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Exact results for a spin-one Ising model with random crystal field

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Abstract. An Ising spin-one model with an arbitrary distribution $P(\Delta)$ of crystal field interaction Δ, described with Blume–Emery–Griffiths Hamiltonian is considered for the annealed case in which the system is in complete thermal equilibrium. The critical temperature, under some restrictive condition on the interaction parameters, is obtained exactly for the honeycomb lattice.

Ising models and their many variations are encountered in different fields of physics and continue to be a subject of current interest. The randomness as a natural phenomenon is omnipresent and difficult to deal with. The theory of random magnets was recently reviewed (Fisher *et al* 1988) considering the frozen-in disorder. In the following we shall be interested in the opposite extreme of annealed disorder in which the system is allowed to reach complete thermal equilibrium. The purpose of this paper is to present some exact results concerning a model with random crystal field.

The specific model under consideration is known as Blume–Emery–Griffiths spin-one model (Blume *et al* 1971) and it is defined by the Hamiltonian

$$\mathcal{H} = \sum_{i,j} \mathcal{H}_{ij} + \sum_{i} \mathcal{H}_i \tag{1}$$

where the pair interaction $\mathcal{H}_{ij}$ includes bilinear (J) and biquadratic (K) exchange interaction between nearest neighbours

$$\mathcal{H}_{ij} = -JS_iS_j + KS_i^2S_j^2 \tag{2}$$

while the single site term

$$\mathcal{H}_i = \sum_k \Delta_k f_k S_i^2 \tag{3}$$

represents the crystal field (Δ_k) interaction energy which is explicitly specified by an indicator function f_k that is 1 if the crystal field strength is Δ_k and 0 otherwise. We shall generally assume that the crystal field strength obeys some arbitrary distribution function $P(\Delta)$ but for convenience, the derivation that follows is given for discrete Δ_k. It is supposed that the spin variables S_i on any lattice site can take three different values 0 and ± 1. It is also supposed that the lattice has a coordination number 3 and the final calculations are carried out for the honeycomb lattice.

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Considering the system in complete thermal equilibrium it is our aim to evaluate the grand partition function

$$\zeta = \sum_{\{S_i, f_k\}} \exp\left(-\beta\mathcal{H} + \beta\sum_k \xi_k f_k\right) \tag{4}$$

where $\beta = 1/kT$, k is the Boltzmann constant, T the absolute temperature, ξ_k the chemical potential coupled to the indicator f_k and the double summation is carried over all possible configurations of the spin variables and indicator functions. Here the calculation closely follows the lines previously set by Thorpe and Beeman (1976) in their consideration of spin-$\frac{1}{2}$ Ising models with random exchange interactions.

Taking the partial trace over $\{f_k\}$, we obtain

$$\sum_{\{f_k\}} \exp\left(-\beta\sum_k \Delta_k f_k S_i^2 + \beta\sum_k \xi_k f_k\right) = \sum_k \exp(-\beta\Delta_k S_i^2 + \beta\xi_k) = C\exp(-DS_i^2) \tag{5}$$

where the last equation defines the functions C and D

$$C = \Sigma_0 \qquad \exp(-D) = \Sigma_1/\Sigma_0 \tag{6}$$

with

$$\Sigma_0 = \sum_k \exp(\beta\xi_k) \qquad \Sigma_1 = \sum_k \exp(-\beta\Delta_k + \beta\xi_k). \tag{7}$$

In this manner the initial problem is reduced to a model defined on the same lattice with an effective crystal-field interaction D which is temperature-dependent function and the elements of randomness are incorporated in its structure. Otherwise D is equal for all lattice sites.

Some exact results for this model were obtained recently: Horiguchi (1986) has mapped the model onto the Kagomé spin-$\frac{1}{2}$ lattice, Wu (1986) gave an independent derivation and subsequently (Wu and Wu 1988) established the equivalence of the model with an external field with an Ising model in a nonzero external field and the author obtained the magnetisation (Urumov 1987) and the critical temperature for the site-diluted model (Urumov 1989). Most of the above results were obtained under some restriction on the parameters of the system, as is the case with the subsequent derivations.

Using the identity (Horiguchi 1986)

$$\exp(\beta JS_iS_j - \beta KS_i^2S_j^2) = \tfrac{1}{2}\sum_{\sigma_{ij}=\pm 1} \exp[A\sigma_{ij}(S_i + S_j) + B(S_i^2 + S_j^2)] \tag{8}$$

which is exact under the conditions

$$\exp\beta K = \cosh\beta J, \tag{9}$$

$$\cosh 2A = \exp 2\beta J, \tag{10}$$

$$B = -(\beta J + \beta K)/2, \tag{11}$$

new spin-like variables σ_{ij} are introduced on each bond connecting two neighbouring

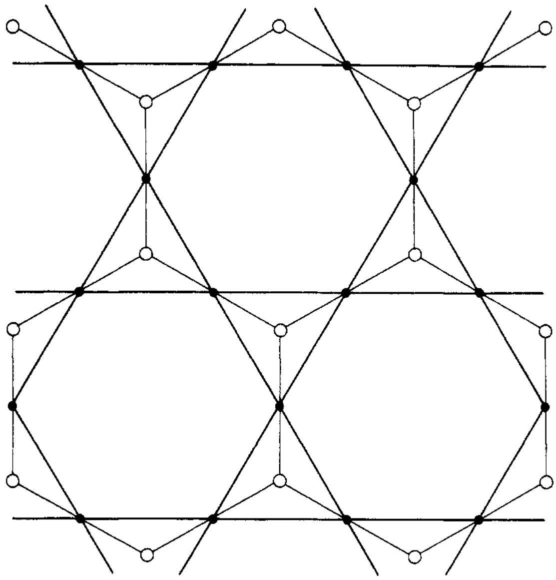

Figure 1. The honeycomb and Kagomé lattices are shown, respectively, by thin and thick lines. The open circles represent the sites occupied by s-spins, which take three values 0, ± 1 and the full circles represent the sites occupied by σ-spins which can have two values, $+1$ or -1.

sites. Figure 1 represents the original honeycomb lattice of $S = 1$ spins together with the σ-spins which are lying on a Kagomé lattice. Interchanging the order of summations and first performing the sums over $\{S_i\}$ and then over the newly introduced σ_{ij}-spins, our model is reduced to the spin-$\frac{1}{2}$ Ising model on the Kagomé lattice.

The grand partition function ζ is expresed exactly by

$$\zeta = 2^{-N_{bh}}(CG)^{N_{sh}} Z_k(F) \tag{12}$$

where N_{sh} and N_{bh} are, respectively, the number of sites and bonds on the honeycomb lattice and

$$G^4 = (\Sigma_0 + 2\Sigma_1 \, e^{3B} \cosh 3A)(\Sigma_0 + 2\Sigma_1 \, e^{3B} \cosh A)^3/\Sigma_0^4, \tag{13}$$

$$e^{4F} = (\Sigma_0 + 2\Sigma_1 \, e^{3B} \cosh 3A)/(\Sigma_0 + 2\Sigma_1 \, e^{3B} \cosh A) \tag{14}$$

and $Z_k(F)$ is the partition function for the Kagomé lattice which is known exactly (Syozi 1972). The partition function $Z_k(F)$ depends on the effective interaction F defined in (14).

It remains to eliminate the chemical potential ξ_k by use of

$$\beta\langle f_k\rangle = \frac{1}{N_{sh}} \frac{\partial \ln \zeta}{\partial \xi_k} \tag{15}$$

which after some manipulation gives

$$\langle f_k\rangle = \frac{e^{\beta\xi_k}}{4(\Sigma_0 + 2\Sigma_1 \, e^{3B} \cosh 3A)} \left\{ \left[1 + \frac{3}{2}\varepsilon(F)\right](1 + 2e^{3B-\beta\Delta_k} \cosh 3A) + 3e^{4F}\left[1 - \frac{\varepsilon(F)}{2}\right](1 + 2e^{3B-\beta\Delta_k} \cosh A)\right\} \tag{16}$$

where

$$\varepsilon(F) = \frac{1}{N_{sk}} \frac{\partial \ln Z_k}{\partial F} \tag{17}$$

is the nearest neighbour pair correlation function on the Kagomé lattice.

The formula for $\langle f_k \rangle$ is now divided by the expression in the braces and the whole expression is summed over k to give

$$\sum_k \langle f_k \rangle / \{[1 + \tfrac{3}{2}\varepsilon(F)](1 + 2\exp(3B - \beta\Delta_k)\cosh 3A) + 3\exp(4F)[1 - \varepsilon(F)/2] \times [1 + 2\exp(3B - \beta\Delta_k)\cosh A]\} = \frac{\Sigma_0}{4(\Sigma_0 + 2\Sigma_1 \exp(3B)\cosh 3A)}. \tag{18}$$

Using (6) and (14) and imposing that $\langle f_k \rangle$ is temperature independent and going to a continuous distribution $P(\Delta)$ we obtain the following relationship

$$\int P(\Delta)\,\mathrm{d}\Delta / \{[1 + \tfrac{3}{2}\varepsilon(F)](1 + 2\exp(3B - \beta\Delta)\cosh 3A) + 3\exp(4F)[1 - \varepsilon(F)/2] \times (1 + 2\exp(3B - \beta A)\cosh A)\} = \frac{2\cosh 2A - 1 - \exp(4F)}{8\exp(4F)(\cosh 2A - 1)}. \tag{19}$$

From (19) in the case without randomness, $P(\Delta) = \delta(\Delta - \Delta_0)$ the result of Horiguchi (1986) is recovered. The last expression represents an integral equation for the effective interaction F between the nearest neighbour σ-spins on the Kagomé lattice. From the relationship (12) it is seen that our model with random crystal field becomes critical when the Kagomé lattice becomes critical. The critical parameters for the Kagomé lattice are known (Syozi 1972) to be

$$\exp(4F_c) = 3 + 2\sqrt{3}, \qquad \varepsilon(F_c) = (1 + 2\sqrt{3})/6. \tag{20}$$

To examine the critical temperature of the random crystal field model, two particular cases for the distribution function $P(\Delta)$ are considered.

In the first the distribution $P_1(\Delta)$ is discrete and the crystal field takes two values $\Delta_0 \pm \Delta_1$ with probability p and $1 - p$, respectively

$$P_1(\Delta) = p\delta(\Delta - \Delta_0 - \Delta_1) + (1 - p)\delta(\Delta - \Delta_0 + \Delta_1). \tag{21}$$

In the second case, uniform distribution is assumed

$$P_2(\Delta) = \frac{1}{2\Delta_1}, \Delta_0 - \Delta_1 < \Delta < \Delta_0 + \Delta_1. \tag{22}$$

The critical temperature, for the case of the discrete distribution $P_1(\Delta)$, as a function of $d = \Delta_1/\Delta_0$ and for various p is shown in figure 2. It is a symmetric function under the substitution $p \to 1 - p$, $\Delta_1 \to -\Delta_1$. Using (10), (20) and (21), the critical temperature in the limit of large fluctuations $d \to \infty$ and for $\Delta_0 < 0$ is found to approach the limiting value given by

$$\exp(2\beta_c J) = \frac{8(1 - p)\,\mathrm{e}^{4F} - (1 + \mathrm{e}^{4F})a}{2[4(1 - p)\,\mathrm{e}^{4F} - a]} \tag{23}$$

where

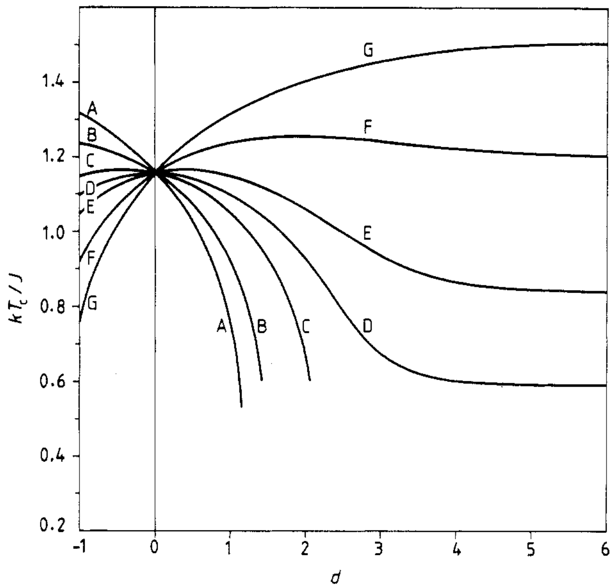

Figure 2. Plots of T_c versus $d = \Delta_1/\Delta_0$ for selected values of p in the distribution function $P_1(\Delta)$ and for $\Delta_0/J = -1$. The curves A, B, C, D, E, F, G correspond, respectively to $p = 0; 0.2; 0.4; 0.5, 0.6; 0.8; 1$.

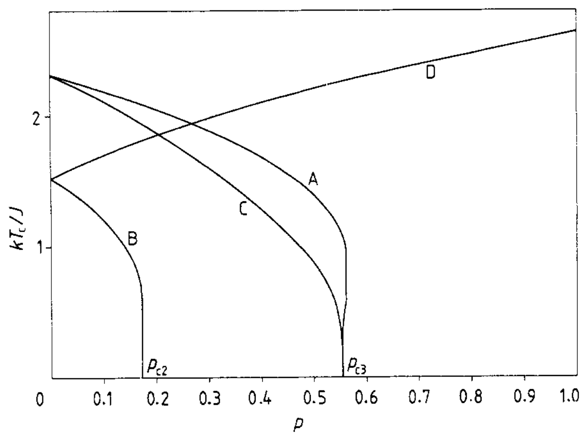

Figure 3. Plots of T_c versus p for $\Delta_0 = 0$, $\Delta_1/J = 1$ (A); $\Delta_0/J = 1$, $\Delta_1/\Delta_0 = 1$ (B); $\Delta_0/J = 1$, $\Delta_1/\Delta_0 = 2$ (C) and $\Delta_0/J = -1$, $\Delta_1/\Delta_0 = 1$ (D) in the distribution function $P_1(\Delta)$.

$$a = b + 3e^{4F}\left[1 - \frac{\varepsilon(F)}{2}\right], b = 1 + \tfrac{3}{2}\varepsilon(F). \qquad (24)$$

The critical temperature vanishes at the critical probability

$$p_{c1} = 1 - a/e^{4F} = 0.447168784. \qquad (25)$$

In figure 3, the critical temperature for the same distribution is shown as a function

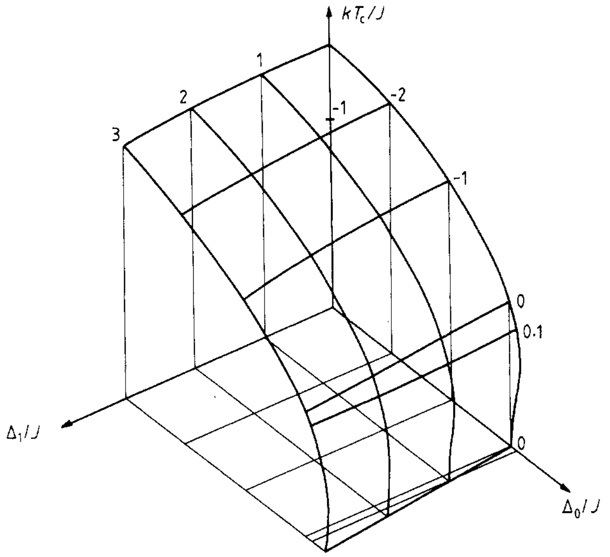

Figure 4. The critical surface kT_c/J as a function of the mean crystal field Δ_0/J and the half-width of its fluctuations Δ_1/J which define the uniform distribution $P_2(\Delta)$ of crystal fields.

of p for several values of Δ_0 and Δ_1. The asymptotic analysis shows that the critical temperature, in the case $\Delta_0 > 0$, $d = 1$, vanishes at

$$p_{c2} = a\left(\frac{1}{e^{4F}} - \frac{1}{8b} + \frac{a}{32b\,e^{4F}}\right) = 0.175240474. \tag{26}$$

For $\Delta_0 > 0$, $d > 1$; $\Delta_0 < 0$, $d < -1$ or $\Delta_0 = 0$, $\Delta_1 > 0$ the critical temperature becomes zero for

$$p_{c3} = \frac{a}{4e^{4F}} = 0.552831216. \tag{27}$$

The critical temperature is finite in the domain $\Delta_0 < 0$, $|d| \leqslant 1$. The critical probabilities for which the critical temperature vanishes, in the remaining cases $\Delta_0 < 0$, $d = 1$ or $d > 1$; $\Delta_0 > 0$, $d < -1$ and $\Delta_0 = 0$, $\Delta_1 < 0$, can be found from the symmetry property.

The distribution $P_1(\Delta)$ for $p = \frac{1}{2}$ is encountered in several recent publications (Kaneyoshi 1988a, b) where the critical temperature is determined within the effective field approximation.

Part of the critical surface as a function of the mean crystal field Δ_0 and the fluctuation range Δ_1 in the case of the uniform distribution is plotted in figure 4. It is a pair function with respect to Δ_1. The critical temperature vanishes along the line

$$\Delta_0 = \left(\frac{a}{2\,e^{4F}} - 1\right)\Delta_1 = 0.105662432\,\Delta_1. \tag{28}$$

It is interesting to note that for positive Δ_0 the domain of the ordered phase is enlarged and T_c is increased with the rise in the range of fluctuations.

In summary, under the restriction (9) on the parameters of the system, the critical temperature for the random crystal field Blume–Emery–Griffiths model in the case of complete thermal equilibrium has been obtained exactly for an arbitrary distribution $P(\Delta)$ of the crystal field interaction. As it was argued by Thorpe and Beeman (1976) for the random exchange interaction model, the results for the annealed case may serve as an approximation for the physically more interesting case of quenched disorder. One may hope that this is the case also when the crystal field is random.

At least two further developments appear to be possible. The essential new ingredient for the exact mapping onto an exactly solved model was the identity (5). This expression can take only two values for $S = 0$ and $S = \pm 1$. The same property exists for similar model with spin-one random biquadratic exchange or for the spin-$\frac{1}{2}$ Ising model in a random field. Unfortunately the latter model would be mapped onto the Ising model in an external field whose exact solution is not known.

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