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Comparison of the exact thermodynamics of the AF Blume–Emery–Grifiths and of the spin-1 ferromagnetic Ising models

E.V. Corrêa Silva [a], M.T. Thomaz [b,*]

[a] Faculdade de Tecnologia, Universidade do Estado do Rio de Janeiro, Rod. Presidente Dutra km 298 s/nº, Pólo Industrial, CEP 27537-000, Resende-RJ, Brazil
[b] Instituto de Física, Universidade Federal Fluminense, Av. Gal. Milton Tavares de Souza s/nº, CEP 24210-346, Niterói-RJ, Brazil

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ABSTRACT

We study in detail the thermodynamics of the anti-ferromagnetic Blume–Emery–Griffiths (AF BEG) model in the presence of a longitudinal magnetic field. Its thermodynamics is derived from the exact Helmholtz free energy (HFE) of the model, valid for $T > 0$. Numerical simulations of this model on a periodic space chain with 10 sites ($N=10$) yield the energy spectra of the model at $\frac{K}{J} = 2$ for $\frac{D}{J} = 1$ and $\frac{D}{J} = 2$, thus helping us compare, for a broad range of temperature, how some (per site) thermodynamic functions with the same value of $\frac{K}{J}$ but distinct values of $\frac{D}{J}$ behave, namely: the z-component of the magnetization, the specific heat and the entropy. These thermodynamic functions of the AF BEG model at $\frac{K}{|J|} = 2$ are compared to those of the spin-1 ferromagnetic Ising model with $\frac{D}{|J|} > 1.5$, for which the $T=0$ phase diagrams of both models are identical. This comparison is done in a large interval of temperature.

1. Introduction

Low-dimensional models are simplified models of real materials which, nevertheless, may show interesting features, e.g. the presence of plateaus in the z-component of the magnetization, as function of the external magnetic field, in spin chain models [1–4]. Those one-dimensional models are in general a mimic of the real materials, since they involve simplifications of the reality. The development of optical devices has allowed the realization of quantum simulators of magnetic theories [5–8], thus bringing the hope that some interesting theoretical features of one-dimensional spin chains may be experimentally detected. In particular, we have the classic spin models with Ising-type of interactions that can be exactly solved by the transfer matrix method [9–11] at any temperature. Their exact thermodynamics permit to derive their features for any desired temperature.

Recently we studied the exact thermodynamics of the ferromagnetic version of the Blume–Emery–Griffiths (BEG) model [12,13], in the presence of a longitudinal magnetic field [14]. Our intention in the present paper is to complement the study of this classic model considering now its anti-ferromagnetic (AF) version at finite temperature.

The exact thermodynamics of the classic BEG model was derived from its Helmholtz free energy (HFE) in Ref. [14], being valid for both the anti-ferromagnetic (AF) ($J > 0$) and ferromagnetic ($J < 0$) versions of the model at finite temperature with $T > 0$.

The AF version can be studied, for $T > 0$, through the dependence on the external longitudinal magnetic field h of the (per site) thermodynamic functions: the z-component of the magnetization, the specific heat and the entropy.

In Section 2 we present the Hamiltonians of the standard and staggered BEG models in the presence of a longitudinal magnetic field h. The staggered version of the AF BEG model has already been discussed in Ref. [14]. In Section 2.1 the phase diagram of the AF BEG model with a longitudinal magnetic field, at $T=0$, and for different intervals of the parameter K, is detailed. Although this model is classic, its phase diagrams are richer than the phase diagrams of the spin-1 AF Ising model ($K=0$) with single-ion anisotropy term and a longitudinal magnetic field. In Section 3 we discuss at distinct finite temperatures the dependence of the z-component of the magnetization and the entropy, both per site, on the value of the external magnetic field at $\frac{K}{J} > 1$ for $\frac{D}{J} = 1$ and $\frac{D}{J} = 2$. In order to explain the behavior of these thermodynamic functions about the values of $\frac{h}{J}$ for a which a phase transition from the ground state occurs, we present in Section 3.1 the numerical simulation of the spectrum of energy per units of J of the AF BEG model in a spatially periodic chain with 10 sites ($N=10$). In Section 4 we compare some thermodynamic functions of the AF BEG model with $\frac{K}{|J|} = 2$ to those of the spin-1 ferromagnetic Ising model

* Corresponding author.
E-mail address: mtt@if.uff.br (M.T. Thomaz).

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$\left(\frac{K}{|J|}=0\right)$, for the same value of $\frac{D}{|J|}$ in both models. In Section 5 we present our conclusions.

For the sake of readability, we include in Appendix A the exact expression of the HFE of the classic BEG model; in Appendix B, the states and energies of the possible dimers for the spin-1 model; in Appendix C, the vector state and respective energies of the ground states of the AF BEG model at $T=0$; and in Appendix D, the values of the degeneracy of the ground state along the transition lines and on the critical points of the phase diagrams of the AF BEG model at $T=0$, besides their respective entropy per site at this temperature.

2. The Hamiltonian of the standard and staggered $1-D$ AF Blume–Emery–Griffiths model in the presence of a longitudinal magnetic field

In order to calculate the HFE of the classical spin models through the transfer matrix method [9–11], we write their Hamiltonians in a symmetrized form to simplify the calculation. For the $1-D$ standard Blume–Emery–Griffiths (BEG) model [12,13], with an external magnetic field h, the symmetrized form reads [14]

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

in which 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. This model includes the single-ion anisotropy term with the crystal field D, the symmetrized external magnetic field h in the nearest neighbors and the term $-K(S_i^z)^2(S_{i+1}^z)^2$ added by Blume et al. [12,13]. The parameters h, D and $K\in\mathbb{R}$. N is the number of sites in the chain, assumed to satisfy the periodic spatial boundary condition, i.e. $S_{N+1}^z=S_1^z$. In the AF version of the BEG model described by the Hamiltonian (1) we have $J>0$. We use the natural units, $e=m=\hbar=1$, throughout this paper.

The symmetrized Hamiltonian of the $1-D$ staggered AF BEG model is [14]

$$\begin{aligned}\mathbf{H}_{BEG}^{stag}(J_s,h_s,D_s,K_s) &= \sum_{i=1}^{N}\left[J_sS_i^zS_{i+1}^z - (-1)^ih_sS_i^z - (-1)^{i+1}h_sS_{i+1}^z + D_s(S_i^z)^2\right. \\ &\quad \left. + D_s(S_{i+1}^z)^2 - K_s(S_i^z)^2(S_{i+1}^z)^2\right],\end{aligned} \tag{2}$$

with $J>0$. This Hamiltonian also satisfies periodic spatial boundary condition, i.e. $S_{N+1}^z=S_1^z$. This condition imposes that we assume that the chain has an even number of sites, so $N=2M$, in which $M\in\mathbb{N}$.

In Ref. [14] it is shown that the staggered AF BEG model is equivalent to the standard ferromagnetic BEG model at any finite temperature. Therefore the thermodynamics of the staggered AF BEG model is given by the results presented in Ref. [14]. From now on we restrict our discussion to the thermodynamics of the $1-D$ standard AF BEG model, given by Hamiltonian (1) with $J>0$. In the following we refer to this model simply as the AF BEG model.

The thermodynamics of the BEG model in the presence of a longitudinal magnetic field was discussed in Ref. [14], and the exact expression of its HFE was calculated therein, being valid for both the ferromagnetic ($J<0$) and the AF ($J>0$) models for $T>0$, in which T is the absolute temperature in kelvin. For completeness, Appendix A of this paper shows the exact HFE, $\mathcal{W}(J,h,D,K;\beta)$ associated to the Hamiltonian (1), for any value of J and for $T>0$. Here, $\beta=\frac{1}{kT}$, in which k is Boltzmann's constant and T is the absolute temperature in kelvin.

2.1. The $T=0$ phase diagrams of the AF BEG model in the presence of a longitudinal magnetic field

The thermodynamic behavior of any model at very low temperatures is ruled by its phase diagram at $T=0$. The energy of the ground state(s) of the quantum system is a function of the parameters of the model. From the Hamiltonian (1) we obtain that the energy of the chain associated to a given vector state can be written as the sum of the energies of N dimers, each one described by the Hamiltonian

$$\begin{aligned}\mathbf{H}_{i,i+1} \equiv J_sS_i^zS_{i+1}^z - h_sS_i^z - h_sS_{i+1}^z + D_s(S_i^z)^2 + D_s(S_{i+1}^z)^2 \\ - K_s(S_i^z)^2(S_{i+1}^z)^2.\end{aligned} \tag{3}$$

The nine possible spin-1 dimer configurations in the AF BEG model, and their respective energy in units of J, are presented in Appendix B. They are the same as the nine possible dimers configurations of the ferromagnetic model, although the energies of four of them are different for the ferromagnetic and AF models.

In Ref. [14] we discussed the spin configurations that minimize the contribution of each term in the Hamiltonian (1) to the partition function of the model for different intervals of the parameters J, h, D and K; we shall not repeat those arguments here.

Looking for the ground state (minimum energy) of the spin configurations in the chain whose dynamics is described by the Hamiltonian (1), we have obtained, with the help of a algebraic computation system, the phase diagrams of the AF BEG model in the presence of a longitudinal magnetic field at $T=0$. We separate these phase diagrams according to the different intervals of the parameter K in Hamiltonian, where $K\in(-\infty,+\infty)$.

In order to simplify the presentation of those phase diagrams in Fig. 1, we let $J=+1$, and have the remaining parameters in (1) written in units of J, i.e.: $\frac{h}{J}$, $\frac{D}{J}$ and $\frac{K}{J}$.

One is reminded that by setting $K=0$ in the Hamiltonian (1), the spin-1 AF Ising model with single-ion anisotropy term and with a longitudinal magnetic field is recovered. The thermodynamics of this model was studied in detail in Ref. [15], including its phase diagram at $T=0$. The presence of the term $-K(S_i^z)^2(S_{i+1}^z)^2$ in the Hamiltonian (1) enriches the phase diagrams of the AF BEG model, which are shown in Fig. 1 for $K\in\mathbb{R}$; we have $J=+1$ and all the other parameters are in units of J, i.e. $\frac{D}{J}$ and $\frac{h}{J}$.

Fig. 1 a shows the phase diagram for $\frac{K}{J}\geq 1$. The vector states associated to the ground state in the phases A, B, C, and G/G' are given by (C.1a), (C.1b), (C.1c), (C.1h) and (C.1i), respectively. The critical points are $Q_a=(\frac{D_1}{J},1)$ and $Q_a'=\left(\frac{D_1}{J},-1\right)$, in which $\frac{D_1}{J}=\frac{1}{2}+\frac{K}{2J}$. Phases A and B are separated by the half-line $\frac{h}{J}\Big|_{A=B}=\frac{1}{2}+\frac{D}{J}-\frac{K}{2J}$, whereas phases A and C are separated by the half-line $\frac{h}{J}\Big|_{A=C}=-\frac{1}{2}-\frac{D}{J}+\frac{K}{2J}$, for $\frac{D}{J}\geq\frac{D_1}{J}$ in both cases. Separating phases B and G/G', we have the horizontal half-line $\frac{h}{J}=+1$, and between phases C and G/G', the horizontal half-line $\frac{h}{J}=-1$; in both cases, $\frac{D}{J}<\frac{D_1}{J}$. The vertical line segment with $\frac{D}{J}=\frac{D_1}{J}$ and $-1<\frac{h}{J}<1$ separates the phases A and G/G'. This type of phase diagram does not occur for the spin-1 Ising model with a longitudinal magnetic field [15].

Fig. 1 b shows the phase diagram for $-1<\frac{K}{J}<1$. The spin-1 AF Ising model, with single-ion anisotropy term and longitudinal magnetic field corresponds to letting $\frac{K}{J}=0$ [15]. In this phase diagram, besides the point $\frac{D_1}{J}$ we also have the point $\frac{D_2}{J}=\frac{K}{J}$. The vector states associated to the phases A, B, C, E/E', F/F' and G/G' are given in Appendix C. There are four tricritical points at $T=0$: $Q_b=\left(\frac{D_1}{J},\frac{h_1}{J}\right)$, $Q_b'=\left(\frac{D_1}{J},-\frac{h_1}{J}\right)$, $\mathcal{P}=\left(\frac{D_2}{J},1\right)$ and $\mathcal{P}'=\left(\frac{D_2}{J},-1\right)$. We have $\frac{h_1}{J}=\frac{D_1}{J}$.