Spontaneous quantum Hall effect in quarter-doped Hubbard model on honeycomb lattice and its possible realization in doped graphene system

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Abstract – We show that a magnetic insulating state with nonzero spin chirality is realized in a quarter-doped Hubbard model on honeycomb lattice as a result of the nesting property of the Fermi surface. This state is topological nontrivial and has a quantized Hall conductance of \( \sigma_{xy} = \frac{e^2}{h} \). We find that such a state is robust against next-nearest-neighboring hopping and we propose that it can be realized in a quarter-doped graphene system. We also show that the quarter-doped Hubbard model on honeycomb lattice is equivalent to a 3/4-filled Hubbard model on triangular lattice in the weak coupling limit, in which a similar effect was predicted previously.

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Electron correlation effect on honeycomb lattice has attracted a lot of interest recently [1–5]. The honeycomb lattice has the smallest coordination number of 3 for a two-dimensional lattice and has Dirac-type dispersion at half filling. It is a nontrivial task to understand the role of electron correlation such systems. As an example, it is reported recently that an exotic spin liquid state can be realized in the half-filled Hubbard model on honeycomb lattice [1].

However, in the two-dimensional graphene sheet [6,7], which is thought to be the most natural realization of an electronic system on honeycomb lattice, the electron correlation effect is believed to be rather weak. This is generally true except for the special case when the Fermi energy is close to the Van Hove singularity (VHS) of the density of state (DOS). In particular, when the system has a nested Fermi surface, an infinitesimally small interaction is enough to induce dramatic correlation effect. Recently, large electron doping on graphene system has been achieved through both chemical doping and electrolytic gating [8,9]. It is also found by angle-resolved-photoemission measurement that the VHS is much more extended than the prediction of band theory.

The DOS of free electron on honeycomb lattice with only nearest-neighboring hopping is shown in fig. 1. The VHS appears on both sides of the half-filled background (at 3/4 or 5/4 band filling)\(^1\). At such special fillings, the system has a nested Fermi surface. In particular, the single particle energy on the Brillouin zone boundary is given by \( \pm t \), where \( t \) is the hopping integral between neighboring sites. It is important to note that rather than one, there are three independent nesting vectors: \( Q_1 = \frac{1}{2} b_1 \), \( Q_2 = \frac{1}{2} b_2 \) and \( Q_3 = \frac{1}{2} (b_1 + b_2) \), where \( b_1 \) and \( b_2 \) are the two elementary reciprocal vectors of the system (see fig. 1). The exact same situation also occurs in \( \frac{3}{4} \)-filled system on triangular lattice. For that case, an interesting magnetic insulating state with nonzero spin chirality and spontaneous quantum Hall effect is predicted previously [11,12]. In this paper, we will show that exactly the same phenomena also occur on the quarter-doped honeycomb lattice. In fact, we find that both systems share the same low-energy theory except for an overall reduction of the energy scale by a factor of 2. We also find that such chiral insulating state is robust against the next-nearest-neighboring hopping. We thus argue that such an exotic state can be realized in a quarter-doped graphene system.

\(^1\)Here the filling fraction is defined as the number of electron per unit cell for each spin. The undoped graphene system thus has a filling fraction of 1. Note this definition is different from that used in [10], in which the undoped system has a filling fraction of 0.5.

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In a magnetically ordered background with nonzero spin chirality, the motion of the electron along a closed loop experiences a Berry phase, the effect of which is indistinguishable from the Aharonov-Bohm phase induced by external magnetic field. Such a quantum phase can induce an anomalous contribution to the Hall coefficient in systems with noncoplanar magnetic order [13–15]. In particular, when the magnetic order opens a full gap in the electron spectrum, such anomalous contribution will have quantized values.

For the $\frac{1}{4}$-filled Hubbard model on triangular lattice, a four-sublattice noncoplanar magnetic order is established for an infinitesimally small value of electron correlation. The ordered moments in the four sublattices point along the normals to the surfaces of a tetrahedron and subtend a solid angle of $\pi$ around each elementary triangular plaquette. In this state, the electron spectrum opens a full gap and the Berry phase effect induces a quantized Hall conductance of $\sigma_{xy} = \frac{e^2}{2h}$ at zero temperature.

Since the system has three independent nesting vectors at the VHS, many different kinds of magnetic orders are possible at low energy. The simplest choice of Bose condensation at a single nesting vector results in a collinear magnetic state, while in the noncoplanar magnetic state with the tetrahedron ordering pattern all the three nesting vectors are involved with the same weight [11]. A realization of the tetrahedron ordering pattern on honeycomb lattice is shown in fig. 2. In such a state, each site is neighbored by three sites in the other three different magnetic sublattices. The system can also be viewed as being composed of two triangular sublattices, on each of which a tetrahedron ordering pattern is established.

To check the stability of the tetrahedron ordering pattern, we have carried out unrestricted mean-field search for the quarter-doped Hubbard model on honeycomb lattice with $12 \times 12 \times 2$ lattice sites. We have included both magnetic and charge order parameters in the optimization. On the $12 \times 12 \times 2$ lattice, there are in total 864 variational parameters for the spin density and 288 variational parameters for the charge density to be optimized. We have used both the conjugate gradient method and the simulated annealing method to find the minimum of the variational energy. Both methods predict that the tetrahedron ordering pattern is the most stable and the charge distribution is always uniform. We now present the mean-field theory of this state.

In the mean-field treatment, the Hubbard model on honeycomb lattice has the form

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,A,\sigma}^\dagger c_{j,B,\sigma} + h.c.) - 4U \sum_i \langle S_{i,A} \rangle \cdot S_{i,A} - 4U \sum_j \langle S_{j,B} \rangle \cdot S_{j,B},$$

where $S_{i,A}$ ($S_{j,B}$) denotes the spin operator on site $i$ ($j$) of sublattice $A$ ($B$).
The ordered moments in the tetrahedron state can be written as
\[
\langle S_{i,A} \rangle = \frac{m}{\sqrt{3}} (\hat{e}_x e^{iQ_3 R_i} + \hat{e}_y e^{iQ_1 R_i} + \hat{e}_z e^{iQ_2 R_i}),
\]
\[
\langle S_{j,B} \rangle = \frac{m}{\sqrt{3}} (\hat{e}_x e^{iQ_3 R_j} - \hat{e}_y e^{iQ_1 R_j} - \hat{e}_z e^{iQ_2 R_j}).
\] (2)

With eq. (2), the mean-field Hamiltonian in the momentum space takes the form
\[
H = \sum_{k \in \text{MBZ}} \psi_{1,k}^\dagger (\Gamma_k - \beta M) \psi_{1,k} + \psi_{11,k}^\dagger (\Gamma_k - \beta M) \psi_{11,k},
\] (3)
in which \( \psi_{1,k}^\dagger = (c_{k+Q_1}^\dagger, c_{k+Q_3}^\dagger, c_{k+Q_3}^\dagger, c_{k+Q_1}^\dagger, c_{k+Q_2}^\dagger, c_{k+Q_2}^\dagger, c_{k+Q_3}^\dagger, c_{k+Q_1}^\dagger, c_{k+Q_2}^\dagger) \), \( \psi_{11,k} = (c_{k}^\dagger, c_{k+Q_1}^\dagger, c_{k+Q_2}^\dagger, c_{k+Q_3}^\dagger, c_{k+Q_1}^\dagger, c_{k+Q_2}^\dagger, c_{k+Q_3}^\dagger) \). The spectrum is thus explicitly twofold degenerate. \( \Gamma_k \) and \( M \) are \( 8 \times 8 \) Hermitian matrices and are given by
\[
\Gamma_k = \begin{pmatrix}
\gamma_k & 0 & 0 & 0 \\
0 & \gamma_k & 0 & 0 \\
0 & 0 & \gamma_k & 0 \\
0 & 0 & 0 & \gamma_k \\
\end{pmatrix},
\]
and
\[
M = \begin{pmatrix}
0 & \sigma_3 & -i\sigma_3 & I \\
\sigma_3 & 0 & -I & i\sigma_3 \\
i\sigma_3 & -I & 0 & \sigma_3 \\
i\sigma_3 & I & \sigma_3 & 0 \\
\end{pmatrix},
\]
in which \( \gamma_k = \left[ \begin{array}{c} \mu g_k \\ \sigma_k \end{array} \right], g_k = 1 + e^{-i2\pi k_1} + e^{-i2\pi k_2}, \sigma = \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right), I \) is the \( 2 \times 2 \) identity matrix, \( \beta = \frac{2U_m}{3\sqrt{3}} \) and \( \mu \) is the chemical potential to be determined by filling concentration.

The self-consistent equation for the order parameter \( m \) is given by
\[
m = \frac{1}{4\sqrt{3}N} \sum_{k \in \text{MBZ}} [\langle \psi_{1,k}^\dagger M \psi_{1,k} \rangle + \langle \psi_{11,k}^\dagger M \psi_{11,k} \rangle].
\] (4)

We have solved this equation as a function of \( U/t \) at zero temperature for the quarter-doped system. The result is shown in fig. 3. The order parameter \( m \) is seen to increase with \( U/t \) from \( U/t = 0 \). This is the result of the nesting property of the Fermi surface. The tetrahedron order is thus a weak-coupling instability of the system.

The tetrahedron state has a nonzero spin chirality, i.e., \( \langle S_i \cdot (S_j \times S_k) \rangle \neq 0 \) for spins on neighboring sites. Electron moving on such a background will experience a nonzero Berry phase, which will induce an anomalous contribution to the Hall response of the electron system. Since the state is fully gapped, such an anomalous contribution must take quantized values of the form of \( \frac{2\pi}{N} \), in which \( n \) is the total Chern-number of all occupied bands. Now we show that \( \sigma_{xy} = \frac{e^2}{h} \) at zero temperature in this state.

The Kubo formula for the Hall conductance \( \sigma_{xy} \) is given by
\[
\sigma_{xy} = 2\pi \frac{e^2}{h} \sum_{k,n,m} \langle j_{n,m}(k) \rangle \langle j_{n,m}(k) \rangle (f(\epsilon_n(k)) - f(\epsilon_m(k))),
\] (5)
in which \( S \) is the area of the system. \( j_{n,m}(k) \) and \( j_{n,m}(k) \) are the matrix elements of the current operators between the \( n \)-th and the \( m \)-th eigenstate of the band Hamiltonian at momentum \( k \). \( f(\epsilon_m(k)) \) is the Fermi distribution function. The current operator \( j^{x} \) is given by
\[
j^{x} = \sum_{k \in \text{MBZ}} \psi_{1,k}^\dagger C_{k}^{x} \psi_{1,k} + \psi_{11,k}^\dagger C_{k}^{x} \psi_{11,k}.
\] (6)

\( j^{y} \) is given by a similar expression with \( C_{k}^{y} \) replaced by \( C_{k}^{x} \). Here \( C_{k}^{x,y} \) is a \( 8 \times 8 \) matrix and is given by
\[
C_{k}^{x,y} = \begin{pmatrix}
0 & c_{k+Q_1}^{x,y} & 0 & 0 \\
c_{k+Q_1}^{x,y} & 0 & 0 & 0 \\
0 & 0 & c_{k+Q_2}^{x,y} & 0 \\
0 & 0 & 0 & c_{k+Q_3}^{x,y} \\
\end{pmatrix},
\]
in which
\[
c_{k}^{x,y} = \begin{pmatrix}
0 \\
c_{k}^{x,y}
\end{pmatrix},
\]
\[
\psi_{k}^{y} = it - \frac{it}{2} (e^{-i2\pi k_1} + e^{-i2\pi k_2}),
\]
\[
\psi_{k}^{y} = \frac{it}{2} (e^{-i2\pi k_1} - e^{-i2\pi k_2}).
\]
Fig. 4: (Colour on-line) The order parameter and the Hall conductance as functions of temperature at $U/t = 4$. Note the close similarity of these results with the results for $3/4$-filled Hubbard model on triangular lattice [11].

To calculate $\sigma_{xy}$, we first solve the mean-field equation at finite temperature. The order parameter as a function of temperature at fixed doping and $U/t = 4$ is shown in fig. 4. The mean-field critical temperature is found to be $T_c \approx 0.09t$ for this set of parameters. The Hall conductance is also shown in fig. 4. $\sigma_{xy}$ is found to be zero above $T_c$ and to increase below $T_c$ in the same manner as the order parameter. It finally saturates to the quantized value of $\sigma_{xy} = e^2/2$ at zero temperature.

The results obtained here are very similar to the results for the 3/4-filled Hubbard model on triangular lattice [11]. For example, the critical temperatures on both lattices are about 0.09t for $U/t = 4$. To understand this close similarity, we note that the honeycomb lattice is actually composed of two interpenetrating triangular lattices, on each of which a tetrahedron ordering pattern is established. Actually, we can show that the quarter-doped Hubbard model on honeycomb lattice and 3/4-filled Hubbard model on triangular lattice are described by the same theory in the low-energy limit except for a reduction of the overall energy scale by a factor of 2. First, we note the dispersion relation of electron on honeycomb lattice has the form

$$E_{k}^h = t|g(k)| = t \sqrt{1 + 3\cos(k_1) + \cos(k_2)},$$

while the dispersion on triangular lattice has the form

$$E_{k}^t = -2t(\cos(k_1) + \cos(k_2) + \cos(k_1 - k_2)).$$

It can be shown then that both lattices have the same dispersion relation near the VHS (where $E_{k}^t = -2t$) except for a reduction of the overall energy scale by a factor of 2.

At the same time, it can be shown that the Hubbard interaction term on both lattices can be rescaled into each other in the low-energy limit and the rescaling factor is also 2.

In the low-energy limit, the Hubbard interaction $H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}$ on triangular lattice reduces to

$$H_U \approx U \sum_{k_i, k'_i} \frac{1}{2} c_{k_i \uparrow} \sqrt{\rho} c_{k'_i \downarrow} c_{k_i \downarrow} c_{k_i \uparrow} + \rho c_{k_i \downarrow},$$

where the sum over $i$ denotes the sum over the three patches of nested Fermi surfaces. $k_i$ and $k'_i$ are the momentums on the $i$-th patch of nested Fermi surface. $\rho$ denotes the nesting vector on the $i$-th patch of nested Fermi surface. On honeycomb lattice, the Hubbard interaction takes the form of $H_U = U \sum_i (n_{i\uparrow} n_{i\downarrow} + n_{i\downarrow} n_{i\uparrow})$. In the low-energy limit, it reduces to

$$H_U \approx U \sum_{k_i, k'_i} \frac{1}{2} c_{A, k_i \uparrow} \sqrt{\rho} c_{A, k'_i \downarrow} c_{A, k_i \downarrow} c_{A, k_i \uparrow} + \rho c_{A, k_i \downarrow} + U \sum_{k_i, k'_i} \frac{1}{2} c_{B, k_i \uparrow} \sqrt{\rho} c_{B, k'_i \downarrow} c_{B, k_i \downarrow} c_{B, k_i \uparrow} + \rho c_{B, k_i \downarrow}.$$ (8)

The free-electron system on honeycomb lattice forms two bands with the dispersion $E_{k} = \pm |t| g(k)|$. If we use $c_{+, k}$ and $c_{-, k}$ to denote the operators of the two bands, we have

$$\begin{pmatrix} c_{+, k} \\ c_{-, k} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & e^{i\phi_k} \\ -e^{-i\phi_k} & 1 \end{pmatrix} \begin{pmatrix} c_{A, k} \\ c_{B, k} \end{pmatrix},$$

in which $\phi_k$ is the phase of $g(k)$. The Fermi surface of the quarter-doped system is given by the three straight line $k_1 = \frac{1}{2}$, $k_2 = \frac{1}{2}$ and $k_1 - k_2 = \frac{1}{2}$. It can be shown then that $\phi_{k_i} = \phi_{k_i + Q_i} = \pi, \pi$, and 0 for $i = 1, 2, 3$. Thus, when the Hubbard interaction term is projected into the subspace of the $E_{+}$ (or $E_{-}$) band, the phase of its matrix element is exactly canceled. Collecting all contributions, we find that in the low-energy limit the Hubbard interaction reduces to

$$H_U \approx \frac{U}{2} \sum_{k_i, k'_i} \frac{1}{2} c_{+, k_i \uparrow} c_{+, k'_i \uparrow} c_{+, k'_i \downarrow} c_{-, k_i \downarrow} + \frac{U}{2} \sum_{k_i, k'_i} \frac{1}{2} c_{-, k_i \uparrow} c_{-, k'_i \uparrow} c_{-, k'_i \downarrow} c_{+, k_i \downarrow}.$$ (10)

Thus in the low-energy limit, the quarter-doped Hubbard model on honeycomb lattice is equivalent to the 3/4-filled Hubbard model on triangular lattice apart from a reduction of the overall energy scale by a factor of 2. This explains the close similarity between the results obtained on both lattices.

Although our calculation is done only at the mean-field level, the prediction of topological insulating ground state for the quarter-doped Hubbard model on honeycomb lattice should be robust for sufficiently small $U/t$, since the magnetic ordering is induced by the Fermi surface.
The situation at finite temperature is more subtle, since the Wagner-Mermin theorem prohibits spontaneous breaking of continuous symmetry at finite temperature in two-dimensional systems. However, as the ordered state also breaks the discrete time reversal symmetry, possibility still exists that the spin chirality may survive even without ordered moment [16].

Finally, we turn to the implications of our results on the physics of graphene. First, we note that the dispersion of the graphene system is not perfectly particle-hole symmetric. Uncertainty remains in the strength of longer range hopping integrals. The next-neighboring hopping integral can also exist [17]. However, we want to emphasize that the nesting property of the quarter-doped system is robust against the introduction of next-nearest-neighboring hopping integral. The perfect nesting will only be destroyed by the next-next-neighboring hopping, which is much smaller than the nearest- and next-nearest-neighboring hopping integrals. We thus believe that our result should be applicable to the graphene system.

To be more specific, we have done the mean-field calculation for nonzero $t'/t$. The order parameter at zero temperature as a function of $U/t$ for $t'/t = 0.2$ and $t'/t = -0.2$ are shown in fig. 5, in which they are compared with the result for $t'/t = 0$. It is seen that the tetrahedron magnetic order still develops at infinitesimally small value of interaction, no matter what is the sign of $t'$. The sign of $t'$ does play a role in reducing or enhancing the magnitude of the order parameter. On the honeycomb lattice, the sign of $t'$ will change under particle-hole transformation. For example, electron doping in a system with positive $t'$ is equivalent to hole doping in a system with negative $t'$. Thus both signs of $t'$ are meaningful for the graphene system.

After the completion of this work [18], we noticed many related recent researches of the same system in which other ordering patterns are proposed [10,19–23]. Especially, a chiral $d$-wave superconducting order is suggested for the ground state of the quarter-doped system by RG analysis [10,22]. However, more recent functional RG study and variational calculation show that for the quarter-doped system, the tetrahedron magnetic ordering pattern proposed in this paper enjoys a much larger condensation energy than the chiral $d$-wave superconducting state [23].

We conclude that the quarter-doped Hubbard model on honeycomb lattice has weak-coupling instability to the formation of a magnetic insulating state with nonzero spin chirality and quantized Hall conductance. We find the nesting property of the quarter-doped system is robust against the introduction of next-nearest-neighbor hopping terms. We thus believe that such an exotic state should be observable in quarter-doped graphene system. Such an exotic state can also act as the parent phase of even more exotic phases if we move slightly away from the VHS.

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