Quantum Phases of Kagome Electron System with Half-Filled Flat Bands

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We study the quantum phase diagram of spinful fermions on kagome lattice with half-filled lowest flat bands. To understand the competition between magnetism, flat band frustration, and repulsive interactions, we adopt an extended $t$-$J$ model, where the hopping energy $t$, antiferromagnetic Heisenberg interaction $J$, and short-range neighboring Hubbard interaction $V$ are considered. In the weak $J$ regime, we identify a fully spin-polarized phase, which can further support the spontaneous Chern insulating phase driven by the short-range repulsive interaction. This phase still emerges with in-plane ferromagnetism, whereas the non-interacting Chern insulator disappears constrained by symmetry. As $J$ gradually increases, the ferromagnetism is suppressed and the system first becomes partially-polarized with large magnetization and then enters a non-polarized phase with the ground state exhibiting vanishing magnetization. We identify this non-polarized phase as an insulator with a nematic charge density wave. At the end, we discuss the potential experimental observations of our theoretical findings.

Introduction—. Kagome lattice featuring Dirac dispersion and flat bands has been extensively studied in transition metal compounds [1–10]. The interplay between strong correlations of $d$ electrons and spin-orbit coupling leads to various magnetic orders and topological phases in compounds with kagome layers of Fe, Co or Cr [1–10]. Specifically, quasi-two-dimensional (2D) massive Dirac dispersion and anomalous Hall effect have been experimentally observed in Fe$_3$Sn$_2$ compound [1–8]. Evidence of flat bands has also been experimentally observed in materials with different magnetisms. The ferromagnetic Co$_3$Sn$_2$S$_2$ exhibits flat bands with strong negative orbital magnetization and anomalous Hall effect, which may originate from the topological band gap opened by spin-orbit coupling [3]. FeSn shows flat bands in a large region of the Brillouin zone [8, 9], where the kagome layer shows in-plane ferromagnetism and is coupled to its neighboring layers anti-ferromagnetically. In YCr$_6$Ge$_6$ and CoSn, however, the magnetism has not yet been observed [10, 11]. Such abundant phases suggest that the synergetic effect of interaction, magnetism, and flat band topology may play a very important role in understanding some of these experimental systems [1–3].

In the presence of strong electron-electron interactions, the instability of Dirac dispersion and flat band with quadratic band touching is of great theoretical interest [12–22]. In the spinless case, the band touching is shown to be unstable against interactions, leading to spontaneous Chern insulator [24–26]. In the spinful case [35–41], kinetic ferromagnetism has been proposed by exact diagonalization study at the half-filled flat band case in the limit of $|t| \ll V < U$, i.e., the hopping energy is much smaller than the on-site ($U$) and the first nearest neighbor Coulomb interaction ($V$) [41]. More numerical evidences are still highly demanded and the intermediate parameter regime of $V \sim t$ has not yet been studied. Inspired by the recent experimental progress on these kagome metals, we explore the quantum phase diagram of kagome system at this regime with half-filled flat bands by including the Coulomb interaction up to the second nearest neighbor.

In this Letter, we theoretically investigate the interplay of topological phases and magnetism in the pres-
ence of strong correlation based on the extended \( t-J \) model on kagome lattice, where \( J \) is the antiferromagnetic exchange interaction between the nearest neighbor sites and \( V \) is the repulsive interaction up to the second nearest neighbor sites. For electrons at the half-filling of the lowest flat band, we identify three phases to be a fully spin-polarized phase with spontaneous Chern insulator, a partially spin-polarized intermediate phase, and a spin-unpolarized phase with symmetry breaking nematic charge density wave as the exchange interaction \( J \) increases. The spontaneous Chern insulator emerges in the fully spin-polarized phase at a small \( J \) and is independent of the direction of spin polarization, which distinguishes itself from the traditional spin-orbit coupling induced Chern insulator. Along with the increase of \( J \), the system first undergoes a quantum phase transition to the partially spin-polarized phase and finally to a non-magnetic phase that exhibits a charge-density-wave order. These different quantum phases exhibit distinct responses by applying an external Zeeman field.

Model and methods—. We consider a kagome lattice of spinful fermions described by an extended \( t-J \) model with the Hamiltonian written as:

\[
H = t \sum_{\langle ij \rangle, \alpha} c_{i,\alpha}^\dagger c_{j,\alpha} + J \sum_{\langle ij \rangle} (S_i \cdot S_j - \frac{1}{4} n_i n_j) + V_1 \sum_{\langle ij \rangle} n_i n_j + V_2 \sum_{\langle \langle ij \rangle \rangle} n_i n_j,
\]

where \( c_{i,\alpha}^\dagger \) (\( c_{i,\alpha} \)) is the creation (annihilation) operator of a fermion with spin \( \alpha = \{\uparrow, \downarrow\} \) at site \( i \) and \( n_i = \sum_{\alpha} c_{i,\alpha}^\dagger c_{i,\alpha} \) is the particle number operator. \( S_i = (S_i^x, S_i^y, S_i^z) = \sum_{\alpha, \beta} c_{i,\alpha}^\dagger \sigma^{x,y,z}_{\alpha,\beta} c_{i,\beta} \) is the spin operator with \( \sigma^{x,y,z} \) being Pauli matrices. The hopping term \( t \) is set to be the energy unit, which makes the lowest energy band flat and quadratically touching with the middle one. The second term represents the exchange interaction with strength \( J > 0 \) (antiferromagnetic type) between each pair of nearest neighbor sites. The third and fourth terms are the repulsive interactions between electrons of first \( \langle \langle ij \rangle \rangle \) and second \( \langle \langle \langle ij \rangle \rangle \rangle \) nearest neighbors with strengths \( V_1 \) and \( V_2 \), respectively. The Hilbert space is constrained by the no-double occupancy condition, \( n_i \leq 1 \), which corresponds to the \( U = \infty \) limit.

We focus on the one-sixth filling case in a finite system of \( N_x \times N_y \) unit cells with total number of sites \( N_s = 3 \times N_x \times N_y \) and the number of fermions \( N_c = 2N_s/6 \). Without loss of generality, we take \( V_1 = 2V_2 = V \) in our calculations. The Zeeman field \( B_0 \) and spin-orbit coupling \( t_{SO} \) are set to zero unless otherwise noted. To characterize the ground states of the system with interactions, we employ the finite density matrix renormalization group (DMRG) algorithm \([12][43]\) on cylinder geometry, where the boundary is open (periodic) along \( x \) (\( y \))-direction, respectively. In DMRG calculations, we set \( N_g \) up to 4 unit cells (8 lattice sites) and keep the DMRG states up to \( M = 12000 \) to guarantee a good convergence (with the truncation error smaller than \( 10^{-5} \)).

Phase diagram—. As each spin component is conserved in our model, the ground states are calculated in sub-Hilbert space with total azimuthal spin \( S_z \) ranging from 0 to \( S_{max} \) with \( S_{max} = N_c/2 \) (results are symmetric about positive and negative total \( S_z \)). For a system of \( N_s = 3 \times 3 \times 4 = 36 \), we numerically calculate the ground-state energies for different \( S_z \) sector in the parameter space spanned by extended Hubbard interaction \( V \) and exchange interaction \( J \). We identify three phases as shown in Fig. 1(a) according to the polarization of the ground state. In phase-I, the system is fully spin-polarized, i.e., the ground states of different spin \( S_z \) ranging from \( -S_{max} \) to \( S_{max} \) are all degenerate with a total spin \( S = N_c/2 \). Our results suggest that the spontaneous ferromagnetization in this system is very strong, which can survive to finite antiferromagnetic coupling \( J \sim 0.4 \). Interestingly, an intermediate interaction strength \( V \sim 0.8 \) can further enlarge the regime of the fully polarized phase. For intermediate \( J \), the ground state jumps from \( S = N_c/2 \) to a partially spin-polarized state with a smaller total \( S \) driven by antiferromagnetic coupling, which is illustrated as phase-II. When \( J \) further increases, the partially polarized phase also becomes excited states and the ground state lies in the spin sector of total \( S = 0 \) labeled as phase-III in Fig. 1.

We further compare results from different system sizes to show the robustness of the quantum phase diagram. As shown in Fig. 1(b) at fixed \( V = 0.6 \), we present the energy difference \( E_{g}\left|\uparrow\downarrow\right> - E_{g}\left|\downarrow\uparrow\right> \) between ground state energy at different \( S_z = 0,1, S_{max} \) as a function of \( J \), for three different system sizes \( N_s = 3 \times 4 \times 3 = 36 \), \( 3 \times 4 \times 4 = 48 \) and \( 3 \times 3 \times 8 = 72 \) sites, respectively. The same energy
evolution with $S_z$ is identified for these different systems. For a smaller $J$, the ground state has a total $S = S_{\text{max}}$ and the lowest energies from each $S_z$ sector has the same energy, representing a $2S + 1$ magnetic degeneracy. For $J = 0.8$ of the phase-II, the ground state has a smaller total $S$, thus $E_g^{S_{\text{max}}} - E_g^0 > 0$ while $E_g^0 - E_g = 0$ representing the same total $S$ states with different $S_z$. For $J > 1.0$, both $E_g^{S_{\text{max}}} - E_g^0 > 0$ and $E_g^0 - E_g > 0$ and the ground state of the whole system is inside the $S = 0$ sector.

Spontaneous chiral current—. In the ferromagnetic phase, the ground state possesses full spin-polarization. This system thus reduces to a $t$-$V$ model of spinless fermions. For this model, the system is a semi-metal with quadratic band crossing at the Fermi point in the non-interacting limit of $V = 0$. In the presence of a finite interaction $V$, a spontaneous Chern insulator can be established as demonstrated in previous work [24], where the ground states show two-fold degeneracy with opposite chiralities. Here, we demonstrate the spontaneous chiral currents for all three phases. We consider a chiral-symmetry-breaking hopping term $h_C = \chi t_C \sum_{\alpha} c_{i,\alpha}^\dagger c_{j,\alpha}$ as a perturbation, where $t_C \ll t = 1$ is small and $\chi = \pm 1$ when the electron hopping is clockwise/anti-clockwise in each triangle. We can then detect the loop current following the Hellmann-Feynman theorem [26, 10, 44] via

$$J(j) = \frac{1}{2N_s} \frac{\partial E(t_C)}{\partial t_C} |_{t_C \to 0},$$

where $E(t_C) = \langle \Psi | H(h_C) | \Psi \rangle$ with $| \Psi \rangle$ being the ground state of the system and $N_s$ is the number of sites. In Fig. 2(a), we show the ground state energy difference $E_g^0(t_C) - E_g^0(t_C = 0)$ as a function of $t_C$ for $N_s = 36$ with $J = 0.4$, 0.8, and 1.4 representing three different phases, respectively. One can find that in the ferromagnetic region, the dependence of ground state energy decreases linearly as a function of $t_C$ (we use small $t_C$ up to 0.008) corresponding to a loop current of $j = 0.028$ for each triangle. The constant current at weak $J$ is robust against the system size $N_s$, as shown in Fig. 2(b) where the scaling behavior of the current as a function of $1/N_s$ is plotted by the red line with solid circles. We find that the current is finite in the order of $10^{-2}$ at the large $N_s$ limit, suggesting the existence of finite current in the thermodynamic limit. The finite current supports the quantum anomalous Hall effect for phase-I with nonzero $V$.

For partially polarized and nonmagnetic phases with $J = 0.8$ and $J = 1.4$, the ground state energy decreases near quadratically with $t_C$ as shown in Fig. 2(a). For $J = 0.8$, the current keeps a small value whereas the current drops a lot at $J = 1.4$ as $N_s$ increases. We caution that because of the quadratic behavior of currents for phase region II and III, we will see much reduced or vanishing current if we take the small $t_C$ limit, which is negligible as it is related to an energy difference at the same order as the relative error in DMRG.

Effect of Zeeman field—. The presence of ferromagnetism indicates that the insulating quantum phases can be tuned by applying external Zeeman field $h_Z = B_z \sum_i S_i^z$ from either external magnetic fields or a proximity effect to ferromagnetic layers nearby. As the Zeeman field term commutes with the Hamiltonian Eq. (1), the calculated ground states of each $S_z$ sector are also eigenstates of the system with the Zeeman field term, but with eigenenergies being shifted by the field. The ground states of each spin $S_z$ sector are calculated for different exchange interaction $J = 0.4$, 0.8, 1.0, and 1.4 for a system with $N_s = 3 \times 3 \times 8 = 72$ as shown in Fig. 3(a) without the Zeeman field. One finds that at $J = 0.4$, all the ground state energies at different $S_z$ are degenerate and thus they show the same total spin $S = N_s/2$. The degeneracy indicates that the ground state will be fully polarized along the field direction in the presence of infinitesimally weak perturbation as illustrated in Fig. 3(b) where the average spin polarization of each unit cell $M$ is plotted as a function of $B_z$. As $J$ increases to around $0.8 \sim 1.0$, the ground states become partially polarized with total spin $S < N_s/2$. When $J$ is further increased to 1.4, the degeneracy is completely lifted and the ground state lives in the $S_z = 0$ sector as a nonmagnetic phase. For these partially polarized and nonmagnetic phases, the presence of a nonzero Zeeman field can enhance the magnetization as shown in Figs. 3(c) and (d), respectively. In the large Zeeman field limit, the ground state

FIG. 3: (a) Energy difference between ground state energy at each spin sector and that at maximal spin sector for different $J = 0.4$, 0.8, 1.0, and 1.4 for $N_s = 72$ site system. (b)-(d) Average magnetization of each electron of the ground state as function of Zeeman field $B_z$ for $J = 0.4$, 1.0, and 1.4. Inset in (b): Schematic plot of splitting of degenerate ground states with spontaneous QAHE of Chern number $C = \pm 1$ due to the presence of spin-orbit coupling as function of its magnitude $t_{SO}$. 

*References:* [24]
will become fully spin polarized, which also has a chiral current and quantum anomalous Hall effect since the nature of this state is identical to the spontaneous polarized state (phase I).

Moreover, in a fully spin-polarized phase with out-of-plane magnetization, the presence of Kane-Mele type spin-orbit coupling \( \Delta \) can lift the two-fold degeneracy between right- and left-handed ground states with Chern numbers of \( \pm 1 \) as illustrated in the inset of Fig. 3(b). This indicates that, by changing the sign of either spin-orbit coupling or Zeeman field, a topological phase transition between ground states with opposite Chern number can be realized, which is in agreement with the experimentally observed spin-dependent orbital-magnetization in CoSbS

**Nematic charge density wave—.** To characterize the quantum phase at phase-III, we measure the density, bond, and current of the ground state. We find that the ground state is a non-magnetic insulator with a nematic charge density wave as illustrated below. In Fig. 4(a), we plot the expectation value of electron number operator \( n_i \) at each site, where the circle size is proportional to the electron number \( \langle n_i \rangle \). One can find that the charge densities for different sublattices are imbalanced, where A and B sites show similar densities, which are much larger than that of sublattice C. The intra-unit cell charge density difference \( \delta n_i = n_{A,i} - n_{C,i} \) at \( i \)th unit cell is plotted as a function of the unit cell position \( i_x \) in the inset of Fig. 4(b). The charge imbalance away from the boundaries shows weak spatial dependence. Such a charge-density pattern preserves the translation symmetry of the system while breaks the rotation symmetry leading to the nematicity. We have checked that such a density pattern is robust as we increase the width \( L_y \) of cylinder systems. The insulating nature of this phase is characterized by a charge excitation gap \( \Delta_{2e} = E^0_g(N_e + 2) + E^0_g(N_e - 2) - 2E^0_g(N_e) \) at ground state spin sector of \( S_z = 0 \) by adding/removing two electrons (one spin up and one spin down). The scaling behavior of the charge gap as a function of \( 1/N_x \) is plotted in Fig. 4(b), where one can find that the charge gap is finite in thermodynamic limit suggesting the system is an insulator.

Since \( J \) represents the strength of the antiferromagnetic coupling, we also check if there is any magnetic order. We show that the state is non-magnetic due to the small site filling number where the antiferromagnetic coupling becomes less efficient. The spin-spin correlation \( \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \) decreases exponentially as a function of the distance between two sites as shown in the lower panel of Fig. 4(c), where the correlation between sites \( i \) and \( j \) with the same \( y \) coordinate is plotted as a function of their distance \( i_x - j_x \) along \( x \)-direction. We also study the single-particle Green function \( G_{ij} \equiv i\langle \mathcal{O}_i \mathcal{O}_j \rangle \) as shown in the upper panel of Fig. 4(c) where the magnitude of \( G_{ij} \) also decreases exponentially as the distance increases, being consistent with a charge insulator state.

**Summary and discussion—.** We have demonstrated the quantum phase diagram of a kagome lattice with 1/6 filling of spinful fermion, where the lowest flat-band is half-filled by considering the extended Hubbard repulsion interaction \( V \) and nearest neighbor antiferromagnetic exchange interaction \( J \). In the weak \( J \) regime, the system exhibits a fully spin-polarized ferromagnetic phase, which hosts a topologically nontrivial spontaneous Chern insulator state in the presence of a finite \( V \). As the antiferromagnetic exchange interaction increases, a quantum phase transition to a partially spin-polarized phase occurs. Further increasing \( J \) leads to a non-magnetic insulating phase with nematic charge density wave order. For these partially polarized and nonmagnetic phases, the presence of a nonzero Zeeman field can enhance the magnetization.

In the fully spin-polarized ferromagnetic phase, the presence of an infinitesimal Zeeman field selects the ground state with spins polarized parallel to the field direction. The spontaneous Chern insulator phase emerges independent of the spin orientation. In contrast, the non-interacting ferromagnetic Chern insulator from spin-orbit coupling shows a strong dependence on the spin polarization, which disappears when the polarization changes to the in-plane direction \( \mathbf{g} = (0,0,\pm 1) \). Our work provides a way to distinguish the physical mechanisms of the Chern insulator for realistic materials. As the quadratic band crossing and flat band features of CoSbS are close to the Fermi energy, we suggest that one can measure the anomalous Hall effect or orbital magnetization when the ferromagnetism is aligned in the plane by external Zee-
man field to detect if there is a spontaneous Chern insulator phase driven by interaction $\Gamma_2$. Besides, kagome lattices in metal-organic frame, monolayers of carbon, and boron exhibiting half-filled flat bands have also been reported [33, 40], which provide ideal platforms to test our theory manifested by Hall effect with in-plane ferromagnetism.

It is noteworthy that one band model is employed in this work that mimics the $d_{z^2}$ orbital in 2D layers. The flat bands contributed from $d_{z^2}$ near the Fermi level have been observed in YCr$_2$Ge$_6$ [10], which however is non-magnetic metal rather than an insulator with charge density wave. The disagreement might be attributed to the multi-band effect and difference of dimensionality. The 3D nature of the kagome metals makes it difficult to tune the carrier density and thus the filling factors of flat bands. Moreover, the flat bands contributed from other $d$-orbitals have also been observed in bulk materials [7–9, 11]. The effects of interaction on those bands are of great theoretical interest and deserve to explore in the future.

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See Supplemental Material for a detailed discussion on the band topology of kagome lattice with spin-orbit coupling and ferromagnetism.