Effective-field model for a spin-1 Ising system with dipolar and quadrupolar interactions

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The effective-field model of a spin-1 Ising system with both dipolar and quadrupolar interactions is studied. From the generalized Suzuki identity the exact expressions for the dipolar and the quadrupolar ordering parameters are found in the form of ensemble averages. Two different operators are introduced to write the above expressions in the form of exponentials, which are then simplified. The transition temperatures for linear, honeycomb, and simple cubic lattices are computed and compared with the results of previous theories.

I. INTRODUCTION

The two-state or spin-$\frac{1}{2}$ Ising model was introduced by Ising[1] in 1925 as a possible model for ferromagnetism. Ising himself solved the model in one dimension and some time later Onsager[2] solved the two-dimensional Ising model exactly. In three dimensions, no exact solution has been obtained. However, several alternative approaches were developed. These are (i) closed-form approximations,[3,4] (ii) Green's-function approximations,[5] (iii) series-expansion method,[6] and (iv) renormalization-group calculations.[7]

It should be appreciated that among the above methods the molecular-field approximation (MFA) is indeed able to give a simple and satisfactory description of the statistical mechanics of the Ising models over a large range of temperatures. One significant defect of MFA is that it leads to the unphysical result for a linear chain. Also, the results for Curie temperatures for different lattices calculated by MFA are much higher than the exact results.

Incorporating the effects of many-body static spin correlations in MFA, Lines[8] developed the correlated effective-field approximation which was later applied to some problems in magnetism. But this method also has some serious drawbacks. Firstly, it predicts a vanishing Curie temperature for a two-dimensional Ising model. Secondly, the results are essentially equivalent to those of the spherical model which provides lower transition temperatures. The exact result should, in fact, lie between those of the spherical model and MFA.

With the motivation of deriving more accurate expressions for the magnetization and Curie temperatures for a spin-$\frac{1}{2}$ Ising system Honmura and Kaneyoshi[9] (HK) developed an effective-field model by introducing an exponential operator technique and by utilizing a correlation identity derived previously by Callen.[10] This technique (which we call HK-MFA) was found by them to yield the transition temperatures which are more accurate than those obtained in MFA. Later, Kaneyoshi and his co-workers[11] developed the technique elaborately. Recently, Taggart[12] and Taggart and Fittipaldi[13] performed calculations for linear, honeycomb, square, and cubic lattices using the Callen identity and an inverse Callen identity. They found that the quantitative agreement with the exact results is better than that obtained in MFA, HK-MFA, and Bethe approximations. The most encouraging feature of the HK technique is that it reproduces the exact results for a linear chain.

The review presented above is concerned only with the spin-$\frac{1}{2}$ Ising model. The Ising model with spins greater than $\frac{1}{2}$ received relatively less attention. The chief difficulty behind this is that the Hamiltonians in these cases are indeed very complicated. The generalized spin-S Ising model as proposed by Taggart[14] is, however, solvable in some special cases. The Blume-Emery-Griffiths (BEG) model[15] and the Blume-Capel (BC) model[16] are two such simple special cases and are spin-1 models. Mukamel and Blume[17] adopted the BEG Hamiltonian and employed the mean-field approximation to study the tricritical points in ternary mixtures. Sivardière and Lajzerowicz[18] and Chakraborty[19] adopted the above Hamiltonian to construct the appropriate lattice gas models for solid, liquid, and gaseous phases and the related phase transitions. The MFA was used by Furman, Dattagupta, and Griffiths[20] to propose the global phase diagram for a ternary system. Renormalization-group calculations for the BEG model have also been performed by some authors.[21,22] Obkata and Oguchi[23] derived the results for Curie temperatures by Bethe approximation. Recently, Tamura and Kaneyoshi[24] utilized the HK technique to study a Blume-Capel model.

The purpose of the present paper is to employ the HK technique to study a spin-1 Ising system described by a Hamiltonian which consists of dipolar and quadrupolar interactions. Using the generalized correlation identity of Suzuki[25] and introducing two exponential operators the HK expressions for dipolar and quadrupolar ordering parameters are worked out. The results for the transition temperatures are computed for linear, honeycomb, and cubic lattices and compared with the results of earlier theories.

II. MOLECULAR-FIELD APPROXIMATION AND SUZUKI'S IDENTITY

We consider a spin-1 Ising system whose spins are coupled by the following Hamiltonian:

$$H = -\sum_{g,f} J_{gf}\vec{S}_g\cdot\vec{S}_f - \sum_{g,f} j_{gf}(S_g^2 S_f^2) \ , \tag{1}$$

where J_{gf} is the dipolar exchange and j_{gf} is the quadrupolar exchange.

The expressions for the magnetization $m=\langle\vec{S}_g\rangle$ and the quadrupolar ordering parameter $Q=\langle S_g^2\rangle$ in MFA applied

to Eq. (1) are[17,18]

$$m=\frac{2e^{2\beta zjQ}\sinh(2\beta Jm)}{1+2e^{2\beta zjQ}\cosh(2\beta zJm)} , \tag{2}$$

$$Q=\frac{2e^{2\beta zjQ}\cosh(2\beta zJm)}{1+2e^{2\beta zjQ}\cosh(2\beta zJm)} , \tag{3}$$

with

$$m=Q\tanh(2\beta zJm) , \tag{4}$$

where z is the number of nearest neighbors; J and j are the nearest-neighbor dipolar and quadrupolar exchange constants, respectively.

Now we want to see whether Eqs. (2)–(4) are derivable from Suzuki's generalized identity. Suzuki considered the following general Hamiltonian:

$$H=\sum_{f>g},\ldots V(S_f,S_g,\ldots) , \tag{5}$$

where $V(S_f,\ldots)$ is the dipolar, quadrupolar, or higher-order function of the spin variables S_f, S_g, etc. Let $-E_g(S_g)$ be the contribution to the energy of the gth spin. For such a system Suzuki derived the following correlation identity:

$$\langle\{f\}(S_g)^p\rangle=\left\langle\{f\}\frac{\mathrm{Tr}_g(S_g)^p e^{\beta E_g(S_g)}}{\mathrm{Tr}_g e^{\beta E_g(S_g)}}\right\rangle , \tag{6}$$

where $p=1$, 2, etc., and $\{f\}$ is any function of S_f's at sites other than the gth. The symbol $\langle A\rangle$ denotes the ensemble average

$$\langle A\rangle=\frac{\mathrm{Tr}(Ae^{-\beta H})}{\mathrm{Tr}e^{-\beta H}} . \tag{7}$$

For a spin-1 Ising model with both dipolar and quadrupolar interactions, the contribution to the energy of the gth spin should consist of dipolar and quadrupolar terms, i.e., we have to replace $E_g(S_g)$ by $[E_d(S_g)+E_q(S_g^2)]$, where d stands for the dipolar and q for the quadrupolar contributions. Hence, considering the case $\{f\}=1$, we get the following identity from Eq. (6):

$$\langle(S_g)^p\rangle=\frac{\mathrm{Tr}_g((S_g)^p\exp\{\beta[E_d(S_g)+E_q(S_g^2)]\})}{\mathrm{Tr}_g(\exp\{\beta[E_d(S_g)+E_q(S_g^2)]\})} . \tag{8}$$

For the spin-1 case above identity leads to the following expressions for m and Q:

$$m=\langle S_g\rangle=\left\langle\frac{2e^{\beta E_q}\sinh(\beta E_d)}{1+2e^{\beta E_q}\cosh(\beta E_d)}\right\rangle , \tag{9}$$

$$Q=\langle S_g^2\rangle=\left\langle\frac{2e^{\beta E_q}\cosh(\beta E_d)}{1+2e^{\beta E_q}\cosh(\beta E_d)}\right\rangle , \tag{10}$$

where

$$E_d=\sum_g J_{gf}S_g , \tag{11}$$

$$E_q=\sum_g j_{gf}S_g^2 . \tag{12}$$

The above type of equations were also obtained by Tamura and Kaneyoshi[24] for a Blume-Capel model.

Now using the approximation $\langle A\rangle/\langle B\rangle\simeq\langle(A/B)\rangle$ one gets from Eqs. (9) and (10)

$$m\simeq Q\langle\tanh(\beta E_d)\rangle . \tag{13}$$

It is evident that if one writes

$$E_d=2zJm,\ E_q=2zjQ \tag{14}$$

then Eqs. (9), (10), and (13) reduce, respectively, to Eqs. (2), (3), and (4). Hence, one should expect that the results would be better than those of MFA if one works with the identities (9), (10), and (13) using the HK technique. We call Eqs. (9) and (10) the individual identities and Eq. (13) the joint identity.

III. EXPONENTIAL OPERATOR TECHNIQUE

The exponential operator technique introduced by Honmura and Kaneyoshi[9] is based on the following identity:

$$\langle e^{D\theta}\rangle\tanh x|_{x\to 0}=\langle\tanh\theta\rangle , \tag{15}$$

where $D\equiv\partial/\partial x$ is a differential operator.

However, since the present problem involves two ordering parameters m and Q we have to introduce two differential operators $D_x\equiv\partial/\partial x$ and $D_y\equiv\partial/\partial y$ such that we arrive at the following two exponential operator identities:

$$\langle e^{D_x\theta+D_y\psi}\rangle\frac{2e^y\sinh x}{1+2e^y\cosh x}\bigg|_{x\to 0,\,y\to 0}=\left\langle\frac{2e^\psi\sinh\theta}{1+2e^\psi\cosh\theta}\right\rangle , \tag{16}$$

$$\langle e^{D_x\theta+D_y\psi}\rangle\frac{2e^y\cosh x}{1+2e^y\cosh x}\bigg|_{x\to 0,\,y\to 0}=\left\langle\frac{2e^\psi\cosh\theta}{1+2e^\psi\cosh\theta}\right\rangle \tag{17}$$

The above identities can be proved in a straightforward manner. We emphasize that since in Eqs. (9), (10), and (13) the parameters m and Q are coupled it is not possible to treat the problem using only a single differential operator as was done by Tamura and Kaneyoshi.

Using (16) and (17) we can transform Eqs. (9), (10), and (13) in the following forms:

$$m=\langle e^{D_x\beta E_d+D_y\beta E_q}\rangle\frac{2e^y\sinh x}{1+2e^y\cosh x}\bigg|_{x\to 0,\,y\to 0} , \tag{18}$$

$$Q=\langle e^{D_x\beta E_d+D_y\beta E_q}\rangle\frac{2e^y\cosh x}{1+2e^y\cosh x}\bigg|_{x\to 0,\,y\to 0} , \tag{19}$$

$$m=Q\langle e^{D_x\beta E_d}\rangle\tanh x|_{x\to 0} . \tag{20}$$

It may be remarked that if one wants to study the individual thermal variations of dipolar and quadrupolar order parameters then one should work with the identities (18) and (19) separately. To find the critical temperature T_c one may work with any one of the above three identities considering the fact that at T_c the dipolar order parameter m vanishes and Q takes the value $\frac{2}{3}$. However, it is much simpler to work with Eq. (20) if one goes to find T_c.

IV. EXPRESSIONS FOR THE ORDER PARAMETERS

From Eqs. (1) and (18) we get the following expression for the magnetization:

$$m = \left\{ \frac{\mathrm{Tr}\exp[2\beta \sum_g [(JD_x + zJm)S_g + (jD_y + zjQ)S_g^2]\}}{\mathrm{Tr}\exp[2\beta \sum_g (zJmS_g + zjQS_g^2)]} \right\} \times \frac{2e^y \sinh x}{1 + 2e^y \cosh x}\bigg|_{x\to 0,\, y\to 0} . \quad (21)$$

For a spin-1 case it reduces to the form

$$m = \lambda^{-z}[1 + 2e^{D_y\psi + b}\cosh(D_x\theta + a)]^z \times \frac{2e^y \sinh x}{1 + 2e^y \cosh x}\bigg|_{x\to 0,\, y\to 0} , \quad (22)$$

where

$$\psi = 2\beta j, \quad b = 2\beta jzQ ,$$
$$\theta = 2\beta J, \quad a = 2\beta zJm , \quad (23)$$
$$\lambda = 1 + 2e^{2\beta zjQ}\cosh(2\beta zJm) .$$

Similarly Eqs. (19) and (20) can be simplified to the following form:

$$Q = \lambda^{-z}[1 + 2e^{D_y\psi + b}\cosh(D_x\theta + a)]^z \times \frac{2e^y \sinh x}{1 + 2e^y \cosh x}\bigg|_{x\to 0,\, y\to 0} , \quad (24)$$

$$m = Q\lambda^{-z}[1 + 2e^b \cosh(D_x\theta + a)]^z \tanh x\,|_{x\to 0} . \quad (25)$$

Equations (22), (24), and (25) are the final expressions for the ordering parameters m and Q in the present effective-field model for a spin-1 Ising model with dipolar and quadrupolar interactions. These are completely different from those of MFA but these are much more complicated and a lot of computational labor is needed. Instead of performing such complicated computations of the thermal variations of m and Q we restrict ourselves to finding the values of $K_c = J/k_B T_c$ for various lattices.

V. RESULTS AND DISCUSSION

Detailed computations of Eqs. (22), (24), and (25) have been carried out to find the Curie temperatures. These equations are first simplified and the limiting condition $m \to 0$, $Q \to \frac{2}{3}$ is imposed and the resulting equations for T_c are computed. We do not present here the simplifications since these can be done in a straightforward manner. Table I shows the values of K_c^{-1} for linear, honeycomb, and simple cubic lattices for the special case where the biquadratic parameter $\alpha = j/J$ is zero. The results are compared with those of MFA, Brown-Luttinger theory,[26] the Obokata-Oguchi generalized Bethe approximation,[23] and the Tamura-Kaneyoshi effective-field model. The values in Table I have been calculated from two equations—values for $z = 2$ and $z = 3$ from Eq. (25) and that for $z = 6$ from Eq. (25). One can alternatively compute the values from Eq. (24). It may be remarked that the value of K_c of the present paper for $z = 6$ as presented in Table I is higher than the value of Tamura and Kaneyoshi. This difference is evidently due to the fact that this value has been computed from the joint identity. We have also performed calculation

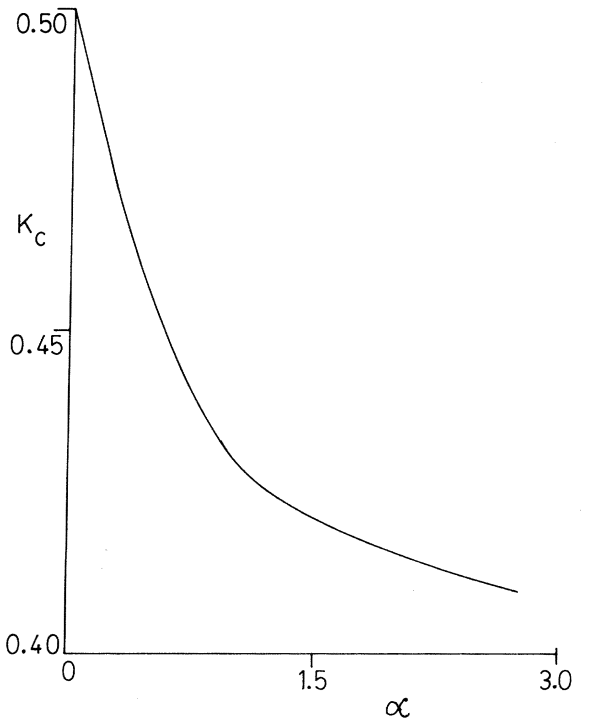

FIG. 1. The nature of variation of K_c with respect to α for a linear Ising chain.

TABLE I. The values of K_c^{-1} for $\alpha = 0$ calculated from the present paper and compared with those of the other theories.

z	2	3	6
MFA	2.667	4.0	8.0
Brown-Luttinger (Ref. 26)			5.4
Obokata-Oguchi (Ref. 23)		2.691	6.876
Tamura-Kaneyoshi (Ref. 24)			7.04
Present paper	No solution	2.3364	7.2464

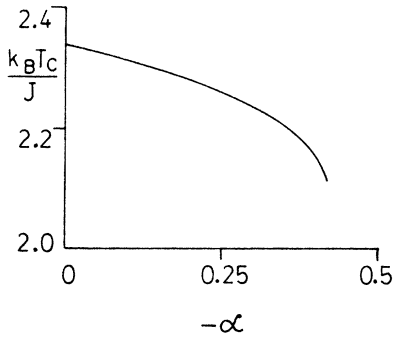

FIG. 2. The nature of variation of $k_B T_c/J$ with respect to $-\alpha$ for a honeycomb lattice.

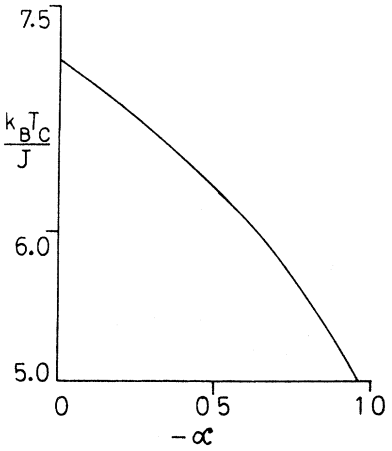

FIG. 3. The variation of $k_B T_c/J$ with $-\alpha$ for a simple cubic lattice.

of K_c^{-1} for $z=6$ from Eq. (22) and we have found that it is exactly identical with the value of Tamura and Kaneyoshi[24] as expected. Table I also shows the self-evident feature of this kind of model, that the phase transition is absent for a linear lattice.

Furthermore, the computations of Curie temperatures for different lattices with nonzero biquadratic parameter α have been carried out and the results are demonstrated in Figs. 1–3. It is seen that for a linear lattice T_c decreases with the increases of α and that a nonzero, real, positive T_c exists for both positive and negative values of α, although $\alpha=0$ does not favor any phase transition. In particular, we have found that for a phase transition the range of α should be

$$-\infty < \alpha < 0; \quad 0 < \alpha \leq \alpha_c \ .$$

α_c has been found to be approximately equal to 7.18. For $\alpha=\alpha_c$ we have found that K_c goes to infinity, i.e., $T_c=0$. In contrast to a linear lattice we have not found any solution for T_c for any positive α in the case of honeycomb and simple cubic lattices. However, solutions exist for negative α in these lattices. The nature of variation of T_c with $-\alpha$ is shown in Figs. 2 and 3 for $z=3$ and $z=6$, respectively. We remark that even such a qualitative nature of the variation of Curie temperature with the biquadratic parameter is completely different from that found in MFA. In this connection it is relevant to mention the work of Takahasi and Tanaka[27] which also shows no phase transition for $\alpha > 0$.

In conclusion, we would like to emphasize that although the HK formalism leads to better accuracy of the values of the Curie temperatures for all lattices it has the major disadvantage that the choice of the effective field even in its simplest form (Weiss field) as used in Eq. (21) leads to much computational labor. So, although the incorporation of the Lines correlated effective-field approximation is able to yield better values, the related equations become so complicated that the computational problem becomes really formidable.

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