From quantum anomalous Hall phases to topological metals in interacting decorated honeycomb lattices

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An analysis of the stability of topological states induced by Coulomb repulsion on decorated honeycomb lattices is presented. Based on a mean-field treatment of a spinless extended Hubbard model on the decorated honeycomb lattice we show how the quantum anomalous Hall (QAH) phase is a robust topological phase which emerges at various electron fillings and involves either quadratic band crossing points (QBCP) or Dirac points of the bands. The topological QAH phase is also found to be most stable against thermal fluctuations up to moderate temperatures when the Coulomb repulsion is maximally frustrated. We show how a topological metal can be induced from the QAH by electron doping the system in a broad electron doping range. Electrons on the Fermi surface of such metallic states are characterized by having a non-zero Berry phase which gives rise to a non-zero intrinsic quantum Hall conductivity.

I. INTRODUCTION

Topological insulators are being intensively studied since their discovery\(^1\). In spite of having a bulk gap, they are conducting in the surface with degenerate edge states crossing the Fermi energy which are protected by time-reversal symmetry (TRS). The associated topological bulk invariant, \(Z_2\), characterizes the Quantum Spin Hall (QSH) phase predicted in graphene in the presence of strong enough spin-orbit coupling (SOC)\(^2,3\). In systems with broken TRS, the Quantum Anomalous Hall (QAH) phase which is characterized by a non-trivial topological invariant, the Chern number\(^4\), can arise. Very recently, both kinds of topological phases have been theoretically predicted in the decorated honeycomb lattice (DHL). In a tight-binding model of the DHL in the presence of SOC, the QSH phase, characterized by a non-vanishing \(Z_2\) invariant, emerges.\(^5\) When the Coulomb interaction is added to the tight-binding model, TRS is spontaneously broken giving way to a QAH phase characterized by a non-zero Chern number.\(^6\) This phase can be associated with the spontaneous generation of finite ‘magnetic’ fluxes piercing the elementary hexagonal plaquettes of the lattice but with zero net flux through the unit cell. This phase is analogous to the quantum Hall phase without an applied magnetic field generated by adding complex next-nearest-neighbors (n.n.n) hopping amplitudes to the tight-binding model on the honeycomb lattice.\(^7\)

The DHL is interesting not only from the theoretical point of view but also because it is realized in actual materials such as the trinuclear organometallic compounds\(^8–11\) e. g. Mo\(_3\)S\(_7\)(dmit)\(_3\), in Iron (III) acetates\(^12\) or in cold fermionic atoms loaded in a decorated honeycomb optical lattice.\(^13\) The hopping parameters, entering the tight-binding Hamiltonian (1), \(H_{tb}\) is shown in Fig. 1(a). The DHL can be seen as interpolating between the honeycomb and the Kagomé lattice.\(^14\) The band structure is richer than on the honeycomb lattice potentially leading to novel topological states of matter. Apart from the Dirac points protected by TRS and inversion symmetry (IS), the band structure also displays quadratic band crossing points (QBCP) which are topologically protected by \(C_6\) or \(C_4\) symmetries\(^15\). The two QBCP’s involve a flat band which in turn leads to divergences in the density of states (DOS) are shown in Fig. 1(c) which are relevant for inducing instabilities of the system, particularly around \(f = 1/2\) and \(f = 5/6\).

Non-trivial topology arises when Coulomb repulsion acts between electrons on the DHL. The off-site Coulomb repulsion in the spinless extended Hubbard model (1) can lead to gaps at \(\Gamma\) and \(K\) (\(K’\)) so that the system becomes an insulator. Such insulator is topologically non-trivial consisting on some bands with non-zero Chern numbers \((\nu_n)\) as displayed in Fig. 1(d), implying topologically non-trivial states arising at certain electron fillings. These states are due to the spontaneous formation of QAH phases induced by the Coulomb repulsion.\(^6\) The two lowest energy bands with Chern numbers: \(\nu_{1,2} = \pm 1\) closely resemble those of the QAH found in a honeycomb lattice when sufficiently strong off-site Coulomb repulsion is considered.\(^4\) In contrast, the bands \(n = 4, 5\) are effectively topologically trivial, \(\nu_{4,5} = 0\), due to the cancellation of the Berry phase (of \(\pm 2\pi\)) involving the QBCP around the \(\Gamma\)-point and the Berry phases of \(\pm \pi\) associated with the Dirac cones at \(K\) and \(K’\).

In the present work, we study the doping and temperature effects on the QAH phase generated by Coulomb repulsion on a DHL. Previous work on the DHL has concentrated on the non-interacting QSH phase induced by SOC and the QAH phase induced by Coulomb repulsion but only at half-filling, \(f = 1/2\). However, little is known about the existence of the QAH at other fillings and/or as temperature is raised. We cover this gap by obtaining the full phase diagram of a spinless extended Hubbard model with nearest-neighbors (n.n), \(V_1\), and n.n.n, \(V_2\) Coulomb repulsion on the DHL at all relevant integer fillings and at certain non-integer fillings.
The paper is organized as follows. In Sec. II we describe the model and the Hartree-Fock method used to analyze the model. In Sec. III we obtain the ground state phase diagram of the model at the filling fractions, \( f \), at which either QBCP or Dirac points are relevant. i.e., for \( f = 1/6 \), \( f = 1/2 \), \( f = 2/3 \) and \( f = 5/6 \). We also explore in Sec. III the thermal stability of the QAH phase found at \( T = 0 \) providing a \( T - V \) phase diagram for specific Coulomb parameters for which the QAH is the ground state. By electron doping the QAH we show how topological metallic phases arise. Finally, in Sec. IV we discuss the implications of our findings on experimental observations of the Hall conductivity and magnetoresistance oscillations. We close up the paper with the conclusions in Sec. V.

II. METHODS

In order to analyze possible topological states emerging from the Coulomb repulsion, we consider a spinless extended Hubbard model on a DHL:

\[
\mathcal{H} = \mathcal{H}_{tb} + \mathcal{H}_{\text{Coul}}
\]

\[
\mathcal{H}_{tb} = -t \sum_{\langle ij \rangle \Delta} c_i^\dagger c_j - t' \sum_{\langle ij \rangle \rightarrow \Delta} c_i^\dagger c_j
\]

\[
\mathcal{H}_{\text{Coul}} = V_1 \sum_{\langle ij \rangle} n_i n_j + V_2 \sum_{\langle i \rangle j \rangle} n_i n_j
\]

where the fermion occupation operator is defined as \( n_i = c_i^\dagger c_i \). We consider the Coulomb repulsion between electrons in nearest and next-nearest neighbour sites parameterized by \( V_1 \) and \( V_2 \), respectively. Since this Hamiltonian is quartic in the fermion operators, it cannot be solved exactly so we apply a Hartree-Fock mean-field decoupling of these terms:

\[
n_i n_j \sim (n_i n_j)_{\text{Hartree}} - (n_i n_j)_{\text{Fock}}
\]

where \( (n_i n_j)_{\text{Hartree}} = n_i \langle n_j \rangle + \langle n_i \rangle n_j - \langle n_i \rangle \langle n_j \rangle \) and \( (n_i n_j)_{\text{Fock}} = c_i^\dagger c_j (c_j^\dagger c_i) + (c_i^\dagger c_j) c_j^\dagger c_i - (c_i^\dagger c_j) (c_j^\dagger c_i) \). We work in the canonical ensemble with a fixed number of electrons \( N_e \). At a given temperature \( \frac{1}{\beta} = k_B T \), the free energy \( \mathcal{F} \) is given by \( \mathcal{F} = \mathcal{F}_T + \mathcal{F}_H + \mathcal{F}_F \), where:

\[
\mathcal{F}_T = -k_B T \sum_{k,n} \log [1 + e^{-\beta (E_{k,n} - \mu)}] + \mu N_e
\]

\[
\mathcal{F}_H = -V_1 \sum_{\langle ij \rangle} \langle n_i \rangle \langle n_j \rangle - V_2 \sum_{\langle i \rangle j \rangle} \langle n_i \rangle \langle n_j \rangle
\]

\[
\mathcal{F}_F = V_1 \sum_{\langle ij \rangle} \langle c_i^\dagger c_j \rangle \langle c_j^\dagger c_i \rangle + V_2 \sum_{\langle i \rangle j \rangle} \langle c_i^\dagger c_j \rangle \langle c_j^\dagger c_i \rangle
\]

with \( \mu \) the chemical potential and \( E_{k,n} \) the Hartree-Fock band dispersions. In order to find the mean field amplitudes that minimize the free energy we solve the following

![Diagram](image-url)
system of coupled equations:
\[
\begin{align*}
\frac{\partial F}{\partial \langle n_i \rangle} &= 0 \quad (6) \\
\frac{\partial F}{\partial \langle c_i^+ c_j \rangle} &= 0 \quad (7) \\
\frac{\partial F}{\partial \langle c_i^+ c_j \rangle} &= 0 \quad (8)
\end{align*}
\]

The number of variables of the whole system is 27 (6 system of coupled equations: \( \eta \) dependence of the band dispersions \( \delta t \) seem to be decoupled. However, due to the decomposition this \( \text{ansatz} \) contribution to the total Hartree-Fock free energy (5) as-
zero due to the periodic boundary conditions. The Fock diagrams of Fig. 2. However, the total flux through the unit cell is zero due to the periodic boundary conditions. The Fock contribution to the total Hartree-Fock free energy (5) assuming this \( \text{ansatz} \) takes the form:
\[
\mathcal{F}_F = 6V_1(\xi_1^2 + \eta_1^2) + 3V_1(\xi_2^2 + \eta_2^2) + 12V_2(\xi_3^2 + \eta_3^2)
\]
\]

(10)

Looking at the free energy expressions (4) and (10), the equations for the densities (6) and for the Fock amplitudes (7) seem to be decoupled. However, due to the dependence of the band dispersions \( E_{k,n}(\langle n_i \rangle, \xi_m, \eta_m) \) on both the local densities and the Fock amplitudes entering the thermal part (3), they form a set of coupled self-consistent equations:
\[
\begin{align*}
V_1 \sum_{j \in \langle ij \rangle} n_j + V_2 \sum_{j \notin \langle ij \rangle} n_j &= \sum_{k,n} \frac{\partial E_{k,n}/\partial \eta_m}{1 + e^{\beta(E_{k,n} - \mu)}} \\
\xi_m &= \frac{1}{a_m V_{1,2}} \sum_{k,n} \frac{\partial E_{k,n}/\partial \xi_m}{1 + e^{\beta(E_{k,n} - \mu)}} \\
\eta_m &= \frac{1}{a_m V_{1,2}} \sum_{k,n} \frac{\partial E_{k,n}/\partial \eta_m}{1 + e^{\beta(E_{k,n} - \mu)}}
\end{align*}
\]

(11)

where \( i \) is the sites index (1 \( \leq i \leq 6 \)) and \( m \) is the Fock \( \text{ansatz} \) index (1 \( \leq m \leq 3 \)). The sums over \( j \in \langle ij \rangle \) and \( j \notin \langle ij \rangle \) refer to the n.n and n.n.n of each site \( i \), respectively. \( a_m \) are coefficients which come from the derivation of (10), and \( V_{1,2} \) is either \( V_1 \) or \( V_2 \) for \( m = 1, 2 \) and \( m = 3 \) respectively (9). The equations are written in a compact way: six equations in the first line corresponding to each site \( i \) while in each resting ones (second and third line), three equations are shown coming from each \( \text{ansatz} \) index, \( m \). This system of 12 equations can be solved iteratively.

Although the system has been simplified through the \( \text{ansatz} \) assumed, in some situations the convergence to one or other minima may depend on the initial guess seeded into the equations. Hence, we proceed as follows. For a given set of \( (V_1, V_2) \), we search for the global minimum by comparing the free energy of the complete set of equations (11) with the free energies obtained with the same set of equations satisfying additional constraints. In this way we can reduce the unwanted dependence of the solution on the initial guess plugged into the system of equations. The first constraint imposed on the equations consists on assuming a pure Hartree decoupling which fixes \( \chi_m = 0 \), so that the system of equations is restricted to the \( (n_i) \) only giving the different possible charge ordering patterns of the model. The second con-
straint consists on imposing Fock amplitudes which are purely imaginary, \( \xi_m = 0 \), giving the contribution to the chiral currents. The third and final constraint restricts the system to solutions of the type: \( \eta_m = 0 \), so that the \( \chi_m \), being real, describe shifts of the hopping parameters \( \delta t_m \): \( t(\triangle) \rightarrow -t + V_1 \delta t_1, t(\triangle \rightarrow \triangle) \rightarrow -t' + V_1 \delta t_2, t(2^\text{nd}) \rightarrow 0 + V_2 \delta t_3 \). As stated above, the free energies \( \mathcal{F} \) are evaluated separately assuming each of the three constraints described above and compared to full set of equations without any constraint imposed. The solution with the lowest free energy provides the ground state for a fixed set of \( (V_1, V_2) \). This allows to construct the phase diagrams of Fig. 2.

The topological properties of the insulating solutions are characterized by calculating the total Chern number (\( \nu \)) of the system. The QAH phase is characterized by having a non-zero Chern number (\( \nu \neq 0 \)) in analogy with the standard Quantum Hall effect as shown in Fig. 3(b). The Chern numbers are evaluated numerically by evaluating the Berry flux through the elementary plaquettes in which the first Brillouin zone is discretized which neutralizes the arbitrary phase coming from the gauge invariance. The topological properties of metallic states are analyzed in a similar way by computing the Berry flux through the \( FS \) defined by the partially filled bands. This gives the non-quantized contribution to the intrinsic Hall conductivity \( \sigma_{xy} \). The details regarding these numerical procedures are given in Appendix A.
III. RESULTS

In this section, we first explore the ground state of the model for different \((V_1, V_2)\) following the procedure described above at each filling fraction, \(f\). Then we check the stability of the QAH phase against thermal fluctuations. This is done for the fixed \(V_2/V_1\) ratio at which the QAH is the ground state of the model. We solve the equations at finite temperature, obtaining a \(T-V\) phase diagram. This allows to extract an estimate of the temperature below which the QAH phase is stable. Finally, we electron dope the system varying the filling between \(f = 1/2\) and \(f = 2/3\) within the \(V_1, V_2\), at which the QAH state is the ground state of the system. In this way we study the evolution of the Fermi surface and the possible topological metallic states emerging in the model.

A. Ground state phase diagram

We first discuss the ground state phase diagram of model (1). We obtain the phase diagrams at four filling fractions, \(f\), at which the conduction and valence bands have either Dirac or quadratic band touching points. We search for the ground state of the model for given \(V_1, V_2\) following the method explained in the previous section (see Fig. 2).

The resulting phase diagrams are shown in Fig. 2. We find uniform charge density (UCD), Charge Density Wave (CDW) and Nematic Insulator (NI) phases. While the uniform charge density (UCD) state preserves the symmetries of the lattice, the CDW phase breaks the \(C_6\) rotational invariance of the lattice reducing it to a mirror symmetry only. The reflection plane goes through either intratriangle (in CDW I and CDW I* phases) or inter-triangle (in CDW II) bonds. These states are three-fold degenerate. Although the charge distribution in the unit cell changes by applying 60 rotations, the total energy is invariant. There are different types of charge ordering patterns in these phases as shown in Fig. 3. The NI phase consists of an almost empty triangle and the rest of the charge uniformly distributed in the other triangle of the unit cell. This state is two-fold degenerate due

![FIG. 2: The \(V_1-V_2\) phase diagrams at various filling fractions, \(f\). (a) At \(f = 1/6\) involving Dirac points: semimetallic (SM) and nematic insulating (NI) phases arise. (b) At \(f = 1/2\) with a QBCP: a quantum anomalous Hall (QAH) phase, two types of charge density wave phases, CDW I and CDW II as well as a NI phase emerge. (c) \(f = 2/3\) with Dirac points: a SM phase which becomes unstable to a QAH phase as well as charge ordered phases such as CDW I* and CDW II and NI* appear. (d) \(f = 5/6\) with a QBCP: a QAH phase and charge ordered phases CDW I and CDW I* are found. Dashed lines denote second order transitions while full lines first order transitions.](image)

![FIG. 3: The different ground states shown in the \(V_1-V_2\) phase diagrams of Fig. 2. (a) Uniform charge density (UCD). The charge density is uniformly distributed in the unit cell and the bonds \(\xi_m \neq 0\) follow the ansatz (9) preserving \(C_6\) symmetry. (b) Quantum anomalous Hall (QAH) phase. This phase preserves \(C_6\) symmetry while TRS is broken by spontaneous chiral currents \(\eta_m \neq 0\) being two-fold degenerate depending on the direction of the current (the represented corresponds to a Chern number, \(\nu = +1\)). (c) Nematic insulator (NI). In this state the charge inside the unit cell is located in one of the triangles of the unit cell. The rotational symmetry is reduced from \(C_6\) to \(C_3\) leading to a two-fold degenerate ground state. (d) Charge density wave I (CDW I). The charge is distributed following the colour patterns displayed. Inside each unit cell nearest-neighbor sites are paired up with the same charge. (e) CDW I*. In this phase the inter-triangle nearest-neighbours sites have different densities. (f) Charge density wave II (CDW II). The densities are associated in pairs but not between nearest-neighbors (except for the n. n. intertriangle sites). In the CDW phases the hamiltonian is invariant under reflection transformations: with respect to the \(x\)-axis for CDW I and CDW I*, and with respect to the \(y\)-axis for CDW II. All these states are three-fold degenerate.](image)
to the reduction of rotational symmetry from $C_6$ down to $C_3$. The transition line separating this phase from the CDW or QAH phases is second order as shown in Fig. 2. When $\sim 90\%$ of the total charge in a unit cell is localized in one of the triangles we assume that the transition has occurred. With four electrons per unit cell, $f = 2/3$, three electrons are located in one triangle while the electron left distributes uniformly among the sites of the other discharged triangle. We denote this phase by NI$^*$. Comparing the phase diagrams at different fillings, we conclude that the QAH phase is robust occurring at all filling fractions except for $f = 1/6$. We can rationalize this from the fact that, at this filling, there is only one electron per unit cell so that the effective Coulomb repulsion is not strong enough to destabilize the semimetallic (SM) phase and turn it into the QAH phase. This has also been found in the Kagomé lattice, in which the emergence of the QAH phase requires a third neighbour interaction. However, at $f = 5/6$ where we only have one hole per unit cell we do find a stable QAH region. This seems to be counter-intuitive if we replace in the above argument particles by holes. However, the different phase diagrams and the larger stability of the QAH at $f = 5/6$ compared to $f = 1/6$ can be attributed to the different density of states (DOS). In particular, the DOS at fillings involving QBCP’s displays a divergence due to the flat bands as shown in Fig. 1(c). Both uniform charge density (UCD) and QAH phases preserve $C_6$ rotational symmetry but the QAH breaks TRS $\eta_0 \neq 0$, as shown in Fig. 3. At filling fractions involving QBCP’s i.e. at $f = 1/2$ and $5/6$ there are no regions UCD phases. Due to the divergence of the DOS, a way to destabilize the QAH phase is through breaking the spatial symmetry caused by charge ordering phenomena.

We finally note that at $f = 1/2$, along the line $V_1/t \sim V_2/t$, the QAH phase is the most stable. This means that the energy difference with the competing UCD state reaches its maximum at this filling (see Fig. 7(a) in Appendix B). Hence, we choose this range of parameters with $f = 1/2$ in order to explore the stability of the QAH against thermal fluctuations.

### B. Finite temperatures

As stated above we analyze the effect of temperature on the QAH phase at $f = 1/2$ for $V = V_1/t \sim V_2/t$. Our mean-field $T - V$ phase diagram is shown in Fig. 4. In the phase diagram temperatures are given in Kelvin using the hopping parameter $t = 0.05$ eV corresponding to Mo$_3$S$_7$(dmit)$_3$ crystals. In the limit $T \to 0$ we do recover the results shown in Fig. 2, as expected. The QAH state is the most stable phase when $V \lesssim 2$, above this value the transition to the CDW I occurs. Subsequently around $V \sim 2.1$, a second order phase transition to the NI phase occurs. Observe in the phase diagram how thermal fluctuations induce a transition from a QAH phase to a UCD for $0 < V < 1.5$ and to a CDW I for $1.5 < V < 2$. In the former case the $C_6$ rotational invariance of the lattice is preserved across the transition whereas the latter transition involves a spontaneous breaking of the rotational symmetry of the lattice. We do not find any further charge ordering transitions beyond the temperature range shown in the figure implying the robustness of the NI and CDW I against thermal fluctuations. From our phase diagram we conclude that the maximum temperature at which we find a stable QAH phase is: $T \sim 84$ K for $V_1 \sim V_2 \sim 1.2t$. In Fig. 7(b) of appendix B we compare the free energies of the UCD and QAH phases. Based on our mean-field theory analysis we conclude that the QAH phase may be most likely found in half-filled isolated layers of Mo$_3$S$_7$(dmit)$_3$ in a broad range of temperatures if the $V_1$ and $V_2$ parameters are tuned through the optimal $V_1 \sim V_2 \sim 1.2t$ values. However, it remains to be seen whether other phases different to the QAH phase become the ground state.

### C. Topological metals

We now explore the possibility of stabilizing a topological metal by doping the QAH state. By raising the Fermi level above zero we partially fill the fourth band in Fig. 1(b) without closing the band gaps. This leads to a topological metallic state with broken TRS since the chiral currents giving rise to the QAH at $f = 1/2$ are found to persist even at non-integer fillings between $f = 1/2$ and $f = 2/3$ and between $f = 2/3$ and $f = 5/6$.

In Fig. 5 we show the Fermi surfaces (FS) corresponding to three different fillings between $f = 1/2$ and $f = 2/3$ for $V_1 \sim 0.5$ and $V_2 \sim 0.2$. For these parameters,
the system is deep in the QAH phase as shown in Fig. 2. We compare the interacting Fermi surface with the non-interacting one corroborating Luttinger’s theorem which states that the area enclosed by the FS should not vary as we increase the Coulomb interaction. Luttinger’s theorem should be satisfied since our calculations are based on a mean-field treatment of the Coulomb interaction. However, the FS can be deformed by the interaction due to the non-local nature of the Fock contribution. A similar deformation of the FS is obtained from the HF approximation to the self-energy, $\Sigma(\omega, k)$, but on the square lattice.\textsuperscript{18}

The topological properties of the metallic state generated from the QAH can be investigated by computing the Berry phase associated with the partially filled fourth band (A3), $\gamma_4$. As shown in Fig. 5, by weakly doping the half-filled system with electrons, the FS consists on a single particle-like loop around the Γ-point. The area of the FS coincides with the number of doped electrons $N_f$ in the system off half-filling quantified by $\gamma$, in the system off half-filling quantified by $\gamma$. Since the spontaneously broken TRS ground state is two-fold degenerate, we have two possible directions of the chiral currents. For the chiral currents shown in Fig. 3(h), the Berry phase is approximately, $\gamma_4 \sim -2\pi$. As the Fermi level is further increased injecting more electrons in the system, the area of the FS increases as expected, with the same Berry phase as shown in Fig. 5(a). However, above $N_f \sim 0.67$ the FS is split into two hole-like loops around the Dirac points at $K$ and $K'$. The area of the FS becomes a single hole-like loop around the Γ-point at larger doping. Increasing the electron doping further, the area of this loop decreases until it disappears when the fifth band becomes completely filled; at this point the hole occupancy of the fifth band: $N_f^{(h)} = 1 - N_f \to 0$. At low dopings the Berry phase of each loop has the same value but opposite to the case discussed previously: $\gamma_5^{(K)} = \gamma_5^{(K')} \sim -\pi$ until $N_f \sim 0.18$ where the Berry phase changes from $\gamma_5 \sim 2\pi$ to $\gamma_5 \sim 2\pi$. Note that the Berry phases obtained are close to but not exactly $2\pi$, and contribute to the non-quantized part of the intrinsic Hall conductivity\textsuperscript{16}, $\sigma_{xy}$, as discussed below.

IV. DISCUSSION

We now discuss the implications of our results on experimental observations. The intrinsic Hall conductivity $\sigma_{xy}$ has two contributions: one coming from the quantized part of the $N_C$ occupied bands with Chern numbers ($\nu_n$) and the other coming from the non-quantized part associated with the Berry phase of the FS of the partially filled band, $\gamma_{N_C+1}$, reading:

$$\sigma_{xy} = -\frac{e^2}{h} \sum_{n=1}^{N_c} \nu_n - \frac{e^2}{h} \frac{\gamma_{N_c+1}}{2\pi}$$

(12)

where $N_c$ is the number of totally occupied bands and $N_c+1$ is the partially filled band. In Fig. 6 we show the dependence of the Hall conductance on the electron doping which we quantify through the occupancies of the fourth and fifth band, $N_{4,5}$. At half-filling, $N_c = 3$, the system consists of three filled bands. Since the two lowest bands have opposite Chern numbers and the third band has a Chern number $\nu_3 = +1$ (see Fig. 1), the system has a net Hall conductivity of $\sigma_{xy} = -\frac{e^2}{\pi}$ which survives as the Fermi energy is moved across the gap as shown in Fig. 6 (around the origin corresponding to $f = 1/2$). Once the gap is crossed and the fourth band becomes gradually filled with electrons the system becomes metallic and the Berry phase of the partially filled band, $\gamma_4 = -2\pi$, contributes to $\sigma_{xy}$ giving a total conductivity, $\sigma_{xy} = 0$. However, if we keep increasing the Fermi energy there is a sudden change of the Fermi surface occurring around $N_f \sim 0.67$, at which the Berry phase $\gamma_4 \sim 2\pi$. This should be added to the $-\frac{e^2}{\pi}$ contribution of the three lowest filled bands giving a total Hall conductance: $\sigma_{xy} \sim -2\frac{e^2}{\pi}$. Hence, around $N_f \sim 0.67$...
we expect a jump in the Hall conductivity from 0 to \(\sim -2\) (in units of \(e^2/h\)) as shown in Fig. 6. A similar jump of the Hall conductivity is found between \(f = 2/3\) and \(f = 5/6\) in a broader doping range than between \(f = 1/2\) and 2/3. This implies that a topological metal emerges. This topological metal is protected by \(C_6\) rotational symmetry since the chiral currents induced at the Hartree-Fock level do not break this symmetry. It is well-known that the Berry phase can manifest itself in metals through magnetic oscillatory phenomena.\(^{19–22}\)

Semi-classical quantization of electron energy levels leads to the magnetoresistance:

\[
\Delta R_{xx} \propto \cos[2\pi \left(\frac{B_F}{B} + \frac{1}{2} + \gamma\right)], \tag{13}
\]

where \(B_F\) is the frequency of the oscillation associated with the area of the electron orbit and \(\gamma\) the Berry phase (in units of \(2\pi\)) picked up by an electron when going around it. For instance, using these measurements, a Berry phase of \(\gamma = 1/2\) around the Dirac cone has been obtained in graphene.\(^{23}\)

Electrons in our topological metal with the FS with closed loops around K and K’ as shown in Fig. 5 would also lead to a Berry phase shift of \(\gamma = 1/2\) in magnetoresistance oscillation experiments. In contrast, the topological metals consisting of a single closed loop FS around the \(\Gamma\)-point shown in Fig. 5 would have \(\gamma \to 1\). This case would be essentially indistinguishable from a topologically trivial metal since it corresponds to an overall shift of \(2\pi\) in the magnetoresistance oscillations described by (13).

V. CONCLUSIONS

In the present work we have analyzed, at the mean-field level, the stability of the topologically non-trivial QAH phase induced by offsite Coulomb repulsion on a decorated honeycomb lattice at different fillings and temperatures. The QAH phase occurs when band touching points between the non-interacting valence and conduction bands exist. Since the band structure of the decorated honeycomb lattice contains both QBCP and Dirac band touching points it allows analyzing different topological states arising from them. This is interesting since Dirac points have Berry phases of \(\pm \pi\) associated with them while the QBCP have a Berry phase of \(\pm 2\pi\).\(^{15}\) In the presence of the Coulomb repulsion a gap can open up around these band touching points. This occurs not only at \(f = 1/2\), as previously reported, but also at \(f = 2/3\) and \(f = 5/6\) as shown in Fig. 2.

An important conclusion derived from our study is that the QAH is found to be most stable at \(f = 1/2\). Also the QAH is more favorable at \(f = 5/6\) than at \(f = 1/6\) in spite of the weak Coulomb repulsion acting between the particles in the two cases. The QAH is not directly correlated to the existence of QBCP’s in the non-interacting bands, since we have also found a QAH phase at \(f = 2/3\) which involves Dirac points. However, the parameter range of \((V_1, V_2)\) in which the QAH phase is stable at \(f = 2/3\) is smaller than for \(f = 1/2\). We believe this is due to the larger effect of charge frustration due to \(V_2\) at \(f = 1/2\) as well as the singular behavior of the non-interacting DOS at the Fermi energy associated with the flat band involved in the QBCP.

The QAH is a topological state protected by \(C_6\) rotational symmetry and spontaneously broken TRS which arises in our mean field treatment due to non-zero imaginary Fock amplitudes. The QAH phase competes with the CDW’s and NI which are topologically trivial insulating phases with the lower reflection and \(C_3\) symmetries, respectively instead of the higher six-fold symmetry. It is even possible to find other charge ordering patterns.\(^{24}\) Based on our mean-field treatment we have also analyzed the stability of the QAH phase with temperature finding that the QAH phase at \(f = 1/2\) is robust up to \(T \sim 90\)K for the optimum choice of Coulomb parameters: \(V_1 \sim V_2 \sim 1.2t\). This temperature can be taken as an overestimation of the actual critical temperature since it is based on a mean-field decoupling of the Coulomb interaction.

We have finally addressed the question of whether a topological metal can be induced by doping the QAH phase. We have explored this by injecting electrons in the \(f = 1/2\) system for Coulomb parameters well in the QAH phase. Interestingly the gaps associated with the QAH phase remain when the system is electron doped between \(f = 1/2\) and \(f = 2/3\) and between \(f = 2/3\) and \(f = 5/6\). This means that the chiral currents giving rise to the QAH are robust also at such partial filling fractions. Our analysis of the Berry phases of the partially
bands indicate that a topological metal with a non-zero quantized Hall conductivity of $\nu = -2e^2/h$ can occur close to $f = 2/3$ and between $f = 2/3$ and $f = 5/6$. The non-zero Berry phases of $\pi$ arising when the occupancy of the fourth band, $N_4 > 0.67$, could be detected through magnetic oscillatory experiments.

Future work should include the spin degeneracy in the model and go beyond the present mean-field treatment taking into account electronic correlations in order to check whether the QAH phase and the topological metal found here remain stable. Recent work on the spinful half-filled Hubbard model \cite{13} (no offsite Coulomb repulsion) on the decorated honeycomb lattice finds a Mott insulator transition between a semimetallic phase and an antiferromagnetic insulator going through an unconventional nematic metallic phase. Both the semimetallic and nematic phases are examples of non-trivial phases emerging from the Coulomb repulsion deserving further characterization.

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**Appendix A: Berry phases and Chern numbers in multiband systems**

In a discretized Brillouin zone, the total Chern number $\nu$ can be calculated from the Berry phases $\gamma_{nl}$ at each elementary placquette $l$. The Berry phase is just the accumulated phase of the wave function along a certain closed $k$-path.

$$\gamma_{nl} = \text{Im} \ln \prod_{j=0}^{N-1} \langle u_{nkj} | u_{nkj+1} \rangle$$  \hspace{1cm} (A1)

where $n$ is the band index and the loop chosen is rectangular with $N = 4$. In the multiband case the wave functions overlap of all possible combinations must be taken into account. So that, if we have $N_c \equiv 6f$ valence bands, we construct a $N_c \times N_c$ matrix at each step of the path. Then, the Berry phase is just the phase of the determinant of the product of these matrices along the loop. The Chern number is nothing else than the sum over the FBZ of all those Berry phases:

$$\nu = \frac{1}{2\pi} \sum_{FBZ} \text{Im} \ln \det \prod_{j=0}^{3} \langle u_{nkj} | u_{nkj+1} \rangle$$  \hspace{1cm} (A2)

where $1 \leq m, n \leq N_c$. The shortest steps the closer to an entire Chern number ($\nu \in \mathbb{Z}$) \cite{25}. If the band is partially filled, for instance by doping the material, the system turns into a conductor. If the Fermi surface (FS) is a simple closed loop, the Berry phase of the metal is determined at this path. Then in (A2) we restrict the sum to the enclosed surface (FS):

$$\gamma_n = \frac{1}{2\pi} \sum_{FS} \text{Im} \ln \prod_{j=0}^{3} \langle u_{nkj} | u_{nkj+1} \rangle$$  \hspace{1cm} (A3)

where $n$ corresponds to the partially filled band. This Berry phase do not have to be a multiple of $2\pi$ contributing to the nonquantized part of the intrinsic Hall conductivity $\sigma_{xy}$ \cite{16}.

**Appendix B: Stability analysis of the ground state**

In the mean-field treatment used in the paper we find that for a given set of parameters $(V_1, V_2)$, there are several solutions having very close free energies.

![Free Energy Difference Between UCD and QAH]

FIG. 7: (a) Dependence of the free energy difference between the two lowest energy states for $V_1/t = V_2/t \equiv V$ and $f = 1/2$. The lowest free energies are found for the UCD with $\eta_1 \equiv 0$ and the QAH with $\eta_m \neq 0$. In the range $0 \lesssim V \lesssim 1.9$, the free energy difference is positive meaning that the QAH phase is the ground state. It presents a maximum at $V \sim 1.4$. (b) The UCD and QAH energies as a function of $T$. The QAH is the ground state up to $T \sim 84 K$ where the UCD becomes the lowest energy phase.

In Fig. 7(a) we show the free energy difference between the UCD and the QAH at $f = 1/2$ for different $V_1/t = V_2/t \equiv V$ in the $T \to 0$ limit. At $V \sim 1.4$ the QAH is the most stable with an energy of 0.0057t below the UCD. This is the maximum energy difference between the UCD and the QAH as $V$ is increased which is consistent with the maximum $T$ at which the QAH phase survives around $V \sim 1.2$ as shown in Fig. 4. In Fig. 7(b) we show the dependence on temperature on the two lowest energy states at fixed $V_1 \sim V_2 \sim 1.2t$. This plot shows how for $T \lesssim 84$ K the QAH has the lowest energy but for $T > 84$ K the UCD becomes the ground state. Hence, $T \sim 84$ K is the maximum temperature estimate at which the QAH is stable as shown in Fig. 4.
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