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Current Perspectives

Comparison of the ferromagnetic Blume–Emery–Griffiths model and the AF spin-1 longitudinal Ising model at low temperature

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ABSTRACT

We derive the exact Helmholtz free energy (HFE) of the standard and staggered one-dimensional Blume–Emery–Griffiths (BEG) model in the presence of an external longitudinal magnetic field. We discuss in detail the thermodynamic behavior of the ferromagnetic version of the model, which exhibits magnetic field-dependent plateaux in the *z*-component of its magnetization at low temperatures. We also study the behavior of its specific heat and entropy, both per site, at finite temperature. The degeneracy of the ground state, at $T=0$, along the lines that separate distinct phases in the phase diagram of the ferromagnetic BEG model is calculated, extending the study of the phase diagram of the spin-1 antiferromagnetic (AF) Ising model in S.M. de Souza and M.T. Thomaz, J. Magn. and Magn. Mater. 354 (2014) 205 [5]. We explore the implications of the equality of phase diagrams, at $T=0$, of the ferromagnetic BEG model with $\frac{K}{|J|} = -2$ and of the spin-1 AF Ising model for $\frac{D}{|J|} > \frac{1}{2}$.

1. Introduction

For a long time simple 1-D spin models have been used as toy models for a better understanding of real systems with coupled spins. Experimental verification of the results derived from those toy spin models is difficult, given the complexity of real spin systems for any spatial dimension. The development of optical devices permitted the simulation of a few 1-D spin models in arrays of cold atoms. In 2011 Simon et al. [1] simulated the 1-D spin-1/2 Ising model in the presence of a magnetic field with longitudinal and transverse components at low temperature. Such possibility encourage us to explore the thermodynamic characteristics of 1-D models.

Recently one of the authors applied the transfer matrix method [2–4] to the calculation of the exact thermodynamics of the 1-D spin-1 Ising model, with single-ion anisotropy term, in the presence of an external longitudinal magnetic field [5]. The present work extends that discussion to the classical 1-D Blume–Emery–Griffiths (BEG) model [6] with external longitudinal magnetic field. This model is classical and its exact thermodynamics can also be derived by the transfer matrix method. The presence of an extra term with respect to the 1-D Ising model with single-ion anisotropy term can modify the behavior of the quantum chain, mainly its phase diagram at $T=0$. In the present paper we study the thermodynamics of the one-dimensional BEG model in the presence of an external longitudinal magnetic field. The phase diagram of the model is discussed in detail for the ferromagnetic case, and for two different regions of the parameter $\frac{K}{|J|}$, and complemented by the discussion on the phase diagram of the spin-1 AF Ising model [5].

In Section 2 we present the Hamiltonian of the standard BEG model in the presence of an external longitudinal magnetic field. We show the relation between the Hamiltonians of the standard and staggered versions of this model, to be used in relating their thermodynamics. In Section 3 we discuss the phase diagram, at $T=0$, of the ferromagnetic BEG model. Its thermodynamics is presented in Section 3.1 through the behavior of three thermodynamic functions per site: the *z*-component of the magnetization, the specific heat and the entropy. The entropy per site along each line that separates distinct phases in the diagram of the ferromagnetic BEG model is calculated at $T=0$. In Section 4 we compare the three previous thermodynamic functions of the ferromagnetic BEG model with $\frac{K}{|J|} = -2$ and the spin-1 AF Ising model at very low temperature. We also extend the discussion on the phase diagram of the spin-1 AF model in Ref. [5] in order to include the degeneracy of the ground state of the model at $T=0$. Our conclusions are presented in Section 5. In Appendix A we present the

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main steps to calculate the exact Helmholtz free energy (HFE) of the standard and staggered one-dimensional BEG model for arbitrary values of the parameters. The states and energies of the dimers present in the spin configurations of the chain are shown in Appendix B. In Appendix C we have the ground states of the BEG model in the presence of an external longitudinal magnetic field and their respective energies. Finally in Appendix D we show how to calculate the degeneracy of the ground state along the lines that separate the different phases along the diagrams of the chain models at $T=0$.

2. The Hamiltonian and HFE of the 1-D Blume–Emery–Griffiths model with a longitudinal magnetic field

Eq. (5) of Ref. [5],

$$\mathbf{H}_I^{S=1}(J, h, D) = \sum_{i=1}^{N}\left[JS_i^z S_{i+1}^z - hS_i^z - hS_{i+1}^z + D(S_i^z)^2 + D(S_{i+1}^z)^2\right], \tag{1}$$

is the Hamiltonian of the one-dimensional classical spin-1 Ising model with the single-ion anisotropy term with the crystal field D, the Blume–Capel model [7,8], in the presence of an external longitudinal (z-axis) magnetic field h, symmetrized in the nearest neighbours. Here, S_i^z is the z-component of the spin-1 operator in the i-th site ($|\vec{S}|^2 = 2$), and J is the exchange strength. For $J > 0$ we have the anti-ferromagnetic (AF) version of the model, whereas for $J < 0$ ferromagnetic version is obtained. We assume that $h \geq 0$, that D may have any real value, and that the chain has N sites and it is periodic, i.e. $S_{N+1}^z = S_1^z$. In this paper we use natural units $e = m = \hbar = 1$.

Adding the term $-K(S_i^z)^2(S_{i+1}^z)^2$ to Hamiltonian (1), with $K \in \mathbb{R}$, yields the Hamiltonian of the Blume–Emery–Griffiths (BEG) model [6,9]

$$\mathbf{H}_{BEG}(J, h, D, K) = \sum_{i=1}^{N} [JS_i^z S_{i+1}^z - hS_i^z - hS_{i+1}^z + D(S_i^z)^2 + D(S_{i+1}^z)^2 - K(S_i^z)^2(S_{i+1}^z)^2]. \tag{2}$$

This Hamiltonian also satisfies the periodic condition. (The Hamiltonian (1) with $L=0$ in Ref. [6] describes the BEG model in a non-symmetrized form.)

Ref. [5] discusses at length which quantum state(s) is (are) favored by each term on the r.h.s. of Hamiltonian (1), regarding the minimization of energy; we will not repeat this discussion here. Let s_i^z be the eigenvalue of the operator S_i^z. In (2), the term in K will, for $K > 0$, favor the dimer states (i.e., relative to two neighboring spins) in which $s_i^z = \pm 1$, independently of their relative orientation (they may be either parallel or anti-parallel). On the other hand, for $K < 0$, the favored dimer states will be those with at least one null eigenvalue, i.e., $s_i^z = 0$. Section 3 will describe how the term in K changes the $T=0$ phase diagrams of the classical ferromagnetic spin-1 Ising models presented in Ref. [5].

The *staggered* BEG model in its symmetrized version reads

$$\mathbf{H}_{BEG}^{stag}(J_s, h_s, D_s, K_s) = \sum_{i=1}^{N}\left[J_s S_i^z S_{i+1}^z - (-1)^i h_s S_i^z - (-1)^{i+1} h_s S_{i+1}^z + D_s(S_i^z)^2 + D_s(S_{i+1}^z)^2 - K_s(S_i^z)^2(S_{i+1}^z)^2\right]. \tag{3}$$

This Hamiltonian will also be subject to the spatial periodic condition. We assume that the chain has an even number of sites, so $N = 2M$, in which $M \in \mathbb{N}$.

The mapping $S_i^z \to (-1)^i S_i^z$ in Hamiltonian (3) yields the relation between the standard and staggered BEG models

$$\mathbf{H}_{BEG}^{stag}(J_s, h_s, D_s, K_s) = \mathbf{H}_{BEG}(-J, h, D, K); \tag{4}$$

hence they have the same thermodynamics if $J_s = -J$, $h_s = h$, $D_s = D$ and $K_s = K$. The ferromagnetic staggered BEG model ($J_s < 0$) has the same thermodynamics as the AF standard BEG model ($J > 0$). The AF staggered BEG model ($J_s > 0$) has the same behavior as the ferromagnetic standard BEG model ($J < 0$) at any finite temperature.

From now on we will restrict our discussion to the thermodynamics of the standard Hamiltonian (2) of the BEG model. The thermodynamic behavior of the staggered BEG models at finite temperature can be obtained from the corresponding standard models by using (4).

In Appendix A we show the calculation of the exact expression of the Helmholtz free energy (HFE) of the ferromagnetic and AF BEG models in the presence of a longitudinal magnetic field by the transfer matrix method [2–4], valid at any finite temperature $T > 0$. In 1975 Krinsky and Furman [10] calculated this thermodynamic function for those BEG models. Our expression of the HFE for non-null external longitudinal magnetic field $h \neq 0$ written differently from that of Ref. [10]; ours has contributions only from real functions of the parameters of Hamiltonian (2) and of $\beta = \frac{1}{kT}$, in which k is Boltzmann's constant and T is the absolute temperature in kelvin. Although the results derived in that appendix are valid for both the ferromagnetic and the AF BEG models, in the following sections of this paper the discussion is restricted to the ferromagnetic case.

3. The phase diagram of the ferromagnetic BEG model at $T=0$

The Hamiltonian (2) can be written as the sum of Hamiltonians of dimers on neighboring sites i and $i+1$, $i \in \{1, 2, \ldots, N\}$. For the dimer composed of the $(i, i+1)$ sites, we have

$$\mathbf{H}_{i,i+1}^{(D)}(J, h, D, K) = JS_i^z S_{i+1}^z - hS_i^z - hS_{i+1}^z + D(S_i^z)^2 + D(S_{i+1}^z)^2 - K(S_i^z)^2(S_{i+1}^z)^2. \tag{5}$$

The ferromagnetic case corresponds to $J < 0$.

Let $|s_i^z\rangle_i$ and s_i^z be the eigenstate and eigenvalue, respectively, of the z-component of the spin operator at i-th site, S_i^z, so that $S_i^z|s_i^z\rangle_i = s_i^z|s_i^z\rangle_i$, with $s_i^z \in \{-1, 0, 1\}$. The energy $\varepsilon_{i,i+1}$ of the dimer $(i, i+1)$, described by the state $|D\rangle_{i,i+1} = |s_i^z\rangle_i \otimes |s_{i+1}^z\rangle_{i+1}$ is, in units of $|J|$,

$$\frac{\varepsilon_{i,i+1}}{|J|} = \frac{{}_{i,i+1}\langle D|\mathbf{H}_{i,i+1}^{(D)}|D\rangle_{i,i+1}}{|J|} = s_i^z s_{i+1}^z - \frac{h}{|J|}(s_i^z + s_{i+1}^z) + \frac{D}{|J|}[(s_i^z)^2 + (s_{i+1}^z)^2] - \frac{K}{|J|}(s_i^z)^2(s_{i+1}^z)^2, \tag{6}$$

with $s_i^z, s_{i+1}^z \in \{0, \pm 1\}$, and $i \in \{1, 2, \ldots, N\}$. All the parameters of the Hamiltonian (2) are scaled in units of $|J|$: $\frac{h}{|J|}$, $\frac{D}{|J|}$ and $\frac{K}{|J|}$; correspondingly, the inverse of the temperature scales as $|J|\beta$.

In Appendix B we present the nine possible dimer configurations of neighbouring sites in the chain and their respective energy per unit of $|J|$. The ground state of the ferromagnetic BEG model is composed of dimer states which minimize the energy at $T=0$.

The value of the parameter $\frac{K}{|J|}$ determines the general structure of the $T=0$ phase diagram of the ferromagnetic BEG model.

(i) *The case* $\frac{K}{|J|} < -1$: The $T=0$ phase diagram for this case is