Dzyaloshinski-Moriya interactions in the kagomé lattice

Maged Elhaja[1], Benjamin Canals, Claudine Lacroix

Laboratoire Louis Néel, 25 avenue des Martyrs, BP 166, 38042 Grenoble Cedex 9, France

August 2001

Abstract

The kagomé lattice exhibits peculiar magnetic properties due to its strongly frustrated crystallographic structure, based on corner sharing triangles. For nearest neighbour antiferromagnetic Heisenberg interactions there is no Néel ordering at zero temperature both for quantum and classical spins. We show that, due to the peculiar structure, antisymmetric Dzyaloshinsky-Moriya interactions ($D_i (S_i \times S_j)$) are present in this lattice. In order to derive microscopically this interaction we consider a set of localized d-electronic states. For classical spins systems, we then study the phase diagram ($T, D/J$) through mean field approximation and Monte-Carlo simulations and show that the antisymmetric interaction drives this system to ordered states as soon as this interaction is non zero. This mechanism could be involved to explain the magnetic structure of Fe-jarosites.

1 Introduction

The kagomé lattice (Fig. 1) with nearest neighbour antiferromagnetic exchange interactions exhibits peculiar magnetic properties, due to geometrical frustration [1]. For classical spins it remains disordered within mean field approximation, reflecting the macroscopic degeneracy of the ground state. Thermal or quantum fluctuations may leave partially this degeneracy, leading to ‘order by disorder’. Here we show that Dzyaloshinski-Moriya interactions (DMI) are present in this system due to the low local symmetry; we discuss the effect of DMI in relation with the magnetic structure observed in Fe-jarosite [2].

The DMI between two spins $S_i$ and $S_j$ was first introduced phenomenologically, using symmetry considerations, by Dzyaloshinski [3], and Moriya showed that it arises from taking into account the spin-orbit coupling ($\lambda L . S$) in the super-exchange interaction between localized magnetic electrons [4]. Including DMI, the Hamiltonian is written as:

$$H = J \sum_{\langle i,j \rangle} S_i . S_j + \sum_{\langle i,j \rangle} D_{ij} (S_i \times S_j) \quad (J > 0)$$

[1] E-mail: elhaja@polycentre-grenoble.fr
The allowed $D$ vectors of the DMI are restricted by the symmetry of the crystal (Moriya’s rules [4]). In the kagomé lattice, there is no inversion symmetry between 2 neighboring sites (see figure 1) and the symmetry of the simple kagomé lattice allows for $D$ perpendicular to the kagomé plane. However, in real compounds such as jarosites (see Ref. [2]), the non-magnetic atoms (which are not on the kagomé lattice) are also relevant, as they contribute to the crystal field and to the super-exchange interaction. Consequently they may lower the symmetry and allow for other directions of $D$.

In any case, applying Moriya’s rules will only restrict the possible $D$, but is not a proof of their existence. This is the reason for the microscopic derivation of the DMI in section 2.

2 Microscopic derivation of Dzyaloshinski-Moriya interaction

We have derived the DMI starting from an (arbitrary) set of localized d electronic states with the crystal electric field shown in Fig. 1a with one electron per magnetic site.

Following Moriya’s formalism [4] we find:

$$
D_x = D_y = 0 \quad D_z = \frac{\lambda \sqrt{3}}{U \Delta_1} \left( \frac{(dd\pi)^2}{2} - (dd\pi)(dd\delta) - \frac{3}{2} (dd\delta)^2 \right)
$$

(2)

where $U$ is the on-site Coulomb repulsion, and $dd\delta$ and $dd\pi$ are the hopping integrals as defined in [3].

In the jarosites (Ref. [2]), each magnetic site is surrounded by an octahedron of oxygen atoms which gives rise to the crystal electric field. The $z$ axis of these octahedra is tilted towards the centers of the triangles of the kagomé structure by an angle $\alpha$. In order to describe these compounds, we have derived the DMI as above but with the local axis on each magnetic site represented on Fig. 1b. In this case, the $D_{ij}$ are in the plane perpendicular to the bond $i-j$. The
expressions of $D_x$, $D_y$, $D_z$ can be obtained as in (2); they depend on $\alpha$ but we do not give them here for simplicity. In the following, we call $\beta$ the angle between $D_{ij}$ and the $z$ axis.

### 3 Low temperature magnetic structure

Looking at the ground state within mean field theory, we observe in both cases ($\beta = 0$ and $\beta \neq 0$) a long range ordered structure. It is a $q=0$ structure (the magnetic cell contains 3 sites). In the case of $D$ perpendicular to the kagomé plane ($\beta = 0$ or $\pi$), all spins lie in the kagomé plane, and only one degree of freedom remains, which corresponds to a ‘global’ rotation of all spins in the plane. In this case the DMI not only acts as an effective easy-plane anisotropy, it also selects one chirality for all the triangles, depending on the sign of $D_z$.

In the case of $D$ not perpendicular to the kagomé plane ($\beta \neq 0$), the effect of the in-plane component of $D$ is the following: the spins are no longer coplanar, each spin is directed in one fixed direction whose projection on the kagomé plane is towards the centers of the triangles (the chirality on the right of Fig. 2 is selected) and all the spins have the same out of plane component giving rise to a weak ferromagnetic magnetization perpendicular to the kagomé plane. This magnetization increases with the in-plane component of $D$ and decreases when $D_z$ increases as it should because isotropic exchange ($J$) selects coplanar magnetic structures. If $D_z > 0$, it selects the same chirality as the in-plane component of $D$, and its effect is to reduce the out of plane magnetization. $D_z < 0$ tends to select the other chirality (on the left of Fig. 2), resulting in a competition with the in-plane component of $D$, and there is a critical value of the angle $\beta$ between $D$ and the $z$ axis, above which the structure becomes coplanar.

In fact such a non-coplanar magnetic structure has been observed in Fe-jarosite (Ref. [3]) and could be due to DMI. In this jarosite it is also observed
that the structure becomes coplanar at lower temperature which could be due
to a small structural change, or possibly due to interplane interactions which
are not taken into account in this work.

In order to study the effect of temperature on this magnetic structure, we
have performed Monté-Carlo simulations with classical Heisenberg spins for dif-
ferent vectors $\mathbf{D}$. In all cases we observe a phase transition. The critical tem-
perature has been obtained as a function of $\frac{D}{J}$, which is represented on Fig. 2 for
the case $\mathbf{D}$ perpendicular to the plane. It is seen that the critical temperature
is of the order of $D$.

Thermal fluctuations also lift the degeneracy of the system without DMI
[6][7], but there is no caracteristic energy scale, i.e, this selection occurs asym-
totically when $T \to 0$. On the other hand, the phase transition due to DMI
occurs at a temperature of the order of $D$. Therefore, we expect that DMI when
present will always dominate the low temperature behaviour.

In conclusion, we have shown that a DMI is relevant for the kagomé lattice
and found that it can induce a phase transition at a temperature of the order
of $D$. It could explain some magnetic structures observed in the Fe-jarosites [2].

References

[1] M.J. Harris, M.P. Zinkin, Mod. Phys. Lett. B 10, 417 (1996).
[2] A.S. Wills, Phys. Rev. B 63, 064430 (2001).
[3] I.E. Dzialoshinskii, Sov. Phys. JETP 5, 1259 (1957).
[4] T. Moriya, Phys. Rev. 120, 91 (1960).
[5] J.C. Slater, G.F. Koster Phys. Rev. 94, 1498 (1954).
[6] J.T. Chalker, P.C.W. Holdsworth, E.F. Shender, Phys. Rev. Lett. 68, 855
(1992).
[7] J.N. Reimers, A.J. Berlinsky Phys. Rev. B 48, 9539 (1993).