Chiral spin density wave order on frustrated honeycomb and bilayer triangle lattice
Hubbard model at half-filling

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We study the ground states of the Hubbard model on the frustrated honeycomb lattice with nearest-neighbor \( t_1 \) and second nearest-neighbor hopping \( t_2 \), which is isomorphic to the bilayer triangle lattice. We show that, at half-filling, the on-site Coulomb interaction \( U \) induces antiferromagnetic (AF) chiral spin-density wave (\( \chi-SDW \)) order in a wide range of \( \kappa = t_2/t_1 \) where both the two-sublattice AF order at small \( \kappa \) and the decoupled three-sublattice 120° order at large \( \kappa \) are strongly frustrated, leading to three distinct phases with different anomalous Hall responses. Increasing \( U \) at fixed \( \kappa \) drives a continuous transition from a \( \chi-SDW \) semimetal with anomalous Hall effect to a topological chiral Chern insulator exhibiting quantum anomalous Hall effect, which undergoes a discontinuous transition to a \( \chi-SDW \) insulator with zero total Chern number but anomalous ac Hall effect. We obtain the phase diagram, discuss its properties, and argue that the AF \( \chi-SDW \) state is a generic phase of strongly correlated and frustrated hexagonal lattice electrons.

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A spin density wave (SDW) refers to the formation of nonzero spin density moments in itinerant electron systems.

The spin texture in a SDW depends on the nature of the electron-electron interaction, the lattice geometry, and the Fermi surface (FS) structure. The ordered moment in a commensurate SDW phase can be written as:

\[
\vec{S}_\ell(r) = \sum_\alpha M_{\ell,\alpha} \cos(\vec{Q}_\alpha \cdot \vec{r} + \theta_\alpha)
\]

where \( \ell \) labels the sublattices in the magnetic unit cell determined by the ordering wavevectors \( \vec{Q}_\alpha \), and \( \theta_\alpha \) is a relative phase. Besides the usual linearly-polarized (collinear) and spiral (coplanar) SDW phases, the textured quantum electronic phase with noncoplanar, chiral SDW (\( \chi-SDW \)) order has attracted great interest recently for its ability to sustain a local spin chirality \( \chi = \vec{S}_{\ell_1} \cdot (\vec{S}_{\ell_2} \times \vec{S}_{\ell_3}) \) that breaks both parity and time-reversal symmetry. Electrons accumulate Berry phase from the spontaneously generated internal magnetic field associated with spin-chirality, leading to the anomalous Hall effect (AHE) [2–3]. A topological phase with quantum anomalous Hall effect (QAHE) can arise in a \( \chi-SDW \) insulator, where the gapped electron bands acquire nonzero Chern numbers.

The spin-chirality mechanism accounts for the AHE in many ferromagnetic materials such as the manganites and the pyrochlores [3]. In this paper, we focus on the antiferromagnetic (AF) \( \chi-SDW \) metals and insulators with \( \sum_\ell \vec{S}_\ell = 0 \) in materials and models with strong electron correlation. They have indeed been discovered in the charge transfer insulator NiS\(_2\) [8–11] and metallic \( \gamma\)-FeMn alloy [12] and related materials, where the magnetic moments reside on the frustrated face-centered-cubic lattice. Neutron scattering experiments observed noncoplanar, AF order with 4-sublattices and 3-ordering wavevectors. The ordered moments on the four sublattices forming a tetrahedron in spin space is a unique character of this triple-Q \( \chi-SDW \) phase. On the theoretical side, it has been shown that frustrated Heisenberg two-spin exchange interactions are insufficient to produce the AF \( \chi-SDW \) order and additional 4-spin exchange interactions are necessary for such a noncoplanar state to emerge as the ground state from the many degenerate magnetic states due to frustration [11,12,13]. In addition, weak-coupling approaches such as nesting based models [15] and band structure (LDA) and LDA+U calculations [11,20,21] have been performed to study the complex magnetic order in these materials. While a microscopic description of the \( \chi-SDW \) order is currently lacking, it is believed that both strong correlation and geometrical frustration play vital roles in its origin.

Recently, it has been shown that the nearest neighbor (NN) Hubbard model on the triangular and the honeycomb lattices has a FS instability at 3/4-band filling due to FS touching the van Hove singularity at the corners of the 2×2 reduced zone boundary [22,23]. In the magnetic channel, this instability leads to the same triple-Q \( \chi-SDW \) order with 4-sublattices spins forming a tetrahe- dron. Several theoretical studies such as renormalization group (RG) [24], functional RG [25], and density matrix RG [26] have been performed to study the competition of the \( \chi-SDW \) state with other forms of FS instabilities such as unconventional superconductivity. These findings raise the exciting possibility of realizing the AHE and the topological QAHE in two-dimensional (2D) or layered quasi-2D materials such as graphene [27] [28], sodium cobaltates [29] [30], and frustrated antiferromagnets [31] [32], and motivate the study of topological AF \( \chi-SDW \) ground states in 2D models with electronic correlation and geometric frustration.

We study in this work the frustrated honeycomb lattice Hubbard model with NN \( t_1 \) and second NN hopping \( t_2 \), and on-site Coulomb repulsion \( U \) shown in Fig. 1a. This
lattice structure is isomorphic to the center-stacked, bilayer triangle lattice with intralayer hopping \( t_2 \) and interlayer hopping \( t_1 \) as indicated by the dashed blue and red lines in Fig. 1a. Materials having such lattice structures include, in addition to graphene and bilayer cobaltates, quasi-2D bilayer triangular lattice chalcogenides \[31\] and layered honeycomb lattice AF compounds \[33, 35–37\]. We study the model at half filling in view of the better control over stoichiometric materials, and address the nature of the magnetic ground states emerging at large enough \( U \) that straddle between the two-sublattice collinear AF order at \( t_2/t_1 \ll 1 \) and one and two decoupled 120° coplanar order at \( t_1/t_2 \ll 1 \). To enable a study of both strong correlation and noncollinear magnetic order, we employ the SU(2) spin-invariant slave boson theory \[38–40\], which has been generalized recently to treat magnetic superstructures \[41\]. Fig. 2 shows our obtained phase diagram in Fig. 1a is

\[
H = \sum_{\langle ij \rangle} t_2 c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\langle i \rangle j} t_1 c_{i\sigma}^\dagger c_{j\sigma} + h.c. + U \sum_n n_i n_i, \quad (1)
\]

where \( t_1 \) and \( t_2 \) describe the inter-sublattice (inter-layer) and intra-sublattice (intra-layer) hopping on the honeycomb (bilayer triangle) lattice. Labeling the two-sublattice (bilayer) as \( A \) and \( B \) and denoting \( C_{k\sigma}^\dagger = (c_{k\sigma,A}^\dagger, c_{k\sigma,B}^\dagger) \), the noninteracting part in Eq. (1) can be written as \[12\]

\[
H_0 = C_{k\sigma}^\dagger H_k C_{k\sigma},
\]

where \( H_k = \left( \begin{array}{cc} t_2 \Delta_k & t_1 \varepsilon_k \\ t_1 \varepsilon_k^* & t_2 \Delta_k \end{array} \right), \quad \varepsilon_k = 1 + e^{-i\hat{a}_1} + e^{-i\hat{a}_2}, \quad (2)
\]

and \( \Delta_k = 2[\cos (\hat{k} \cdot \hat{a}_1) + \cos (\hat{k} \cdot \hat{a}_2) + \cos (\hat{k} \cdot (\hat{a}_1 - \hat{a}_2))]. \) Diagonalizing \( H_k \) gives two noninteracting bands,

\[
E_k^\pm = t_2 \Delta_k \pm t_1 \sqrt{3 + \Delta_k}.
\]

For \( t_2 < t_1/3 \), the two subbands cross at the Dirac points \( (K' \text{ and } K') \) that pin the Fermi level at half-filling. However, when \( t_2 > t_1/3 \), the subbands overlap, giving rise to three FS sections: a hole pocket around zone center \( \Gamma \) and two electron pockets around \( K \) and \( K' \) as shown in Fig. 3(a). Increasing \( t_2/t_1 \) further, the FS pockets grow in size and the Fermi level rises toward the van Hove (vH) singularity at \( M \) point with energy \( E_M^\pm = t_1 - 2t_2 \). Fig. 3(b) shows that at half-filling, the Fermi level touches the vH points at \( t_2^\pm \approx 0.85t_1 \) where...
the electron pockets. For $t_2 > t_2^*$, the electron pockets coalesce to produce the large hexagonal electron FS (Fig. 3c), while the smaller hole FS pocket grows continuously around $\Gamma$. A weak-coupling theory of itinerant electrons would predict that on top of the PM hole FS will be an SDW instability of the hexagonal electron FS at $t_2/t_1 \approx 0.85$, involving some or all of the wavevectors $Q_{1,2,3}$ connecting the vH points in Fig. 3(a).

To treat Coulomb interaction nonperturbatively and study noncollinear spin order, we represent the local Hilbert space by a spin-1/2 fermion $f$, and six bosons $e$, $d$, and $p_{\mu}$ ($\mu = 0, 1, 2, 3$) for empty, doubly-occupied, and singly occupied sites respectively [38–41]: $|0\rangle = e^\dagger |\text{vac}\rangle$, $|\uparrow\downarrow\rangle = d^\dagger f_1^\dagger f_1^\dagger (\text{vac})$, and $|\sigma\rangle = \frac{1}{\sqrt{2}}f_{\sigma}^\dagger p_{\mu}^\dagger \sigma_{\sigma}^\dagger |\text{vac}\rangle$ where $\sigma_{1,2,3}^\dagger$ and $\sigma^0$ are Pauli and identity matrices. The completeness of the Hilbert space, and the equivalence between boson and fermion representations of the particle and spin density impose three local constraints:

\[
\begin{align*}
Q_1 &= e_{\downarrow}^\dagger e_{\downarrow} + p_{\downarrow0}^\dagger p_{\downarrow0} + \vec{p}_{\downarrow} \cdot \vec{d}_{\uparrow} + d_{\uparrow}^\dagger d_{\uparrow} - 1 = 0, \\
Q_0 &= p_{\downarrow0}^\dagger p_{\downarrow0} + p_{\uparrow}^\dagger \vec{p}_{\downarrow} + d_{\uparrow}^\dagger d_{\uparrow} - f_{\downarrow\uparrow}^\dagger f_{\downarrow\uparrow} = 0, \\
Q_\alpha &= p_{\downarrow0}^\dagger p_{\uparrow0} + p_{\uparrow}^\dagger \vec{p}_{\downarrow} + i(p_{\downarrow}^\dagger \times \vec{p}_{\downarrow})_\alpha - f_{\downarrow\uparrow}^\dagger \tau_{\sigma\sigma}^\dagger f_{\downarrow\uparrow} = 0.
\end{align*}
\]

The Hubbard Hamiltonian thus becomes,

\[
H = \sum_{\langle ij \rangle} t_{ij} \psi_i^\dagger g_i \psi_j + \sum_{\langle\langle ij \rangle\rangle} t_{ij} \psi_i^\dagger g_i \psi_j + U \sum_i d_{i}^\dagger d_i - \mu_0 \sum_{i} f_{\downarrow\uparrow}^\dagger f_{\downarrow\uparrow} + \sum_i \lambda_i Q_i + \sum_{i} \lambda_{\mu} Q_i^\mu,
\]

where the fermion spinor $\psi_i = (f_{\uparrow i}^\dagger, f_{\downarrow i}^\dagger)$; $\lambda_i$ and $\lambda^\mu_i$ are Lagrange multipliers enforcing the constraints. The hopping renormalization factors $g_i$, $g_j$ are $2 \times 2$ matrices involving the bosons $g_{ij}[39, 40]$. We found that due to the particle-hole symmetry at half-filling, $g_i$ simplifies considerably and $g_i = g_{0\alpha}^\dagger$ where $g_{0\alpha}$ is the corresponding hopping renormalization of Kotliar and Rukenstein [39]. We solve the self-consistency equations that minimize Eq. 5 with the bosons condensed in a general spin and charge configuration in an up to 8-sites per unit cell. To determine the ground state properties accurately, we use the supercell construction [41] and discretize the reduced zone with $600 \times 600 k$-points in all calculations.

The obtained results show that for $t_2/t_1 < 0.55$, the bipartite collinear AF insulator remains the ground state as in the unfustrated case at $t_2 = 0$ and $U/W \geq 0.57$. In the opposite limit, when $t_2/t_1 > 1.3$, the 120° coplanar AF state becomes ground state, which is analytically connected to the decoupled 120° states in the limit $t_1 \to 0$ and $U/W \geq 0.80$. Remarkably, we find that in the wide region $0.55 < t_2/t_1 < 1.3$ the effects of frustration and vH singularity give rise to three new SDW phases as shown in the phase diagram (Fig. 2). They are described by

1Q Stripe, $\vec{S}_i = m(\pm e^{i\vec{Q}_1 \cdot \vec{r}_i}, 0, 0)$,

2Q Spiral, $\vec{S}_i = \frac{m}{\sqrt{2}}(\pm e^{i\vec{Q}_1 \cdot \vec{r}_i}, \pm e^{i\vec{Q}_2 \cdot \vec{r}_i}, 0)$,

3Q $\chi$–SDW, $\vec{S}_i = \frac{m}{\sqrt{3}}(\pm e^{i\vec{Q}_1 \cdot \vec{r}_i}, \pm e^{i\vec{Q}_2 \cdot \vec{r}_i}, \pm e^{i\vec{Q}_3 \cdot \vec{r}_i})$,

with $\pm$ for $i \in A, B$ respectively and $Q_{1,2,3}$ depicted in Fig. 3a. Let us fix the degree of frustration at $t_2/t_1 = 0.85$ and increase the correlation strength $U/W$. Fig. 2 shows that the PM metal undergoes two sequential discontinuous transitions to the 1Q-strip and then the 2Q-spiral phases. These phases are metallic due to the partial gapping of the FS and break the $C_3$ symmetry.

Increasing $U/W$ further leads to the onset of the triple-Q $\chi$–SDW order through a discontinuous transition. We
find that a non-zero spin chirality $\chi$ alone is insufficient to specify the ground state and there are three distinct $\chi$-SDW phases characterizable by their intrinsic Hall responses. The latter can be calculated using the Kubo formula:

$$\sigma_{xy}(\omega) = \frac{e^2}{\hbar} \sum_{k,n \neq m} \frac{f(\varepsilon_{kn}) - f(\varepsilon_{km})}{(\varepsilon_{kn} - \varepsilon_{km})^2 - (\omega + i\delta)^2} \text{Im} \left[ v_x^{mn} v_y^{nm} \right],$$

where $\varepsilon_{kn}$ is the dispersion of the $n$th band $|nk\rangle$, $f(x)$ is the Fermi function, and $v_{x(y)}^{mn} = \langle km | \hat{v}_{x(y)} | kn \rangle$ is the matrix element of the velocity operator. In Fig. 4, we plot the calculated anomalous Hall response and the spin chirality $\chi$ as a function of $U/W$. As the system enters the $\chi$-SDW phase, the triple-Q order parameter gaps out the vH points of the outer FS in Fig. 3b; but the overlap of the inner FS with the $2 \times 2$ hexagonal reduced zone boundary truncates it into electron and hole FS pockets via umklapp scattering. This $\chi$-SDW-I semimetal phase exhibits dc AHE with an unquantized value of $\sigma_{xy}$ as shown in Fig. 4. As the ordered moments grow with increasing $U$, the FS pockets shrink and disappear when the system makes a continuous transition into the insulating $\chi$-SDW-II phase (Fig. 2) that is characterized by a QAHE with $\sigma_{xy} = C e^2/h$ and $C = 2$ as can be seen in Fig. 4. Indeed this topological phase is a Chern insulator (CI), since all bands acquire a nonzero Chern number and the total Chern number of all occupied bands is $C = 2$ as displayed in Fig. 5a. Note that the quantization of the Hall conductance is not affected by the presence of spin-waves since the lattice do not carry charge. One would usually expect that this topological phase to remain stable unless the insulating single-particle gap closes, such as at the edges of the sample where gapless surface states emerges. Quite surprisingly, Fig. 4 shows that the $\sigma_{xy}$-plateau collapses above $U = 7.2t_1$ where a third $\chi$-SDW-III insulating phase sets in and occupies most of the large-$U$ region on the phase diagram in Fig. 2. In this phase, each band still carries a nonzero Chern number, as shown in Fig. 5b, but the total Chern number $C = 0$ below the Fermi level leading to $\sigma_{xy} = 0$. We find that the CIs with $C = 2$ and $C = 0$ are separated by a discontinuous topological transition, as detailed in Fig. 4, accompanied by a hysteretic jump in the spin chirality $\chi$ without symmetry change in the order parameter or gap-closing. Although the anomalous dc Hall response is zero in the $C = 0$ CI phase, the Chern bands shown in Fig. 5b give rise to an intrinsic AHE in the ac Hall response $\sigma_{xy}(\omega)$, which is also related to nontrivial optical dichroism, through interband transitions, as shown in the inset of Fig. 4.

To summarize, we have shown that, at half-filling, the ground state of the Hubbard model on frustrated honeycomb and bilayer triangular lattices exhibit the triple-Q, $\chi$-SDW order over a wide region where frustration is strongest. The latter leads to three distinct $\chi$-SDW phases with different intrinsic AHE, QAHE, and ac AHE responses, and a discontinuous topological transition between the $C = 2$ and $C = 0$ Chern insulators where the ordered spin chirality shows hysteresis. Our findings provide insights into the different roles played by itinerancy, frustration, and correlation. While the existence of the vH singularity and umklapp scattering near $t_2/t_1 = 0.85$ pulls down the nearby magnetic phase boundaries toward small $U$ and produces the intervening 1Q-strip and 2Q-spiral phases, the emergence of the $\chi$-SDW order at intermediate $U$ is a consequence of AF frustration. Indeed, Fig. 2 shows that direct transitions from the PM phase to the $\chi$-SDW insulator take place generically away from such special band structure point, and the phase boundary of the $C = 0$ $\chi$-SDW insulator on the phase diagram is essentially insensitive to the band parameters $t_1$ and $t_2$ in this region. An important corollary of our findings is that the insulating magnetic phases of the Hubbard model are not necessarily connected adiabatically to those of the Heisenberg model with quadratic spin exchange interactions. Indeed, recent studies of the $J_1$-$J_2$ Heisenberg model on the honeycomb lattice have not found the $\chi$-SDW phase. At least for the intermediate range of $U$ studied here, additional spin-spin interactions involving four or more spins are important to uncover the $\chi$-SDW ordered phases, consistent with the conclusions drawn from studies of the 3D $\chi$-SDW insulator NiS$_2$ using spin models. It is hoped that the findings reported here will further stimulate the search for topological AF $\chi$-SDW phases in the wide parameter range of 2D or layered hexagonal materials with both strong correlation and magnetic frustration.

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