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Magnetizaition plateau of the compound $K_3Cu_3AlO_2(SO_4)_4$

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Abstract. Using the density matrix renormalization group method of the spin 1/2 magnetic behavior of the compound $K_3Cu_3AlO_2(SO_4)_4$, which represents the physical realization of the diamond chain, was studied. For the values $J_1 = J_3 = 132K, J_2 = 336K$ of coupling constants we obtained the magnetization plateau in the region 50-300 T of the external magnetic field. We used the ALPS (Algorithms and Libraries for Physics Simulations) library for the numerical calculations.

Keywords: magnetization plateau, diamond chain, DMRG

1. Introduction

Low-dimensional systems are particularly attractive since they provide opportunities for approbation of condensed-state physics models. The fact is that models for low-dimensional systems can be more easily analyzed than large-scale model, on the one hand, on the other hand, they reveal a wide range of the most diverse and interesting physical properties, being, thus, a touchstone for the above-mentioned field. The more interesting are the physical implementations of low-dimensional systems, which make it possible to compare theoretical results with experimental ones.

The so-called diamond chain model, which is a quasi-one-dimensional structure, was proposed to explain the properties of the compound $Cu_3Cl_6(H_2O)_2\cdot 2H_8C_4SO_2$ [1]. Presently, more than a dozen compounds having the structure of parallel located diamond chains are known [2, 3, 4, 5]. Among them – the long-known natural mineral azurite $Cu_3(CO_3)_2(OH)_2$ [2, 3], attracted the great interest both in the experimental and theoretical sectors. Such interest was caused by the following reasons. On the one hand, attempts have been made to describe the azurite in the approximation of parallel placed diamond chains, such that the interaction between them is much smaller than the interactions inside the diamond chain, or the effect of the inter-chain couplings is transferred to the couplings inside the diamond chain (the effective diamond chain model). On the other hand, within the framework of this model, the researchers, using various theoretical approaches, came to different, sometimes contradictory, values for coupling constants, nevertheless, with good consistency of theoretical to particular experimental results. For example, the Kikuchi group established $J_1 : J_2 : J_3 = 1 : 1.25 : 0.45$ [2, 3], Gu and Su [6, 7] proposed the anisotropy of the Heisenberg bond, with the presence of a ferromagnetic component, for the best coincidence with the experimental magnetic susceptibility: $J_1 : J_2 : J_{3z} = 1 : 1.9 : -0.3$ and $J_{3x}/J_{3z} = J_{3y}/J_{3z} = 1.7$. In the researches, for the couplingJ_3, both antiferromagnetic [8, 9] and ferromagnetic [10, 11] values were proposed. Extensive research undertaken by a group of researchers [12] established the values of the coupling constants for the model of an effective diamond chain, in which the best consistency with all experimental data is observed. Taking into account direct nodal couplings here was significant. A number of theoretical works should be also noted directly related to experimental data, or revealing the properties of diamond chains with an arbitrary spin in general, without binding them to specific materials [13] – [22]. Recently, a group of Japanese researchers synthesized a compound $K_3Cu_3AlO_2(SO_4)_4$ with diamond chain structure [5]. The dependence of the magnetic susceptibility on temperature was measured in the work, as well as the dependence of the magnetization on the external magnetic field up to 50 T.

In Section 2 of this paper the Hamiltonian for an antiferromagnetic diamond chain studied. In Section 3, for numerical values of the coupling constants obtained in [5], we numerically calculate the magnetization curve using DMRG method for 300 spins (100 diamonds) by means of the ALPS (Algorithms and Libraries for Physics Simulations) library. The Conclusion contains the main results.

2. The Hamiltonian of the model

On the basis of the result of Ref. [23], using the high-temperature series expansion method, one can, under the assumption of symmetric diamond chain, obtain the coupling constants values for which the best fit of the theoretically calculated magnetic susceptibility curve is observed with the experimental curve in the temperature range from 100 to 300 K.

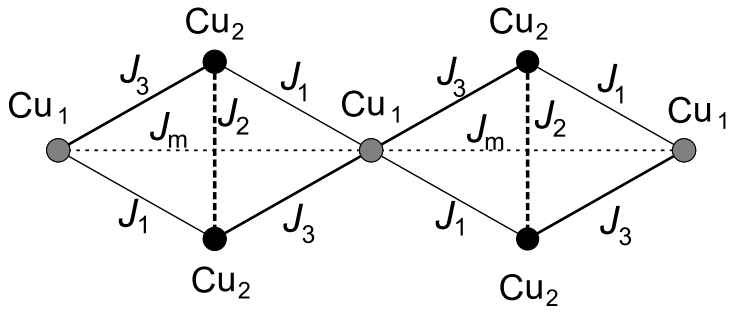

Figure 1: Structure of the rhombus.

We use the antiferromagnetic Heisenberg Hamiltonian with spins 1/2 for our diamond chain:

$$H = J_1 \sum_i \left(\vec{S}_{3i-1}\vec{S}_{3i} + \vec{S}_{3i}\vec{S}_{3i+1}\right) + J_2 \sum_i \vec{S}_{3i+1}\vec{S}_{3i+2} + \\ + J_3 \sum_i \left(\vec{S}_{3i-2}\vec{S}_{3i} + \vec{S}_{3i}\vec{S}_{3i+2}\right) + J_m \sum_i \vec{S}_{3i}\vec{S}_{3i+3} - g\mu_B h \sum_i S_j^z. \quad (1)$$

where $\vec{S}_i$ are the spin operators 1/2, J_i are the interaction constants between the Cu^{2+} ions. h, μ_B and g is the value of the z projection of the external magnetic field, the Bohr magneton and the gyromagnetic ratio g=2.3, respectively. The Figure 1 illustrates two diamonds clusters from the chain.

3. Magnetic properties of the model

For the values of $J_1 = J_3 = 132K$, $J_2 = 336K$ and $J_m = 40K$ (symmetric diamond chain) taken from [5], we performed a numerical calculation using the density matrix renormalization group method (DMRG) [24] and the matrix product of states method (MPS) [25, 26] diamond chain containing 300 spins (100 diamond clusters). For the calculations, we used the ALPS library [27, 28]. The calculations were performed on a super cluster of the Yerevan Physical Institute (SuperServer 7047GR-TRF) using parallel computations. The code is given in Appendix.

The Figure 2 shows the magnetization curve. It can be seen that it has a 1/3-plateau in the 50-300 T region. According to the experimental results obtained in the above work, the magnetic plateau is not observed up to 70 T. According to this, we can say that fitting the coupling constants and the gyromagnetic ratio, using

only the behavior of the magnetic susceptibility, turns out to be insufficient for a correct description of the magnetic behavior of the mentioned compound.

Quite recently a publication [29] appeared, in which the model of an asymmetric diamond chain for the compound $K_3Cu_3AlO_2(SO_4)_4$ is considered. In this publication, along with antiferromagnetic, ferromagnetic interactions are also introduced, and the value of the gyromagnetic ratio is also revised. Calculations were made at zero temperature by the renormalization-group approach of the density matrix (DMRG) at 120 spins. In the article the 1/3-plateau of magnetization appears in the region 110-250T of the external magnetic field.

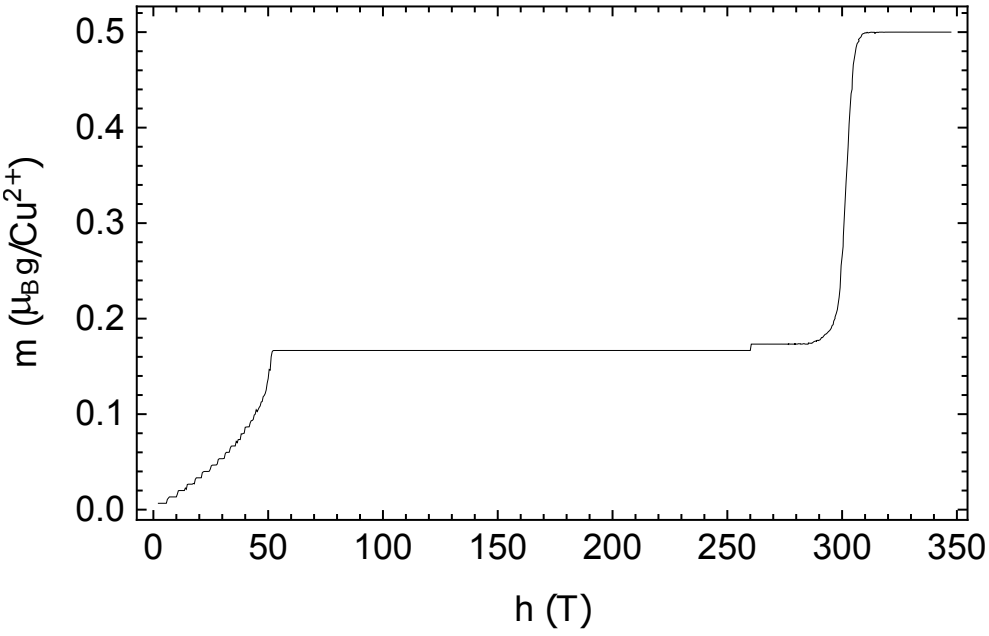

Figure 2: Magnetization curve of the rhombus.

4. Conclusion

We obtained the magnetization curve for the $K_3Cu_3AlO_2(SO_4)_4$ compound model using the density matrix renormalization group (DMRG) method and the matrix product state (MPS) method exploiting the ALPS library. The chosen number of spins of a periodic and symmetrical diamond chain in our model is quite sufficient to predict with great accuracy the appearance of a magnetic 1/3 plateau on the magnetization curve in the framework of this model. Thus, we show that the values obtained in Ref. [5] cannot be correct and in spite of the fact that they provide good coincidence of the magnetic susceptibility in the temperature range 100-300 K, nevertheless they contradict the experimental data on the magnetization, leading to the appearance of 1/3-plateau with external magnetic field from 50T in the model, whereas in the experiment it is not observed up to 70T. Taking out the nodal-nodal

interaction J_m constant between the Cu^{2+} ions would bring the results that agree better with the experimental data.

5. Appendix

The code of the program for calculating the magnetization of a cyclical symmetrical diamond chain consisting of 300 spins (Python, ALPS library):

```
import pyalps
import numpy as np
import matplotlib.pyplot as plt
import pyalps.plot

def frange(x, y, jump):
   while x < y:
      yield x
      x += jump

# preparation of calculation parameters

parms = []
hstart=0
hend=1
hdelta=0.1
hcount=(hend-hstart)/hdelta

for sz in frange(hstart,hend,hdelta):
   parms.append( {
      'LATTICE' : "mylattice",
      'LATTICE_LIBRARY' : "dd-graph1.xml", # diamond chain model
      'MODEL' : "Heisenberg_1",
      'MODEL_LIBRARY' : "model-dspin1.xml", # Hamiltonian
      'CONSERVED_QUANTUMNUMBERS': 'N,Sz',
      'h' :  sz,
      'local_S0' :  0.5,
      'local_S1' :  0.5,
      'J1' :  132.0/336.0,
      'J2' :  1,
      'J3' :  132.0/336.0,
      'J4' :  40.0/336.0,
      'Delta1' :  1,
      'Delta2' :  1,
      'Delta3' :  1,
      'Delta4' :  1,
```

```
      'SWEEPS' : 4,
      'NUMBER_EIGENVALUES' : 1,
      'L' : 100, # number of clusters
      'MAXSTATES' : 1200,
      'MEASURE_AVERAGE [magnetization]' :  'Sz'
   } )

# creating of input files and starting a simulation

input_file = pyalps.writeInputFiles('parm_spin_one_half',parms)
res = pyalps.runApplication('mps',input_file,writexml=True)
```

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