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Physica A 374 (2007) 173–178
PHYSICA A
www.elsevier.com/locate/physa

Thermodynamic properties of a uniform and nonuniform spin-$\frac{1}{2}$ chain as a model for the oxalate-bridged Cu(II) complexes

Y.C. Li[a,*], K.L. Yao[a,b], Z.L. Liu[a]

[a]*Department of Physics and State Key Lab of Laser Technology, Huazhong University of Science and Technology, Wuhan 430074, China*
[b]*The International Center of Materials Physics, Chinese Academic of Science, Shenyang 110015, China*

Received 22 May 2006; received in revised form 1 July 2006
Available online 4 August 2006

Abstract

By using the transfer matrix renormalization group method, we studied the magnetic and thermodynamic properties of the uniform and the nonuniform quantum Heisenberg spin chain with $S = \frac{1}{2}$. Compared with experiment results of some compounds, we investigated the effects of different interactions among the magnetic irons of the quantum system, and it is found that the ferro- and antiferromagnetic interaction affect the magnetic characteristics of the system and play important roles in determining the internal energy and the specific heat at finite temperature.

Keywords: Transfer matrix renormalization group; Internal energy; Specific heat

1. Introduction

The design and synthesis of molecular-based magnetic materials with different properties, especially with ferromagnetic coupling is one of the major challenges in molecular materials research [1,2]. The polynuclear oxalate-bridged complexes have been a focus of magnetic studies [3–5] for the past decades due to the capability of the oxalate ligand (ox) to adopt the bis-bidentate bridging mode together with its remarkable ability to mediate electronic effects between paramagnetic metal ions separated by more than 5 Å. Recently, Castillo et al. [8] synthesized a series of oxalate-bridged copper(II) complexes, with general formula *Cu* (μ-ox) $(n\text{-ampy})_2 \cdot x\mathrm{H_2O}$, where $n = 2, 3, 4$ and $x = 0, 1.5$.

The bridged copper(II) binuclear system is of particular interest, not only because only one electron per magnetic center participates in the magnetic interaction, but also because there are different properties of materials with different bridging ligands. Such molecular-based magnetic materials can provide a good example to understand the internal mechanism of different properties of materials.

In Refs. [6,7] the authors used the renormalization-group method to study the finite-temperature properties of quantum mechanical systems. In this paper, we use recently developed quantum transfer matrix renormalization group (TMRG) method [9–11], which is a finite-temperature extension of the powerful

*Corresponding author. Tel.: +86 027 87556264.
E-mail address: hustliyan@163.com (Y.C. Li).

0378-4371/$ - see front matter
doi:10.1016/j.physa.2006.07.008

density matrix renormalization group method, to investigate the magnetic and thermodynamic properties of three oxalate-bridged chain-like polymers of copper(II) [8]. The paper is organized as follows: the model Hamiltonian and the aspects of computational method are given in Section 2. In Section 3, the magnetic susceptibility, the magnetic specific heat and the internal energy are calculated and discussed. Conclusions are given in Section 4.

2. Theoretical model and numerical method

As mentioned in Ref. [8], according to the X-ray crystal structure determination, all the three complexes are comprised of one-dimensional chains in which Cu(n-ampy)$_2^{2+}$ unites are sequentially bridged by bis-bidentate oxalate ligands with different Cu–Cu intrachain distances. Thus we assume that it is the different superexchange interactions from the bridging oxalate ligands that lead to the different magnetic properties of the there compounds. So we describe the systems (Figs. 1–3) as an alternating ferro- and antiferromagnetic $S=\frac{1}{2}$ chain. Then the adopted spin Hamiltonian in the presence of external field B reads

$$H=-\sum_{i=1}^{N}(J_1S_{2i}S_{2i-1}+J_2S_{2i}S_{2i+1})-\sum_{i}^{2N}g\mu_BBS_i^Z. \tag{1}$$

Here S denotes the spin-$\frac{1}{2}$ operator and J_1 and J_2 are isotropic with different sign. J_1 negative corresponds to antiferromagnetic coupling, while J_2 positive corresponds to ferromagnetic coupling. In order to describe easily, we define $\alpha=J_{1/}J_2$. In our calculations, we apply the same Trotter-decomposition strategy as that in Ref. [12]. The Hamiltonian is transformed to the following form:

$$H=H_1+H_2, \tag{2}$$

$$H_1=-\sum_{i=\mathrm{odd}}^{N}\left[J_1S_iS_{i+1}-g\mu_BB\frac{(S_i^z+S_{i+1}^z)}{2}\right], \tag{3}$$

$$H_2=-\sum_{i=\mathrm{even}}^{N}\left[J_2S_iS_{i+1}-g\mu_BB\frac{(S_i^z+S_{i+1}^z)}{2}\right]. \tag{4}$$

The TMRG uses the second-order approximation of the Trotter formula

$$Z=\mathrm{Tr}(-\mathrm{e}^{\beta\mathrm{H}})=\mathrm{Tr}(\mathrm{e}^{-\varepsilon(H_1+H_2)})^M+\mathrm{o}(\varepsilon^2), \tag{5}$$

where $\varepsilon=\beta/M$, and M is the Trotter number in TMRG method. The partition function can be calculated by means of the quantum transfer matrix. The thermodynamic properties can then be obtained from the maximum eigenvalue and the corresponding right and left eigenvectors of the transfer matrix. The magnetic field is expressed in a dimensionless form $h=g\mu_BB/|J_2|$. For all calculations, we keep 60 states in the

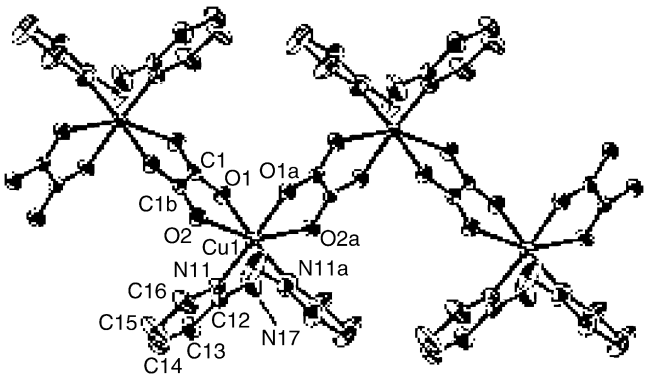

Fig. 1. The polymeric chain of 3[Cu(μ-ox)(2-ampy)]$_2$.