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High-field Magnetization Study of the S = 1/2 antiferromagnetic Heisenberg chain $Cu(C_6H_5COO)_2 \cdot 3H_2O$

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Abstract

We present a temperature dependent high-field magnetization study of the S = 1/2 antiferromagnetic Heisenberg chain $Cu(C_6H_5COO)_2 \cdot 3H_2O$ along the magnetically characteristic axis a''. The data are analyzed on basis of the Bethe ansatz equations and via exact diagonalization of a linear spin chain with 20 sites, respectively. Overall, we find a very good agreement between experimental data and theoretical calculations, and extract a magnetic coupling strength J/k_B along the chain of 18.8(1) K. We discuss our results in context with the possibility for a magnetocaloric effect during the magnetization process of S = 1/2 antiferromagnetic Heisenberg chain systems.

Key words: Cu Benzoate, pulsed-field magnetization, antiferromagnetic Heisenberg chain
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Motivated by the rich variety of different and exotic magnetic ground states, quasi-one-dimensional quantum magnets have been the focus of intense experimental and theoretical research efforts in recent years [1,2]. Here, in order to gain deeper insight into the physics of such systems, the uniform S = 1/2 antiferromagnetic Heisenberg chain (AFHC) is of particular interest, since it is exactly solvable using the Bethe ansatz equations. This way, the thermodynamic properties of the S = 1/2 AFHC have been calculated for arbitrary temperatures T and magnetic fields H [3]. As we will see below, exact diagonalization of large but finite chains is quite capable of accounting for the experimental data in the accessible temperature range.

As yet, the theoretical predictions have been tested in experiments only for limited ranges of the H/T parameter space [4,5]. Further, recently it has been claimed that in pulsed-field experiments on a S = 1/2 AFHC magnetocaloric effects can be detected [6]. In this situation, in order to extend our studies on such systems [5], and to test the notion of a sizeable magnetocaloric effect in pulsed-field experiments, we have carried out a detailed study of the magnetization of a S = 1/2 AFHC, *viz.*, Cu Benzoate $Cu(C_6H_5COO)_2 \cdot 3H_2O$.

This material has previously been described as a *staggered S = 1/2 AFHC* [7,8]. Here, with respect to the magnetic properties there are two main crystallographic directions, a'' and c'', as result of the Dzyaloshinskii-Moriya interaction and a staggered g tensor. While along c'' the effects of the staggering are most prominent, along a'' the system behaves like a perfect S = 1/2 AFHC. Here, we present high-field magnetization experiments for $H \| a''$ of Cu Benzoate at temperatures $0.1J \leq k_BT \leq 1.3J$ (J: magnetic coupling constant) and up to $H > H_{sat}$ (H_{sat}: saturation

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field). We compare our data with the results of calculations obtained from exact diagonalization of a linear spin chain and based on the Bethe ansatz, respectively.

Single crystals of copper benzoate have been grown as described in Ref. [9]. The crystals show well-defined facets and the principal axes can be identified easily. By comparing low-field magnetization measurements for our samples with those published in the Refs. [7,9] we find some sample dependency, as evidenced by a variation of J by ~ 10 % around its average value, but overall a matching behavior for the different sets of data. A more detailed account of our experiments will be given elsewhere [10].

For the magnetization measurements the samples were oriented along the a'' axis (misalignment $< 5^\circ$), glued onto a plexi glass rod, which was fixed inside a gel capsule, and placed inside a thin walled teflon cylinder. The magnetization signal of the sample holder was also measured and corrected for in the data analysis. Magnetization measurements were carried out at the LNCMP in Toulouse in pulsed magnetic fields up to 37 T (details of the procedure are described in Ref. [5]). For signal calibration additional measurements were performed in fields up to 5 T in a commercial SQUID.

In the Figs. 1 and 2 we plot the overall field dependence and the low field range of the magnetization of Cu Benzoate at temperatures 1.7 to 25 K (solid lines). The T dependence is that expected from a S = 1/2 AFHC, with the pronounced rounding in $M(H)$ at the saturation field H_{sat} at low T, while at highest T a Brillouin-like behavior is observed.

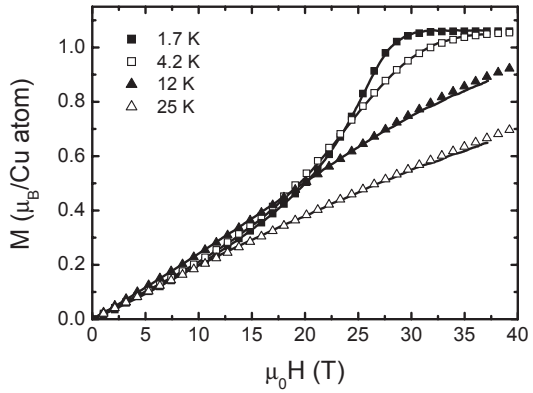

Fig. 1. The magnetization for $H \| a''$ of Cu Benzoate as function of temperature; experimental data as solid lines, markers denote the calculated magnetization based on exact diagonalization; for details see text.

Quantitatively, we can perfectly describe our data at all temperatures by means of exact diagonalization of a linear spin chain with 20 sites (for a description of such calculations see Ref. [5]). For the quantitative comparison we use values for g of 2.117 and J of 18.8(1) K

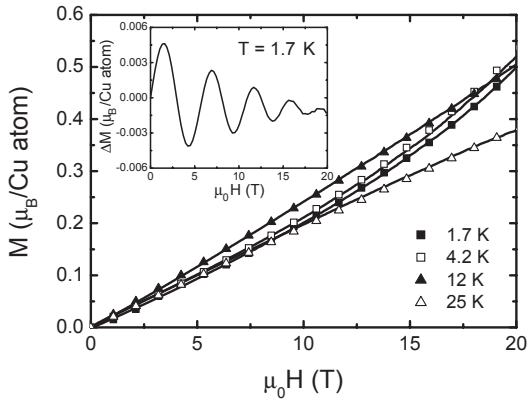

Fig. 2. The low field range of the data from Fig. 1. In the inset the difference of the calculated magnetization based on Bethe ansatz and exact diagonalization is shown; for details see text.

($H_{sat} = 26.5$ T), in good agreement with previous reports [7]. The results of the calculations are included in the figures and denoted by the markers. The fact that we have perfect matching between theory and experiment at all temperatures implies that in our pulsed-field experiments magnetocaloric effects play no role.

We also compared our experimental data with results from thermodynamic Bethe ansatz calculations [3]. Overall, the matching between the Bethe ansatz results and our data is as good as via exact diagonalization. In comparison, only for $k_B T \leq 0.1J$ small finite size effects are observable in the exact diagonalization approach. This is illustrated in the inset of Fig. 2, where we plot the difference between exact diagonalizations of finite chains and the Bethe ansatz calculation. As can be seen, the difference is less than ~ 0.005 μ_B/ Cu atom, and vanishes above 20 T.

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References

[1] H.-J. Mikeska and A. K. Kolezhuk, *One-Dimensional Magnetism*, Lect. Notes Phys. **645** (2004) 1.

[2] M. Kenzelmann et al., Phys. Rev. Lett. **93** (2004) 017204.

[3] A. Klümper, Eur. Phys. J. B **5** (1998) 677; A. Klümper and D. C. Johnston, Phys. Rev. Lett. **84** (2000) 4701.

[4] P. R. Hammar et al., Phys. Rev. B **59** (1999) 1008.

[5] A. U. B. Wolter et al., Phys. Rev. B **68** (2003) 220406(R).

[6] B. Wolf et al., Phys. Rev. B **69** (2004) 092403.

[7] D. C. Dender et al., Phys. Rev. B **53** (1996) 2583.

[8] M. Oshikawa and I. Affleck, Phys. Rev. Lett. **79** (1997) 2883; I. Affleck and M. Oshikawa, Phys. Rev. B **60** (1999) 1038.

[9] M. Date et al., Suppl. Progr. Theor. Phys. **46** (1970) 194.

[10] S. Glocke, A. U. B. Wolter, et al., to be published.