

Efficient transfer matrix simulations for quantum molecular-based chains [★]

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Abstract. In the field of molecule-based magnetism materials composed of magnetically isolated chains have become the main research trend in last years. The quantum transfer matrix (QTM) method based on a checkerboard structure has been applied to the one-dimensional Heisenberg model with Dzyaloshinskii-Moriya interaction in the $S = 1/2$ spin chain. This model with the transverse staggered magnetic field and uniform magnetic field has been applied to the semimetallic compound Yb_4As_3 . Our simulations results have been compared with the available experimental results of the field dependent specific heat and a quantitative agreement has been established. A new approach to the analysis of the QTM simulation results (based on a polynomial extrapolation) has significantly improved the accuracy of results, which permitted getting reliable numerically extrapolated results for temperatures lower than hitherto considered. Moreover the new version of the QTM method was studied, where only one column is considered. In order to increase the length of the transfer matrix in Trotter direction we apply the density-matrix renormalization technique.

Key words: Molecular magnetism; Heisenberg model; numerical simulations

1 Introduction

Computer modelling of the finite-temperature properties of the Yb_4As_3 is based on the $S = 1/2$ anisotropic Heisenberg model with the antisymmetric Dzyaloshinskii-Moriya (DM) interaction. The DM interaction is eliminated by rotating the spins in the x-y plane by the angle θ . Then the model is mapped onto [1]

$$\mathcal{H} = -J \sum_{i=1}^N \mathbf{S}_i \mathbf{S}_{i+1} - g_{\perp} \mu_B B^x \sum_{i=1}^N S_i^x - g_{\perp} \mu_B B_s^y \sum_{i=1}^N (-1)^i S_i^y. \quad (1)$$

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In our simulations for Yb_4As_3 in an external magnetic field, we assumed the intrachain exchange coupling $J/k_B = -28$ K, the g -factors parallel and perpendicular to the spin chain of Yb_4As_3 were estimated as $g_{\parallel} = 3.0$, $g_{\perp} = 1.3$ and $\tan(\theta) = 0.19$ [1].

For the spin system described in (1) we can calculate the canonical partition function $\mathcal{Z} = \text{Tr} e^{-\beta\mathcal{H}}$. The values of matrix elements of $e^{-\beta\mathcal{H}}$ cannot be calculated for large N because of noncommuting operators in (1). To eliminate this restriction, we look for systematic approximants to the partition function \mathcal{Z} . We express Hamiltonian (1) as a sum of the spin-pair operators $\mathcal{H}_{i,i+1}$ and in the check-board decomposition we divide the Hamiltonian (1) into two noncommuting parts [2] each part defined by the commuting spin-pair operators $\mathcal{H}_{i,i+1}$. Then the series of the classical approximants of the quantum thermal values can be found, using the general Suzuki-Trotter formula [2]. The partition function is calculated from the expression

$$\mathcal{Z} = \lim_{m \rightarrow \infty} \mathcal{Z}_m = \lim_{m \rightarrow \infty} \text{Tr} \left[\prod_{i=1}^{N/2} \mathcal{V}_{2i-1,2i} \prod_{i=1}^{N/2} \mathcal{V}_{2i,2i+1} \right]^m, \quad (2)$$

where $\mathcal{V}_{i,i+1} = e^{-\beta\mathcal{H}_{i,i+1}/m}$, $i = 1, 2, \dots, N$ and m is a natural number (referred to as the Trotter number).

The approximant \mathcal{Z}_m can be calculated numerically, without any restrictions on the value of N , by the quantum transfer-matrix (QTM) method. The computation of \mathcal{Z}_m is possible for relatively small values of m , because of computer storage limitation, but the leading errors in taking a finite m approximant are of the order of $1/m^2$ and therefore, extrapolations to $m \rightarrow \infty$ can be performed. For infinite chains (the macroscopic limit) it is better to reverse the transfer direction and to calculate the partition function from the largest eigenvalue of the transfer matrix. In order to reverse the transfer direction we must define a new local transfer matrix (TM) $\mathcal{L}_{r,r+1}$ and a unitary shift operator \mathcal{D} [3]. These operators act in a Hilbert space \mathcal{H}^{2m} whose dimension is independent of N . In this case the global TMs can be expressed in terms of two operators $\mathcal{L}_{1,2}$ and $\mathcal{L}_{2,3}$: $\mathcal{W}_r = (\mathcal{L}_{r,r+1}\mathcal{D}^+)^m$ ($r = 1, 2$) and the m -th classical approximant to the partition function can be written as:

$$Z_m = \text{Tr} (\mathcal{W}_1\mathcal{W}_2)^{N/2}. \quad (3)$$

In the limit $N \rightarrow \infty$ the partition function \mathcal{Z} is equal to the highest eigenvalue of the global transfer matrix $\mathcal{W} = \mathcal{W}_1\mathcal{W}_2$.

2 Description of the extrapolation method

In order to obtain a certain value of specific heat or any other thermodynamical quantity calculated from the partition function (3), one should analyze for a given temperature the dependence of the calculated specific heat on Trotter index m and extrapolate the dependence $C(1/m^2)$ in the limit $m \rightarrow \infty$. For

low temperatures the dependence $C(1/m^2)$ significantly deviates from linear character and with increasing m the specific heat values change significantly, so the accuracy of the estimated specific heat is affected.

In order to improve the accuracy of this estimation for low temperatures, the analysis of the specific heat as a function of $1/m^2$ was made as follows. A function described by the extrapolation polynomial of the degree k ($k = 1, \dots, k_{max}$) in the form $C_m/T = \sum_{j=0}^k a_j \cdot (\frac{1}{m^2})^j$ was developed to fit all the points C_m corresponding to m_{min}, \dots, m_{max} . The extrapolation procedure starts with $m_{min} = 2$ and is continued till $m = m_{max} - 1$. In each step the number of fitted points n ($n = m_{max} - m_{min} + 1$) is fixed and a number of extrapolations are performed with polynomials of the degree k ($1 \leq k \leq n - 1$, but not more than 10). In this way for a given field and temperature we obtain a set of extrapolated values for different values of n and k and we can present the variation of the data with n for the fixed degree k of the polynomial. We observed that the variation of the data decreases with increasing degree k and the reliability of the estimates increases for $k \geq 4$.

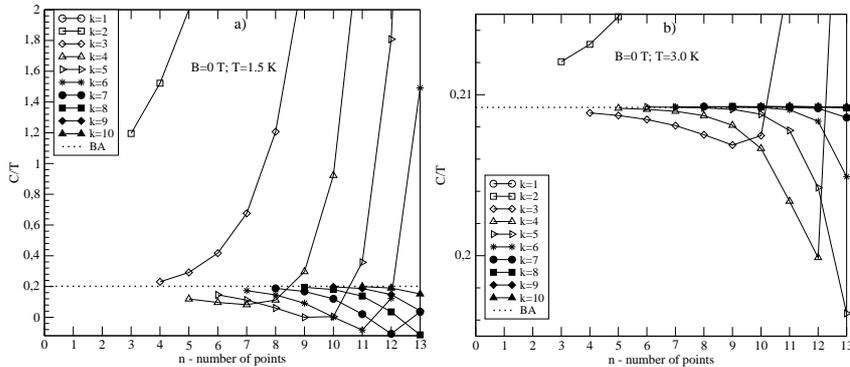


Fig. 1. The extrapolated values of specific heat versus the number points n for which the polynomials are constructed. Each particular plot corresponds to the polynomial of a given degree k . The figures have been drawn for different temperatures $T = 1.5$ K (a) and $T = 3.0$ K (b). The Bethe ansatz results [4] is shown as a dotted line.

The extrapolated specific heat values obtained from the above procedure are shown in Fig. 1 and 2, correspond to the vanishing magnetic field and two different temperatures ($T = 1.5$ K, $T = 3.0$ K). To check the accuracy of the extrapolations, the plots were referred to the value obtained on the basis of the Bethe ansatz (BA) [4] which is shown as a dotted line in Fig. 1 and 2. As shown, the convergence depends significantly on the degree k of the polynomial. The curves corresponding to $k = 1$ cannot be shown here. The convergence is much better for higher temperatures, which confirms high accuracy of the extrapolation results.

Recently the new version of the QTM method has been proposed [5], where the TM pattern is only one column wide. This saves the storage space and simplify the calculation of correlation functions. As in the typical QTM method the density-matrix renormalization-group method (DMRG) [6] can be applied to increase the size of the system along the Trotter direction. It is interesting to test both approaches for quantum spin models related to molecular-based chains.

3 Results and conclusions

In order to calculate the magnetic contribution to the specific heat corresponding to the experimental results for the polydomain sample, the following simulation was performed. It was assumed that 25% of the domains are oriented in parallel to the direction of the spin chain, and the external magnetic field B is also applied in parallel to the chain direction. For the 75% of domains the effective magnetic field $B_{eff} = B \cdot \sin(70^\circ)$ is assumed to be oriented in perpendicular to the direction of the chain. $C/T(B) = 0.75 \cdot C_{\perp}/T(B_{eff}) + 0.25 \cdot C_{\parallel}/T(B)$.

The results of our numerical extrapolations and the estimated errors have been compared with the literature values [1, 4]. The above analysis reveals an excellent agreement between our results and those obtained by other methods: Bethe ansatz [4] and the DMRG [1]. The accuracy of the present QTM results is comparable with that of DMRG results for temperature $T = 2$ K, ($k_B T/J = 0.077$) and exceeds 1%. This confirms that our QTM technique is a reliable tool for analysis of the specific heat measurements.

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