Physica A 387 (2008) 5117–5126

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Thermodynamics of the quantum and classical Ising models with skew magnetic field

E.V. Corrêa Silva [a], James E.F. Skea [b], Onofre Rojas [c], S.M. de Souza [c], M.T. Thomaz [d,*]

[a] *Universidade do Estado do Rio de Janeiro, Estrada Resende-Riachuelo, s/nº, Morada da Colina, CEP 27523-000, Resende-RJ, Brazil*

[b] *Grupo de Física Matemática e Computacional, Departamento de Física Teórica, Instituto de Física, Universidade do Estado do Rio de Janeiro, R. São Francisco Xavier 524, CEP- 20559-900, Rio de Janeiro-RJ, Brazil*

[c] *Departamento de Ciências Exatas, Universidade Federal de Lavras, Caixa Postal 3037, CEP 37200-000, Lavras-MG, Brazil*

[d] *Instituto de Física, Universidade Federal Fluminense, Av. Gal. Milton Tavares de Souza s/nº, CEP 24210-346, Niterói-RJ, Brazil*

ARTICLE INFO

Article history:
Received 19 February 2008
Received in revised form 13 May 2008
Available online 28 May 2008

PACS:
75.10.Jm
05.30.-d
05.50.+q

Keywords:
Quantized spin models
Classical spin models
Statistical mechanics
Ising model
High-temperature expansion

ABSTRACT

The thermodynamics of the unitary (normalized spin) quantum and classical Ising models with skew magnetic field, for $|J|\beta \lesssim 0.9$, is derived for the ferromagnetic and antiferromagnetic cases. The high-temperature expansion (β-expansion) of the Helmholtz free energy is calculated up to order β^7 for the quantum version (spin $S \geq 1/2$) and up to order β^{19} for the classical version. In contrast to the $S = 1/2$ case, the thermodynamics of the transverse Ising and that of the XY model for $S > 1/2$ are *not* equivalent. Moreover, the critical line of the $T = 0$ classical antiferromagnetic Ising model with skew magnetic field is absent from this classical model, at least in the temperature range of $|J|\beta \lesssim 0.9$.

1. Introduction

The one-dimensional Ising model is the simplest model with first-neighbor spin interactions. The exact thermodynamics of the $S = 1/2$ model with longitudinal magnetic field was derived in 1925 by Ising in his original paper [1]. The case of a transversal magnetic field was treated by Pfeuty [2] in 1970; in this case, many thermodynamical functions (e.g. the specific heat and magnetization) of the ferromagnetic and antiferromagnetic cases are identical. In 1978, Fogedby [3] discussed the behavior of the $S = 1/2$ ferromagnetic model with skew magnetic field (i.e., with both longitudinal and transversal components) at $T = 0$ K. The corresponding $S = 1/2$ antiferromagnetic case had its phase diagram presented by Ovchinnikov et al. [4] in 2003, who also showed that at $T = 0$ K a critical line exists for both the quantum model and its classical limit.

Only recently Rojas et al. [5] calculated the high-temperature expansion (β-expansion), up to order β^{40}, of the Helmholtz free energy (HFE) of the arbitrary spin-S Ising model, where $S = 1/2, 1, \ldots, \infty$ (classical limit), in the absence of external magnetic field. In Ref. [6] we calculated the β-expansion of the HFE for the antiferro and ferromagnetic $S = 1/2$ Ising model in a skew magnetic field, up to order β^7. We also showed the equivalence of the transversal Ising model and the XY model, both with $S = 1/2$.

* Corresponding author. Tel.: +55 21 2629 5807; fax: +55 21 2629 5887.
E-mail address: mtt@if.uff.br (M.T. Thomaz).

0378-4371/$ – see front matter
doi:10.1016/j.physa.2008.05.033

The current techniques of synthetization of magnetic materials allow the construction of "single chain magnets" [7–10], with one-dimensional behavior. Due to the high spin in each chain site, those materials show a classical behavior. Some of them can be well described, in some suitable interval of temperature, by the classical Ising model [10].

As to the β-expansion of the HFE for the quantum Ising model with skew magnetic field, a severe computational limitation in reaching high orders in β is imposed by the non-commutative terms of the hamiltonian. In the present work, we apply the method exposed in Ref. [11] to calculate the expansion of the HFE of the classical version of the model. The order in β we have reached for the classical version is more than twice as much as that of the quantum version.

The objective of this paper is threefold: (i) to calculate the β-expansion of the HFE of the quantum and classical one-dimensional Ising model in a skew constant magnetic field (with $|J|\beta \lesssim 0.9$) up to order β^7 and β^{19}, respectively, and determine the minimum value of the spin-S for which the quantum model can be well approximated by its classical limit; (ii) to check if the duality of the transversal Ising model and the XY model, valid for $S = 1/2$, still holds for higher values of spin; (iii) to verify if for $|J|\beta \lesssim 0.9$ the classical antiferromagnetic Ising model in a skew magnetic field has any trace of the critical line it exhibits at $T = 0$ K. The existence of analytical expansions makes it easier to fit experimental data and determine the value of J for a given magnetic material.

In Section 2 we present the hamiltonian of the Ising model with normalized but otherwise arbitrary spin and the main features of the β-expansion of its HFE. We also check if the spin-S transversal Ising model is equivalent to the spin-S XY model for $S > 1/2$. In Section 3 we compare several thermodynamical functions of the antiferromagnetic and ferromagnetic cases of the quantum and classical models, for $|J|\beta \lesssim 0.9$. In Section 4 the $T = 0$ K critical line of the classical antiferromagnetic Ising model in a skew magnetic field is shown to be absent in the high-temperature regime. Section 5 contains our conclusions. In Appendix A the reader finds the expression of the β-expansion of the HFE for the quantum Ising model with arbitrary normalized spin and skew magnetic field, up to order β^5. In Appendix B we rewrite the hamiltonian (1) in terms of the spherical angular coordinates that characterize the orientation of the classical normalized spin vector in space, with respect to the chain axis; we also present the β-expansion up to order β^8 of the HFE for the classical model.

2. The Ising model with arbitrary normalized spin and skew magnetic field

Upon a suitable choice of the coordinates axes, the hamiltonian of the one-dimensional quantum Ising model with arbitrary normalized spin-S and constant external magnetic field with arbitrary orientation is

$$\mathbf{H} = \sum_{i=1}^{N} \left(J s_i^z s_{i+1}^z - h_y s_i^y - h_z s_i^z \right), \tag{1}$$

where s_i^y and s_i^z stand for the y- and z-components, respectively, of the *arbitrary normalized spin operator*, defined as $\vec{s}_i \equiv \frac{\vec{S}_i}{\sqrt{S(S+1)}}$, $i \in \{1, 2 \dots N\}$. The components of $\vec{S}_i$ are the spin-S matrices, with norm $\|\vec{S}\|^2 = S(S+1)$, $S = 1/2, 1, 3/2, \dots, \infty$.

The chain has N spatial sites and satisfies periodic spatial boundary conditions. The coupling strength J between first-neighbor z-components of spin can either be positive (antiferromagnetic case) or negative (ferromagnetic case). Due to the rotational symmetry of the hamiltonian with respect to the z-axis (the easy-axis), the most general constant external magnetic field that we must consider is: $\mathbf{h} = h_y\hat{j} + h_z\hat{k}$, where h_y and h_z are constants.

By taking the limit $S \to \infty$ in Eq. (1) we recover the classical version of the model; its corresponding thermodynamics is finite. When Eq. (1) is written in terms of the non-normalized operators S_i^y and S_i^z, the coupling constant becomes $J' = J/S(S+1)$ and the components of the magnetic field are $h'_y = h_y/\sqrt{S(S+1)}$ and $h'_z = h_z/\sqrt{S(S+1)}$ [5,12].

In the present work, the method exposed in Ref. [11] is applied to the quantum hamiltonian (1) for arbitrary normalized spin-S in order to calculate the β-expansion of its HFE up to order β^7, in the thermodynamical limit ($N \to \infty$). One is reminded that $S(S+1)$, the squared norm of spin at each site, is a constant of motion of the system; it turns out that each coefficient in the β-expansion of the HFE is a polynomial of $(m-1)$th degree in $[S(S+1)]^{-1}$, i.e., of the form $\sum_{k=0}^{m-1} C_k\,[S(S+1)]^{-k}$, where the C_k's are functions of the parameters of the model. We have calculated the HFE for nine distinct values of spin, namely, $S = 1/2, 1, 3/2, \dots, 9/2$, so that fitting the coefficients of the series allowed us to determine the series for arbitrary values of spin. The whole expression of the HFE is too large; Appendix A shows this expansion up to order β^5 only. (The authors would be glad to send the complete expression to the interested reader, upon request.) By letting $h_y = 0$ in Eq. (A.1) we recover the expansion, up to order β^5, obtained from the XYZ model for $J_x = J_z = D = 0$ in Ref. [13].

The HFE of the classical model can be obtained from (A.1) by taking the limit $S \to \infty$. A different way to obtain the same result is to apply the method of Ref. [11] directly to the hamiltonian (B.2), where the components of the classical spins are given by Eqs. (B.1). All the terms in this classical hamiltonian are c-numbers, thus simplifying the computational task and allowing us to calculate the β-expansion of its HFE up to order β^{19}. This expression is also very lengthy and is shown in Appendix B up to order β^8 only. (For the complete expression, the interested reader is welcome to contact the authors.) Ref. [14] presents a survey of the method applied here.

The expansions (A.1) (for the quantum models) and (B.3) (for the classical model) are equally valid for the ferromagnetic ($J < 0$) and antiferromagnetic ($J > 0$) cases and have the following features:

1. they are even functions of h_y and h_z, reflecting the rotation symmetry of the system with respect to the easy-axis;