Journal of Magnetism and Magnetic Materials 414 (2016) 180–186

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Order-by-disorder effects in antiferromagnets on face-centered cubic lattice

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ARTICLE INFO

Article history:
Received 5 February 2016
Received in revised form
5 April 2016
Accepted 17 April 2016
Available online 23 April 2016

Keywords:
"order by disorder" phenomena
Antiferromagnets
Spin waves
Frustration
Quantized spin models

ABSTRACT

We discuss the role of quantum fluctuations in Heisenberg antiferromagnets on face-centered cubic lattice with small dipolar interaction in which the next-nearest-neighbor exchange coupling dominates over the nearest-neighbor one. It is well known that a collinear magnetic structure which contains (111) ferromagnetic planes arranged antiferromagnetically along one of the space diagonals of the cube is stabilized in this model via order-by-disorder mechanism. On the mean-field level, the dipolar interaction forces spin to lie within (111) planes. By considering $1/S$ corrections to the ground state energy, we demonstrate that quantum fluctuations lead to an anisotropy within (111) planes favoring three equivalent directions for the staggered magnetization (e.g., $[11\bar{2}]$, $[1\bar{2}1]$, and $[\bar{2}11]$ directions for (111) plane). Such in-plane anisotropy was obtained experimentally in related materials MnO, α-MnS, α-MnSe, EuTe, and EuSe. We find that the order-by-disorder mechanism can contribute significantly to the value of the in-plane anisotropy in EuTe. Magnon spectrum is also derived in the first order in $1/S$.

1. Introduction

Frustrated spin systems have attracted a great deal of interest in recent years [1]. In many of them, classical ground state has a degeneracy which can be lifted by quantum or thermal fluctuations who thereby select and stabilize an ordered state. This is the so-called "order by disorder" phenomenon [2–4]. One of such spin systems is the Heisenberg antiferromagnet (AF) on face-centered cubic (fcc) lattice in which the next-nearest-neighbor AF exchange coupling (i.e., that along the cube edge) dominates over the nearest-neighbor one [5]. Although this model describes a number of prototypical AFs (e.g., MnO), some open problems remain in this field.

AF on fcc lattice can be viewed as four interpenetrating AF cubic sublattices (see Fig. 1(a)) [5,6]. Any spin from a sublattice locates at zero molecular field of spins from three other sublattices. As a result, staggered magnetizations of these sublattices can be oriented arbitrary relative to each other that leads to an infinite ground state degeneracy. However, quantum fluctuations make staggered magnetizations of all sublattices parallel to each other [5]. Besides, among two possible collinear arrangements, they select that presented in Fig. 1(b) which is referred to in the literature as AF structure of the second kind, type A (fluctuations make unfavorable type B structure) [5,6]. This AF structure contains (111) ferromagnetic (FM) planes arranged antiferromagnetically along one of $\langle 111\rangle$ directions. As soon as $[111]$, $[\bar{1}11]$, $[1\bar{1}1]$, and $[11\bar{1}]$ directions are equivalent, there are four equivalent spin arrangements of this type which are described by vectors of the magnetic structure $\mathbf{k}_0 = (\pi, \pi, \pi)$, $(\pi, 0, 0)$, $(0, \pi, 0)$, and $(0, 0, \pi)$ (hereafter we set to unity the cube edge length). This symmetry breaking by fluctuations is naturally accompanied by appearance of gaps induced by fluctuations in some magnon branches (not all the magnon branches acquire gaps because the continuous symmetry remains related to a rotation of all spins by any angle about any axis) [5]. It can be shown also that the selection of collinear spin structures can be described phenomenologically on the mean-field level by introducing to the Hamiltonian a biquadratic interaction between spins from different sublattices having the form $-Q(\mathbf{S}_i\mathbf{S}_j)^2$, where $Q > 0$ [5,7].

Unfortunately, it is often difficult to confirm unambiguously the presence of order-by-disorder effects in real materials because small anisotropic interactions cannot be generally excluded which are able to lift the classical ground state degeneracy explicitly (see also discussion in Ref. [8]). (In particular, one always expects the biquadratic exchange in real substances bearing in mind that it arises naturally in the Hubbard model in high orders in t/U, where t is the hoping constant and U is the on-site repulsion energy [9]). However, there are some compounds in which low-symmetry interactions are ruled out [8] or they are strongly suppressed for

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http://dx.doi.org/10.1016/j.jmmm.2016.04.052
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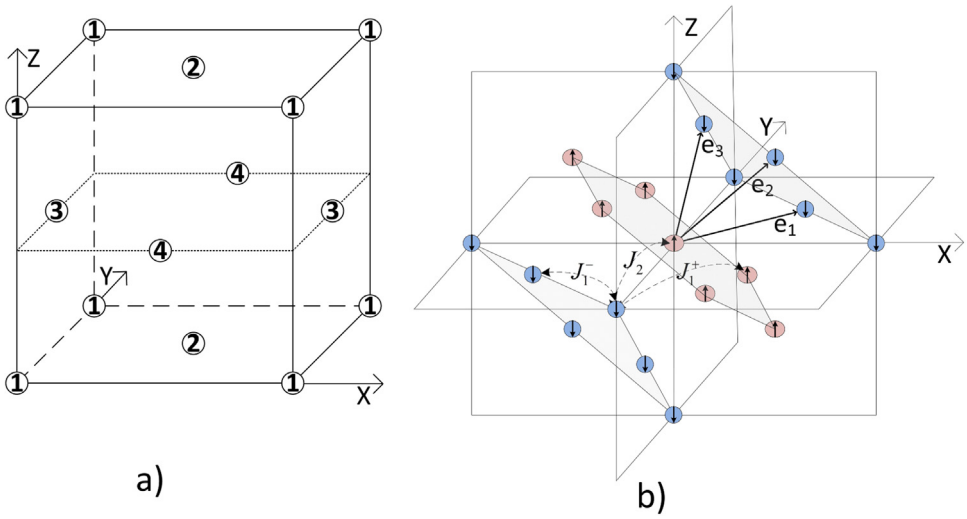

Fig. 1. (Color online.) (a) Classical AF on fcc lattice at $T=0$. Number indicates which of four AF cubic sublattices the given spin belongs to. (b) Magnetic structure of AF on fcc lattice which is realized in the considered model via order-by-disorder mechanism (which is referred to in the literature as AF structure of the second kind, type *A*). Spins belonging to different (111) FM planes (shaded) arranged antiferromagnetically along [111] direction are shown in different colors and are denoted by arrows ↑ and ↓. Exchange coupling constants $J_1^{\pm}, J_2$ and lattice vectors $\mathbf{e}_{1,2,3}$ are also presented.

some reason. Order-by-disorder effects contribute noticeably to properties of such materials.

One expects this situation in the following AFs on fcc lattice which show the spin structure presented in Fig. 1(b) at small T: MnO, [10,11] α-MnS, [12] α-MnSe, [12] EuTe, [13] and EuSe [14,15]. Four types of domains were observed in these materials at small T in which four equivalent (111) planes are FM planes. As soon as magnetic ions Mn^{2+} and Eu^{2+} are in isotropic states characterized by zero orbital moment in these compounds, the anisotropy arisen from spin–orbit interaction is expected to be very small. The main source of anisotropy is the dipolar interaction in these materials. It was found in Refs. [16–18] that anisotropic corrections to the classical ground state energy from dipolar interaction make (111) planes to be easy planes in accordance with experimental results. Dipolar forces make also more favorable type *A* AF structure of the second kind rather than the type *B* one (see Ref. [18] and references therein), as quantum fluctuations do. However, dipolar interaction does not select the collinear spin arrangement which is observed experimentally. In MnO, the selection of the collinear magnetic structure was attributed to dipolar anisotropy arisen due to small lattice rhombohedral distortion [18]. But such lattice distortions were not observed in other compounds. It should be noted also that the biquadratic exchange was suggested phenomenologically well before Ref. [5] to explain the temperature dependence of the order parameter and some other experimental findings in MnO and EuTe [13,19–21]. Particular estimations using equations from Ref. [5] give for the value of the effective biquadratic interaction $Q\sim 0.1$ K and 10^{-3} K for MnO and EuTe, respectively. These values are of the same order of magnitude as those proposed in Refs. [13,19–21] for description of experimental data. Then, the order-by-disorder mechanism has a large impact on magnetic properties of these materials.

Experimental data show also that there is a small anisotropy within (111) planes of unknown origin in all materials mentioned above. In particular, directions $[11\bar{2}]$, $[1\bar{2}1]$, and $[\bar{2}11]$ are three equivalent easy axes within (111) plane. It is the aim of the present paper to demonstrate that the order-by-disorder mechanism contributes to this anisotropy. For this purpose, we consider the first $1/S$ correction to the ground state energy of AF on fcc lattice with dipolar forces. We find below that due to the dipolar interaction this correction is anisotropic and it contributes to the in-plane anisotropy. Actually, we extend the analysis of order-by-disorder phenomena carried out in Ref. [5] by inclusion of the small dipolar interaction in the model. The obtained values of the in-plane anisotropy (and values of the gap in the magnon spectrum related to the in-plane anisotropy) are compared with those measured experimentally in considered substances. We point out that the order-by-disorder mechanism can contribute noticeably to the anisotropy in EuTe.

The rest of the present paper is organized as follows. We discuss the Hamiltonian transformation and technique in Section 2. The classical magnon spectrum is analyzed in Section 3. The spectrum renormalization in the model without dipolar forces is discussed in Section 4. The order-by-disorder effects in the model with dipolar forces are considered in Section 5, where we derive an expression for the in-plane anisotropy. Section 6 contains comparison with available experimental data in MnO, α-MnS, α-MnSe, and EuTe. A summary and our conclusion can be found in Section 7.

2. Hamiltonian transformation

We discuss Heisenberg AF on fcc lattice with dipolar interaction whose Hamiltonian has the form

$$\mathcal{H}=\frac{1}{2}\sum_{l\neq m}(J_{lm}\delta_{\alpha\beta}-Q_{lm}^{\alpha\beta})S_l^{\alpha}S_m^{\beta}, \tag{1}$$

where the summation over repeated Greek letters is implied,

$$Q_{lm}^{\alpha\beta}=\frac{\omega_0}{4\pi}\frac{3R_{lm}^{\alpha}R_{lm}^{\beta}-\delta_{\alpha\beta}R_{lm}^2}{R_{lm}^5}, \tag{2}$$

$$\omega_0=4\pi\frac{(g\mu_B)^2}{v_0}, \tag{3}$$

v_0 is the unit cell volume, and non-zero exchange constants are