Spontaneous symmetry breakings in two-dimensional kagome lattice

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We study spontaneous symmetry breakings for fermions (spinless and spinful) on a two-dimensional kagome lattice with nearest-neighbor repulsive interactions in weak coupling limit, and focus in particular on topological Mott insulator instability. It is found that at \(1/3\)-filling where there is a quadratic band crossing at \(\Gamma\)-point, in agreement with Ref\textsuperscript{1}, the instabilities are infinitesimal and topological phases are dynamically generated. At \(2/3\)-filling where there are two inequivalent Dirac points, the instabilities are finite, and no topological phase is favored at this filling without breaking the lattice translational symmetry. A ferromagnetic quantum anomalous Hall state with infinitesimal instability is further proposed at half-filling of the bottom flat band.

Introduction. —Recent interests have been revived in Fermi surface instabilities in connection with dynamic generation of topological Mott insulators\textsuperscript{1–4}. The first step is forwarded by Wu and Zhang\textsuperscript{3,4} where a new mechanism of generating spin-orbit coupling in strongly correlated, nonrelativistic systems is proposed. Attention is then focused in particular when the Fermi surface shrinks into discrete points, usually as band-crossing points (BCP), where the quasi-particle excitations are not described by the Fermi liquid theory. Two examples are discussed in two-dimensional (2-D) honeycomb\textsuperscript{5} and checkerboard lattices\textsuperscript{6} with \(C_6\) and \(C_4\) rotational symmetry respectively. In the honeycomb lattice, the BCPs have linearly vanishing density of states (DOS) at the Dirac points. Therefore only a full gap opening at the filling to the Dirac points could facilitate gaining energy, and the nodal phase becomes unstable only above finite critical interactions. While in the checkerboard lattice, the BCP has quadratic dispersion with constant DOS in 2-D, so that any gap opening at the BCP would help to gain energy and lead to the infinitesimal instabilities of the spontaneous breaking of rotational or time-reversal symmetries (TRS).

Infinitesimal instabilities were proposed in 2-D systems with a quadratic BCP, which is protected by TRS and \(C_4\) or \(C_6\) rotational symmetry\textsuperscript{1,5}. In the explicit example with \(C_4\) symmetry in checkerboard lattice\textsuperscript{6} unequal next-nearest neighbor hoppings connected and not by diagonal bonds are required to make the BCP quadratic, which makes it hard to search for real materials. In this work, we suggest to realize the infinitesimal topological instabilities in 2-D kagome lattice with \(C_6\) symmetry, where the kagome compound herbertsmithite\textsuperscript{10–12} appears to be a good candidate. The kagome lattice is a triangular lattice with three sites per unit cell, see Fig[1] Within only the nearest-neighbor (nn) hopping, it has three bands, the top two bands cross at two inequivalent Dirac points and the bottom is a flat band. However, interestingly, by considering a small next-nearest neighbor (nnn) hopping, the flat band becomes dispersive, and its band structure shows both quadratic and Dirac BCPs at \(1/3\) and \(2/3\)-fillings separately, which facilitates us to stress the differences of these two types of BCPs in a very same system. Although the magnetic properties of kagome lattice were studied extensively\textsuperscript{13–15}, only little attention has been paid to its nonmagnetic insulating behavior, especially the physics near the quadratic BCP. Recently, topological phases with broken TRS and quantized Hall conductance on kagome lattice have been studied for non-interacting fermions\textsuperscript{16–18}, while interacting fermions with broken symmetries are rarely explored. Finally, we propose that a ferromagnetic quantum anomalous Hall phase with infinitesimal instability can be naturally realized at the half-filling of the bottom flat band.

Symmetries and order parameters. —Before discussing specific models we first analyze the symmetries and define order parameters. The symmetries of importance on kagome lattice under considerations are i) reflection symmetry between up (dark) and down (gray) triangles, by breaking which together with TRS, a quantum anomalous Hall state is spontaneously generated.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.jpg}
\caption{Kagome lattice. There are three sites (“A, B, C”) per unit cell, \(b_1, b_2\) are bravais vectors. The arrows on the links represent currents respecting the reflection symmetry between up (dark) and down (gray) triangles, by breaking which together with TRS, a quantum anomalous Hall state is spontaneously generated.}
\end{figure}

\(K_1 - K_2\)
in the susceptibilities, where \( \mathbf{K}_1 \) and \( \mathbf{K}_2 \) are the two Dirac points. This is always true at \( \frac{\pi}{3} \)-filling because there is only one BCP at \( \Gamma \)-point, and the instabilities occur only at \( q = 0 \) which preserves the lattice translational symmetry. Based on the symmetry considerations, we introduce the order parameters as below. Note that in the case of spinless fermions, since the order parameters, defined only in the sublattice space with \( \Psi_k = (C_{kA}^\dagger C_{kB}^\dagger C_{kC}^\dagger) \), have the same form as those in the spinful case, we only write down the order parameters in spinful case explicitly. For site order, the order parameters are \( N^\nu(n^\nu) = \langle \Psi | \tau^\nu \otimes I_z(R_s) | \Psi \rangle \), where \( \nu = 0, 1, 2, 3 \) and \( \Psi_k = (C_{kA}^\dagger C_{kB}^\dagger C_{kC}^\dagger C_{kA} C_{kB} C_{kC}) \). Here \( \tau^\nu \) are Pauli matrices in spin space, and \( I_z = \text{diag}(1 1 1) \). The order parameters under considerations are \( \Delta^u_{n(d)} \) which don’t break any symmetry. While \( \Delta^d_{n} \) is responsible for the bond density wave (BDW) phase at \( \frac{\pi}{3} \)-filling, the nematic order parameters pull the two Dirac points closer for small \( V \). While at large \( V \), the two Dirac points with opposite Berry phases annihilate each other and open a full gap to gain energy. Therefore the nematic order is always a competing phase at both fillings. The phase transition into nematic phase is of first order.

For bond order, due to the frustration of the nn repulsive interactions, we consider the possibilities of breaking reflection symmetry (or parity) between up and down triangles and TRS, while conserve the \( C_3 \) rotational symmetry (\( S_{\nu}^u(0) = 0 \)). The order parameters, \( \Delta^u_{n(d)} \), lead to four independent ones, \( \Delta_{R_L} = \frac{1}{2} \text{Re}(\Delta_u) \pm \text{Re}(\Delta_d) \) and \( \Delta_{L \pm} = \frac{1}{2} \text{Im}(\Delta_u) \pm \text{Im}(\Delta_d) \). Among these, \( \Delta_{R+} \) is only a renormalization of the nn hopping energy \( t \) and doesn’t break any symmetry. While \( \Delta_{R-} \) breaks the parity and is responsible for the bond density wave (BDW) phase where the hopping amplitude differs in up and down triangles. This order parameter will remain the degeneracy of \( \Gamma \)-point at \( \frac{\pi}{3} \)-filling, but opens a full gap at \( \frac{\pi}{3} \)-filling thus gain energy. For the imaginary parts which break the TRS generally, \( \Delta_{L \pm} \) respects the parity and corresponds to a staggered flux picture, this order parameter won’t open a gap at \( \Gamma \)-point, and only shifts up-and-down the energies at the two Dirac points. While \( \Delta_{L \pm} \) breaks both parity and TRS giving rise to the quantum anomalous Hall (QAH) phase with topologically protected edge states and opens a full gap at both fillings.

The mean-field Hamiltonian for spinless fermions with only nn repulsive interactions is

\[
H = t \sum_{\langle ij \rangle} (c_{ij}^\dagger c_{ij} + h.c.) - t' \sum_{\langle ij \rangle} (c_{ij}^\dagger c_{ij} + h.c.) + V \sum_{\langle ij \rangle} n_i n_j
\]

where \( t' \cdot t > 0 \) is a small nnn hopping which is taken according to the transfer integrals in a natural spin-1/2 kagome compound known as herbertsmithite. The nnn hopping term makes the bottom flat band dispersive and quadratic at the \( \Gamma \)-point with which the Fermi surface crosses at \( \frac{\pi}{3} \)-filling. However this term won’t affect the low energy expansion near the Dirac points at \( \frac{\pi}{3} \)-filling. The nn repulsive interactions for side order will in general favor the nematic phase, which breaks the \( C_3 \) rotational symmetry, with complex order parameter \( n = \langle n_A \rangle + e^{i\omega_0} \langle n_B \rangle + e^{2i\omega_0} \langle n_C \rangle \), where \( \langle n_A \rangle = \langle c_{iA}^\dagger c_{iA} \rangle \). There are two independent order parameters in this phase, the real part of \( n \) depicts the picture that the charge densities are equal on sites \( B \) and \( C \) but different on site \( A \), while the imaginary part of \( n \) visualizes that the charge densities on the three sites are all different. At \( \frac{\pi}{3} \)-filling, the nematic order parameters split the quadratic touching at \( \Gamma \)-point with \( 2\pi \) Berry phase into two Dirac points with \( \pi \) Berry phase each, thus open a gap at \( \Gamma \)-point to gain energy. At \( \frac{\pi}{3} \)-filling, the nematic order parameters pull the two Dirac points closer for small \( V \). While at large \( V \), the two Dirac points with opposite Berry phases annihilate each other and open a full gap to gain energy. Therefore the nematic order is always a competing phase at both fillings. The phase transition into nematic phase is of first order.

Our numerics show that the nematic phase will stabilize at large \( V \) for both fillings with \( \text{Re}(n) = \pm 1 \) respectively, where the charge densities reside all in \( A \)-site at \( \frac{\pi}{3} \)-filling and equally in \( B \)- and \( C \)-sites at \( \frac{\pi}{3} \)-filling.

For bond order, due to the frustration of the nn repulsive interactions, we consider the possibilities of breaking reflection symmetry (or parity) between up and down triangles and TRS, while conserve the \( C_3 \) rotational symmetry (\( S_{\nu}^u(0) = 0 \)). The order parameters, \( \Delta^u_{n(d)} \), lead to four independent ones, \( \Delta_{R_L} = \frac{1}{2} \text{Re}(\Delta_u) \pm \text{Re}(\Delta_d) \) and \( \Delta_{L \pm} = \frac{1}{2} \text{Im}(\Delta_u) \pm \text{Im}(\Delta_d) \). Among these, \( \Delta_{R+} \) is only a renormalization of the nn hopping energy \( t \) and doesn’t break any symmetry. While \( \Delta_{R-} \) breaks the parity and is responsible for the bond density wave (BDW) phase where the hopping amplitude differs in up and down triangles. This order parameter will remain the degeneracy of \( \Gamma \)-point at \( \frac{\pi}{3} \)-filling, but opens a full gap at \( \frac{\pi}{3} \)-filling thus gain energy. For the imaginary parts which break the TRS generally, \( \Delta_{L \pm} \) respects the parity and corresponds to a staggered flux picture, this order parameter won’t open a gap at \( \Gamma \)-point, and only shifts up-and-down the energies at the two Dirac points. While \( \Delta_{L \pm} \) breaks both parity and TRS giving rise to the quantum anomalous Hall (QAH) phase with topologically protected edge states and opens a full gap at both fillings.

The mean-field Hamiltonian for spinless fermions is

\[
H_{MF} = E_0 + \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} [h_0(\mathbf{k}) + h_1(\mathbf{k})] \Psi_{\mathbf{k}}
\]

The first term in the Hamiltonian includes the nn and nnn hoppings, and

\[
h_1(\mathbf{k}) = -V \begin{pmatrix}
2\langle n_A \rangle & \Delta_u^* + \Delta_d e^{-i\pi_2} & \Delta_u + \Delta_d e^{i\pi_1} \\
\Delta_u^* + \Delta_d e^{i\pi_2} & 2\langle n_B \rangle & \Delta_u^* + \Delta_d e^{-i\pi_3} \\
\Delta_u^* + \Delta_d e^{-i\pi_1} & \Delta_u^* + \Delta_d e^{i\pi_3} & 2\langle n_C \rangle
\end{pmatrix}
\]

with \( E_0 = \frac{4V}{3} [\text{Re}(n)^2 + \text{Im}(n)^2] + 6V[\Delta_{R+}^2 + \Delta_{R-}^2 + \Delta_{L+}^2 + \Delta_{L-}^2] \).
FIG. 2: (Color online). Finite temperature mean-field phase diagram for spinless fermions in kagome lattice at $\frac{1}{3}$-filling with $t'/t = 0.3$. Thick and thin lines are respectively second and first order transitions.

The mean-field free energy is obtained as

$$F(n, \Delta_u, \Delta_d) = E_0 - \frac{1}{\beta L^2} \sum_{\text{all}} \log \left(1 + e^{-\beta E_i}\right)$$

where $\beta = 1/k_B T$, and $L^2$ is the number of unit cells. Since the order parameters are classified by different symmetries they usually order at different $T_c$, therefore by minimizing the free energy with respect to the order parameters separately, we could study the mean-field phase diagram at finite temperatures. The phase diagram at $\frac{1}{3}$-filling is shown in Fig. 2 where we see that the instabilities are infinitesimal at this filling, i.e., the symmetries are broken at low temperatures for arbitrarily weak interactions. However this infinitesimal instability is absent in the phase diagram at $\frac{2}{3}$-filling due to the vanishing DOS at Fermi level. Our numerics show that at zero temperature, there are two quantum phase transition points. For small $V$, the system remains in the semi-metal phase, till $V_{c1} = 1.85t$, the system goes into the BDW phase, and finally stabilizes in the nematic phase for $V \geq V_{c2} = 2.55t$. Note that the QAH phase never dominates in the phase diagram at $\frac{1}{3}$-filling near the Dirac points without breaking the lattice translational symmetry.

The infinitesimal instabilities are predicted in Ref. 3 in both checkerboard and kagome lattices with $C_4$ and $C_6$ symmetries, where the phase diagram is obtained in checkerboard lattice at half-filling. Here we see that for spinless fermions on kagome lattice, similar phase diagram is obtained at $\frac{1}{3}$-filling by lifting the degeneracies of the flat band and make it quadratic at $\Gamma$-point. The infinitesimal instability at $\frac{1}{3}$-filling on kagome lattice can be seen more clearly by projecting the mean-field Hamiltonian into the two low energy states $\Phi = (\phi_1 \phi_2)$ near $\Gamma$-point as

$$H_{\text{eff}} = \frac{1}{L^2} \sum_k \Phi_k \left[ h_0^{\text{eff}} - \frac{V}{2} (Q_1 \sigma_z + Q_2 \sigma_x + \Delta \sigma_y) \right] \Phi_k + \frac{V}{4} (Q_1^2 + Q_2^2 + \Delta^2)$$

where $h_0^{\text{eff}} = d_0 \sigma_0 + d_z \sigma_z + d_x \sigma_x$ with $d_0 = (t - 2t')k^2$, $d_x = -2(t + t')k_x k_y$, and $d_z = -(t + t')k^2$, which have $d$-wave symmetry, and $Q_1 = \langle \Phi \sigma_y \Phi \rangle$, $Q_2 = \langle \Phi \sigma_x \Phi \rangle$ are the effective nematic order parameters, $\Delta = \langle \Phi \sigma_y \Phi \rangle$ is the QAH order parameter. Here $\sigma_i$’s are Pauli matrices in quasi-particle space. For weak coupling, the ground state of Hamiltonian (4) is QAH phase with the gap function at $T = 0$ given by $\Delta \propto -\frac{1}{\rho_0} \exp[-\frac{\Lambda}{\sigma_0}]$, where $\rho_0$ is the constant DOS for a 2-D quadratic system. We see that at the phase boundary the interactions have infinitesimal instability, and the phase transition is of the second order. In contrast, by projecting the original Hamiltonian into the two high energy states near Dirac points, we have $d_0 = t + 2t'$, $d_x = -\sqrt{3} t k_x$, and $d_z = \sqrt{3} t k_y$, which has $p$-wave symmetry. In this case, the gap function for QAH phase is $\Delta \propto 1 - \frac{t'}{\Lambda}$ where $\Lambda$ is the momentum cutoff, we see that at the phase boundary $V_c \sim \Lambda$, which is finite. We also perform the renormalization (RG) group analysis based on the projected interacting model at both fillings. Specifically, the result is very similar to that obtained in Ref. 4 at $\frac{1}{3}$-filling. The interaction is marginal at the tree level, as expected from the constant DOS at the quadratic BCP; while it is marginally relevant at the one-loop level, which makes the system flow to strong coupling, supporting our mean-field results for symmetry broken phases. Except for the proportional constant which is model-dependent, the beta function is qualitatively the same as that given in Ref. 4. However at $\frac{1}{3}$-filling, the interaction is irrelevant at the one-loop level of the RG and higher loops are quite involved.

Spinful fermions. —Now we take the spin degrees of freedom into account and discuss the spin-$\frac{1}{2}$ fermions on kagome lattice. In addition to the nn repulsive interactions, we also include an on-site repulsive Hubbard term as well as an nn exchange term,

$$H = t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - t' \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_i \mathbf{n}_{i\uparrow} + V \sum_{\langle ij \rangle} n_i n_j + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$. For site order, besides the nematic order $n^{\text{ns}}$ as discussed in the spinless case where there is no spin order, there is a spin-triplet order parameter $\mathbf{n}$, nematic-spin-nematic phase, where there is no charge order. Different from the checkerboard lattice with $C_4$ symmetry, the spin degrees of freedom won’t restore the $C_6$ symmetry of kagome lattice in charge sector, therefore we expect both nematic and NSN phases in the phase diagram. With the spin degrees of freedom, the nematic order has contributions from both the spin-singlet
channel of Hubbard term $t_i n_i n_i$, and the nn repulsion term $V n_i n_j$, which together form an effective nn repulsion $V' = V - \frac{U}{2}$, mimicking the nematic phase in the spinless model, therefore the nematic phase exists only in the region $0 < U < 4V$ in the $U - V$ plane. For the NSN order, it comes only from the spin-triplet channel in the Hubbard term $-\frac{U}{3} S_i S_j$, where $S_i = \frac{1}{2} \epsilon_{\alpha \beta} c_i^\dagger \alpha c_i^\dagger \beta$. The NSN order parameters shift the two degenerate quadratic touching points into four Dirac points and open a gap at $\Gamma$-point thus gain energy. At $\frac{2}{3}$-filling, the NSN order parameters split the two Dirac points into four at small $U$, one of the Kramer’s pair will go closer and annihilate to open a gap as $U$ increases, but the other two still remain linear touching and no full gap is opened, so that not like the nematic order, the NSN order is not competitive at $\frac{2}{3}$-filling.

The bond order all come from the nn repulsive interactions $V$. The spin-singlet ones $\Delta_{R, d}^0$ are the order parameters of QAH phase as discussed in the spinless model, while the spin-triplet ones $\Delta_{R, d}^3$ are the order parameters responsible for quantum spin Hall (QSH) phase. The QSH phase can be visualized as double QAH layers with opposite flux, and in each layer, it is a QAH phase in the entire $U - V$ plane. However, the spin-singlet and spin-triplet QAH phases gain equal energies in the nn repulsion. In the region $0 < U < 4V$ respectively, but keeps the quadratic point touched. So the gap opened at $\Gamma$-point of magnitude $2V$ is attractive, only the NSN and the QAH/QSH orders compete. Starting from the $U = 0$ axis, the topological phases win first for arbitrarily weak nn repulsion $V$, and then be suppressed by the NSN phase at large $U$. When $0 < U < 4V$ where all nematic, NSN and topological phases compete, the NSN order is completely suppressed. The topological phase dominates at small $V$ but then be taken over by the nematic phase, as seen in the spinless case, and the large on-site $U$ helps to reduce the nematic order further. At $\frac{2}{3}$-filling, all the instabilities are finite again, and the topological phases are not favored at all. Compared with the phase diagram in spinless case, we notice that at $U = 0$, the multi-channel repulsions $\uparrow\uparrow$, $\downarrow\downarrow$, $\uparrow\downarrow$ and $\downarrow\uparrow$ in the nn repulsion $V$ in spinful model, facilitate the ordering of nematic phase relative to BDW phase, therefore the BDW phase disappears in the $U = 0$ axis, and the nematic phase begins to order at a finite interaction $V > V_c = 1.25t$. However, this multi-channel advantage is suppressed by large on-site Hubbard term, and the BDW appears for $U \geq U_c = 2.44t$. In the phase diagram at $\frac{2}{3}$-filling, we need to point out that the nodal phase at $V > V_c$ in Fig. 3(a) at $\frac{1}{2}$-filling and in Fig. 3(b) at $\frac{3}{4}$-filling. At $\frac{1}{2}$-filling, it is seen again that all the broken symmetries have infinitesimal instabilities.
small-$V$ and large-$U$ should not be taken too seriously. Since there are two Dirac points at this filling, the system could in principle gain energy by breaking the lattice translational symmetry and nesting between them, which is the case we do not consider in our discussions.

Finally we discuss in brief the idea of ferromagnetic QAH state with infinitesimal instabilities at half-filling of the bottom band on kagome lattice. If we consider only the nn hopping $t$, the bottom band is completely flat. In the presence of an on-site repulsive Hubbard term, its ground state is ferromagnetic at $\frac{1}{6}$-filling. Now if we turn on the nn repulsion $V$, where the physics is effectively depicted by the spinless model at $\frac{1}{2}$-filling discussed before, the QAH state with infinitesimal instabilities will be favored in the ferromagnetic background. The ferromagnetic QAH phase is a topological state with quantized Hall conductivity $\sigma_{xy} = \frac{e^2}{h}$, it is stable even in the presence of a small nnn hopping $t'$. The ferromagnetic QAH state has been proposed in Hg$_{1-y}$Mn$_y$Te quantum wells with Mn-doped impurities, where a small magnetic field is still needed to polarize the Mn moments. However, on kagome lattice, we only need to tune the filling to right to realize the ferromagnetic QAH state. The detail study of the ferromagnetic QAH state on kagome lattice will be presented in a separate work.

The material ZnCu$_3$(OH)$_6$Cl$_2$, known as herbertsmithite, appears to be an excellent realization of the 2-D spin-$\frac{1}{2}$ kagome lattice. This material consists of Cu kagome layers separated by nonmagnetic Zn layers, structurally with space group $R\bar{3}m$ and lattice parameters $c = 14.049\,\text{Å}$ which is twice of $a = b = 6.832\,\text{Å}$. The transfer integrals $t$ and $-t'$ of this material are 87meV and -10meV respectively, which implies the opposite sign between nn and nnn hoppings and their ratio is quantitatively in agreement with that taken in our numerics. We suggest to realize all the symmetry broken phases on spin-$\frac{1}{2}$ kagome lattice by tuning the filling, say replacing the Cl$^-$ ions with sulfur (S) or oxygen (O), in this kind of material.

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