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A Spin-1 Ising Model in the Presence of the Magnetic Fields Due to the Dipole and Quadrupole Moments

Mustafa KESKİN
Department of Physics, Gaziosmanpaşa University,
60110 Tokat-TURKEY
Hüseyin ARSLAN
Department of Physics, Kahramanmaraş
Sütçü İmam University,
46100 Kahramanmaraş-TURKEY

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Abstract

The spin-1 Ising model with bilinear (J) and biquadratic (K) exchange interactions is studied for magnetic fields due to the dipole and quadrupole moments, H_S and H_Q respectively, by using the lowest approximation of the cluster variation method. Stable, metastable and unstable solutions of order parameters are found and the behaviours of the thermal variations of these solutions as a function of the reduced temperature are investigated. These solutions and their classifications are checked by displaying the contour mapping of the free energy surfaces in the two dimensional phase space.

1. Introduction

The spin-1 Ising model Hamiltonian with nearest-neighbour exchange interactions, both bilinear and biquadratic, and with a crystal-field interaction is known as the Blume-Emery-Griffiths (BEG) model. It was introduced by Blume, Emery and Griffiths [1] to study phase separation and superfluid ordering in $He^3 - He^4$ mixtures. With vanishing biquadratic exchange interactions the model is called the Blume-Capel model [2]. The model was subsequently reinterpreted to describe phase transitions in simple and multicomponent fluids [3]. It has become very attractive because of its simplicity and rich fixed-point structure. The model has been studied by the mean-field approximation [1-3], high-and low-temperature series expansions [4], the constant coupling approximation [5],

Monte Carlo simulations [6], renormalization group methods [7], the effective-field theory [8] and Monte Carlo renormalization group techniques [9]. In this contex the exact solution of the model on the Bethe lattice [10], the honeycomb lattice [11] and the square lattice [12] could be mentioned. Due to their intrinsic complexity, spin-1 quantum models have also been investigated extensively [13].

Nonequilibrium properties of a spin-1 Ising system has been also studied by the path probability method [14], and multidimensional kinetic model based on the Glauber model [15], and the real-space renormalization group technique [16].

Recently stable, metastable and unstable solutions of a spin-1 Ising model with arbitrary J and K pair interactions has been studied for zero magnetic field [17]as well as the external magnetic field is present [18].

The purpose of the present paper is to study the spin-1 Ising model Hamiltonian with arbitrary bilinear and biquadratic exchange interactions for the magnetic fields due to the dipole and quadrupole moments, H_S and H_Q respectively. Especially, find the stable, metastable and unstable solutions of order parameters and investigate the behaviours of the thermal variations of these solutions as a function of the reduced temperature.

Our plan of exposition is as follows: In section 2, the model description is given. In section 3, the set of self-consistent equations is obtained in order to analyze the equilibrium properties of the system. Finally, the discussion of the results is presented in the last section.

2. Description of the spin-1 Ising model

The spin-1 Ising system is a three-state and two-order parameters system. The average value of each of the spin states will be indicated by X_1, X_2 and X_3, which are also called the state or point variables. X_1 is the average fraction of spins with value $+1$, X_2 is the average fraction of spins that have the value 0, and X_3 is the average fraction of spins that have the value -1. These variables obey the following normalization relation:

$$\sum_{i=1}^{3} X_i = 1. \tag{1}$$

Two long-range order parameters are introduced as follows: (1) The average magnetization $< S >$, which is the excess of one orientation over the other orientation, also called dipole moment, and (2) the quadrupole moment Q, which is a linear function of the average of squared magnetization $< S^2 >$, written as

$$Q = 3 < S^2 > -2. \tag{2}$$

The order parameters can be expressed in terms of the internal variables and are given by

$$S \equiv < S > = X_1 - X_3,$$
$$Q \equiv < Q > = X_1 - 2X_2 + X_3. \tag{3}$$

Using Eqs. (1) and (3), the internal variables can be expressed as linear combinations of the order parameters

$$\begin{aligned} X_1 &= \frac{1}{3} + \frac{1}{2}S + \frac{1}{6}Q \\ X_2 &= \frac{1}{3}(1 - Q) \\ X_3 &= \frac{1}{3} - \frac{1}{2}S + \frac{1}{6}Q \end{aligned} \tag{4}$$

The Hamiltonian of the spin-1 Ising model with bilinear and biquadratic exchange interactions for magnetic fields due to the dipole and quadrupole moments is

$$\beta\mathcal{H} = -\frac{1}{2}\sum_{<ij>}(JSiSj + KQiQj) - \sum_i (H_S Si + H_Q Q_i), \tag{5}$$

where J is the exchange coupling and K is the quadrupole coupling. We have introduced coupling parameters J and K that depend on the temperature $J => J/kT$ and $K => K/kT$, where T is the absolute temperature and k is the Boltzmann factor and $\beta = 1/kT$. H_S is the magnetic field which corresponds to S and H_Q is the field corresponding to Q.

Besides the spin interpretation, one can also use a description in terms of the lattice gas, introducing both vacant and occupied sites. Particles in the occupied site can have two internal states, say orientations corresponding to spin values of plus and minus one, and the spin value zero corresponds to vacant sites. Furthermore, K is related to the inteparticle interaction which is independent of the relative orientation and J is the orientation-dependent part of the coupling.

3. Solutions for the system at equilibrium

The equilibrium properties of the system are determined by means of the lowest approximation of the cluster variation method [19]. The method consists of the following three steps:

(1) consider a collection of weakly interacting systems and define the internal variables;

(2) obtain the weight factor W in terms of the internal variables;

(3) find the free energy expression and minimize it. The internal variables X_1, X_2 and X_3 have been defined in section 2. The weight factor W can be expressed in terms of the internal variables as

$$W = \frac{N!}{\prod_{i=1}^{3}(X_i N)!}, \tag{6}$$

where N is the number of lattice points. A simple expression for the internal energy of such a system is found by working out Eq. (5) in the lowest approximation of the cluster variation method. This leads to:

$$\frac{\beta E}{N} = -\frac{1}{2}JS^2 - \frac{1}{2}KQ^2 - H_S S - H_Q Q \tag{7a}$$

Substituting Eq. (4) into Eq. (7a), the internal energy can be written as

$$\begin{aligned} \frac{\beta E}{N} &= -\frac{1}{2}J(X_1 - X_3)^2 - \frac{1}{2}K(X_1 - 2X_2 + X_3)^2 \\ &- H_S(X_1 - X_3) - H_Q(X_1 - 2X_2 + X_3) \end{aligned} \tag{7b}$$

The entropy S and the free energy F are given by

$$S = k \ln W \quad \text{and} \quad F = E - TS. \tag{8}$$

Using Eqs. (5)-(8) and making use of the Stirling approximation, the free energy F can now be written as

$$\begin{aligned} \Phi &= -\frac{\beta F}{N} = \frac{1}{2}J(X_1 - X_3)^2 \\ &+ \frac{1}{2}K(X_1 - 2X_2 + X_3)^2 + H_S(X_1 - X_3) + H_Q(X_1 - 2X_2 + X_3) \\ &- \sum_{i=1}^{3} X_i(\ln X_i - 1) + \beta\lambda(1 - \sum_{i=1}^{3} X_i) \end{aligned} \tag{9}$$

where λ is introduced to maintain the normalization condition. The first four terms of Eq. (9) are the internal energy of system and the fifth term gives the entropy of the system in this approximation.

The minimization of Eq. (9) with respect to X_i gives

$$\frac{\partial \Phi}{\partial X_i} = 0 \qquad (i = 1, 2, 3). \tag{10}$$

Using Eqs. (1), (9) and (10), the internal variables are found to be

$$X_i = \frac{e_i}{Z}, \tag{11}$$

where

$$e_i = \exp(-\frac{\beta}{N}\frac{\partial E}{\partial X_i}) \quad \text{and} \quad Z = \sum_{i=1}^{3} e_i \ \ (i = 1, 2, 3).$$

Z represents the partition function, e_1, e_2 and e_3 are calculated using Eq. (7) as follows:

$$\begin{aligned} e_1 &= \exp(JS + KQ + H_S + H_Q) \\ e_2 &= \exp[-2(KQ + H_Q)] \\ e_3 &= \exp(-JS + KQ - H_S + H_Q) \end{aligned} \tag{12}$$

One can easily find the following set of self-consistent equations by using Eqs. (3), (11) and (12):

$$\begin{aligned} S &= \frac{2Sinh(\alpha KS + H_S)}{\exp[-3(KQ + H_Q)] + 2Cosh(\alpha KS + H_S)}, \\ Q &= \frac{Cosh(\alpha KS + H_S) - \exp[-3(KQ + H_Q)]}{Cosh(\alpha KS + H_S) + 1/2\exp[-3(KQ + H_Q)]} \end{aligned} \tag{13}$$

where $\alpha = J/K$ is called the ratio of the coupling constants or the relative energy barrier. These two nonlinear algebraic equations are solved by using the Newton-Raphson method. Thermal variations of the order parameters S and Q for various values as α, H_S and H_Q are plotted in Figures 1-2. Besides the stable solutions, the metastable and unstable solutions, which are very important for many experimental and theoretical works, such as metallic glasses, binary alloys, superfluids, superconductors, gels, lasers, magnetic systems, astrophysics, glasses and crystalline ceramics, etc. [20], are also found. In these figures, subscript 1 indicates the stable solutions (drawn lines), 2 the metastable solutions (dashed lines) and 3 the unstable solutions (dotted lines). It can be seen from the figures that below a cretain reduced temperature two more solutions, namely metastable and unstable solutions of S and Q exist. This temperature is called the quasicritical temperature, Tqc. The discussion of these solutions will be given in the last section.

4. Results and Discussions

Thermal variations of stable, metastable and unstable solutions of the order parameters S and Q as a function of reduced temperature for various value of α, H_S and H_Q are shown in Figures 1-2.

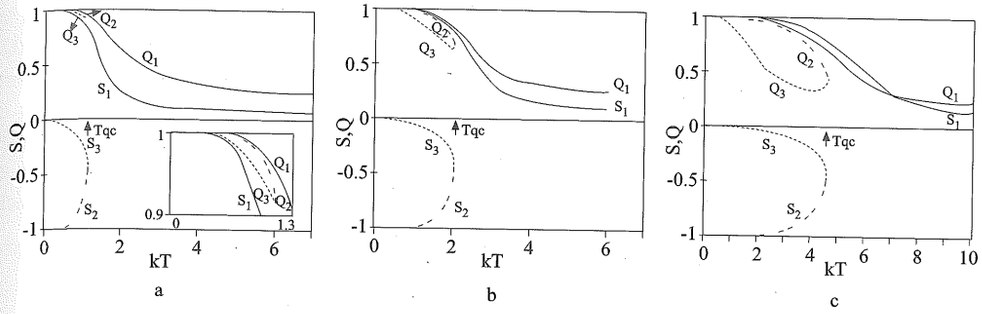

Figure 1. Thermal variations of order parameters S and Q as a function of the reduced temperature. Subscript 1 indicates the stable solutions (drawn lines), 2 the metastable solutions (dashed lines) and 3 the unstable solutions (dotted lines). Tqc is the quasicritical temperature. a) $\alpha = 1.5$, $H_s = 0.1$, $H_Q = 0.1$; b) $\alpha = 3.0$, $H_S = 0.1$, $H_Q = 0.1$; c) $\alpha = 7.5$, $H_S = 0.1$, $H_Q = 0.1$;

From Figure 1, one can see that for small values of α, keeping H_S and H_Q constants, the stable solutions of S and Q become zero more rapidly above the quasicritical temperature, Tqc, and the metastable and unstable solutions occur at the low reduced temperatures. Therefore, if one wants to obtain metastable and unstable solutions at high temperatures, he has to take big values of α. For big values of H_S and small values of H_Q, the Tqc occurs at low temperatures, that means one cannot obtain metastable and unstable solutions at the high temperatures, seen in Figure 2a.

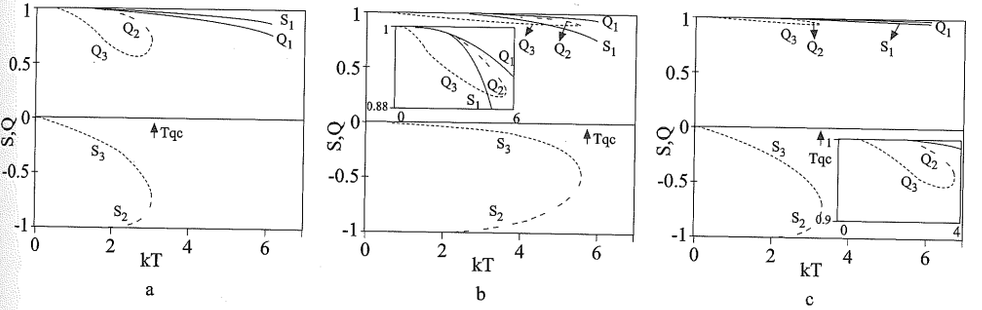

Figure 2. Same as Figure 1, but a) $\alpha = 7.5$, $H_S = 0.7$, $H_Q = 0.1$; b) $\alpha = 7.5$, $H_S = 0.1$, $H_Q = 0.7$; c) $\alpha = 7.5$, $H_S = 0.7$, $H_Q = 0.7$.

On the other hand, if values of H_S and H_Q are vice versa, Tqc occurs at high temperatures, shown in Figure 2b. Moreover, Figure 1a and Figure 2c illustrate that the metastable and unstable solution can be found at the high reduced temperature for small values of $H_S = H_Q$ than big values of $H_S = H_Q$.

Finally, in order to see that these three solutions and their classifications are correct, the free energy surfaces are displayed by means of the contour mapping in the

two dimensional phase space of S and Q. Figure 3 illustrates the free energy surface in the form of the contour mapping for $\alpha = 7.5, H_S = H_Q = 0.1, kT = 3.5$ and $N = 1000$. In the contour mapping, the open circle corresponds to the stable which is the lowest values of free energy, the closed square corresponds to the metastable solutions which is the second lowest value of free energy and the closed circle is the unstable solution which is a higher value of free energy. If one compares Figure 1c with Figure 3 at kT = 3.5, it is easily seen that stable, metastable and unstable solutions coincide exactly with each other in both methods of the calculation.

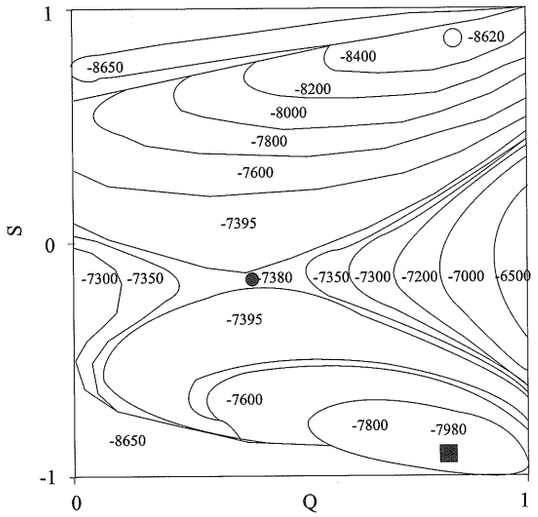

Figure 3. Contour mapping of the free energy surfaces for $\alpha = 7.5, H_S = H_Q = 0.1, kT = 3.5$ and $N = 1000$. The open circle corresponds to the stable solution, the closed square to the metastable solution, and the closed circle is the unstable solution

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