Spontaneous formation of kagome network and Dirac half-metal on a triangular lattice

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(Dated: December 12, 2014)

In spin-charge coupled systems, geometrical frustration of underlying lattice structures can give rise to nontrivial magnetic orders and electronic states. We here explore such a possibility in the Kondo lattice model with classical localized spins on a triangular lattice by using a variational calculation and simulated annealing. As a result, we find that the system exhibits a four-sublattice collinear ferrimagnetic phase at 5/8 filling for a large Hund’s-rule coupling. In this state, the system spontaneously differentiates into the up-spin kagome network and the isolated down-spin sites, which we call the kagome network formation. In the kagome network state, the system becomes Dirac half-semimetallic: the electronic structure shows a massless Dirac node at the Fermi level, and the Dirac electrons are almost fully spin-polarized due to the large Hund’s-rule coupling. We also study the effect of off-site Coulomb repulsion in the kagome network phase where the system is effectively regarded as a 1/3-filling spinless fermion system on the kagome lattice. We find that, at the level of the mean-field approximation, a $\sqrt{3} \times \sqrt{3}$-type charge order occurs in the kagome network state, implying the possibility of fractional charge excitations in this triangular lattice system. Moreover, we demonstrate that the kagome network formation with fully-polarized Dirac electrons is controllable by an external magnetic field.

PACS numbers: 71.10.Fd, 71.27.+a, 72.25.Dc

I. INTRODUCTION

The ferromagnetic (FM) Kondo lattice model, often called the double-exchange (DE) model, is one of the fundamental models for correlated electron systems. It has been extensively studied for a long time, mainly for understanding the physical properties of perovskite manganese oxides. The phase transition to the FM metallic state by decreasing temperature and the colossal negative magnetoresistance are well explained by the DE mechanism: an effective FM interaction is induced by the kinetic motion of electrons under the influence of the large Hund’s-rule coupling to localized magnetic moments. On the other hand, the competition between the FM DE interaction and the antiferromagnetic (AFM) superexchange (SE) interaction between the localized spins has also been studied intensively. In the early stage, a spin canting state with a spin-flip type ordering was predicted in the lightly doped region, which smoothly connects the AFM insulating state at half filling and a hole-doped FM metal. Later, the scenario was revisited: a phase separation (PS) was found to take place between the AFM insulator and FM metal, and hinders the canting state. In addition, at the commensurate 1/4 filling, the magnetic competition leads to the first-order transition from the FM metal to an insulator with a peculiar “flux”-type magnetic ordering.

Recently, the FM Kondo lattice model has been attracted renewed interest from the viewpoint of geometrical frustration in underlying lattice structures. In general, the geometrical frustration leads to competition between different magnetic orders, resulting in peculiar states, such as a complicated ordering, liquid-like, and glassy states. Such peculiar magnetism significantly affects the electronic state of itinerant electrons and gives rise to peculiar transport phenomena. A typical example is the unconventional anomalous (or topological) Hall effect discovered in some pyrochlore oxides. Theoretically, the topological Hall effect is caused by the coupling of itinerant electrons to a noncoplanar spin configuration with nonzero spin scalar chirality. Indeed, such mechanism was investigated in many frustrated systems, such as triangular, kagome, face-centered-cubic, and pyrochlore lattices. Fermi surface properties are important for stabilizing such noncoplanar orders. Another interesting phenomena is the unconventional anomalous (or topological) Hall effect discovered in some pyrochlore oxides. The competition between the FM DE interaction and the AFM SE interaction has also been studied in geometrically frustrated systems. For instance, a variety of magnetic phases were predicted by the mean-field analysis in kagome and pyrochlore lattice systems. Monte Carlo studies were done for a pyrochlore lattice system, and unveiled bad-metallic behavior, a peculiar PS, and a spontaneous spin Hall effect by inversion symmetry breaking. Triangular and checkerboard lattice systems were also studied by Monte Carlo simulation, and scalar chiral ordered phases were found. Furthermore, the lightly-electron doped region in the triangular lattice system was studied by variational calculations, and a noncoplanar three-sublattice spin canting order was found adjacent to a PS. These results indicate that the competition between the FM DE and AFM SE interactions leads to much richer physics in geometrically frustrated systems.

In this paper, we investigate new magnetic and electronic phases induced by the competition between the
FM DE and AFM SE interactions on a triangular lattice. We study the ground state of the FM Kondo lattice model with the AFM SE interaction by complementarily using the variational calculation and the simulated annealing. As a result, we find that a new four-sublattice collinear ferrimagnetic phase appears in the large Hund’s-rule coupling region at a commensurate 5/8 filling. In this phase, the triangular lattice system is spontaneously differentiated into a kagome network (KN) composed of up-spin sites and isolated down-spin sites. Under the KN formation, the electronic structure shows a Dirac node with linear dispersion, and the Fermi level at 5/8 filling is located just at the Dirac node. The Dirac electrons are almost fully spin-polarized by the large Hund’s-rule coupling. A similar Dirac half-semimetal was also found at 1/3 filling in a different ferrimagnetic phase in the absence of the AFM SE interaction [40]. In our KN state, however, excess electrons over half filling are effectively regarded as spinless fermions on the kagome lattice at 1/3 filling. This leads us to study the effect of the off-site Coulomb repulsive interaction between itinerant electrons in the KN phase from the interest of a fractional charge excitation on a triangular lattice. We also clarify the effect of an external magnetic field on the KN formation with half-metallic Dirac electrons.

The organization of this paper is as follows. In Sec. II we introduce the model and theoretical methods used in this paper. After introducing the FM Kondo lattice model in Sec. II A, we describe the details of the variational calculation and simulated annealing in Secs. II B and II C respectively. In Sec. III we present the results for the KN phase. We discuss the ground-state phase diagram obtained by the variational calculation (Sec. III A), the electronic structure in the KN phase (Sec. III B), and the stability of the KN phase examined by the simulated annealing (Sec. III C). In Sec. III D we present the mean-field results for the effect of the electron-electron interaction between nearest-neighbor sites and discuss the possibility of fractional charge excitations. Moreover, we discuss the effect of an external magnetic field by using the simulated annealing in Sec. III E. Finally, Sec. IV is devoted to a summary.

II. MODEL AND METHOD

In this section, we introduce the model and methods. The model is given in Sec. II A. Details of the variational calculation and the simulated annealing are described in Sec. II B and Sec. II C respectively.

A. Kondo lattice model

We consider a Kondo lattice model on a triangular lattice, whose Hamiltonian is given by

\[ \mathcal{H}_{KL} = -t \sum_{\langle i,j \rangle, \alpha} (c_{i,\alpha}^\dagger c_{j,\alpha} + h.c.) - J_H \sum_{i,\alpha,\beta} \sigma_{\alpha\beta} c_{i,\alpha}^\dagger \mathbf{S}_i + J_{AF} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \] (1)

The first term describes the hopping of itinerant electrons; \( c_{i,\alpha}^\dagger c_{i,\alpha} \) is a creation (annihilation) operator for an itinerant electron with spin \( \alpha \) on site \( i \), and \( t \) is the transfer integral. The sum \( \langle i,j \rangle \) is taken over the nearest-neighbor sites on the triangular lattice. The second term denotes the FM Hund’s-rule coupling between itinerant electron spins and localized spins: \( J_H \) is the coupling constant, \( \sigma_{\alpha\beta} = (\sigma_+^\alpha, \sigma_-^\alpha, \sigma_\times^\alpha) \) are Pauli matrices, and \( \mathbf{S}_i \) is a localized spin on site \( i \). The last term describes the AFM SE interaction with the coupling constant \( J_{AF} \) between the nearest-neighbor localized spins (\( J_{AF} \geq 0 \)). Here, we consider classical spins for \( \mathbf{S}_i \) with \( |\mathbf{S}_i| = 1 \). Note that the sign of \( J_H \) is irrelevant at \( J_{AF} = 0 \). Therefore, we take \( t = 1 \) as the unit of energy, the lattice constant \( a = 1 \), and the Boltzmann constant \( k_B = 1 \).

B. Variational calculation

In the present study, we clarify the ground-state phase diagram of the model in Eq. (1) in the parameter space of the electron filling \( n = \frac{1}{2N} \sum_i \langle c_{i,\alpha}^\dagger c_{i,\alpha} \rangle \) (\( N \) is the total number of sites), \( J_H \), and \( J_{AF} \) [see Figs. II A and II B]. In order to obtain the global structure of the phase diagram, we adopted a variational method in which we compare the ground state energies of possible ordered states. The method is the same as those used in the previous studies [17, 39], but we describe the details below for making the paper self-contained.

For the current model on the triangular lattice, we consider 13 different types of ordered states up to four-site unit cell, as shown in Fig. II C. Figure II C(1a) shows a FM order. Figures II C(2a) and II C(2b) show two-sublattice orders: (2a) a collinear stripe order and (2b) a stripe order with a canting angle \( \theta \). Figures II C(3a)-II C(3d) show three-sublattice orders: (3a) a 120° non-collinear order, (3b) a noncoplanar umbrella-type order with angle \( \theta \) (canted in the normal direction to the coplanar plane from the 120° order) which was discussed in Ref. 39, (3c) a coplanar order with canting angle \( \theta \) for two spins from 120° order, and (3d) a 2:1-type order with two parallel spins that have angle \( \theta \) to the remaining one. Figures II C(4a)-II C(4f) show four-sublattice orders: (4a) an all-out-type order which was discussed in detail in Ref. 17 and 20, (4b) a two-in two-out-type order, (4c) a three-in one-out-type order, (4d) an all-out-type order with canting angle \( \theta \) for three spins, (4e) a
FIG. 1. (Color online) Ground-state phase diagrams for the model \( J_{AF} = 0.14 \) and \( J_H \) at \( n = 5/8 \). The vertical dashed lines at \( n = 1/4, 1/2, \) and \( 3/4 \) in (a) indicate gapful insulating regions. PS stands for phase-separated region. In (b), we ignore the possibility of PS. (c) Ordering patterns of localized spins used in the variational calculations: (1a) FM order, (2a) and (2b) two-sublattice orders, (3a)-(3d) three-sublattice orders, and (4a)-(4f) four-sublattice orders (see the text in Sec. II B for details). The numbers in (3a) and (4a) indicate the sublattices at which the spins are located on the two-dimensional lattice shown in each left.

3:1 collinear order, and (4f) a coplanar order with a 90° flux-type configuration.

Among the various ordered states, we focus on the four-sublattice ferrimagnetic order (4e) in this paper. The magnetic ordering structure is collinear with three-up one-down spin configuration per four sites; the up-spin sites comprise a kagome lattice in the triangular lattice, and the down-spin sites are at the centers of the six-site hexagons in the up-spin kagome network, as shown in Fig. 1(c)(4e). We call this state (4e) the kagome network (KN) phase hereafter.

In the calculations of the ground state energy, we computed the integral over the first Brillouin zone by approximating it by the sum over grid points of \( 1600 \times 1600 \). We carefully checked the possibility of electronic PS by comparing the grand potential as a function of the chemical potential \( \mu \). For the states (2b), (3b), (3c), (3d), and (4d), we optimized the canting angle \( \theta \). Note that (2b) with \( \theta = \pi \), (3b) with \( \theta = \pi/2 \), (3c) with \( \theta = 0 \), (4d) with \( \theta = \cos^{-1}(-1/3) \), \( \theta = \cos^{-1}(+1/3) \), and \( \theta = \pi \) are equivalent to (2a), (3a), (3a), (4a), (4c), and (4e), respectively. Although an incommensurate order might take place for a general filling, we focus on uniform \( q = 0 \) orders with the magnetic unit cells listed above.

C. Simulated annealing

In order to check the stability of the KN state (4e) against other ordered states having more larger unit cells, we used the simulated annealing method. The simulated annealing is a technique for the optimization of a given function in the large parameter space \( [41] \). In the present case, we considered an enlarged magnetic unit cell including 12 sites (see the inset of Fig. 4), and optimized the localized spin configuration by the simulated annealing. Namely, temperature \( T \) is decreased gradually, and at each \( T \), the spin configuration is updated by the Monte Carlo method.
Carlo sampling. The cooling process is done in the geometrical way, i.e., \( T_{k+1} = \alpha T_k \) \((0 < \alpha < 1)\), where \( T_k \) is the temperature in the \( k \)-th step. For instance, we take \( \alpha = 0.93 \), the initial temperature \( T^i = 0.1 \), and \( k = 132 \) for the final step of cooling in the calculations (the final temperature is \( T_{132} \approx 7.4 \times 10^{-6} \)) in Secs. IIIC and IIIE.

In the Monte Carlo sampling at each \( T \), we take the summation over grid points of \( 10 \times 10 \) in the (folded) first Brillouin zone, which means that the effect of the electron-electron interaction between nearest-neighbor sites, \( \delta \), at the level of mean-field approximation. We present the phase diagram as a function of the electron filling \( n \) on the 5/8-filling KN state hereafter. This is related with the peculiar electronic structure of this state, as discussed in Sec. IIIE. At \( n = 5/8 \), however, the KN phase is stabilized in a wide region of the parameter space of \( J_{AF} \) and \( J_H \).

A. Phase diagram by the variational calculation

Figure 1(a) shows the result of the ground-state phase diagram as a function of the electron filling \( n \) and the Hund’s-rule coupling \( J_H \) at \( J_{AF} = 0.14 \). As the AFM SE interaction \( J_{AF} \) favors the 120° Néel order on the triangular lattice, the (3a) state appears in a broad parameter region as shown in the figure. The phase diagram shares many aspects with the previous results in Refs. 17 and 39: for instance, (4a) all-out chiral phases at \( n = 1/4 \) and 3/4, and (3b) umbrella-type ordered phase in the lightly-doped region.

The new finding, however, is the KN state (4e) emerging at \( n = 1/8 \) and 5/8. As described in Sec. IIIB, the magnetic structure consists of the up-spin kagome network in the triangle lattice and the down-spins at the remaining sites, as shown in Fig. 1(c) (4e). To further confirm the stability of the KN phase within the variational calculation, we consider all the possible magnetic orders in a larger 12-site unit cell (see the inset of Fig. 3) by replacing the localized spins by the Ising spins. Namely, we calculate the energies for \( 2^{12} \) states (including the equivalent states from the symmetry point of view) and compare them to find the lowest energy state. This procedure corresponds to the full parameter search within the 12-sublattice collinear spin configurations. As a result, we find that the KN state is the lowest energy state at \( n = 5/8 \), while it is not at \( n = 1/8 \). The result suggests that the (4e) phase at \( n = 1/8 \) is taken over by another ordered state with a larger unit cell, but that at 5/8 filling is stable, at least, up to the 12-site unit cell in the Ising limit. The stability of the 5/8-filling phase will be further confirmed by the simulated annealing in the Heisenberg case in Sec. IIIC. For these reasons, we focus on the 5/8-filling KN state hereafter.

As shown in Fig. 1(a), the (4e) KN state is not limited just at \( n = 5/8 \) but appears in a narrow filling region around 5/8 filling. This is related with the peculiar electronic structure of this state, as discussed in Sec. IIIE. At \( n = 5/8 \), however, the KN phase is stabilized in a wide region of the parameter space of \( J_{AF} \) and \( J_H \).

B. Dirac electrons in the kagome network phase

The KN phase found at \( n = 5/8 \) has a peculiar electronic structure at the Fermi level: the Dirac node with linear dispersion. In other words, the system is a Dirac semimetal in the KN phase. This is understood as follows. First, let us discuss the limit of \( J_H \rightarrow \infty \). In this limit, the hopping amplitude between up- and down-
spin sites becomes zero; the up-spin KN and the isolated
down-spin sites are completely separated. Consequently,
ethe electronic structure consists of two independent con-
tributions from them. The isolated down-spin sites give
rise to a flat band at $\varepsilon = \pm J_H$. Meanwhile, the up-spin
KN leads to two copies of the band structure, each of
which has the same form as that for the non-interacting
tight-binding model on the kagome lattice. The band
structure consists of two dispersive bands in the energy
range of $-4t \pm J_H \leq \varepsilon \leq 2t \pm J_H$, in addition to a flat
band at $\varepsilon = 2t \pm J_H$. Each pair of the two dispersive
bands comprises a Dirac node at $\varepsilon = \pm t \pm J_H$ at the K’
point in the Brillouin zone. At $n = 5/8$, the lower four
bands (two dispersive and two flat bands) are fully oc-
cupied, while the upper bands are occupied only up to
the Dirac point; hence, the Fermi level is located at the
Dirac node in the upper two dispersive bands.

The similar situation is seen in the KN phase for finite
but much larger $J_H$ than the noninteracting bandwidth.
Figure 2 shows the electronic structure in the KN state at
$J_H = 10$ (note that $J_{AF}$ does not change the electronic
structure up to a constant energy shift). As shown in
the figure, the electronic structure splits into two bands:
the upper (lower) band centered at $\varepsilon \simeq J_H$ ($\varepsilon \simeq -J_H$).
Each band consists of two parts: one is similar to the
kagome lattice electronic structure with the Dirac node
at $\varepsilon \simeq -t \pm 10$, and the other is a nearly-flat mode at
$\varepsilon \simeq \pm 10$, as expected from the above consideration in
the limit of $J_H \rightarrow \infty$. Although the form of each band
is modified because of nonzero hopping between up- and
down-spin sites allowed for finite $J_{AF}$, the Dirac node with
linear dispersion is preserved and the Fermi level is just
at the Dirac node, as shown in Fig. 2 [45].

The interesting point of the Dirac node is that the
Dirac electrons are almost perfectly spin-polarized; e.g.,
over 99% of the full moment at $J_H = 10$ (fully polarized
in the limit of $J_H \rightarrow \infty$). Namely, this KN state pro-
vides a half-semimetal with Dirac electrons. The Dirac
semimetal has been extensively studied from the discov-
er of graphene, from the potential for applications to
electronic devices [44]. In addition, the half-metallicity
will also be beneficial for spintronics, as the electronic
state can be manipulated by an external magnetic field.
In Sec. III E we will demonstrate such magnetic field
control. We note that a similar Dirac half-semimetal was
discussed for a three-sublattice ferrimagnetic state at 1/3
filling [40].

Now, let us discuss the stabilization mechanism of the
KN phase at 5/8 filling. The KN phase is a zero-gap semi-
conductor with the Dirac node at 5/8 filling, as shown
above. In many cases, a magnetically ordered phase is
stabilized by opening an energy gap. Indeed, in the phase
diagram in Fig. 1(a), the (4a) scalar chiral phases at 1/4
and 3/4 filling appear with opening an energy gap. The
Dirac node is not a full gap, but it may give rise to an
energy gain for the KN phase. The difference between
the full-gap insulator and zero-gap semiconductor is seen
in the phase diagram; the gapped chiral phases are lim-
ited just at 1/4 and 3/4 filling in the large $J_H$ region, as
shown in Figs. 1(a) and 1(b) (see also Fig. 3 in Ref. [17]),
whereas the zero-gap semiconducting KN phase appears
in a very narrow but a finite range of the electron filling
around $n = 5/8$ [see Fig. 1(a)]. The narrow $n$ range might
be a footprint of the fact that the Dirac node formation
contributes to the stabilization of the KN phase.

C. Stability of the kagome network phase: simulated annealing results

Next, we examine the stability of the KN phase at
5/8 filling by the simulated annealing for the enlarged
12-sites magnetic unit cell, as described in Sec. II C. We
find that it is difficult to obtain a converged result at 5/8
filling, suggesting (quasi)degeneracy with other states or
the possibility of a larger sublattice order than the 12
sites [45]. In Sec. III A however, we found that the KN
state is the lowest-energy state in the Ising limit within
the 12-site unit cell. We, therefore, performed the sim-
ulated annealing by adding the spin anisotropy in the
model (1) as

$$\mathcal{H} = \mathcal{H}_{KL} - D \sum_i (S_i^z)^2, \quad (2)$$

where the first term is the Hamiltonian in Eq. (1) and the
second term denotes the single-ion anisotropy ($D > 0$); $S_i^z$ is the $z$ component of $S_i$. Note that the limit of
$D \rightarrow \infty$ corresponds to the Ising limit.

As a result, we find that the KN state is stabilized
when we introduce a small single-ion anisotropy $D$. As
the demonstration, in Fig. 3 we show the cooling process
in the simulated annealing at $D = 0.044$. The calculation was done at $J_{H} = 10$, $J_{AF} = 0.12$, and $n = 5/8$. Figure 3 shows the energy per site, $\langle H \rangle / N$, and the spin structure factor $S(q)$ at $q = (0,0)$ as functions of cooling step (temperature) in the simulated annealing. The spin structure factor is defined as $S(q) = \frac{1}{N} \sum_{i,j} S_{i} \cdot S_{j} \exp (i q \cdot r_{ij})$, where $r_{ij}$ denotes the position vector from $i$ to $j$th site. The KN state is signaled by peaks of $S(q)$ at $q = (0,0)$, $\pm (0, 2\pi/\sqrt{3})$, $\pm (\pi, -\pi/\sqrt{3})$, and $\pm (\pi, \pi/\sqrt{3})$ with equal weights. As shown in the figure, the energy and $S(0,0)$ converge to the values expected in the KN state (dashed lines) as $T \to 0$. During the cooling process, $S(0, 2\pi/\sqrt{3})$, $S(\pi, -\pi/\sqrt{3})$, and $S(\pi, \pi/\sqrt{3})$ have the same values as $S(0,0)$ within the errorbars. The results clearly indicate that the KN state found at 5/8 filling in the variational calculation remains stable within the 12-site unit cell, at least, in the presence of a small Ising-type anisotropy.

**D. Effect of off-site Coulomb repulsion**

As discussed in Sec. III in the KN phase at 5/8 filling in the large $J_{H}$ region, the lower four bands are fully occupied and the upper bands are occupied up to the Dirac node. This electronic state is approximately regarded as the 1/3-filling state in the spinless fermion model on a kagome lattice: the doped electrons in the upper bands are almost confined in the KN with aligning their spins antiparallel to the localized up-spins because of the large $J_{H}$, and the band filling corresponds to 1/3 in the bands originating from the KN. The mapping becomes exact in the limit of $J_{H} \to \infty$. In the spinless fermion model at 1/3 filling, it was pointed out that a fractional charge excitation ($\pm e/2$, $e$ is the elementary charge) emerges when the system has a strong Coulomb repulsion between nearest-neighbor sites $\text{KL}$.

Bearing such a possibility in mind, we investigate the effect of a nearest-neighbor Coulomb repulsion on the KN formation. The Hamiltonian is given by

$$H = H_{KL} + V \sum_{\langle i,j \rangle} n_{i} n_{j},$$

where $V$ is the Coulomb repulsion between nearest-neighbor sites, and $n_{i} = \sum_{\alpha} c_{i,\alpha}^{\dagger} c_{i,\alpha}$ is a number operator for itinerant electrons on site $i$. Here, we study the effect of the $V$ term by means of the mean-field approximation. Namely, we decouple the interaction term by using the standard Hartree-Fock approximation as

$$n_{i} n_{j} \approx n_{i} \langle n_{j} \rangle + \langle n_{i} \rangle n_{j} - \langle n_{i} \rangle \langle n_{j} \rangle - \sum_{\alpha \beta} \langle c_{i,\alpha}^{\dagger} c_{j,\beta} \rangle c_{j,\beta}^{\dagger} c_{i,\alpha} - \langle c_{i,\alpha}^{\dagger} c_{j,\beta} \rangle c_{j,\beta}^{\dagger} c_{i,\alpha}.$$  

(4)

In the mean-field analysis, we assumed that configurations of the classical localized spins are (1a), (2a), (3a), (3d), and (4e) in Fig. 1(c), as these orderings appear in Fig. 1(b). In the calculation, we take 200×200 grid points in the folded first Brillouin zone.

Figure 4 shows the ground-state phase diagram at 5/8 filling obtained by the mean-field approximation. At $V = 0$, there are three phases, (1a), (4e), and (3d), while changing $J_{AF}$. The (4e) and (3d) states exhibit a charge disproportionation even at $V = 0$, because of the translational symmetry breaking by magnetic ordering; the local charge density at up-spin sites are higher than that at down-spin sites. While increasing $V$, however, an additional translational symmetry breaking appears in each region by charge ordering, i.e., a superstructure of charge density distinct from the magnetic one.

Among various charge ordered phases, we here focus on the (4e-CO) phase, which emerges from the (4e) KN phase through a second-order phase transition while increasing $V$. The (4e-CO) phase is the KN state accompanied by charge ordering with the wave number $q = (2\pi/3, 2\pi/\sqrt{3})$, that is the so-called $\sqrt{3}$ type. The charge ordering pattern is the same as that discussed for the spinless fermion model on a kagome lattice at 1/3 filling [47]. The charge-ordered state in the spinless fermion system can exhibit fractional charge excitations when an electron (a hole) is added to the 1/3-filling state [48]. Therefore, it is expected that our mean-field state (4e-CO) is connected to the phase with fractional charge excitations. In fact, a “defect” by electron (hole) doping in the (4e-CO) state can propagate without energy loss, at least for $V \gg t$ (see also Fig. 4 in Ref. [49]).
Although it is necessary to go beyond the mean-field approximation to clarify whether the KN state accommodates fractional charge excitations, this is an interesting issue since fractional charge excitations usually emerge in the systems whose lattice structures consist of corner-sharing units. The possibility in the current system on the edge-sharing triangular lattice is left for future study.

### E. Effect of external magnetic field

![Fig. 5](image.png)

**FIG. 5.** (Color online) Magnetization per site as a function of an external magnetic field in the \(z\) direction obtained by the simulated annealing supplemented by variational calculations. The data are calculated for \(J_H = 10\) and \(J_{AF} = 0.12\) at \(n = 5/8\). The (4e), (3d) and (1a) phases appear for \(0.04 \lesssim h^z \lesssim 0.16\), \(0.38 \lesssim h^z \lesssim 0.58\), and \(0.58 \lesssim h^z\), respectively. In \(0.16 \lesssim h^z \lesssim 0.38\), the 3:1 canted phase emerges. The first-order transition occurs near \(h^z \sim 0.38\). Others are continuous transition. In shaded area for \(0 \leq h^z \lesssim 0.04\), it is hard to obtain good convergence; we plot the magnetization for the 12 sublattice chiral order [45] appearing as the solution in the simulated annealing.

Finally, we discuss the effect of an external magnetic field on the KN state. We consider the Zeeman coupling to a magnetic field applied in the \(z\) direction,

\[
\mathcal{H}_Z = -h^z \sum_i S_i^z, \tag{5}
\]

as an additional term to Eq. (1). For simplicity, we neglect the coupling of orbital motion of itinerant electrons to the magnetic field.

We investigate the effect of the Zeeman term in Eq. (5) on the model in Eq. (1) by using the simulated annealing. As a result, we find that the external magnetic field stabilizes the KN phase as in the case of the single-ion anisotropy \(D\) discussed in Sec. III C. Figure 5 shows the magnetization curve calculated by combining the simulated annealing and variational calculations [46]. Here, the magnetization is defined by \(M = \sum_i S_i^z/N\). As shown in the figure, the KN phase appears for \(0.04 \lesssim h^z \lesssim 0.38\).
$h^2 \lesssim 0.16$, with exhibiting magnetization plateau at $M = 1/2$. As further increasing $h^2$, the KN phase changes into the $3\text{:}1$ canted phase for $0.16 \lesssim h^2 \lesssim 0.38$ [a four-sublattice version of the $(3d)$ phase in Fig. 1(c)], $(3d)$ phase for $0.38 \lesssim h^2 \lesssim 0.58$ [49], and finally turns into the FM phase for $h^2 \gtrsim 0.58 \sim 5J_{AF}$. The transitions at $h^2 \sim 0.16$ and 0.58 are both continuous, whereas at $h^2 \sim 0.38$ is of first order. We note that both the $3\text{:}1$ and $(3d)$ $2\text{:}1$ canted phases are magnetic counterparts of supersolid [51, 52].

The result suggests an interesting controllability of the Dirac electronic state; i.e., one can destroy and create the Dirac electrons by sweeping the magnetic field. While increasing the magnetic field, it shows a transition to a magnetic supersolid phase, in which exotic behavior is expected as well. Furthermore, once the KN phase exhibits fractional charge excitations in the presence of $V$ (see Sec. III), there is the possibility of controlling the appearance of fractional charge excitations by magnetic field.

IV. SUMMARY

We have investigated the Kondo lattice model on a triangular lattice by using the variational calculation and the simulated annealing method. As a result, we found that the system exhibits the kagome network state at a special filling $n = 5/8$ for the large Hund’s-rule coupling. In the kagome network state, the system is spontaneously divided into two parts by the four-sublattice collinear ferromagnetic order: one is the kagome lattice composed of up-spin sites, and the other is isolated down-spin sites in the hexagons of the kagome lattice. This peculiar magnetism gives rise to an unusual electronic state: a Dirac half-semimetallic state. The semimetallic dip of the density of states due to the Dirac node formation contributes to the stabilization of the kagome network phase. We have also found that a $\sqrt{3}\times\sqrt{3}$-type charge order occurs in the kagome network state as the mean-field solution when we include the Coulomb repulsion between nearest-neighbor sites. This charge ordering pattern is the same as that for the spinless fermion model on a kagome lattice at $1/3$ filling discussed from the interest of fractional charge excitations. Moreover, we have found that the emergence of the kagome network Dirac half-semimetal can be controlled by an external magnetic field. Considering real materials, the parameters used in the present calculations are reasonable to some extent: the Hund’s-rule coupling $J_H$ is dozens of times larger than the transfer integral, and it is one- or two-orders of magnitude larger than the antiferromagnetic superexchange interaction $J_{AF}$ and the single-ion anisotropy $D$. These energy scales are seen in some real materials, such as manganese oxides. It is desired to explore the kagome network phase discussed in the paper in real systems as a candidate for the peculiar Dirac half-metal and possible fractional charge excitations.

ACKNOWLEDGMENTS

We acknowledge helpful discussions with Chisa Hotta, Takahiro Misawa, and Masafumi Udagawa. Y.A. thanks Satoru Hayami, Ryu Ki Kaneko, Yuichi Motoyama, and Junki Yoshitake, and Hiroaki T. Ueda for helpful comments. Y.A. was supported by Grant-in-Aid for JSPS Fellows. Y.A. acknowledges support from Okinawa Institute of Science and Technology Graduate University. This work was supported by Grants-in-Aid for Scientific Research (Grant Nos. 21340090, 22540372, and 24340076) Global COE Program “the Physical Sciences Frontier,” the Strategic Programs for Innovative Research (SPIRE), MEXT, and the Computational Materials Science Initiative (CMSI), Japan.

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