Magnetic model for $Ba_2Cu_3O_4Cl_2$

J.Richter, A.Voigt, J.Schulenburg, N.B.Ivanov* and R. Hayn**

Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Postfach 4120, 39106 Magdeburg, Germany

* Georgi Nadjakov Institute for Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko chaussee blvd., 1784 Sofia, Bulgaria

** Fachbereich Physik, TU Dresden, Germany

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Abstract

$Ba_2Cu_3O_4Cl_2$ consists of two types of copper atoms, $Cu(A)$ and $Cu(B)$. We study the corresponding Heisenberg model with three antiferromagnetic couplings, $J_{AA}$, $J_{BB}$ and $J_{AB}$. We find interesting frustration effects due to the coupling $J_{AB}$.

Keywords: antiferromagnetism, quantum fluctuations, frustration, phase transition

I. INTRODUCTION

The exciting collective magnetic properties of layered cuprates have attracted much attention over the last decade. Recent experiments on $Ba_2Cu_3O_4Cl_2$ [1] show magnetic properties of this quasi 2d quantum antiferromagnet which differ from the well studied antiferromagnetism of the parent cuprates like $La_2CuO_4$. Most interesting is the observation of two magnetic critical temperatures ($T^c_A \sim 330K$, $T^c_B \sim 40K$) and of a weak ferromagnetic moment [1], where a simple explanation of the ferromagnetic moment by a Dzyaloshinsky-Moriya exchange can be ruled out [2].

The important difference between the parent cuprates and $Ba_2Cu_3O_4Cl_2$ is the existence of additional $Cu(B)$ atoms located at the centre of every second $Cu(A)$ square. The coupling
between the $A$ spins $J_{AA}$ is strongly antiferromagnetic. The observation of a smaller second critical temperature $T_c^B$ indicates a weaker antiferromagnetic coupling $J_{BB}$ between the $B$ spins. Additionally, there is a competing coupling $J_{AB}$ between $A$ and $B$ spins giving rise for interesting frustration effects.

II. THE MODEL

We consider the classical and the quantum (spin $1/2$) version of the Heisenberg model

$$H = J_{AA} \sum_{<i \in A, j \in A>} S_i S_j + J_{BB} \sum_{<i \in B, j \in B>} S_i S_j + J_{AB} \sum_{<i \in A, j \in B>} S_i S_j$$

where the sums run over nearest neighbour bonds of type $A-A$, $B-B$, $A-B$. Tight binding calculations and the large $T_c^A$ indicate a strong antiferromagnetic $J_{AA}$. Because the couplings $J_{BB}$ and $J_{AB}$ are of higher order of the hopping integrals they can be assumed as (much) smaller than $J_{AA}$. In this paper we focus our interest on antiferromagnetic $J_{BB}$, $J_{AB} < J_{AA}$ and discuss the magnetic properties in dependence on $J_{AB}$ and $J_{BB}$ for fixed $J_{AA} = 1$. Since the copper spin is $1/2$ the quantum nature of the spins is of great importance. To take into account full quantum fluctuations we use an exact diagonalization algorithm to calculate data for two finite lattices of $N = 12$ sites ($8A$ spins and $4B$ spins) $N = 24$ sites ($16A$ spins and $8B$ spins). For comparison we present also some data for the corresponding classical systems.

III. RESULTS

The ground state results for small $J_{BB}$ and $J_{AB}$ are as follows:

- Classical model: Starting from the point $J_{AB} = 0$ we have Néel ordering in the subsystems $A$ and $B$. These two Néel states are decoupled and can rotate freely with respect to each other, i.e. the ground state is highly degenerated.

Increasing the frustrating $J_{AB}$ there is a first order transition to a non-planar canted state at $J_{AB}^c = 2\sqrt{J_{AA}J_{BB}}$ (see Fig.1). In this non-planar state the $A$ spins form a slightly tilted
Néel state, where the sublattice magnetization $M_{s,A}$ is lowered to about 90% for $J_{AB} \gtrsim J_{c,AB}$ and decreases with increasing $J_{AB}$. In the $B$ subsystem the angle between neighbouring spins is $\pi/2$ and the spins build a planar state perpendicular to the sublattice magnetization axis of the $A$ subsystem. However, due to the canting of $A$ spins there is a correlation between $A$ and $B$ spins. There is no ferromagnetic moment in the non-planar canted state. However, an almost degenerated classical planar state exists with a weak ferromagnetic moment which increases with $J_{AB}$. Quantum fluctuations may change this situation and could select a planar state instead of a non-planar ground state. For larger $J_{AB}$ further transitions to other ground states take place, which are not considered here.

- Quantum model: We focus our consideration on the lattice with $N = 24$ sites. The results for $N = 12$ are comparable supposing a relation of $J_{BB}^{12} = 2J_{BB}^{24}$. (Notice, that for $N = 12$ the $B$-spins have only two nearest $B$ neighbors instead of four.) First we consider the antiferromagnetic ground state ordering for small $J_{AB}$, where the two subsystems order in a quantum Néel state. In contrast to the classical case the quantum fluctuations cause a typical 'order from disorder' effect and lift the classical degeneracy by selecting a state with a collinear structure of two sublattice magnetizations. This is accompanied by the development of a magnetic coupling between $A$ and $B$ subsystems. A similar 'order from disorder' phenomenon is well-known from the $J_1 - J_2$ antiferromagnet on square lattice for $J_2/J_1 \sim 0.65$ [4]. The stability of the Néel state is supported by quantum fluctuations (Fig.1). The transition line to a canted state lies well above the classical instability line and for small $J_{BB} < 0.07J_{AA}$ the line follows approximately the relation $J_{c,AB} \approx 2.7\sqrt{J_{AA}J_{BB}}$. A detailed analysis of the canted state gives indications for planar structure which is, however, slightly different from that classical planar state which is almost degenerated with the non-planar classical ground state. The ground state order parameters for the $N = 24$ site lattice are shown in Fig.2 for $J_{BB} = 0.1J_{AA}$ which corresponds to the relation of critical temperatures. Obviously, both systems are antiferromagnetically ordered. However, the antiferromagnetic order in the $B$ system is weakened by $J_{AB}$ and drops down dramatically.


at the critical line. This is accompanied by an increase of the square of the total magnetic moments \( M_B^2, M_A^2 \) indicating the possibility of a weak ferromagnetic moment in the quantum system.

Let us finally present the temperature dependence of the specific heat \( c(T) \) for the quantum case (Fig. 3). The exact calculation of \( c(T) \) needs the complete diagonalization of the Hamiltonian and is restricted to very small system, i.e. to \( N = 12 \) in our case. We find two peaks in \( c(T) \) indicating the two transition temperatures. The peak positions \( T_A \) and \( T_B \) correspond to the coupling strengths \( J_{AA} \) and \( J_{BB} \). The frustrating coupling \( J_{AB} \) causes a decrease of \( T_A \) and \( T_B \). For the parameters used in Fig. 3 we have \( T_A(J_{AB} = 0.5)/T_A(J_{AB} = 0) = 0.99 \) and \( T_B(J_{AB} = 0.5)/T_B(J_{AB} = 0) = 0.87 \).

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REFERENCES

[1] S.Noro et al., Mater.Sci.Eng. B 25 (1994), 167; K.Yamada et al. Physica B 213-214 (1995), 191.

[2] F.C.Chou et al. Phys.Rev.Let. 78 (1997), 535.

[3] H.Rosner and R.Hayn, Physica B (1997), to be published.

[4] K.Kubo, T.Kishi, J.Phys.Soc.Jap. 60 (1991), 567; J.Richter, Phys.Rev.B 47 (1993), 5794.
FIGURES

FIG. 1. Transition line between the Néel phase and the canted phase (see text) for small $J_{AB}$ and $J_{BB}$ ($N = 24$). Notice that for larger $J_{AB}$ several other phases appear which are not considered here.

FIG. 2. Square of magnetic order parameters versus $J_{AB}$ for $J_{BB} = 0.1$ ($N = 24$). $M_{s,A}^2$ ($M_{s,B}^2$) - staggered magnetic moment of subsystem $A$ ($B$), $M_A^2$ ($M_B^2$) - total magnetic moment of subsystem $A$ ($B$).

FIG. 3. Specific heat versus temperature for $J_{BB} = 0.25$ ($N = 12$) and two different $J_{AB}$. 
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