Thermodynamics of the one-dimensional $s=1$ XXZ Heisenberg model: analytical results

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We apply the results derived by Rojas et al. to derive the $\beta$-expansion of the Helmholtz free energy of the spin-1 XXZ Heisenberg model up to order $\beta^5$. The analytical expansion obtained is valid for all phases of this model. Our curves of the specific heat fit well Blöte's numerical results in the high temperature regime.

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The spin-1 XXZ Heisenberg model is non-integrable and therefore cannot be solved by the algebraic Bethe ansatz method. Since the 70’s its thermodynamics has been studied numerically. More recently, Yamamoto and Miyashita applied a Monte Carlo method to study the specific heat, static magnetic susceptibility and magnetization of rings and chains of different sizes as a function of temperature and extended those results to the thermodynamic limit. Bao et al. derived a set of self-consistent equations to approximately obtain the thermodynamics of this model for all range of temperature, and solved those equations numerically.

The cumulant series yields a $\beta$-expansion of the Helmholtz free energy for exact integrable as well as for non-integrable models. Recently Rojas et al. showed for any one-dimensional chain model with periodic boundary condition, invariance under spatial translation and interaction between nearest neighbours that, in the thermodynamic limit, the coefficient of the high temperature expansion of arbitrary order $\beta^n$ can be derived from an auxiliary function $\varphi$.

Our aim in this work is to apply the results of Ref. to derive an analytical $\beta$-expansion of the Helmholtz free energy per site of the anisotropic spin-1 XXZ Heisenberg model with single-ion anisotropy, up to order $\beta^5$.

The hamiltonian of the spin-1 XXZ Heisenberg model with anisotropy is

$$H = \sum_{i=1}^{N} \left( J \left( S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) + \Delta S_i^z S_{i+1}^z - h S_i^z + D (S_i^z)^2 \right),$$

where $N$ is the number of sites in the periodic chain, $\Delta$ the anisotropy constant, $h$ the external magnetic field in the $z$-axis and $D$ the single-ion anisotropy parameter. We have $S_i^z \equiv \frac{1}{\sqrt{2}} \left( S_i^x \pm i S_i^y \right)$. We do not fix the sign of any constant in eq.(1).

Applying the results of Ref. to the spin-1 XXZ Heisenberg model with single-ion anisotropy, we obtain its Helmholtz free energy $W(\beta)$ up to order $\beta^5$:

$$W(\beta) = - \frac{\ln(3)}{\beta} \frac{2}{3} D + \left( \frac{1}{9} D^2 - \frac{4}{9} J^2 - \frac{1}{3} h^2 - \frac{2}{9} \Delta^2 D(\varphi) \right) \beta + \left( \frac{1}{81} D^3 + \frac{4}{9} \Delta h^2 + \frac{4}{27} \Delta^2 D - \frac{4}{27} J^2 D + \frac{1}{9} h^2 D - \frac{1}{9} J^2 D^3 \right) \beta^2 + \left( \frac{1}{36} h^4 - \frac{1}{54} \Delta^4 + \frac{1}{234} D^4 + \frac{13}{81} J^2 \Delta^2 + \frac{1}{54} h^2 D^2 + \frac{7}{162} J^4 - \frac{8}{27} \Delta h^2 D + \frac{5}{72} J^2 h^2 \right) \beta^3 + \left( \frac{7}{243} J^2 D^2 + \frac{1}{18} J^4 \Delta + \frac{1}{972} D^5 \right) \beta^4 + \left( \frac{1}{27} D J^2 h^2 + \frac{1}{81} J^2 D^2 - \frac{1}{81} D \Delta^4 \right) \beta^5 + \left( \frac{11}{162} D J^2 \Delta^2 - \frac{4}{243} \Delta^2 D^3 + \frac{22}{81} h^2 \Delta^3 \right) \beta^6 + \left( \frac{10}{27} J^2 \Delta h^2 - \frac{1}{36} D h^4 + \frac{8}{27} \Delta^2 h^2 D \right) \beta^7 + \left( \frac{1}{162} D^3 h^2 + \frac{1}{36} J^2 \Delta^3 + \frac{13}{162} D J^4 + \frac{4}{27} h^4 \Delta \right) \beta^8 + \cdots$$

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We point out that this analytic expansion is valid for any arbitrary set of values of the parameters \( J, \beta, D \) and \( h \) in the high temperature regime. Therefore it applies equally well to any phase of the one-dimensional spin-1 XXZ Heisenberg model. Each coefficient in expansion (2) is exact and valid for any \( \beta \) order of the phase of the model.

A numerical work by Blöte [2] confirms the validity of the expansion in powers of \( (\beta^2) \) for the isotropic Heisenberg model with single-ion anisotropy and in the presence of an external magnetic field. However, we do not agree with the high temperature limit of the correlation function for the \( z \)-component of spin between nearest neighbors \( \langle S_0^z S_1^z \rangle \) of Ref. [3]. The correct limit is \( \langle S_0^z S_1^z \rangle \approx -\frac{1}{2} \Delta \beta \).

In summary, in this letter we applied the method of Ref. [2] to a non-integrable spin-1 XXZ Heisenberg model with single-ion anisotropy in the presence of an external magnetic field in the \( z \)-direction. We obtained the analytical \( \beta \)-expansion of the Helmholtz free energy per site \( f(\beta) \) of the model up to order \( \beta^5 \). Each coefficient in expansion (2) is exact and valid for any phase of the model.

Our curves in the high temperature region fit well Blöte’s numerical results for the spin-1 XXZ Heisenberg model. We recover the few analytical results known in the literature [4] about the isotropic spin-1 Heisenberg model. We correct the high temperature limit of \( \langle S_0^z S_1^z \rangle \) of Ref. [3]. For the first time in the literature we have analytical results easily handled for the anisotropic spin-1 Heisenberg model with single-ion anisotropy and in the presence of an external magnetic field.

Finally, we should mention that our calculation procedures have been implemented in the symbolic computational language Maple [4]. Currently, refinements are being made so that the expansion of the Helmholtz free energy (2) for the \( s = 1 \) Heisenberg model can be extended to higher orders in \( \beta \).

An enlarged version of this letter will be published elsewhere.

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Specific Heat

$\Delta = +2$
$D = 0$
$h = 0$

FIG. 1: Comparison of our analytic expression for the specific heat and Blöte’s numerical result\cite{1} for the anisotropic Heisenberg model with different anisotropies and $h = 0$. Solid lines stand for the specific heat of our analytical result and dotted lines correspond to data from Ref. 1.

Specific Heat

$J = -2$
$\Delta = -2$
$h = 0$

FIG. 2: Comparison of our analytic expression for the specific heat and Blöte’s numerical results\cite{1} for the isotropic Heisenberg model with different single-ion parameters and $h = 0$. Solid lines stand for our results and dotted lines correspond to data from Ref. 1.