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Magnetic competition with different spin chiralities in kagome magnets

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Abstract. Using the Bogoliubov variational method we study the magnetic competition in a minimal model proposed for kagome magnets. The minimal model consists of itinerant electrons with their spin-orbit coupling and localized electrons with their anisotropic spin exchange. A spin exchange between localized and itinerant electrons is also included into the model, and it is anisotropic. At half filling and in the region of stable in-plane antiferromagnetism, a magnetic competition between antiferromagnetic phases with different spin chiralities is found. Depending on the sign of the hopping integral and the spin-orbit coupling, either the 1×1 or $\sqrt{3} \times \sqrt{3}$ in-plane antiferromagnetism is established. These in-plane antiferromagnetic states are characterized by distinguishable spin chiralities.

1. Introduction

The interplay between magnetism, correlation, and topology has attracted a lot of research attention [1–3]. Kagome magnets provides a fertile platform for investigating the interplay. The principal feature of the kagome magnets is the two-dimensional lattice of triangles with sharing corners. Due to the special geometric frustration, various exotic states including Dirac electrons [4], flat band [5], quantum spin liquids [6], unconventional magnetism [7–10], and the quantized Hall conductivity [11, 12] can be realized in the kagome lattice. Recently, a magnetic phase transition between the out-of-plane ferromagnetism (O-FM) and the in-plane antiferromagnetism (I-AFM) and its flexible tunability were experimentally observed in kagome magnets [13–16]. The kagome magnets also often exhibit a large anomalous Hall conductance [13, 14]. This indicates an impact of nontrivial topology on the magnetic phase transition. Since the discovery of the $\mathcal{Z}_2$ topological insulator, the spin-orbit coupling (SOC) is an essential ingredient for maintaining the topological ground state [17–19]. In the electron structure it creates a gap between the valence and conduction bands and induces a band inverting [17, 18]. Incorporating the SOC into the kagome lattice, a topological state is also achieved [11, 12]. Recently, the magnetic competition between the O-FM and I-AFM in kagome magnets can be analyzed within a minimal model, that includes anisotropy in the spin exchange between itinerant and localized electrons, as well as in the spin exchange among localized electrons [9, 10]. However, the impact of the SOC on the magnetic competition is not yet studied.

In this paper we report the change of the spin chirality in the magnetic competition between different I-AFM states in the kagome lattice. The spin chirality characterizes the spin rotation in the lattice, and it is a trace of the SOC impact. The minimal model that we use to study the magnetic competition was previously proposed [10]. The Bogoliubov variational calculations reveal the magnetic competition between the O-FM and I-AFM and its universality in the regime of strong spin exchange [10]. Applying the Bogoliubov variational method, we find the dependence of the stable phase and its spin chirality on the SOC. This yields the impact of the SOC on the magnetic competition. This paper is a complement to the previous work [10].

The present paper consists of 4 sections. In Sec. 2 we introduce the minimal model, which describes the dynamics of itinerant and localized electrons together with their spin exchanges in the kagome magnets. The numerical results of the Bogoliubov variational calculations are presented in Sec. 3. Finally, the conclusion is presented in Sec. 4.

2. Model

In the previous work, we proposed a minimal model, which could describe the electrons dynamics in the kagome magnets [10]. The model is based on the tight-binding itinerant electrons with their SOC, and localized electrons with their anisotropic spin exchange on the kagome lattice. An anisotropic spin exchange between localized and itinerant electrons is also included. In the second quantization, the model Hamiltonian is

$$\begin{aligned} H &= -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - i\lambda \sum_{\langle i,j\rangle,s,s'} c^\dagger_{is} c_{js'} \sigma^z_{ss'} \nu_{ij} \\ &\quad - \sum_{i,\alpha,ss'} c^\dagger_{is} c_{is'} S^\alpha_i \sigma^\alpha_{ss'} h_\alpha - \sum_{\langle i,j\rangle,\alpha} S^\alpha_i S^\alpha_j J_\alpha. \end{aligned} \tag{1}$$

Here we have used the conventional notations: i, j are the lattice site indices, σ, s, s' are the spin indices, σ^α ($\alpha = x, y, z$) is the component of the Pauli matrices. The first term in Hamiltonian (1) is the nearest-neighbor hopping of itinerant electrons with the hopping parameter t and the conventional notations $c^\dagger_{i\sigma}$, $c_{i\sigma}$ for the creation and the annihilation operators of itinerant electrons. The second term is the SOC of itinerant electrons with its parameter λ. It is actually the nearest-neighbor direction-dependent hopping with the sign $\nu_{ij} = 1$ (-1) for the counterclockwise (clockwise) hopping direction (see figure 1(a)). The third term is the spin exchange between itinerant and localized electrons with the strength h_α in the α axis and the conventional notation S^α_i for the localized electron spin in the α axis. The last term in Hamiltonian (1) is the Heisenberg spin exchange of localized electrons with strength J_α in the α axis. We will consider the case where the spin exchanges are the same in the xy plane, but not in the z direction. We denote $h_{xy} \equiv h_x = h_y$, and $J_{xy} \equiv -J_x = -J_y$. The spin exchange between itinerant and localized electrons describes the double-exchange mechanism of long-range magnetic ordering [20, 21]. The Heisenberg spin exchange of localized electrons describes a magnetic phase transition from the O-FM to an I-AFM states at $J_{xy} = 2J_z$ [7–9]. In the double-exchange mechanism, both itinerant electrons and magnetic moments are together magnetically ordered, therefore the change of magnetic moment ordering due to the spin exchange also gives rise to a change of the magnetic ordering of itinerant electrons. This yields the magnetic phase transition in the kagome magnets [10].

The SOC of itinerant electrons can be encoded into a complex spin-dependent hopping $t_{ij\sigma} = t + i\nu_{ij}\sigma\lambda = r\exp(\pm i\Phi/3)$, where $r = \sqrt{t^2+\lambda^2}$ is its module, and $\Phi = 3\arg(t + i\lambda)$ is its argument. The argument Φ can be considered as a magnetic flux penetrating the corner-sharing triangles of the kagome lattice. This indicates that the SOC plays like a magnetic flux. Therefore the impact of the SOC on the magnetic competition is like the impact of the magnetic flux on the magnetic competition. With the notation of the complex hopping, we rewrite the first two terms in Hamiltonian (1) as a tight-binding Hamiltonian

$$H_0 = -\sum_{\langle i,j\rangle,\sigma} t_{ij\sigma} c^\dagger_{i\sigma} c_{j\sigma}. \tag{2}$$

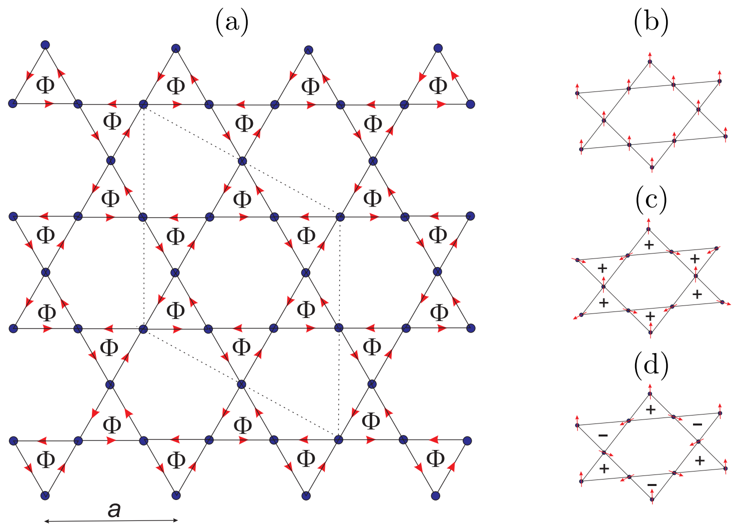

Figure 1. (a) The geometric structure of the kagome lattice. The SOC sign $\nu_{ij} = 1$ is indicated by the arrows on the lattice edges, and the magnetic flux penetrating the lattice induced by the SOC is Φ. The $\sqrt{3} \times \sqrt{3}$ unit cell is denoted by the dotted rhombus. (b) Out-of-plane FM state. (c) & (d) 1×1 and $\sqrt{3} \times \sqrt{3}$ in-plane AFM states, respectively. The spin chiralities $\chi = \pm 1$ of the in-plane AFM states are denoted by the sign $\pm$ in each triangle. The lattice parameter is set $a = 1$.

This Hamiltonian can be considered as the spinful model for the quantum anomalous Hall effect [12, 17]. Its spin component can be obtained from the double exchange model in the limit of strong spin exchange [11]. However, in our work it just describes the tight-binding dynamics of itinerant electrons with their SOC. In each spin sector the band structure consists of three bands, which are separated by two gaps [11]. The lowest band carries the Hall conductance $\sigma^{\sigma}_{xy} = (e^2/h)C_{\sigma}$, where $C_{\sigma} = \sigma$ is the Chern number [11]. Therefore, at filling 2/3 or 4/3, the ground state exhibits the quantized spin Hall effect and it actually yields a Z_2 topological insulator [11, 12, 17]. At half filling the ground state is metallic. However, when the spin exchange is included, it exhibits a large anomalous spin Hall conductance, and agrees well with experimental observations [10, 13–15]. In the following we will consider the half filling case, and use $r = 1$ as the unit of energy.

3. Bogoliubov variational principle and numerical results

We will use the Bogoliubov variational method to find the stable phases. It is based on the Bogoliubov inequality

$$\Omega \leq \langle H - H_{tr} \rangle_{tr} + \Omega_{tr} \equiv \tilde{\Omega}, \tag{3}$$

where H and H_{tr} are the original and trial Hamiltonians, respectively. Ω, Ω_{tr} are the grand potentials of the statistical ensembles, where Hamiltonian defining their statistical dynamics is given by H and trial H_{tr}, respectively [35, 36]. The statistical average is performed over the trial ensemble. The trial Hamiltonian is chosen by an appropriate phase ansatz, which is relevant to the consideration. The stable phase is found by minimizing $\tilde{\Omega}$. It would be the lowest grand potential among the ansatz phases defined by the trial ensemble. In zero-temperature limit $T = 0$, $\tilde{\Omega}$ is reduced to the ground state energy $\tilde{\Omega} \to E - \mu n N$, where E and n are the energy and the electron filling of the trial state, and μ is the chemical potential. The details of numerical calculations are presented elsewhere [10]. Actually, we treat the localized electron spin classically and set $\mathbf{S}_i^2 = 1$ as usually adopted in many studies of magnetic materials [20–33]. We calculate $\tilde{\Omega}$

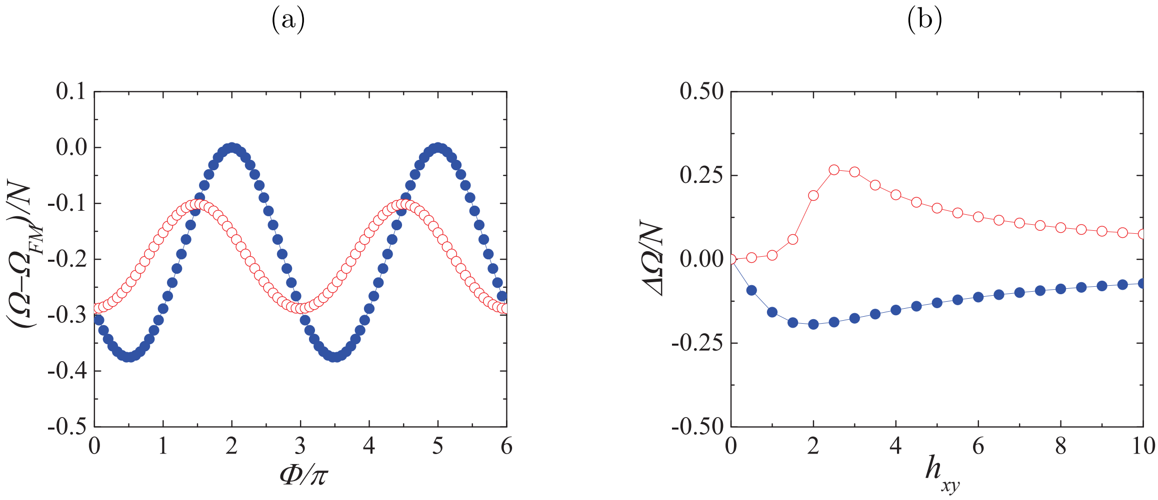

Figure 2. (a) The grand potential difference $\Omega - \Omega_{FM}$ from the O-FM state as a function of Φ at fixed $h_{xy} = 5$. The filled blue (open red) disks are the grand potential of the 1×1 ($\sqrt{3} \times \sqrt{3}$) I-AFM. (b) The difference of the grand potential between the 1×1 and $\sqrt{3} \times \sqrt{3}$ I-AFM states as a function of the in-plane spin exchange h_{xy} at fixed Φ. The filled blue (open red) disks are the grand potential difference at $\Phi = \pi/2$ ($\Phi = 2\pi$). Both figures present the numerical results at zero temperature, half filling, and model parameters: $J_z = 1$, $J_{xy} = 3$ and $h_z = 6$.

for different trial states which are generated by all arranges of localized electron spins within the 3×3 unit cell, and find its lowest value [10]. The Bogoliubov variational calculations reveal that at half filling the O-FM and the I-AFM are most stable [10]. The O-FM state is characterized by the parallel of all spins in the z direction. The in-plane magnetic states are characterized by fact that all spins are within the xy plane, and the spin directions are arranged at angle 120° in respect of each other (see figure 1(b)-(d)). Depending on the model parameters, the O-FM and the I-AFM compete each other, and the magnetic phase transition occurs [10]. However, there are two different stable I-AFM states, which are characterized by different vector chiralities. The vector chirality is defined within each lattice triangle by

$$\boldsymbol{\chi} = \frac{2}{3\sqrt{3}} \sum_{(i \neq j)=1,2,3} \mathbf{S}_i \times \mathbf{S}_j. \tag{4}$$

This vector chirality is parallel to the z axis $\boldsymbol{\chi} = \mathbf{e}_z \chi$, where $\mathbf{e}_z$ is the z axis unit [37]. It characterizes the non-collinearity and rotation of spins. The vector chirality is uniform $\chi = 1$ in the 1×1 AFM, and staggered $\chi = \pm 1$ in the $\sqrt{3} \times \sqrt{3}$ AFM. These I-AFM states are schematically presented in figures 1(c)-(d).

At half filling a magnetic transition between the O-FM and the I-AFM occurs at h^*_{xy} [10]. The ground state is O-FM when $h_{xy} < h^*_{xy}$, and I-AFM when $h_{xy} > h^*_{xy}$ [10]. The numerical calculations reveal a universality of the critical in-plane spin exchange h^*_{xy} in the strong out-of-plane spin exchange regime [10]. This finding agrees well with the experimental observation of the magnetic tunability [16]. In this paper we will focus our study to the regime $h_{xy} > h^*_{xy}$. In this regime the I-AFM is stable. In figure 2(a) we plot the flux dependence of the grand potential at half filling. One can notice that the grand potential is periodic in flux Φ. The period in Φ is 3π. It is clear from the complex hopping of itinerant electrons $t_{ij\sigma} = r \exp(\pm i\Phi/3)$ in the presence of the SOC. When $\Phi \to \Phi + 3\pi$, $t_{ij,\sigma} \to t_{ij,-\sigma}$, thus the two spin components of electrons change their role. Therefore we can consider the impact of the SOC in the range $0 \leq \Phi < 3\pi$. Figure 2(a) shows the competition between the 1×1 and the $\sqrt{3} \times \sqrt{3}$ I-AFM states. In the flux range $0 \leq \Phi \leq 3\pi/2$, the grand potential of the 1×1 I-AFM state has a lower value, while in the flux range $3\pi/2 \leq \Phi < 3\pi$, the grand potential of the $\sqrt{3} \times \sqrt{3}$ I-AFM state has a lower value. This indicates that the ground state is the 1×1 I-AFM when $0 \leq \Phi \leq 3\pi/2$, and the $\sqrt{3} \times \sqrt{3}$ I-AFM when $3\pi/2 \leq \Phi < 3\pi$. The phase transition occurs at $\Phi^* = 0, 3\pi/2$. The flux $\Phi = \Phi^*$ only when either the SOC or the hopping integral vanishes. Note that when the flux Φ crosses Φ^*, either the SOC or the hopping integral change their sign. Therefore when $\lambda \cdot t$ changes its sign, the ground state changes from the 1×1 to the $\sqrt{3} \times \sqrt{3}$ I-AFM. The phase boundary Φ^* is independent on the spin exchange, as one can see in figure 2(b). When $0 \leq \Phi \leq 3\pi/2$, $\Delta\Omega \equiv \Omega_{1\times1} - \Omega_{\sqrt{3}\times\sqrt{3}} < 0$, and when $3\pi/2 \leq \Phi < 3\pi$, $\Delta\Omega > 0$ for all values of the in-plane spin exchange h_{xy}. Only in the limit of strong spin exchange, the grand potentials of both 1×1 and $\sqrt{3} \times \sqrt{3}$ I-AFM states approach each other.

4. Conclusion

In this work we study the magnetic competition in the kagome magnets based on a minimal model. The minimal model includes the nearest-neighbor hopping, the SOC, the anisotropic spin exchanges. We use the Bogoliubov variational method to find the stable phase. The variational calculations reveal that in the regime of strong in-plane spin exchange, where the I-AFM is stable, a competition between the 1×1 and the $\sqrt{3} \times \sqrt{3}$ I-AFM states occurs. These I-AFM states are distinguishable by the vector chirality. The phase transition between the the 1×1 and the $\sqrt{3} \times \sqrt{3}$ I-AFM states occurs when either the hopping integral or the SOC changes their sign. The finding shows that the vector spin chirality is sensitive to the sign of the hopping integral or of SOC.

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References

[1] Keimer B and Moore J 2017 Nat. Phys. **13** 1045
[2] Sachdev S 2018 Rep. Prog. Phys. **82** 014001
[3] He K, Wang Y and Xue Q-K 2018 Annu. Rev. Condens. Matter Phys. **9** 329
[4] Mazin I I, Jeschke H O, Lechermann F, Lee H , Fink M, Thomale R and Valenti R 2014 Nat. Commun. **5** 4261
[5] Leykam D, Andreanov A and Flach S 2018 Adv. in Phys. X **3** 677
[6] Balents L 2010 Nature **464** 199
[7] Sachdev S 1992 Phys. Rev. B **45** 12377
[8] Reimers J N and Berlinsky A J 1993 Phys. Rev. B **48** 9539
[9] Legendre J and Le Hur K 2020 Phys. Rev. Res. **2** 022043(R)
[10] Thanh-Mai Thi Tran, Duong-Bo Nguyen, Hong-Son Nguyen and Minh-Tien Tran 2021 Mater. Res. Express **8** 126101
[11] Ohgushi K, Murakami S and Nagaosa N 2000 Phys. Rev. B **62** R6065
[12] Guo H M and Franz M 2009 Phys. Rev. B **80** 113102
[13] Nakatsuji S, Kiyohara N and Higo T 2015 Nature **527** 212
[14] Liu E, Sun Y, Kumar N, Muechler L, Sun A, Jiao L, Yang S Y, Liu D, Liang A, Xu Q, Kroder J, Süß V, Borrmann H, Shekhar C, Wang Z, Xi C, Wang W, Schnelle W, Wirth S, Chen Y, Goennenwein S T B and Felser C 2018 Nat. Phys. **14** 1125
[15] Wang Q, Xu Y, Lou R, Liu Z, Li M, Huang Y, Shen D, Weng H, Wang S and Lei H 2018 Nat. Commun. **9** 3681
[16] Guguchia Z, Verezhak J A T, Gawryluk D J, Tsirkin S S, Yin J X, Belopolski I, Zhou H, Simutis G, Zhang

S S, Cochran T A, Chang G, Pomjakushina E, Keller L, Skrzeczkowska Z, Wang Q, Lei H C, Khasanov R, Amato A, Jia S, Neupert T, Luetkens H and Hasan M Z 2020 Nat. Commun. **11** 559
[17] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 226801
[18] Bernevig B A, Hughes T L and Zhang S 2006 Science **314** 1757
[19] König M, Wiedmann S, Brüne C, Roth A, Buhmann H, Molenkamp L W, Qi X L and Zhang S C 2007 Science **318** 766
[20] Zener C 1951 Phys. Rev. **82** 403
[21] Dagotto E 2003 *Nanoscale Phase Separation and Colossal Magnetoresistance*, *Springer Series in Solid-State Sciences* Vol. **136** (Springer, Berlin, Heidelberg)
[22] Furukawa N 1994 J. Phys. Soc. Jpn. **63** 3214
[23] Furukawa N 1994 J. Phys. Soc. Jpn. **64** 2754
[24] Furukawa N 1996 J. Phys. Soc. Jpn. **65** 1174
[25] Yunoki S, Hu J, Malvezzi A L, Moreo A, Furukawa N and Dagotto E 1998 Phys. Rev. Lett. **80** 845
[26] Kogan E and Auslender M 2003 Phys. Rev. B **67** 132410
[27] Phan V N and Tran M T 2003 Mod. Phys. Lett. B **17** 39
[28] Minh-Tien T 2003 Phys. Rev. B **67** 144404
[29] Phan V N and Tran M T 2005 Phys. Rev. B **72** 214418
[30] V.-N. Phan and M.-T. Tran, Phys. Rev. B 2015, 92, 155201.
[31] Phan V N, Ninh Q H and Tran M T 2016 Phys. Rev. B **93** 165115
[32] Tran M T, Nguyen H S and Le D A 2016 Phys. Rev. B **93** 155160
[33] Tran T T M, Le D A, Pham T M, Nguyen T K T and Tran M T 2020 Phys. Rev. B **102** 205124
[34] Wu F Y 1982 Rev. Mod. Phys. **54** 235
[35] Feynman R P 1972 *Statistical Mechanics* (Addison-Wesley, Reading, MA, USA)
[36] Callen H B 1985 *Thermodynamics and an Introduction to Thermostatistics* (Wiley, New York, USA)
[37] Grohol D, Matan K, Cho J H, Lee S H, Lynn J W, Nocera D G and Lee Y S 2005 Nat. Mat. **4** 323