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Critical temperature for a spin-1 Ising model with dipolar and quadrupolar interactions

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The critical temperature for an isotropic Blume-Emery-Griffiths model is discussed in a new type of effective-field approximation. The method, which can systematically include correlation effects, is illustrated by applying to linear, honeycomb, and simple-cubic lattices. The relation between the present method and that very recently proposed by Chakraborty is widely discussed.

In a recent report,[1] Chakraborty, using an effective-field model of a spin-1 Ising system with both dipolar and quadrupolar interactions [isotropic Blume-Emery-Griffiths (BEG) model], which is described by the Hamiltonian

$$H=-\sum_{g,f} J_{gf}S_gS_f-\sum_{g,f} j_{gf}S_g^2S_f^2 \ ,$$

drew the following basic conclusions about the transition temperature.

(i) For a linear chain, a nonzero, real, positive critical temperature T_c exists for both positive and negative values of α [where $\alpha=j/J$ is the quadrupolar (j) and dipolar (J) interactions ratio], although $\alpha=0$ does not favor any phase transition.

(ii) For both honeycomb and simple-cubic lattice structures no solution is found for T_c for any positive values of α.

$$m=\langle S_f\rangle=\left\langle \prod_g \exp(\beta J_{gf}S_gD_x)\prod_{g'}\exp(\beta j_{g'f}S_{g'}^2D_y)\right\rangle f(x;y)\Big|_{x=0;y=0} \ , \tag{1a}$$

$$Q=\langle S_f^2\rangle=\left\langle \prod_g \exp(\beta J_{gf}S_gD_x)\prod_{g'}\exp(\beta j_{g'f}S_{g'}^2D_y)\right\rangle g(x;y)\Big|_{x=0;y=0} \ , \tag{1b}$$

where the functions $f(x,y)$ and $g(x,y)$ are defined as

$$f(x,y)=2e^y\sinh x/(1+2e^y\cosh x)$$

and

$$g(x,y)=2e^y\cosh x/(1+2e^y\cosh x)$$

and $D_x\equiv\partial/\partial_x$ and $D_y\equiv\partial/\partial_y$ are the two differential operators. Now, by using the van der Waerden identities for the spin-1 Ising systems (i.e.,

$$\exp(\lambda S_g)=1+S_g\sinh(\lambda)+S_g^2[\cosh(\lambda)-1]$$

and $\exp(\lambda S_g^2)=1+S_g^2[\exp(\lambda)-1]$ $A\lambda$), Eqs. (1a) and (1b) may be rewritten in a more useful and elegant form

$$m=\left\langle \prod_g F(D_x;S_g,S_g^2)\prod_{g'} G(D_y;S_{g'}^2)\right\rangle f(x,y)\Big|_{x=0;y=0} \ , \tag{2a}$$

We should like to point out that the results obtained by the use of Chakraborty's approach[1] provide no reliable information about the nature of the transition temperature of the BEG model. His drastic assumption $\langle A\rangle/\langle B\rangle \cong \langle (A/B)\rangle$ is not appropriate and leads to unphysical results in both a qualitative and quantitative point of view. The usual Honmura and Kaneyoshi mean-field approximation[2] (HK-MFA, as he calls it), does not need so drastic a supposition.

In fact, Eqs. (18) and (19) of Chakraborty's paper are correct; however, his development beyond that point, based in his Eq. (13), introduces modifications in the original HK-MFA procedure and, as a consequence, spurious results may occur.[3] In order to clarify this, firstly we should note that the summations appearing in Eqs. (18) and (19) through the definitions of $E_d=\sum_g J_{gf}S_g$ and $E_q=\sum_g j_{gf}S_g^2$ can be transformed in products over the nearest neighbors of the site f, as follows:

$$Q=\left\langle \prod_g F(D_x;S_g,S_g^2)\prod_{g'} G(D_y;S_{g'}^2)\right\rangle g(x,y)\Big|_{x=0;y=0} \ , \tag{2b}$$

where the operators functions $F(D_x;S_g,S_g^2)$ and $G(D_y;S_g^2)$ are defined by

$$F(D_x;S_g,S_g^2)=1+S_g\sinh(\beta J_{gf}D_x)+S_g^2[\cosh(\beta J_{gj}D_x)-1] \ , \tag{3a}$$

$$G(D_y;S_g^2)=1+S_g^2[\exp(\beta j_{gf}D_y)-1] \ . \tag{3b}$$

The exact set of mutually coupled Eqs. (2a) and (2b) is particularly amenable to systematic approximations and will be used here as the basis for the present formalism. Firstly, we should note that the exact Eqs. (2a) and (2b) provide a set of relations between the two relevant statistical-

mechanical quantities m and Q and associated multispin correlation functions of the various sites. Thus, if we try to exactly take into account all these spin-spin correlations, the problem quickly becomes mathematically untractable, so that some approximations have to be done. However, as has already been pointed out in earlier works on both spin-$\frac{1}{2}$ (Refs. 4–9) and spin-1 Ising systems[10] as well as in other models,[11] this kind of exact formal set of identities can be used as a basis for various approximate schemes which can explicitly and systematically include effects of correlations. On the other hand, a first obvious attempt to deal with it is to *ignore correlations*. It is clear that within this approximation, the strict criticality of the system is lost (in particular, the critical exponents are going to be the classical ones), and the real dimensionality of the system is only partially taken into account through the coordination number z. Nevertheless, this kind of approximate procedure is quite superior to the ordinary MFA, and this is so because, in the present framework relations like $S_g^2=0,1$ are taken exactly into account (and, as a consequence, neglects only correlations between different spin variables), whereas the usual mean-field approximation neglects all correlations.

Based in this approximation (where spin-spin correlations are neglected) the two statistical-mechanical quantities m and Q pertinent to the BEG model can be evaluated from the following set of equations:

$$m=[F(D_x;m,Q)G(D_y;Q)]^z f(x,y)|_{x=0;y=0} , \tag{4a}$$

$$Q=[F(D_x;m,Q)G(D_y;Q)]^z g(x,y)|_{x=0;y=0} , \tag{4b}$$

where now

$$F(D_x;m,Q)=1+m\sinh(\beta J_{gf}D_x)+Q[\cosh(\beta J_{gf}D_x)-1]$$

and

$$G(D_y;Q)=1+Q[\exp(\beta j_{gf}D_y)-1] .$$

Thus, by using the property of the exponential operator [namely, $\exp(\lambda D_x)f(x,y)=f(x+\lambda,y)$], Eqs. (4a) and (4b) can be transformed for any lattice structure, characterized by the coordination number z, into polynomial expressions of the general form

$$m=\sum_{\nu} A_{\nu z}m^{\nu}, \quad \nu=1,3,5,\ldots,\ \nu\leq z \tag{5a}$$

$$Q=\sum_{\nu'} B_{\nu' z}m^{\nu'}, \quad \nu'=0,2,4,6,\ldots,\ \nu'\leq z , \tag{5b}$$

where the coefficients $A_{\nu z}$ and $B_{\nu z}$, which are not explicitly presented here, are dependent on the variables Q and T.

With the Eqs. (5a) and (5b) the computation of the relevant thermodynamical quantities for different lattice structures, with nonzero biquadratic parameter α, have been carried out, and the main conclusions are summarized as follows.

(i) For a linear chain ($z=2$), in contrast to Chakraborty's results, we found no solution for $T_c\neq 0$ for any value of α. $Q=1$ and $m=1$ is a solution only for $T_c=0$.

(ii) For honeycomb ($z=3$) and simple-cubic ($z=6$) lattices, we have found that a nonzero, real, positive solution for T_c always exists for both *positive* and negative values of α.

In fact, our conclusion (i) is in complete agreement with the exact result obtained by means of the transfer matrix[12] and by the use of other approximate methods.[13] Moreover, we also note that our conclusion (ii) is in qualitative disagreement with Chakraborty's results[1] once he predicts no solution for T_c for any positive α in both cases of honeycomb and simple-cubic lattices.

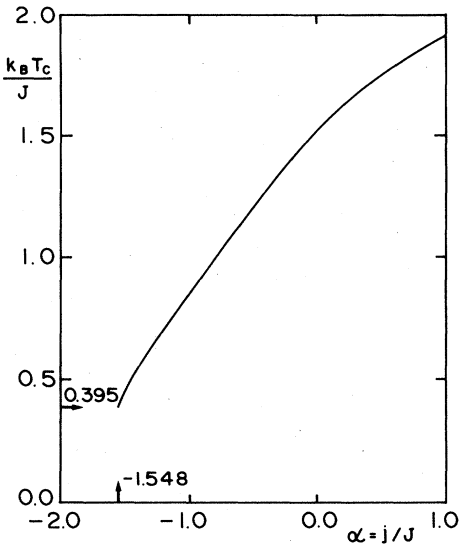

FIG. 1. Nature of variation of $k_B T_c/J$ with respect to α over the range $-\alpha_c\leq\alpha\leq 1$ for a honeycomb lattice. The curve refers to the second-order phase transition and the critical point (T_c^*,α_c) is indicated by arrows.

In Fig. 1 the results of our calculation for the critical frontier in the (T,α) space—which determines the limit of stability of the long-range ferromagnetic order—is illustrated for the case of a honeycomb lattice. We find that there exists a certain critical negative value of α ($\alpha_c=-1.548$) below which the set of Eqs. (5a) and (5b) does not exhibit solutions with $m=0$. In fact, we have found that for $\alpha<\alpha_c$ the magnetization exhibits a discontinuity which goes from certain finite value m_c to zero, at a certain temperature T_c, suggesting a first-order phase transition, which characterizes a different behavior of the system over the range $-\infty<\alpha<-1.548$. The fact that the present system undergoes the first-order or the second-order phase transition according to the value of the biquadratic parameter α, is also provided by the usual MFA[14] as well as other approximate schemes.[13]

Let us conclude by saying that our results support the belief that the present framework provides qualitative and to a certain extent quantitative confidence. So, as a main conclusion we would like to emphasize that the discrepancies we have found between our results and those from Chakraborty's work are basically due to his drastic assumption $\langle A\rangle/\langle B\rangle\cong\langle A/B\rangle$. Finally, we should also mention that, owing to their simplicity, the method developed here can be used to study more complex problems associated with the Ising spin-1 Hamiltonian. In a forthcoming paper we intend to discuss thermodynamical properties which have not been analyzed herein, such as the thermal behavior of the m and Q order parameters, internal energy, specific heat, and so on.

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