Hamiltonian of the spin-S Ising model with a single-ion anisotropy term in the presence of a longitudinal magnetic field

This text is part of section 3 of Ref. [1].

The Hamiltonian of the spin-S Ising model with a single-ion anisotropy term in the presence of a longitudinal magnetic field is[2]

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

where (S_i^z, S_i^y, S_i^z) are the components of the spin $\vec{S}$ operator with norm: $||\vec{S}||^2 = S(S+1)$, $S = \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots$, at the i-th site at the chain. J' is the exchange strength and it can have negative value (ferromagnetic model) or positive value (anti-ferromagnetic model). In Refs. [2] and [3] we studied the exact thermodynamics of this model for $S = \frac{1}{2}$ and 1, respectively.

The classical version of model (1) is obtained by taking the limit of $S \to \infty$. If this limit is done directly in Hamiltonian (1) all the classical thermodynamic functions diverge. In order to keep the classical functions finite, we study the normalized version of the Hamiltonian (1), that is,

$$\mathbf{H}_s = \sum_{i=1}^{N} \left[J s_i^z s_{i+1}^z - h s_i^z + D(s_i^z)^2 \right], \qquad s = \frac{1}{2}, 1, \frac{3}{3}, 2, \cdots, \tag{2}$$

with s_i^z being the z-component of the spin operator $\vec{s}$ that has norm 1. The $\vec{s}$ operator is defined as

$$\vec{s} \equiv \frac{\vec{S}}{\sqrt{S(S+1)}}, \qquad S = \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots \tag{3}$$

Making $S \to \infty$ in the Hamiltonian (2) we obtain its classical limit.

The Hamiltonians (1) and (2) are identical when

$$J = S(S+1)J', \quad h = \sqrt{S(S+1)}h' \quad \text{and} \quad D = S(S+1)D', \tag{4}$$

with $S = \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots$

Let $\mathcal{Z}'_S(J', h', D'; \beta)$ be the partition function derived from Hamiltonian (1),

$$\mathcal{Z}'_S(J', h', D'; \beta) = Tr\left[e^{-\beta \mathbf{H}'_S} \right]. \tag{5}$$

Its HFE, in the thermodynamic limit, is called $\mathcal{W}'_S$, where

$$\mathcal{W}'_S(J', h', D'; \beta) = -\lim_{N\to\infty} \frac{1}{N}\,\frac{1}{\beta}\;\; \ln\left[\mathcal{Z}'_S(J', h', D'; \beta)\right]. \qquad (6)$$

The analogous functions for the normalized Hamiltonian (2) are

$$\mathcal{Z}_s(J, h, D; \beta) = Tr\left[e^{-\beta \mathbf{H}_s}\right] \qquad (7a)$$

and

$$\mathcal{W}_s(J, h, D; \beta) = -\lim_{N\to\infty} \frac{1}{N}\,\frac{1}{\beta}\;\; \ln\left[\mathcal{Z}_s(J, h, D; \beta)\right]. \qquad (7b)$$

For arbitrary spin value S, the relation between the HFE's (6) and (7b) is

$$\mathcal{W}'_S(J', h', D'; \beta) = \mathcal{W}_s(S(S+1)J', \sqrt{S(S+1)}h', S(S+1)D'; \beta). \qquad (8)$$

We calculate the β-expansion of $\mathcal{W}_s(J, h, D; \beta)$, for arbitrary value S of the spin, up to order β^{17}. The relation (8) can be applied to obtain the β-expansion of $\mathcal{W}'_S(J', h', D'; \beta)$ from the expansion of $\mathcal{W}_s(J, h, D; \beta)$.

We should note that this β-expansion is valid for positive, null or negative values of J, and for arbitrary values of S, h and D. The HFE of the classical model of Hamiltonian (2) is calculated from the β-expansion of $\mathcal{W}_s(J, h, D; \beta)$ by taking the limit of $S \to \infty$.

In the link: `http://www.proac.uff.br/mtt/thermodynamics-low-dimensional-systems/Helmholtz-free-energies-list`, in this web page, we have the data files with the quantum (arbitrary spin-S) and the classical HFE's of the normalized Hamiltonian (2) up to order β^{17}.

References

[1] M.T. Thomaz and O. Rojas, "*The β-expansion of the quantum and classical Ising model with S_z^2 term*", submitted to publication.

[2] W.A. Moura-Melo *et al.*, Phys. A **3**22 (2003) 393.

[3] O. Rojas *et al.*, Braz. J. Phys. **3**1 (2001) 577.
We have a misprint in the expression of the HFE in this reference. In this reference, the constant Δ in eq. (25) should be replaced by $\frac{\Delta}{2}$.

[4] O. Rojas *et al.*, Eur. Phys. J. B **4**7 (2005) 165.