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Modeling and Simulations of Complex Low-Dimensional systems: Testing the Efficiency of Parallelization

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***Abstract*—**The deterministic quantum transfer-matrix (QTM) technique and its mathematical background are presented. This important tool in computational physics can be applied to a class of the real physical low-dimensional magnetic systems described by the Heisenberg hamiltonian which includes the macroscopic molecular-based spin chains, small size magnetic clusters embedded in some supramolecules and other interesting compounds. Using QTM, the spin degrees of freedom are accurately taken into account, yielding the thermodynamical functions at finite temperatures.
In order to test the application for the susceptibility calculations to run in the parallel environment, the speed-up and efficiency of parallelization are analyzed on our platform SGI Origin 3800 with $p = 128$ processor units. Using Message Parallel Interface (MPI) system libraries we find the efficiency of the code of 94% for $p = 128$ that makes our application highly scalable.

***Keywords*—**Deterministic simulations, low-dimensional magnets, modeling of complex systems, parallelization.

I. Introduction

In this article we describe numerical simulation based on the quantum transfer-matrix (QTM) method, we present some applications in computational physics and analyze the characteristics of parallelization which make our code suitable to run in the parallel environment. The domain of applications of the QTM method is very wide and includes not only simulations of the thermodynamic properties of the low-dimensional systems [1], but also phase transitions [2].

Before presenting the modeling and the simulation QTM technique, we review physical systems belonging to the class of low-dimesional magnets, in particular the molecular magnets. First we consider the compound $[Mn(hfac)_2NITPh]_6$ (hfac, hexafluoroacetyl acetonate; NITPh, 2-phenyl-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxy-3-oxide) belonging to a class of nano-compounds actively investigated for their magnetic properites [3], [4]. Synthesis of polynuclear metal complexes with oxygen atom bridges has resulted in a series of new molecules with unusual geometric symmetries and patterns [5]. Their magnetic properties, associated to a large number of interacting paramagnetic centers in a single aggregate, have significantly stimulated the research effort with the prospect of technological applications [3]. The interest in spin assemblies stems from the fact that they set the low-size limit for magnetic nanoparticles. They can display magnetic quantum tunneling [5] and quantum-size effects in the thermodynamic properties [6].

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II. Microscopic Model and Simulation Technique

To simulate the finite-temperature properties of low-dimensional magnetic systems, we model rings or chains in the framework of the spin Hamiltonian with the nearest neighbour interaction, which can be described by the following operator:

$$\mathbf{H} = J\sum_{i=1}^{N}\mathbf{S}_i \cdot \mathbf{S}_{i+1} - D\sum_{i=1}^{N}\left(\mathbf{S}_i^z\right)^2 - g_\nu \mu_B B\sum_{i=1}^{N}\mathbf{S}_i^\nu , \qquad (1)$$

where $\mathbf{S}_i$ is interpreted as the spin located at the i-th site of a one-dimensional lattice of N equally spaced sites. N may become infinite for the macroscopic chain. J denotes the nearest neighbour exchange integral (negative for the antiferromagnetic coupling) and D stands for the anisotropy parameter. B is the external magnetic field which can be applied along the chain $\nu = z$ or in the perpendicular direction ($\nu = x, y$), g_ν is the corresponding gyromagnetic ratio and N is the size of a given one-dimensional system (the chain or the ring). The spin values S_i may be uniform or non-uniform and define the matrix representation of the corresponding non-commuting operators.

We calculate the thermodynamic properties from the derivatives of the free energy related to the partition function Z. For the spin system described in (1) we can calculate the canonical partition function Z from the definition

$$Z = \mathbf{Tr}\left\{e^{-\beta\mathbf{H}}\right\} \qquad (2)$$

The Hilbert space of states of an N-site low-dimensional system is a direct product of single spin spaces, therefore, the

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base states can be labelled by the N-tuple of the eigenvalues of the z component of the single spin operator

$$\left|S_i^z \ldots S_N^z\right\rangle \equiv \left|S_i^z\right\rangle \ldots \left|S_N^z\right\rangle \tag{3}$$

The values of matrix elements of $e^{-\beta \mathbf{H}}$ cannot be calculated for large N because of non-commuting operators in (1). Thus, to eliminate this restriction, we look for systematic approximants to the partition function Z.

We express Hamiltonian (1) in terms of the spin-pair operators $\mathbf{H}_{i,i+1}$ as

$$\begin{aligned}\mathbf{H} = \sum_{i=1}^{N} \Big\{ & J\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \tfrac{1}{2} D\left[\left(\mathbf{S}_i^z\right)^2 + \left(\mathbf{S}_{i+1}^z\right)^2\right] + \\ & + \tfrac{1}{2} g_v \mu_B B\left(\mathbf{S}_i^v + \mathbf{S}_{i+1}^v\right)\Big\}\end{aligned} \tag{4}$$

In the checker-board decomposition (CBD) we divide the Hamiltonian (4) into two non-commuting parts [7]

$$\begin{aligned}H &= H^{odd} + H^{even} = \\ &= \left(H_{1,2} + \ldots + H_{N-1,N}\right) + \left(H_{2,3} + \ldots + H_{N,1}\right),\end{aligned} \tag{5}$$

each part defined by the commuting spin-pair operators $\mathbf{H}_{i,i+1}$. Then the series of the classical approximants of the quantum thermal values can be found, using the general Suzuki-Trotter formula [7]. The partition function is calculated from the expression

$$Z = \lim_{m\to\infty} Z_m = \lim_{m\to\infty} \mathbf{Tr}\left\{\prod_{i=1}^{N/2} \mathbf{V}_{2i-1,2i} \prod_{i=1}^{N/2} V_{2i,2i+1}\right\}, \tag{6}$$

where $\mathbf{V}_{i,i+1} = \exp\left(-\beta \mathbf{H}_{i,i+1}/m\right)$ $i = 1,2,\ldots,N$ and m is a natural number (reffered to as the Trotter number).

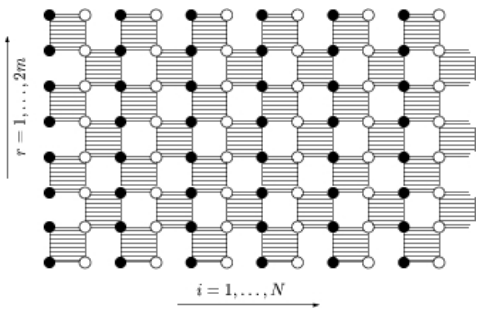

Fig. 1 The structure of the classical map of the quantum ring of the alternating spins in the checker-board decomposition. The shaded squares denote the Boltzmann vertices, whereas the full circles and the open circles stand for spins at the odd and even sites of chain.

The approximant Z can be calculated numerically, without any restrictions on the value of N, by the quantum transfer-matrix method. The computation of 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 $m \to \infty$ can be performed.

The trace in (6) is taken over all the configurations of the classical Ising variable $S_{i,r}$ (the eigenvalues of $\mathbf{S}_{i,r}^z$) on a planar lattice of the size $N \times 2m$. The lattice is obtained in the checker-board decomposition and sketched in Fig. 1. The shaded squares denote the corresponding Boltzmann weights $\mathbf{V}_{i,i+1}$ present in (6) which are determined by some 4-spin operators.

The thermodynamic functions for all systems described by Hamiltonian (1) are related to the free energy which can be calculated from the formula $F = -k_B T \cdot \ln Z$. The specific heat is given as its second derivative with respect to temperature, the magnetization is then evaluated from the first and the zero-field susceptibility from the second derivative with respect to the field.

III. Simulation Results

The QTM method has been applied to simulation of the $S = 1/2$ and $S = 1$ one-dimensional Heisenberg model and our results are compared with the experimental results for many compounds [1]. We have studied the finite temperature static properties in wide ranges of temperatures and the single-ion anisotropy (the D parameter in (1)).

The simulations of the finite chains with arbitrary size N are challenging due to the experimentally observed effects of the non-magnetic dilution of Yb_4As_3. The specific heat data calculated for the finite segments $N = 20$ and $N = 29$, are plotted in Fig. 2 in order to show the sizeable dependence on N at low temperatures and applicability of our method for a diluted system.

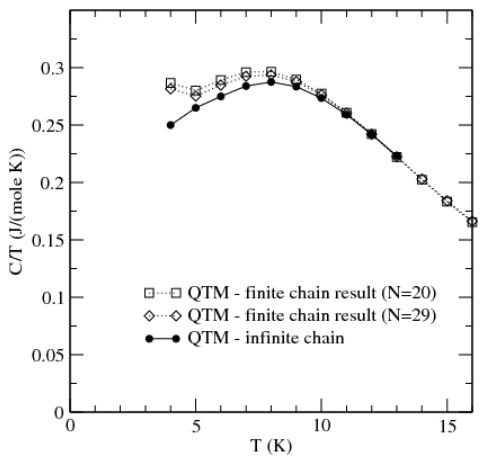

Fig 2 Temperature dependence of the specific heat numerical results for finite chains ($N = 20$ and $N = 29$ spins) and infinite chain.

Here we report the susceptibility of the Mn_6 molecule [1]. Depending on temperature and the number n of the spin pairs $S = 1/2$ and $S = 5/2$, in some cases the calculations preserving 5 decimal places required as many as $m = 900$ steps in the Trotter direction. To save the supercomputer time, for temperatures higher than $k_B T/|J| = 0.05$ we performed our simulations only up to $n = 5$ pairs. Then we extrapolated the estimates of the zero-field susceptibility to $n = 6$ which corresponded to Mn_6. The uncertainties, smaller than 1% at

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higher temperatures, reached the order of 5% for about $k_B T/|J| = 0.05$ and at this point the QTM simulations were performed for $n = 6$ pairs.

The measured susceptibility of Mn_6 [8] is drawn for the monomeric formula in Fig. 3 by small circles. To fit our theoretical data, we have fixed $g = 2.0$ due to the negligible spin-orbit coupling for Mn ion. The best fit has been found for the isotropic parameter $J/k_B = -350(K) \pm 10(K)$, which is consistent with the existing qualitative estimates [3]. Our "exact" estimate for $n = 6$ (the large full circle) at $k_B T/|J| = 0.05$ is also depicted in Fig. 3. and confirms the approximate extrapolated results.

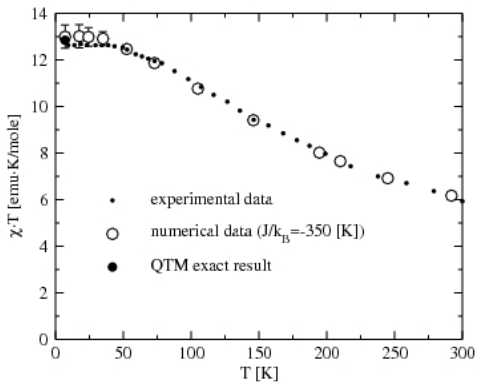

Fig. 3 The temperature dependence of the product $\chi \cdot T$ for Mn_6 in molar units (emu K mole^{-1}) divided by the number of pairs. The experimental data are given by small full circles and the extrapolated QTM results by open circles. The large full circle shows the numerically exact QTM estimate at $k_B T/|J| = 0.05$. The error bars are indicated where they exceed the size of the symbols.

From the computational point of view, the diagonal elements of the transfer matrix with size $12^{n=6} = 2\,985\,984$ had to be calculated. Their number was reduced approximately by a factor of 6 due to the symmetry considerations so that we had to evaluate about $0.5 \cdot 10^6$ matrix elements. It is a formidable task typical for the currently sinthesized magnetic supramolecules [9] and needs effectives methods of parallelization on the large number of processors and ultimately the grid environment.

In the remaining part of our work we analyze the properties of our code with respect to the distribution of the computational task over a number of processors available in the Supercomputing and Networking Centre in Poznan.

We have performed tests for a model molecule consisting of $n = 4$ pairs with $S_1 = 1/2$ and $S_2 = 5/2$ corresponding to the real Mn_6 cluster. The size of the transfer matrix is equal 20736 and a number of independent diagonal matrix elements amounts to about 5000.

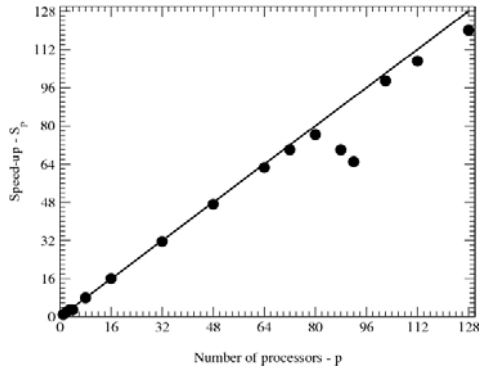

Fig 4 The speed-up p of the parallel computation for the number of processors $p \le 128$ tested on the SGI Origin 3800 supercomputer. The line describe the function $S_p = p$.

The performance of our parallelized code is presented in Fig. 4. We have run the program in the SGI Origin 3800 supercomputer. To reach the convergence for our simplified model system, we need in the sequential version of the algorithm about 14600 CPU seconds for the SGI platform. The speed-up of the parallelization based on the MPI librares is drawn by circles in Figure 4. The speed-up has been computed as the quotient of the CPU time of the sequential version of the algorithm divided by the maximum CPU time used by the slave processes plus the master process CPU time [10], [11].

IV. Conclusion

We have worked out QTM approach to characterize the finite temperature magnetic properties of the high nuclearity cyclic spin clusters with large and alternating spins and a number of the macroscopic quasi-one-dimensional magnets.

We have carried out large-scale computations obtaining high resolution data for the $S = 1$ spin chains down to low temperatures and in the wide range of single-ion anisotropy parameters. For Mn_6 cluster the QTM technique provides the numerically exact results [1].

Our simulations demonstrate that the QTM approach is a valuable tool for calculations of the finite-temperature properties of the low-dimensional magnetic systems. This approach is also expected to be effective for magnetic properties of large clusters of interacting magnetic centers.

The computational complexity of our numerical problems is exponential so that for the finite ring simulations we are limited by the CPU time resources and a new grid environment should be envisaged. The efficiency of the parallel computation is diminished from 100% for $p \le 4$ to 94 % for $p = 128$ but still very high and efficiently scalable.

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