Hamiltonian of the quantum and classical XYZ model with a single ion-anisotropy term

This text is part of Ref.[1] and section 2 of Ref.[2].

The Hamiltonian of the spin-S XYZ quantum periodic chain with N sites reads

$$\begin{aligned} \mathbf{H} &= \sum_{i=1}^{N} \big[J'_x S_i^x S_{i+1}^x + J'_y S_i^y S_{i+1}^y + J'_z S_i^z S_{i+1}^z \\ &- h' S_i^z + D' (S_i^z)^2 \big], \end{aligned} \tag{1}$$

where S_i^α, $\alpha \in \{x, y, z\}$, are the spin matrices at the i-th site, the J'_α are the exchange interaction couplings between first neighbors, and h' is the external magnetic field along the z-axis. We also include the single ion-anisotropy D' parallel to the external magnetic field.

In order to render the thermodynamic functions to be finite, even in the classical limit ($S \to \infty$), we define a scaled spin operator $\mathbf{s}$ with unitary norm[3] as $\mathbf{s} \equiv \mathbf{S}/\sqrt{S(S+1)}$. In order to write explicitly the effect of the anisotropy in the x and y directions in relation to the XXZ model[3], we rewrite the hamiltonian (1) in terms of the spin operators s_i^z and $s_j^{\pm} \equiv \frac{1}{\sqrt{2}}(s_j^x \pm i s_j^y)$, with $j = 1, \cdots, N$,

$$\begin{aligned} \mathbf{H} &= \sum_{i=1}^{N} \{ J[s_i^- s_{i+1}^+ + s_i^+ s_{i+1}^- + \delta(s_i^+ s_{i+1}^+ \\ &+ s_i^- s_{i+1}^-) + \Delta s_i^z s_{i+1}^z] - h s_i^z + D (s_i^z)^2 \}. \end{aligned} \tag{2}$$

The relations among the constants in hamiltonians (1) and (2) are: $J \equiv (S/2)(S+1)(J'_x + J'_y)$, $\delta \equiv (J'_x - J'_y)/(J'_x + J'_y)$, $\Delta \equiv 2J'_z/(J'_x + J'_y)$, $h \equiv \sqrt{S(S+1)}h'$ and $D \equiv S(S+1)D'$.

The classical version of the hamiltonian of the anisotropic XYZ chain with unitary spin-S, as shown in Eq.(2) of Ref. [1], is

$$\begin{aligned} \mathbb{H} = \sum_{i=1}^{N} \mathbf{H}_{i,i+1} &= \sum_{i=1}^{N} \{ J_x s_i^x s_{i+1}^x + J_y s_i^y s_{i+1}^y + J_z s_i^z s_{i+1}^z \\ &\qquad - h s_i^z + D (s_i^z)^2 \}, \end{aligned} \tag{3}$$

where

$$\begin{aligned} s_i^x &= \sin(\theta_i)\,\cos(\phi_i), \;\; s_i^y = \sin(\theta_i)\,\sin(\phi_i), \\ s_i^z &= \cos(\theta_i); \end{aligned} \tag{4}$$

θ_i and ϕ_i are the polar and azimuthal angles, respectively, of the classical spin $\vec{s}_i$; N is the number of sites in the periodic chain; h is the magnitude of the external magnetic field along the z-axis and D is the single-ion anisotropy parameter. The constants J_x, J_y and J_z give the strength of first-neighbour interactions between the spins components.

References

[1] Onofre Rojas, S.M. de Souza, E.V. Corra Silva and M.T. Thomaz, "*High-temperature series expansion of the Helmholtz free energy of the quantum spin-XYZ chain*", Physical Review B vol. 72 (2005) 172414 (1-4). [http://dx.doi.org/10.1103/PhysRevB.72.172414]

[2] E.V. Corrêa Silva, Onofre Rojas, James E.F. Skea, S.M. de Souza and M.T. Thomaz, "*The high temperature expansion of the classical XYZ chain*", Physica A vol. 375 (2007) 185-198. [http://dx.doi.org/10.1016/j.physa.2006.09.015]

[3] O. Rojas, S. M. de Souza, E. V. Corrêa Silva and M. T. Thomaz, The European Physical Journal- Condensed Matter and Complex Systems B vol. 46 (2005) 385-398.