reach the equilibrium state. The annealed case is easier to deal with and it is treated with the methods of equilibrium statistical mechanics.

The subject of dilute magnetism, where the impurities are of non-magnetic nature, was reviewed by Stinchcombe (1983). The exact results are essentially restricted to the case of bond disorder in which the interaction parameters between two neighbouring spins can take random values according to some distribution law. The decorated models (and models on bipartite lattices) in which only the decorating sites are occupied by magnetic or non-magnetic atoms (on bipartite lattices only one of the sublattices can host the impurities) can be related to the corresponding pure models (Syozi 1965, Syozi and Miyazima 1966, Wu 1980). It is the purpose of this Letter to present some exactly obtained results for a model with natural disorder, extended to all the sites of the lattice.

The model at hand is the Blume–Emery–Griffiths (BEG) spin-one model defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{i,j} s_i s_j c_i c_j + K \sum_{i,j} s_i^2 s_j^2 c_i c_j + \Delta \sum_i s_i^2 c_i \tag{1}$$

where the first two summations are carried out over all the pairs of nearest neighbours on a honeycomb lattice, and the last term is a sum over all sites of the lattice. The presence or absence of a spin on the lattice site i is accounted for by c_i, a spin-like variable correspondingly taking two values, 1 or 0. The spin s_i at site i can have three orientations

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0, +1 and −1 and the neighbouring pairs of spins interact via bilinear (J) and biquadratic (K) exchange. The single-site interaction energy $\Delta s_i^2 c_i$ represents the interaction with the crystal field. Originally the model (Blume *et al* 1971) without impurities was proposed to discuss the phase separation and superfluid ordering in ^{3}He–^{4}He mixtures. Recently, Horiguchi (1986) obtained an exact expression for the partition function of the pure BEG model on the honeycomb lattice under the restriction

$$\exp(\beta K) = \cosh(\beta J) \tag{2}$$

where $\beta = 1/kT$ (k is the Boltzmann constant and T the absolute temperature), and I (Urumov 1987) calculated the magnetisation under the same restriction.

We can obtain the grand partition function for the model

$$\zeta = \sum_{\{s_i, c_i\}} \exp\left(\beta J \sum_{i,j} s_i s_j c_i c_j - \beta K \sum_{i,j} s_i^2 s_j^2 c_i c_j - \beta \Delta \sum_i s_i^2 c_i + \xi \sum_i c_i\right) \tag{3}$$

where the summations $\{s_i, c_i\}$ are carried out over all the possible configurations of the variables s_i, c_i. The last term in the exponent is introduced to keep count of the number of occupied sites. The variable ξ is eliminated using

$$p = (1/N_h)(\partial/\partial\xi) \ln \zeta \tag{4}$$

where N_h is the number of sites on the honeycomb lattice and p is the concentration of sites occupied by magnetic atoms.

An essential step for the calculation is the identity

$$\exp(\beta J s_i s_j c_i c_j - \beta K s_i^2 s_j^2 c_i c_j) = \tfrac{1}{2} \sum_{\sigma_{ij} = \pm 1} \exp[A\sigma_{ij}(s_i c_i + s_j c_j) + B(s_i^2 c_i + s_j^2 c_j)] \tag{5}$$

which effectively introduces the spin-like variable $\sigma_{ij} = \pm 1$ on each bond connecting two neighbouring sites. The lattice of σ-spins is known as the Kagomé lattice. It is shown in figure 1 together with the original honeycomb lattice of s-spins.

From all the possible values of s_i and c_i for a pair of neighbouring sites we obtain the following equations for the effective interaction parameters A and B in (5):

$$\begin{aligned} &\exp(\beta J - \beta K) = \cosh(2A) \exp(2B) \\ &1 = \cosh A \exp B \\ &\exp(-\beta J - \beta K) = \exp(2B). \end{aligned} \tag{6}$$

Their solution

$$A = 0.5 \cosh^{-1} \exp(2\beta J) \qquad B = -0.5(\beta J + \ln(\cosh \beta J)) \tag{7}$$

introduces the restriction (2) for the validity of the identity (5). The temperature-dependent effective interaction parameters A and B and the restrictive condition (2) are exactly the same as those found for the pure system (Horiguchi 1986). The presence of impurities manifests itself in the subsequent transformations.

Substitution of the identity (5) in the grand partition function permits one to interchange the order of summations

$$\zeta = \sum_{\{\sigma_{ij}\}} \prod_{i,j} \frac{1}{2^{N_b}} \sum_{\{c_i\}} \sum_{\{s_i\}} \exp[A s_i c_i(\sigma_{ij_1} + \sigma_{ij_2} + \sigma_{ij_3}) + 3B s_i^2 c_i - \beta \Delta s_i^2 c_i + \xi c_i] \tag{8}$$

first eliminating the s-spins on the honeycomb lattice. Here N_b is the number of bonds

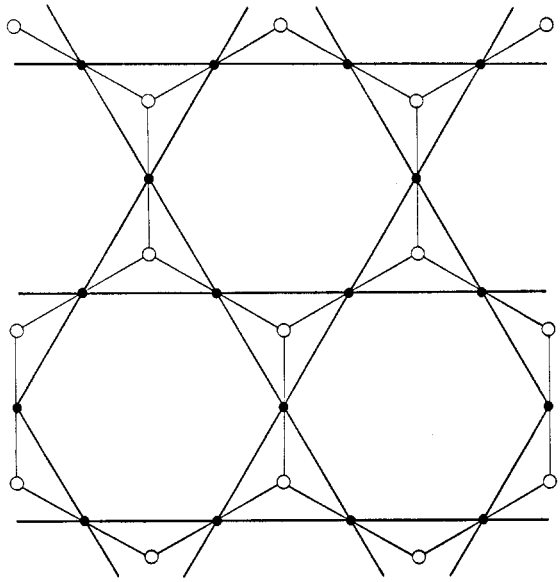

Figure 1. The honeycomb lattice is shown by thin lines. The open circles represent the sites that can be occupied either by s-spins, which can take the values 0, ± 1, or by non-magnetic impurities free from interactions with their neighbours. The Kagomé lattice is given in thick lines that connect the sites occupied by σ-spins (full circles) which can have only two orientations, $+1$ or -1.

on the honeycomb lattice and σ_{ij_1}, σ_{ij_2}, σ_{ij_3} are the σ-neighbours of s_i. The internal summations over $c_i = 0, 1$ and $s_i = 0, 1$ can be represented as

$$1 + \exp\xi + 2\exp(\xi + 3B - \beta\Delta)\cosh[A(\sigma_{ij_1} + \sigma_{ij_2} + \sigma_{ij_3})]$$
$$= D\exp[F(\sigma_{ij_1}\sigma_{ij_2} + \sigma_{ij_2}\sigma_{ij_3} + \sigma_{ij_3}\sigma_{ij_1})] \tag{9}$$

with the effective interaction between the pairs of nearest-neighbour spins on the Kagomé lattice given by

$$\exp(4F) = (1 + \exp\xi + 2\exp(\xi + 3B - \beta\Delta)\cosh 3A)$$
$$\times (1 + \exp\xi + 2\exp(\xi + 3B - \beta\Delta)\cosh A)^{-1} \tag{10}$$

and

$$D^4 = (1 + \exp\xi + 2\exp(\xi + 3B - \beta\Delta)\cosh 3A)$$
$$\times (1 + \exp\xi + 2\exp(\xi + 3B - \beta\Delta)\cosh A)^3. \tag{11}$$

Introducing (9) in (8) we find that the grand partition function of our model is expressed by the partition function $Z_K(F)$ for the Kagomé lattice

$$\zeta = 2^{-N_b} D^{N_h} Z_K(F). \tag{12}$$

Equation (4) leads to

$$p = \frac{1 + \frac{3}{2}\varepsilon_K}{4}\frac{q + 2q\exp(3B - \beta\Delta)\cosh 3A}{1 + q + 2q\exp(3B - \beta\Delta)\cosh 3A}$$
$$+ \frac{3 - \frac{3}{2}\varepsilon_K}{4}\frac{q + 2q\exp(3B - \beta\Delta)\cosh A}{1 + q + 2q\exp(3B - \beta\Delta)\cosh A} \tag{13}$$

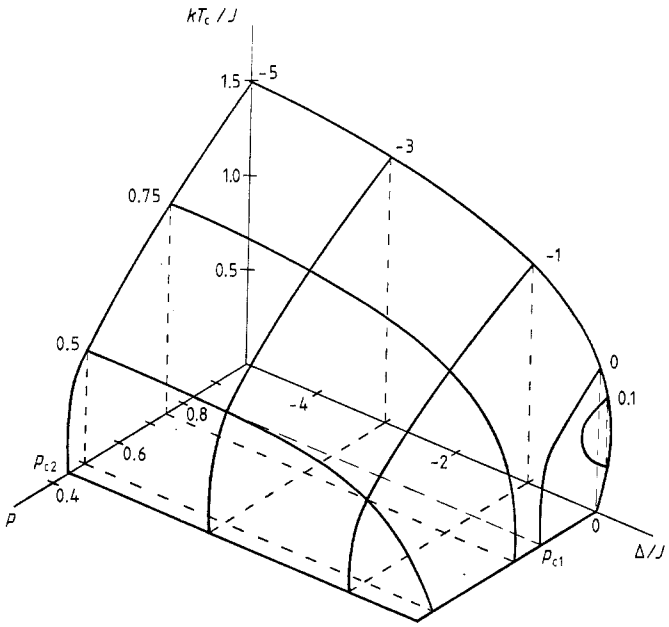

Figure 2. The reduced critical temperature kT_c/J as a function of p (the number density of magnetic atoms) and Δ/J (the reduced crystal field parameter).

where $\varepsilon_K = \varepsilon_K(F) = (1/N_K)\,\partial \ln Z_K(F)/\partial F$ and the factor of 3/2 in front of $\varepsilon_K(F)$ stems from the relation $N_K = \frac{3}{2}N_h$ giving the number of sites N_K on the Kagomé lattice. The parameter $q = \exp \xi$ can be expressed using (10) as

$$q = \frac{1 - \exp(4F)}{\exp(4F)\,(1 + 2\exp(3B - \beta\Delta)\cosh A) - (1 + 2\exp(3B - \beta\Delta)\cosh 3A)}. \tag{14}$$

Equations (13) and (14) give in implicit form the effective interaction F as a function of the temperature, the concentration of magnetic atoms p and the parameters of the Hamiltonian J, K and Δ.

To determine the critical temperature of the model, use should be made of the critical parameters F_c, ε_c of the Kagomé lattice which are known (Syozi 1972) to be

$$\exp(4F_c) = 3 + 2\sqrt{3} \qquad \varepsilon_c = (1 + 2\sqrt{3})/6. \tag{15}$$

With such substitutions in (13) and (14), the equation was solved numerically for various values of the parameters p and Δ/J. The critical surface is displayed in figure 2. It is folded for positive Δ/J giving two critical temperatures between which there is magnetic order in the system. We should stress here again that along the axis of the critical temperature the ratio K/J of the exchange interaction parameters changes according to the restrictive condition (2).

The critical concentration p_c, which limits the phase with magnetic order to $p > p_c$, can be evaluated from (13) and (14), examining the asymptotic region when the critical temperature tends to 0. The analysis gives two critical concentrations, one for $\Delta = 0$ when

$$p_{c1} = \frac{1 + 3\varepsilon_c/2}{4}\frac{9q}{1 + 9q} + \frac{3(1 + \varepsilon_c/2)}{4}\frac{q}{1 + q} \tag{16}$$

with $q = (1 - \exp 4F_c)/(\exp 4F_c - 9)$ leading to $p_{c1} = 0.824759527$ and the other for negative Δ/J given by

$$p_{c2} = \frac{1 + 3\varepsilon_c/2}{4}(1 - \exp(-4F_c)) = 0.447168784. \tag{17}$$

In conclusion, under the restrictive condition (2), an exact mapping of the dilute BEG spin-one model on a honeycomb lattice with site disorder onto the pure Kagomé lattice Ising model with usual $\sigma = \pm 1$ spins and effective temperature and concentration dependent interaction was achieved. An essential feature for the preceding calculation to be possible is that the honeycomb lattice has a coordination number $z = 3$. Exactly the same calculation can be done for any lattice with coordination number $z = 3$ if at the same time the critical parameters F_c and ε_c are known for the lattice of σ-spins obtained by their introduction in the middle of each bond of the basic lattice (the 3–12 lattice is such a candidate). The calculation can also be extended to the evaluation of the specific heat (Syozi 1965, 1972), to the magnetisation (Urumov 1987) and the correlation function and it is hoped to address these questions in the future.

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