A spin-1/2 model for CsCuCl\textsubscript{3} in an external magnetic field

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Abstract. CsCuCl\textsubscript{3} is a ferromagnetically stacked triangular spin-1/2 antiferromagnet. We discuss models for its zero-temperature magnetization process. The models range from three antiferromagnetically coupled ferromagnetic chains to the full three-dimensional situation. The situation with spin-1/2 is treated by expansions around the Ising limit and exact diagonalization. Further, weak-coupling perturbation theory is used mainly for three coupled chains which are also investigated numerically using the density-matrix renormalization group technique. We find that already the three-chain model gives rise to the plateau-like feature at one third of the saturation magnetization which is observed in magnetization experiments on CsCuCl\textsubscript{3} for a magnetic field perpendicular to the crystal axis. For a magnetic field parallel to the crystal axis, a jump is observed in the experimental magnetization curve in the region of again about one third of the saturation magnetization. In contrast to earlier spinwave computations, we do not find any evidence for such a jump with the model in the appropriate parameter region.

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1 Introduction

CsCuCl\textsubscript{3} is in several respects a quite unusual stacked triangular (anti)ferromagnet (see e.g. [1] for a review of the subject). Among others, three-dimensional features are vital in this compound: The ferromagnetic stacking is just an order of magnitude larger than the antiferromagnetic in-plane coupling while in most other materials the coupling constants differ at least by two orders of magnitude. Furthermore, the smaller antiferromagnetic coupling is crucial since it gives rise to a non-trivial behaviour of CsCuCl\textsubscript{3} in the presence of an external magnetic field.

The behaviour of CsCuCl\textsubscript{3} in strong external magnetic fields and at low temperatures has been studied already some time ago (see e.g. [2]). One observes different behaviour, depending on whether the magnetic field is applied along or perpendicular to the c (crystal)-axis. For a magnetic field along the c-axis, there is a jump in the magnetization curve at values of the magnetization of about one third of the saturation value. In contrast, one finds a plateau in the same area if the magnetic field is applied perpendicular to the c-axis\textsuperscript{1}.

The spin in CsCuCl\textsubscript{3} is carried by Cu\textsuperscript{2+} ions and thus is a spin 1/2. So, a proper treatment of quantum fluctuations is important. However, in order to be able to treat the three-dimensional situation, most theoretical approaches have so far been either phenomenological [4–6] or used first-order spinwave theory [7–10,5].

The goal of the present paper is to treat directly a spin-1/2 model with realistic XXZ-anisotropies. We will use series expansions around the Ising limit, numerical diagonalization and degenerate second-order weak-coupling perturbation theory.

When one solves a classical or Ising-version of this model, it becomes clear that essential features are already captured by a three-chain variant. The bulk of our paper will therefore concentrate on three antiferromagnetically coupled ferromagnetic chains. The simplification to a one-dimensional situation also opens the possibility of applying methods which work particularly well in one dimension like the density-matrix renormalization group (DMRG) method [11,12].

The purpose of the present paper is to gain some qualitative insight and demonstrate that new theoretical approaches to CsCuCl\textsubscript{3} are viable. It should be possible to

\textsuperscript{1} Actually, a plateau with \langle M \rangle = 1/3 can also be observed in other triangular antiferromagnets (see e.g. [3] for recent rather clear examples).
develop all these approaches further to improve the accuracy of the results, to obtain a more realistic modeling or to compute other quantities.

2 The model

Now we proceed to give a more accurate description of our model and the parameter region we are interested in. We model CsCuCl₃ by a stacked triangular lattice antiferromagnet as sketched in Figure 1.

The quantum-spin Hamiltonian corresponding to Figure 1 is given by (compare also [8]):

\[ H = J \sum_{i=1}^{N} \sum_{x=1}^{L} \Delta_1 S_{i,x}^z S_{i,x+1}^z + \frac{1}{2} \left( S_{i,x}^+ S_{i,x+1}^- + S_{i,x}^- S_{i,x+1}^+ \right) \]

\[ + J' \sum_{(i,j)} \sum_{x=1}^{L} \Delta_2 S_{i,x}^z S_{j,x}^z + \frac{1}{2} \left( S_{i,x}^+ S_{j,x}^- + S_{i,x}^- S_{j,x}^+ \right) \]

\[ -h \sum_{i,x} S_{i,x}^z, \]  

(2.1)

where the \( S_{i,x} \) are spin-1/2 operators and \( h \) is a dimensionless magnetic field. The notation \( (i,j) \) denotes neighbouring pairs of the \( N \) chains. Here, the number of chains \( N \) will be kept fixed while we are interested in the limit of infinite \( L \). Mostly, we choose \( \Delta_1 = \Delta_2 \) and then denote both of them just by “\( \Delta \”).

Quite often, CsCuCl₃ is modeled by a Hamiltonian which includes a Dzialoshinski-Moriya interaction with a vector pointing along the ferromagnetic chains in order to account for a modulation in the magnetic structure with a period of slightly more than 70 layers along the \( c \)-axis [13]. However, by a local unitary transformation this can be traded for a contribution to the anisotropy \( \Delta_2 \) and a surface term which is then discarded (see e.g. [8]). Further contributions to the anisotropies come from crystal fields. In this way, the \( z \)-direction in spin space is identified with the direction along the ferromagnetic chains (the \( c \)-axis) in real space.

\( J \) will be ferromagnetic (\( J < 0 \)) and \( J' \) antiferromagnetic (\( J' > 0 \)). In order to describe the material CsCuCl₃ one uses \( J' \approx -J/6 \) and \( \Delta \) slightly less than one [14-17]. The actual values used should not matter so much; it should however be noted that CsCuCl₃ is described by weakly coupled ferromagnetic chains — though not so weakly coupled as is the case for many other triangular lattice antiferromagnets [1]. A Monte-Carlo simulation of an \( XY \)-model takes \( J' = -J/10 \) [18] showing the influence the weaker coupling has on the critical behaviour of triangular antiferromagnets. To make the situation clearer in the study of the few-chain problem we choose a bit stronger interchain coupling, e.g. \( J' = -J/3 \) to compensate partially for the missing neighbouring chains.

The \( \langle i,j \rangle \)-summation in (2.1) should run over a triangular lattice as sketched in Figure 1. However, since \( J' \ll |J| \), a reasonable first approximation should be obtained by retaining only one site as a representative for each of the three sublattices of the triangular lattice. This leads to the model of three coupled chains which is indicated by the bold lines in Figure 1.

Since we are interested in the behaviour of CsCuCl₃ at low temperatures, we actually simplify to zero temperature in the present paper. We further restrict to magnetic fields applied along the anisotropy axis. The magnetization

\[ \langle M \rangle = \frac{2}{NL} \left( \sum_{i=1}^{N} \sum_{x=1}^{L} S_{i,x}^z \right) \]

(2.2)

is then given as the expectation value of a conserved operator. This is technically useful since it permits one to relate all quantities in a magnetic field \( h \) to those with a given magnetization \( \langle M \rangle \) at zero field. In the presence of an anisotropy \( \Delta \neq 1 \), the effect of a magnetic field along the \( z \)-axis is different from a magnetic field in the \( xy \)-plane. Because of the aforementioned simplification we consider only the former case in the present paper.

Possible plateaux in the magnetization curve can be most easily read off in the strong-coupling limit \( J' \gg |J| \). For a fixed number \( N \) of coupled chains one finds [19, 20] that for \( J = 0 \) the only possible values of the magnetization are \( \langle M \rangle = -1, -1 + 1/2N, ..., 1 - 2/N, 1 \). In particular, for all \( N \) that are divisible by three, a plateau with \( \langle M \rangle = 1/3 \) is possible (the simplest case is \( N = 3 \)). However, this strong-coupling argument does not ensure that a certain plateau actually does occur for given values of the parameters — this issue requires a computation of the magnetization curve (at least in the vicinity of the plateau-value of the magnetization).

Before we proceed with the discussion of the magnetization process, we note that a straightforward computation yields the upper critical field for \( N = 3 \) cyclically coupled chains

\[ h_{uc} = J'(\Delta_2 + \frac{1}{2}) + J(\Delta_1 - 1) \]

(2.3)

for \( J' > 0 \) and \( J < 0 \). This result is based on the assumption that the transition proceeds with a single spin flip and is therefore valid for \( \Delta_1 \) small enough (in particular \( \Delta_1 \leq 1 \)). If the transition to saturation becomes first order, (2.3) ceases to be valid.