Spontaneous order in the highly frustrated spin-1/2 Ising-Heisenberg model on the triangulated Kagomé lattice due to the Dzyaloshinskii-Moriya anisotropy

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Abstract. The spin-1/2 Ising-Heisenberg model on the triangulated Kagomé (triangles-in-triangles) lattice is exactly solved by establishing a precise mapping correspondence to the simple spin-1/2 Ising model on Kagomé lattice. It is shown that the disordered spin liquid state, which otherwise occurs in the ground state of this frustrated spin system on assumption that there is a sufficiently strong antiferromagnetic intra-trimer interaction, is eliminated from the ground state by arbitrary but non-zero Dzyaloshinskii-Moriya anisotropy.

1. Introduction
The antiferromagnetic quantum Heisenberg model (QHM) on geometrically frustrated planar lattices is currently at a forefront of theoretical research interest as it exhibits a variety of unusual ground states owing to a mutual interplay between quantum fluctuations and geometric frustration [1, 2, 3]. The intensive efforts aimed at better understanding of this peculiar interplay are closely related to several transition-metal magnetic materials, which are topologically prone to the geometric frustration due to a connectivity of their underlying magnetic lattice [4, 5]. One of the most interesting geometrically frustrated magnetic structures is the triangulated Kagomé (triangles-in-triangles) lattice (Fig. 1), which resembles the magnetic structure of a series of polymeric coordination compounds Cu$_9$X$_2$(cpa)$_6$.nH$_2$O (X=F, Cl, Br) [6, 7, 8].

It is worthy to notice, however, that the spin-1/2 QHM on the triangulated Kagomé lattice is not amenable to exact analytical treatment on account of mathematical complexities closely connected to a non-commutability of spin operators. Contrary to this, the spin-1/2 Ising model on the triangulated Kagomé lattice can be rather straightforwardly solved by establishing a precise mapping relationship to the spin-1/2 Ising model on Kagomé [9] or honeycomb [10] lattice exactly solved many years ago. The Ising model might unfortunately fail in describing many important features of the copper-based coordination compounds as it entirely neglects quantum fluctuations firmly associated with a quantum nature of the paramagnetic Cu$^{2+}$ ions having the lowest possible quantum spin number 1/2. Nevertheless, it has been recently shown that the approach based on exact mapping relations can also be applied to the spin-1/2 Ising-Heisenberg model on triangulated Kagomé lattice, which correctly takes into account the intra-trimer Heisenberg interaction and approximates merely the monomer-trimer interaction by the
Ising-type coupling \[11, 12\]. In the present work, we shall provide a further extension of this model by accounting for the antisymmetric Dzyaloshinskii-Moriya interaction as well.

The rest of this paper is so organized. In Section 2, we briefly describe the investigated model system and we also recall the most important steps of exact mapping method. Section 3 deals with a discussion of the most interesting results and it also summarizes main conclusions.

2. Ising-Heisenberg model and its exact solution

Consider the spin-1/2 Ising-Heisenberg model on the triangulated Kagomé lattice, which consists of two different lattice sites diagrammatically depicted in Fig. 1 as open and full circles. Assign the Heisenberg spin \(S = 1/2\) to all lattice sites shown as full circles and the Ising spin \(\mu = 1/2\) to all lattice sites shown as full circles. The spin-1/2 Ising-Heisenberg model on the triangulated Kagomé lattice can be then viewed as the Kagomé lattice of the Ising spins (monomers), which contains inside of each triangle unit a smaller triangle of the Heisenberg spins (trimer). The total Hamiltonian of the model under investigation can be for further convenience written as a sum over all Heisenberg trimers \(\mathcal{H}_k\), where each Hamiltonian \(\mathcal{H}_k\) involves all the interaction terms associated with three Heisenberg spins from \(k\)th trimer

\[
\mathcal{H}_k = \sum_{i=1}^{3} \left\{ -J_H \left[ \Delta \left( \hat{S}_{k,i}^x \hat{S}_{k,i+1}^x + \hat{S}_{k,i}^y \hat{S}_{k,i+1}^y \right) + \hat{S}_{k,i}^z \hat{S}_{k,i+1}^z \right] \
- D \left( \hat{S}_{k,i}^y \hat{S}_{k,i+1}^y - \hat{S}_{k,i}^z \hat{S}_{k,i+1}^z \right) - J_I \hat{S}_{k,i}^z \left( \hat{\mu}_{k,i}^z + \hat{\mu}_{k,i+1}^z \right) \right\}. \tag{1}
\]

The parameter \(J_H\) denotes the intra-trimer Heisenberg interaction, \(\Delta\) is the spatial anisotropy in this interaction, \(D\) labels the intra-trimer Dzyaloshinskii-Moriya interaction, \(J_I\) stands for the monomer-trimer Ising interaction and \(\hat{S}_{k,3} \equiv \hat{S}_{k,1}, \hat{\mu}_{k,3} \equiv \hat{\mu}_{k,1}\).

Exact solution for the aforesaid model system can be achieved by following the same procedure as developed in our earlier work \[11\]. In fact, the exact mapping correspondence to the simple spin-1/2 Ising model on Kagomé lattice can be established by adopting the star-triangle transformation given by Eq. \(4\) of Ref. \[11\] with the modified parameters \(P\) and \(Q_{\pm}\)

\[
P = \left( \frac{J_I}{3} \right)^2 \left[ \frac{3}{4} - \left( \mu_{k,1}^z \mu_{k,2}^z + \mu_{k,2}^z \mu_{k,3}^z + \mu_{k,3}^z \mu_{k,1}^z \right) \right] + \left( \frac{J_H \Delta}{2} \right)^2 + \left( \frac{D}{2} \right)^2, \tag{2}
\]
In the critical condition disordered states of the Ising-Heisenberg model can be obtained by solving numerically the lattice becomes critical if and only if the corresponding spin-1/2 Ising model on the Kagomé lattice becomes critical as well. Consequently, the critical temperature between ordered and disordered states of the Ising-Heisenberg model without the Dzyaloshinskii-Moriya term is the spontaneously long-range ordered unless the geometric frustration is strong enough to raise the disordered spin liquid ground state for $J_H/|J_1| < -2/(2 + \Delta)$. On the other hand, it surprisingly turns out that the ground state of the Ising-Heisenberg model with arbitrary but non-zero Dzyaloshinskii-Moriya anisotropy is spontaneously long-range ordered independently.

In the spirit of this transformation, the spin-1/2 Ising-Heisenberg model on the triangulated Kagomé lattice is mapped to the corresponding spin-1/2 Ising model on the simple Kagomé lattice with the effective nearest-neighbour interaction $\beta J_{\text{eff}}^\text{kag} = \ln(V_1/V_2)$ given by

$$V_1 = 2 \exp(\beta J_H) \cosh\left(\frac{3\beta J_I}{2}\right) + 2 \cosh\left(\frac{\beta J_I}{2}\right) \sum_{n=0}^{2} \exp\left[-2\beta \text{sgn}(q_1) \sqrt{p_1} \cos\left(\phi_1 + \frac{2\pi n}{3}\right)\right].$$  

$$V_2 = 2 \exp(\beta J_H) \cosh\left(\frac{\beta J_I}{2}\right) + \exp\left(\frac{\beta J_I}{6}\right) \sum_{n=0}^{2} \exp\left[-2\beta \text{sgn}(q_2^+) \sqrt{p_2} \cos\left(\phi_2^+ + \frac{2\pi n}{3}\right)\right]$$

$$+ \exp\left(-\frac{\beta J_I}{6}\right) \sum_{n=0}^{2} \exp\left[-2\beta \text{sgn}(q_2^-) \sqrt{p_2} \cos\left(\phi_2^- + \frac{2\pi n}{3}\right)\right],$$

where $\beta = 1/(k_B T)$, $k_B$ is Boltzmann’s constant, $T$ absolute temperature and the parameters

$$p_1 = \left(\frac{J_H \Delta}{2}\right)^2 + \left(\frac{D}{2}\right)^2, \quad q_1 = \left(\frac{J_H \Delta}{2}\right) \left[3 \left(\frac{D}{2}\right)^2 - \left(\frac{J_H \Delta}{2}\right)^2\right], \quad \phi_1 = \frac{1}{3} \arctan\left(\frac{\sqrt{p_1^2 - q_1^2}}{q_1}\right);$$

$$p_2 = p_1 + \left(\frac{J_I}{3}\right)^2, \quad q_{1,2}^\pm = q_1 \pm \left(\frac{J_I}{3}\right)^2, \quad \phi_{1,2}^\pm = \frac{1}{3} \arctan\left(\frac{\sqrt{p_2^3 - (q_{1,2}^\pm)^2}}{q_{1,2}^\pm}\right).$$

As a result of this mapping, the spin-1/2 Ising-Heisenberg model on the triangulated Kagomé lattice becomes critical if and only if the corresponding spin-1/2 Ising model on the Kagomé lattice becomes critical as well. Consequently, the critical temperature between ordered and disordered states of the Ising-Heisenberg model can be obtained by solving numerically the critical condition $\beta \cdot J_{\text{eff}}^\text{kag} = \ln(3 + 2\sqrt{3})$, where $\beta = 1/(k_B T_c)$ and $T_c$ is the critical temperature.

3. Results and discussion

Let us turn our attention to a discussion of the most interesting numerical results obtained for the finite-temperature phase diagrams. Before starting our discussion, however, it is worthwhile to remark that the most interesting results for the Ising-Heisenberg model without the Dzyaloshinskii-Moriya term has been detailed examined in our preceding paper [11] to which the interested reader is referred to for more details. In the present work, we therefore aim to investigate mostly the effect of Dzyaloshinskii-Moriya interaction on the critical behaviour.

In Figs. 2 and 3, the dimensionless critical temperature $k_B T_c/|J_1|$ is plotted against the ratio $J_H/|J_1|$ between intra-trimer and monomer-trimer interactions for several values of the Dzyaloshinskii-Moriya term $D/|J_1|$ and two different values of the exchange anisotropy $\Delta = 0.0$ and 1.0, respectively. As it can be clearly seen, the displayed critical lines terminate at a certain value of the ratio $J_H/|J_1|$, below which the system becomes disordered at all temperatures, just when the Dzyaloshinskii-Moriya anisotropy completely vanishes (i.e. for $D/|J_1| = 0.0$). This observation is fully consistent with previously published results [11, 12], which serve in evidence that the ground state of the spin-1/2 Ising-Heisenberg model without the Dzyaloshinskii-Moriya term is the spontaneously long-range ordered unless the geometric frustration is strong enough to raise the disordered spin liquid ground state for $J_H/|J_1| < -2/(2 + \Delta)$. On the other hand, it surprisingly turns out that the ground state of the Ising-Heisenberg model with arbitrary but non-zero Dzyaloshinskii-Moriya anisotropy is spontaneously long-range ordered independently.
of $J_H/|J_I|$ and $\Delta$. As a matter of fact, the critical temperature tends asymptotically to some constant non-zero value for any $D/|J_I| \neq 0$ even for highly frustrated case to be achieved in the limit $J_H/|J_I| \rightarrow -\infty$, whereas the asymptotical value of critical temperature is being the greater, the stronger is the Dzyaloshinskii-Moriya anisotropy $D/|J_I|$. It should be also mentioned that the aforementioned critical behaviour represents a rather general feature of the considered model that holds irrespective of the exchange anisotropy $\Delta$. Another striking observation for the highly frustrated region ($J_H/|J_I| \ll 0.0$) follows from a direct comparison of Figs. 2 and 3. It seems that quantum fluctuations support the spontaneous ordering, which is demonstrated by an increase of the critical temperature acquired through an increase of the parameter $\Delta$.

In conclusion, we have studied the spin-1/2 Ising-Heisenberg model on the triangulated Kagomé lattice within an exact method based on the generalized star-triangle mapping transformation. The most interesting result to emerge from our study is that the Dzyaloshinskii-Moriya anisotropy prohibits an existence of the disordered spin liquid ground state in spite of the high geometric frustration caused by the antiferromagnetic intra-trimer interaction. The more comprehensive investigations of spontaneously ordered state(s) to appear in the highly frustrated region and of thermodynamics are left as challenging tasks for future work.

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