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NUMERICAL STUDY OF WEAK FERROMAGNETISM IN 2D J_1–J_2 HEISENBERG MODEL WITH DZYALOSHINSKII–MORIYA INTERACTION

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By means of exact diagonalization we consider the groundstate of the J_1–J_2 spin 1/2 Heisenberg model with an anisotropic interaction term of Dzyaloshinskii–Moriya type. We find that a Dzyaloshinskii–Moriya interaction may create a weak ferromagnetic moment. The interplay between the quantum nature of the groundstate of the pure J_1–J_2 model and the anisotropic Dzyaloshinskii–Moriya interaction favour energetically a well-defined direction of spin alignment creating anisotropic correlations.

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1. Introduction

The $s = 1/2$ J_1–J_2 Heisenberg model on the square lattice has attracted a considerable interest in connection with the magnetic properties of the high-temperature superconductors in recent time [1]. The groundstate properties of this model are widely discussed in the last years, mainly with respect to a possible breakdown of the magnetic long-range order (LRO) due to the combined influence of quantum fluctuations and frustration (see [2] and references therein). However, there are also indications for additional anisotropic terms in the Hamiltonian which could explain the experimentally observed weak ferromagnetism (FM) for instance in La_2CuO_4 [3]. In general, a small FM moment in antiferromagnets (AFM) may appear in materials with a low crystal symmetry. The tilting of the spins can be described by adding the so-called anisotropic Dzyaloshinskii–Moriya (DM) interaction to the isotropic Heisenberg model [4,5]. The occurring additional interaction term in the Hamiltonian is proportional to the DM vector $\boldsymbol{D}$. In some recent publications [6–8] one has examined the origin and the structure of $\boldsymbol{D}$. Here we discuss the occurring weak FM of the J_1–J_2 model on the square lattice.

2. Model

In this paper we want to consider the following Hamiltonian:

$$\hat{H} = \sum_{\langle NN\rangle} J_1(\boldsymbol{S}_i \boldsymbol{S}_j) + \sum_{\langle NNN\rangle} J_2(\boldsymbol{S}_i \boldsymbol{S}_j) + \sum_{\langle NN\rangle} \boldsymbol{D}_{i,j}(\boldsymbol{S}_i \times \boldsymbol{S}_j) - \boldsymbol{h}\sum_{i=1}^{N} \boldsymbol{S}_i. \quad (1)$$

$\boldsymbol{S}_i$ denotes the spin-1/2 operator on site i. J_1 and J_2 are the nearest- and next--nearest-neighbour (diagonal) Heisenberg interactions, $\boldsymbol{D}_{ij}$ is the site dependent DM vector and $\boldsymbol{h}$ is an homogeneous magnetic field.

The vector $\boldsymbol{D}_{ij}$ is determined through the symmetry of the underlying crystal. In Ref. [6] Coffey and coworkers consider orthorhombic and tetragonal symmetries of La_2CuO_4 and get $\boldsymbol{D}_{ij}$ for the whole lattice by requiring for the vector $\boldsymbol{D}_{ij}$ that the energy of any configuration of spins is invariant under the symmetry transformations of the crystal structure. One could show that only a vector $\boldsymbol{D}_{ij}$ which varies from a bond to a bond corresponds to the crystal structure and is able to describe the observed weak FM. In this paper we focus our interest on the orthorhombic symmetry, since this symmetry is valid for low doping in $La_{2-x}Ba_xCuO_4$ [9]. If we fix $\boldsymbol{D}_{A,B} = (d_1, d_2, 0)$, then for the entire lattice one can construct $\boldsymbol{D}_{ij}$ through the symmetry considerations: $\boldsymbol{D}_{A,C} = (-d_2, -d_1, 0)$, $\boldsymbol{D}_{B,D} = -\boldsymbol{D}_{A,C} = (d_2, d_1, 0)$, $\boldsymbol{D}_{C,D} = -\boldsymbol{D}_{A,B} = (-d_1, -d_2, 0)$, $\boldsymbol{D}_{C,E} = -\boldsymbol{D}_{A,C} = (d_2, d_1, 0)$ and so on. Following the arguments of Ref. [6] we will restrict our considerations to d_1 and d_2 of the equal strength. Hence we consider two different cases for the parameters: case I: $d_1 = +d_2 = d$ and case II: $d_1 = -d_2 = d$. The

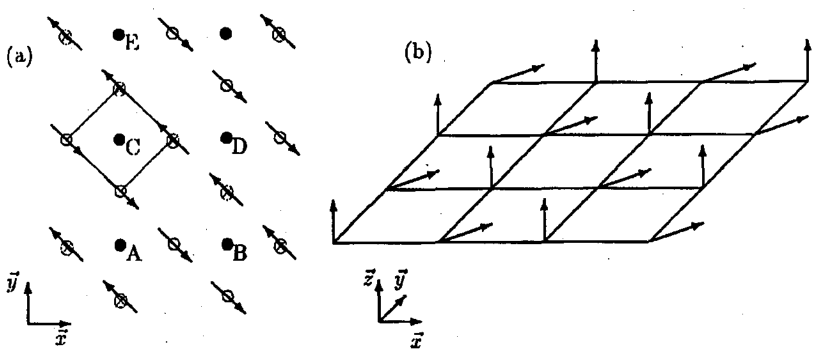

Fig. 1. (a) The orthorhombic arrangements of the CuO-octahedra in CuO-plane. The filled circles are the copper sites which carry the spins, the open circles are oxygen sites, which are tilted up out of the plane and the crossed circles are oxygen sites, which are tilted down out of the plane. The square represents one tilted CuO-octahedron. The points A–E denote certain copper sites used in the text. The arrows show one particular arrangement of the DM vector $\boldsymbol{D}_{ij}$ for this lattice (cases II); (b) The respective classical spin configurations for the DM-Hamiltonian for the case II with a 2-sublattice configuration and with a net ferromagnetic moment (all spins are aligned either along the z-axis or in the xy-plane).

main groundstate features for a classical DM-Hamiltonian ($J_1 = J_2 = h = 0$), where $\boldsymbol{S}_i$ and $\boldsymbol{S}_j$ are classical 3D vectors are as follows: For the case I we find a four-sublattice configuration without a net FM moment and for the case II a two-sublattice configuration with a net FM moment. The arrangement of $\boldsymbol{D}_{ij}$ for the case II is presented in Fig. 1a. The respective classical spin configuration is shown in Fig. 1b. Now we turn to the quantum system.

3. Numerical results

We have used a modified Lanczos procedure to calculate the groundstate for square lattices with $N = 16$ and $N = 20$ sites. In the figures we present the data for $N = 16$. The corresponding data for $N = 20$ are qualitatively the same. The Hamiltonian (1) contains terms of the form $S_i^{\pm} S_j^z$ which do not commute with the z-component of the total spin $\boldsymbol{S}$. Hence we have to take **all** 2^N-Ising states in the calculations.

In the pure model ($\boldsymbol{D}_{i,j} = 0,\ \boldsymbol{h} = 0$) the Hamiltonian (1) commutes with $\boldsymbol{S}^2$ and S^z and the groundstate is isotropic with $\boldsymbol{S}^2 = 0$. If we now put on the anisotropic DM interaction ($\boldsymbol{D}_{i,j} \neq 0$) the Hamiltonian does not commute with $\boldsymbol{S}^2$. Thus we may expect that the square of the magnetization $(M^\gamma)^2 = \langle \left[\frac{1}{N} \sum_{i=1}^N S_i^\gamma\right]^2 \rangle$ with $\gamma = x, y, z$ is not zero. Moreover, if we put on an external magnetic field we could measure a magnetization:

$$(S^\gamma) = \left\langle \frac{1}{N} \sum_{i=1}^{N} S_i^\gamma \right\rangle, \quad \gamma = x, y, z. \tag{2}$$

For the pure J_1–J_2 model and finite systems the magnetization is a step function of the external magnetic field because the magnetic field does not change the eigenstates but alters the eigenvalues. If we put on the DM interaction the situation changes basically. The Hamiltonian does not commute with the field term and the magnetization becomes a smooth function of $\boldsymbol{h}$. Due to the symmetry of the DM interaction some directions of spin alignment are preferred. This can be illustrated as follows [8, 11]: Consider a classical spin system without DM interaction and a collinear spin structure. The DM term contains the cross product of the spins so it vanishes. If now the quantum fluctuations are put on, the DM interaction favours the direction of spin fluctuations with minimal energy. From the classical picture follows that the minimum in the energy is reached, if the spins are perpendicular to the vector $\boldsymbol{D}_{i,j}$, i.e. are aligned in a plane with a normal vector parallel to $\boldsymbol{D}_{i,j}$. If the external magnetic field is directed parallel to this plane, the total magnetization $\langle S \rangle$ reaches a maximum. For both cases I and II we can chose the z-direction as an optimal direction for $\boldsymbol{h}$.

In Fig. 2a we present the z-components of the magnetization $\langle S^z \rangle$ ($\langle S^x \rangle$ and $\langle S^y \rangle$ are zero) as a function of the external magnetic field $\boldsymbol{h} = h\boldsymbol{z}$ for the case I and case II. The magnetic field together with the DM interaction causes a small magnetization in z-direction which increases almost linearly with growing h. The magnetization is much larger for the case II than for the case I. This is in accordance with the classical model (net FM for the case II, no net FM for the case I).

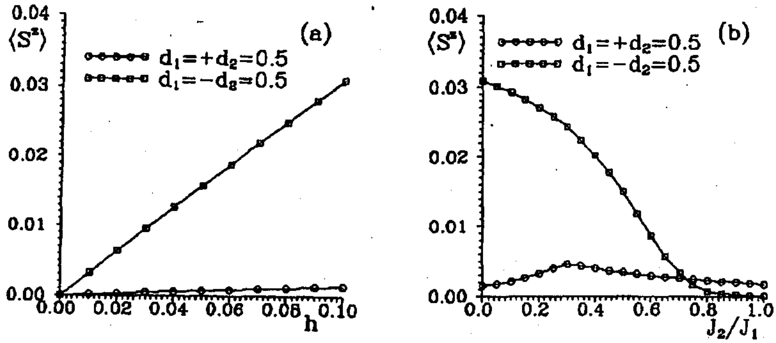

Fig. 2. (a) The z-component of the magnetization as a function of the external magnetic field $\boldsymbol{h} = h\boldsymbol{z}$ ($N = 16,\ J_1 = 1,\ J_2 = 0$); (b) The z-component of the magnetization as a function of the frustrating J_2 ($N = 16,\ J_1 = 1,\ \boldsymbol{h} = 0.1\boldsymbol{z}$).

Now we will discuss the influence of the J_2 term on the magnetization. The influence on the spin-liquid region of the pure model is a shift to lower or higher values of J_2/J_1. But this is beyond the scope of this paper and will be reported elsewhere [10]. Here we are interested how the weak FM is changed. In Fig. 2b the same parameter as in Fig. 2a is presented as a function of the frustrating J_2. The J_2 term favours a four-sublattice structure, which should not have a weak FM. Hence for increasing J_2 the magnetization decreases to very small values. For the case I there is a small increase in the magnetization in the spin-liquid region.

4. Summary

We have reported how the DM interaction influences the J_1–J_2 model. First the DM interaction creates an anisotropy in the spin correlations. Which components are enhanced and which are suppressed is a result of the interplay between quantum fluctuations, the particular symmetry of the DM vector as well as the underlying magnetic structure of the pure model. Second the DM interaction may create a weak FM moment. In accordance with the classical picture the case II yields the strongest FM moment and might indicate the existence of weak FM in the thermodynamic limit just for this symmetry of $\boldsymbol{D}_{i,j}$. This weak FM is suppressed by frustrating J_2.

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