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Abstract. An integral equation of the Curie temperature for the Blume–Emery–Griffiths model is derived. Numerical integration is carried out and the results for SC, BCC and FCC lattices are presented.

The spin-1 Ising model with both bilinear and biquadratic interactions along with the single-ion anisotropy is expressed by

$$H = -\sum_i h_i S_i^z - D\sum_i (S_i^z)^2 - \tfrac{1}{2}\sum_{ij} J_{ij} S_i^z S_j^z - \tfrac{1}{2}\sum_{ij} J'_{ij}(S_i^z)^2 (S_j^z)^2 \tag{1}$$

where h_i is the external field acting on site i, D is the strength of the single-ion anisotropy, and J_{ij} and J'_{ij} represent the bilinear and biquadratic exchange integrals respectively. The above equation is usually referred to as the Blume–Emery–Griffiths (BEG) (1971) model and has been studied by several workers during the past few years (Chakraborty 1984, 1988, Chakraborty and Morita 1984, 1985, Chakraborty and Tucker 1986, Tucker 1987, 1988, 1989, Siqueira and Fittipaldi 1985, Fittipaldi and Siqueira 1986, Kaneyoshi 1987, Kaneyoshi and Sarmento 1988, Ziegler 1986, Wang *et al* 1987, Wang and Wentworth 1987, De Alcantara Bonfim and Sa' Barreto 1985, 1986). The purpose of the present paper is to employ the cumulant expansion technique (Horwitz and Callen 1961, Frank and Mitran 1977, 1978, Frank *et al* 1982). Such formalism for the BEG model has not been carried out in the past.

Kubo's (1957) correlation identities are expressed as

$$\langle [A(t), B] \rangle = \int_{-\infty}^{\infty} I_{AB}(\omega)[\exp(\beta\omega) - 1]\exp(-i\omega t) \tag{2a}$$

$$\langle [A(t), B] \rangle_+ = \int_{-\infty}^{\infty} I_{AB}(\omega)[\exp(\beta\omega) + 1]\exp(-i\omega t) \tag{2b}$$

where [ ] is the commutator and [ ]$_+$ is the anticommutator, and A and B are any two quantum mechanical operators; $A(t) = \exp(iHt)A\exp(-iHt)$ is the operator A in the Heisenberg representation. The angular brackets denote thermal averages. I_{AB} is the spectral density of the correlation function $\langle B(O)A(t) \rangle$. The symbol β stands for $1/k_{\rm B}T$, $k_{\rm B}$ being the Boltzmann constant.

Using the relations

$$S_i^+(t) = \exp\left[-it(h_i + O_i)\right](S_i^+ - \sigma_i^+) + \exp\left[-it(h_i + O_i + D + Q_i)\right]\sigma_i^+ \quad (3a)$$

$$\sigma_i^+(t) = \exp\left[-it(h_i + O_i)\right]\exp\left[-it(D + Q_i)\right](2S_i^z - 1) - 2(S_i^z - 1)\sigma_i^+ \quad (3b)$$

where

$$\sigma_i^\pm = S_i^z S_i^\pm + S_i^\pm S_i^z \tag{4a}$$

$$O_i = \sum_j J_{ij} S_j^z \tag{4b}$$

$$Q_i = \sum_j J'_{ij}\left(S_j^z\right)^2 \tag{4c}$$

and, considering $A = S_i^+$, $B = S_i^-$ and $A = S_i^+$, $B = \sigma_i^-$ we arrive at the following equation for the order parameters $\langle S_i^z \rangle$ and $\lambda = \langle 3(S_i^z)^2 - 2\rangle$:

$$\langle S_i^z \rangle = 4I_0 / \left[(1-I)(3+I) + I_0^2\right] \tag{5}$$

$$\lambda = \left[4I(1-I) + 4I_0^2\right] / \left[(1-I)(3+I) + I_0^2\right]. \tag{6}$$

Other pairs $A = \sigma_i^+$, $B = \sigma_i^-$ and $A = \sigma_i^+$, $B = S_i^-$ also lead to the same expressions as above. I_0 and I are given by

$$I_0 = -\frac{i}{\beta} \int_{-\infty}^{\infty} dt \ \mathrm{cosech}\left(\frac{\pi t}{\beta}\right) \langle \exp\left[it(h_i + O_i)\right]\rangle \tag{7}$$

$$I = -\frac{i}{\beta} \int_{-\infty}^{\infty} dt \ \mathrm{cosech}\left(\frac{\pi t}{\beta}\right) \langle \exp\left[it(h_i + O_i)\right]\exp\left[it(D + Q_i)\right] - 1\rangle. \tag{8}$$

The averages are expressed in terms of semi-invariants or cumulants (Horwitz and Callen 1961):

$$\langle \exp ax \rangle = \exp\left(\sum_{n=1}^{n=\infty} \frac{a^n}{n!} M_n(x)\right) \tag{9}$$

where $M_n(x)$ denote the semi-invariants. For two variables x and y, one has the relation $M_n(x+y) = M_n(x) + M_n(y)$. Let $x = O_i$, $y = Q_i$. Following Frank and Mitran (1977) we obtain after necessary simplification the following integral equation for the Curie temperature T_C:

$$\frac{k_B T_C}{ZJ} = \frac{8}{A} \int_0^\infty dz \ \mathrm{cosech}(\pi z)\left(a_1 z + a_2 z^3 + a_3 z^5\right)\exp\left(b_1 z^2 + b_2 z^4 + b_3 z^6\right) \tag{10}$$

where Z is the number of nearest neighbours, J is the exchange constant and

$$a_1 = 1 \qquad a_2 = \tfrac{1}{3}bK_C^2 \qquad a_3 = \tfrac{1}{20}b^2 K_C^4$$

$$b_1 = -\tfrac{1}{2}bK_C^2 \qquad b_2 = -\tfrac{1}{12}b^2 K_C^4 \qquad b_3 = -\tfrac{1}{120}b^4 K_C^6 \tag{11}$$

$$A = 8/(1-I^C)(3+I^C)$$

where I^C is the value of the integral I at T_C, $K_C = ZJ/k_B T_C$ and T_C is the transition temperature. b is given by

$$b = \tfrac{1}{3}(2 + \lambda_C)\{[F(1) - 1]/F(1)\}. \tag{12}$$

Approximations used in deriving equation (10) are

$$
\begin{aligned}
M_2^C(x) &= (\lambda_C + 2)\{[F(1) - 1]/F(1)\} J^2 Z^2/3 \\
\langle x^{2n} \rangle &= b^n J^{2n} Z^{2n} \qquad \text{for } n > 1 \\
\langle y^n \rangle &= \alpha^n b^n J^n Z^n
\end{aligned} \tag{13}
$$

where $\alpha = J'/J$, J' and J being the nearest-neighbour bilinear and biquadratic exchange constants. We have also used the symbol $\alpha' = D/J$ which has been, however, taken to be zero in the results of computation. The quantity λ_C denotes the value of λ at T_C.

Table 1. Values of $k_B T_C/J$ for various values of α and for SC, BCC and FCC lattices obtained from the present calculations.

α	$k_B T_C/J$		
	SC	BCC	FCC
1.0	3.877	5.086	7.569
0.8	3.743	4.929	7.350
0.6	3.618	4.785	7.150
0.4	3.502	4.655	6.972
0.2	3.398	4.540	6.815
0	3.305	4.438	6.675
−0.2	3.223	4.348	6.555
−0.4	3.151	4.270	6.449
−0.6	3.089	4.202	6.357
−0.8	3.035	4.142	6.276
−1.0	3.000	4.090	6.205

Equation (10) is to be computed in conjunction with equations (6) and (8) in the limit T approaching T_C. Considering the leading terms in equations (6) and (8) and using them in equation (10), numerical integration has been carried by the Gaussian quadrature formula. The computation was done for SC, BCC and FCC lattices up to the sixth-order cumulants. The values of the Watson sum $F(1)$ have been taken as 1.51638, 1.39320 and 1.34466 for SC, BCC and FCC lattices, respectively. For simplicity we have concentrated only on the nature of variation in T_C with α. The results are summarized in table 1. From the table we note that as α decreases, the Curie temperature decreases and, as the number of nearest neighbours increases, T_C increases. We note that the values of the Curie temperature obtained in the present calculations are lower than those obtained by the cluster variation method in the pair approximation (Tucker 1988) and the Bethe lattice solution (Chakraborty and Tucker 1986). The absence of a re-entrant phenomenon in the present calculations is to be noted and needs further investigations considering higher-order cumulants.

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