Ordered-Current State of Electrons in Bilayer Graphene

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(Dated: December 12, 2013)

PACS numbers: 73.22.Pr,71.70.Di,71.10.-w,71.27.+a

I. INTRODUCTION

The study of bilayer graphene (BLG) is a focused area in the condensed-matter physics because of the potential application of BLG to new electronic devices\(^1\). One of the fundamental subjects is to explore the physics of the ground state of electrons in BLG. A number of experiments\(^2\) performed on high quality suspended BLG samples have provided the evidence that the ground state is gapped at the charge neutrality point (CNP). In particular, a recent experiment by Velasco et al.\(^7\) has observed that (i) the ground state is insulating in the absence of external electric and magnetic fields, with a gap \(E_{\text{gap}} \approx 2\) meV that can be closed by a perpendicular electric field of either polarization, (ii) the gap grows with increasing magnetic field \(B\) as \(E_{\text{gap}} = \Delta_0 + \sqrt{a^2 B^2 + \Delta_0^2}\) with \(\Delta_0 \approx 1\) meV and \(a \approx 5.5\) meVT\(^{-1}\), and (iii) the state is particle-hole asymmetric. On the other hand, theories have predicted various gapped states, such as a ferroelectric-layer asymmetric state\(^3,4\) or quantum valley Hall state (QVH)\(^5,6\) a layer-polarized antiferromagnetic state (AF)\(^5\) a quantum anomalous Hall state (QAH)\(^6\) a quantum spin Hall state (QSH)\(^6\) and a superconducting state in coexistence with antiferromagnetism (SAF)\(^6\). The ferroelectric-layer asymmetric and QAH and QSH states all have been ruled out by the experiment\(^2\). The SAF state is excluded because the real system is an insulator. The AF state cannot reproduce the gap behavior with varying the magnetic field. Recently, the loop-current state has been studied by reducing the gap behavior with varying the magnetic field.

Based on the four-band continuum model, we study the ordered-current state (OCS) for electrons in bilayer graphene at the charge neutrality point. The present work resolves the puzzles that (a) the energy gap increases significantly with increasing the magnetic field \(B\), (b) the energy gap can be closed by the external electric field of either polarization, and (c) the particle-hole spectrum is asymmetric in the presence of \(B\), all these as observed by the experiment. We also present the prediction of the hysteresis energy gap behavior with varying \(B\), which explains the existing experimental observation on the electric conductance at weak \(B\). The large energy gap of the OCS is shown to originate from the disappearance of Landau levels of \(n = 0\) and \(1\) states in conduction/valence band. By comparing with the existing models and the experiments, we conclude that the OCS is a possible ground state of electrons in bilayer graphene.

II. FOUR-BAND CONTINUUM MODEL

The lattice structure of a BLG is shown in Fig. 1. The unit cell of BLG contains four atoms denoted as \(a_1\) and \(b_1\) on top layer, and \(a_2\) and \(b_2\) on bottom layer with interlayer distance \(d \approx 3.34\) Å. The lattice constant defined as the distance between the nearest-neighbor (NN) atoms of a sublattice is \(a \approx 2.4\) Å. The energies of intralayer NN [between \(a_1\) (\(a_2\)) and \(b_1\) (\(b_2\))] and interlayer NN (between \(b_1\) and \(a_2\)) electron hopping are \(t \approx 2.8\) eV and \(t_1 \approx 0.39\) eV, respectively.

The first Brillouin zone and the two valleys \(K\) and \(K'\) in the momentum space are depicted in Fig. 2. For the carrier concentration close to the CNP, we need to consider only the states with momenta close to the Dirac points \(K = (4\pi/3,0)\) and \(K' = -K\). We here define the operator \(C_{vkl}^\dagger = (c_{l}^\dagger_{a_1,v+k+\sigma}, c_{l}^\dagger_{b_1,v+k+\sigma}, c_{l}^\dagger_{a_2,v+k-\sigma}, c_{l}^\dagger_{b_2,v+k-\sigma})\), where \(v = K\) or \(K'\), \(c_{l}^\dagger_{v+k+\sigma}\) creates a spin-\(\sigma\) electron of momentum \(k\) in valley \(v\) of \(l\) sublattice, and \(k\) is measured from the Dirac point \(K\) (\(K'\)) and confined to a circle \(k \leq 1/a\) in \(K\)
\( \text{(K')} \) valley. With the operator \( C^\dagger_{\nu k\sigma} \), the Hamiltonian describing the noninteracting electrons is given by

\[
H_0 = \sum_{\nu k\sigma} C_{\nu k\sigma}^\dagger H^0_{\nu k} C_{\nu k\sigma} \tag{1}
\]

with

\[
H^0_{\nu k} = \begin{pmatrix}
0 & e_{\nu k} & 0 & 0 \\
e^{\ast}_{\nu k} & 0 & -t_1 & 0 \\
0 & -t_1 & 0 & e_{\nu k} \\
0 & 0 & e^{\ast}_{\nu k} & 0
\end{pmatrix} \tag{2}
\]

where \( e_{\nu k} = \epsilon_0 (s_\nu k_x + ik_y) \), \( s_\nu = 1 \) \((-1)\) for \( k \) in the valley \( K \) \((K')\), and \( \epsilon_0 = \sqrt{3}t/2 \). We hereafter use the units of \( \epsilon_0 = 1 \) and \( a = 1 \).

The interaction Hamiltonian is

\[
H' = U \sum_{l_j} \delta n_{l_i\uparrow} \delta n_{l_j\downarrow} + \frac{1}{2} \sum_{l_i \neq l_j} v_{l_i, l_j} \delta n_{l_i\uparrow} \delta n_{l_j\downarrow} \tag{3}
\]

where \( \delta n_{l_i\sigma} \) is the number deviation of electrons with spin \( \sigma \) from its average occupation at site \( i \) of sublattice \( l \) (hereafter denoted as \( l_i \) for short), \( \delta n_{l_i} = \delta n_{l_i\uparrow} + \delta n_{l_i\downarrow} \), \( U \) is the on-site interaction, and \( v_{l_i, l_j} \) is the interaction between electrons at sites \( l_i \) and \( l_j \). Within the mean-field approximation (MFA), since the interaction \( v_{l_i, l_j} \) appears in the exchange self-energy, it can be considered as a finite-range interaction by taking into account the screening effect due to the electronic charge fluctuations. The total Hamiltonian \( H_0 + H' \) satisfies the particle-hole symmetry.

**III. ORDERED-CURRENT STATE**

In the ordered-current state for which there is no antiferromagnetism, the effective interaction under the MFA is given by

\[
H' \approx \sum_{l_i \neq l_j} v_{l_i, l_j} \langle c_{l_i\sigma} c_{l_j\sigma}^\dagger \rangle \langle c_{l_i\sigma} c_{l_j\sigma} \rangle \exp(i\vec{K} \cdot \vec{d}) \tag{4}
\]

where the self-energy \( \Sigma_{l_i,l_j}(k) \) is defined by

\[
\Sigma_{l_i,l_j}(k) = \sum_{\vec{d} \neq \vec{0}} v_{l_i, l_j} \langle c_{l_i\sigma} c_{l_j\sigma}^\dagger \rangle \exp(i\vec{K} \cdot \vec{d}) \tag{5}
\]

and \( \vec{d} \) is the vector from the position \( l_i \) to \( l_j \). First, we consider the diagonal self-energy and denote \( v_{l_i, l_j} \) by \( v(d) \) for brevity. Now, the function \( R_{l_i}(d) + iI_{l_i}(d) \) can be written as

\[
R_{l_i}(d) + iI_{l_i}(d) = \langle c_{l_i\sigma} c_{l_i\sigma}^\dagger \rangle \\
= \frac{1}{2} (\langle c_{l_i\sigma} c_{l_i\sigma}^\dagger \rangle - \langle c_{l_i\sigma}^\dagger c_{l_i\sigma} \rangle) |i\neq j| \\
= \frac{1}{N} \sum_k \left( \frac{1}{2} - \langle c_{l_i\kappa\sigma} c_{l_i\kappa\sigma}^\dagger \rangle \right) \exp(-i\vec{K} \cdot \vec{d}) \tag{6}
\]

where the \( k \) summation runs over the first Brillouin zone, and \( N \) is the total number of unit cells on single layer graphene. Note that the function \( 1/2 - \langle c_{l_i\kappa\sigma} c_{l_i\kappa\sigma}^\dagger \rangle \) in the integrand in Eq. 6 is sizable only in areas close to the two Dirac points. Figure 3 shows the typical behaviors of the two functions

\[
f_{K,K'}(k) = \frac{1}{2} - \langle c_{l_iK(K')}^{\dagger} c_{l_iK(K')} \rangle \bigg|_{l=1} \tag{7}
\]

defined in the two valleys \( K \) and \( K' = -K \), respectively. The result in Fig. 3 is obtained by the self-consistent
Therefore, we can write the formulas for \( \mathbf{k} \) charge-fluctuation screening, the phase exchange interaction can be confined to two valleys. Since the range of the \( k \) the lattice constant. Then, the \( k \) integration in Eq. (6) can be confined to two valleys. Since the range of the \( k \) momenta close to the Dirac points. Then by expanding the self-energy with respect to the momentum \( k \) the average electron doping concentration on sublattice \( \mathbf{r} \),

\[
R_{l}(d) = \frac{1}{N} \sum_{k} (1 - \langle c_{lK+k\sigma}^\dagger c_{lK+k\sigma} \rangle - \langle c_{lK'+k\sigma}^\dagger c_{lK'+k\sigma} \rangle) cos(\mathbf{K} \cdot \mathbf{d})
\]

\[
I_{ll}(d) = \frac{1}{N} \sum_{k} (\langle c_{lK+k\sigma}^\dagger c_{lK+k\sigma} \rangle - \langle c_{lK'+k\sigma}^\dagger c_{lK'+k\sigma} \rangle) \sin(\mathbf{K} \cdot \mathbf{d})
\]

where the \( k \) summation is confined to a single valley, and the quantities \( r_l \) and \( d_l \) are defined by

\[
r_{l} = \frac{1}{N} \sum_{k} (1 - \langle c_{lK+k\sigma}^\dagger c_{lK+k\sigma} \rangle - \langle c_{lK'+k\sigma}^\dagger c_{lK'+k\sigma} \rangle)
\]

\[
d_{l} = \frac{1}{N} \sum_{k} (\langle c_{lK'+k\sigma}^\dagger c_{lK'+k\sigma} \rangle - \langle c_{lK+k\sigma}^\dagger c_{lK+k\sigma} \rangle).
\]

The quantity \( r_l \) can be written as \( r_l = -\delta_l/2 \) with \( \delta_l \) as the average electron doping concentration on sublattice \( l \). For the doping concentration close to the CNP, we need to consider only the low energy quasiparticles with momenta close to the Dirac points. Then by expanding the self-energy with respect to the momentum \( k \) in the two valleys and taking only the leading terms, we get

\[
\Sigma_{ll}(\pm K) = r_{l} v_{c} \pm d_{l} v_{s}
\]

Physically, the imaginary part \( I_{ll}(d) \) is proportional to a bond current. All the bond currents in the lattice constitute to the current loops. The existence of the bond currents breaks the time-reversal symmetry. In Fig. 4, we draw out some of the bond currents on the same sublattice connected to a given site \( i \). Clearly, the total current density at site \( i \) is zero.

Next, we consider the quantity \( I_{ll}(d) \) with \( l \neq l' \). For example, consider the case for \( l = a_1 \) and \( l' = b_1 \) on the top layer. Suppose the quantity is not vanishing. As shown in Fig. 5, the bond currents all with a fixed bond length \( d = |i-j| \) result in three kinds of hexagon current loops with positive, negative, and zero fluxes [supposing the flux is positive (negative) for counterclockwise (clockwise) current loop, respectively. From the particle conservation law, the current along the boundary between the positive and the negative flux hexagons is two times of that along the boundary between the zero and the positive/negative flux ones. The hexagon current loops imply not only the breaking of time-reversal symmetry but also the breaking of translational invariance (homogeneity). The breaking of translational invariance to a low symmetry state requires the relevant interaction strong enough. Note that there is no a common periodicity for the two kinds of hexagon current loops with different side length \( d \) in the lattice. The coexistence of the different hexagon current loops corresponds to completely an inhomogeneous system and cannot be realized for the electrons with finite-range interactions. The most

![Figure 3](image-url) FIG. 3: (Color online) Behaviors of functions \( f_{K}(k) \) (red circles) and \( f_{K'}(k) \) (green squares) defined by Eq. (7).

![Figure 4](image-url) FIG. 4: (Color online) Some of the bond currents connected to the black site on a sublattice. The sign factor \( \pm \) in \( I_{ll}(d) \) is defined by Eq. (9) as \( \pm J_{l}((l'-l)) \) for the electron motion from the black site \( i \) to the red (white) site \( j \). There are no currents between the black site and the blue sites.
favorable case is the smallest hexagon loops may exist when the interaction between the NN a₁ and b₁ atoms is strong enough. The argument applies to all \( I_{L}(d) \) with \( l \neq l' \). For weak to medium interactions, we here assume all the currents between the sites of different sublattices are negligible small. On the other hand, the off-diagonal averages \( \langle c_{i\sigma}c_{j\sigma}^{\dagger} \rangle \) with \( l \neq l' \) can be pure real quantities without breaking homogeneity of the system. The real quantities describe the electron hopping and renormalize the noninteracting Hamiltonian. We here assume that such renormalization has already been included in \( H_{0} \), we therefore do not take into account these hopping processes more again. (In the presence of external electric or magnetic field, even if the renormalization depends on the field, we will neglect the field effect.)

We suppose \( d_{a_{1}}v_{s} = -d_{b_{2}}v_{s} \equiv -\Delta_{1} \) and \( d_{b_{1}}v_{s} = -d_{a_{2}}v_{s} \equiv -\Delta_{2} \) that means the breaking of the layer inversion symmetry. For the homogeneous system at the CNP, we have \( r_{1} = 0 \). As a result, the effective MFA Hamiltonian \( H_{0} \) is obtained by adding the diagonal matrix \( \text{Diag}(-s_{c}\Delta_{1}, s_{v}\Delta_{2}, -s_{v}\Delta_{2}, s_{c}\Delta_{1}) \) to \( H_{0}^{0} \):

\[
H_{0} = \begin{pmatrix}
-s_{c}\Delta_{1} & e_{k} & 0 & 0 \\
e_{k}^* & s_{v}\Delta_{2} & -t_{1} & 0 \\
0 & -t_{1} & -s_{v}\Delta_{2} & e_{k} \\
0 & 0 & e_{k}^* & s_{c}\Delta_{1}
\end{pmatrix}.
\]

Note that the matrices \( H_{0} \) and \( H_{-0} \) are related by \( H_{0} = S H_{-0} S \), where \( S \) is a \( 4 \times 4 \) matrix

\[
S = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}.
\]

If \( \psi_{k}^{\mu} \) is an eigenfunction of \( H_{0} \) with eigenvalue \( E_{k}^{\mu} \) (with \( \mu = 1, 2, 3, 4 \)), then \( S\psi_{-k}^{\mu} \) is an eigenfunction of \( H_{-0} \) with the same eigenvalue. Therefore, the whole energy spectra can be obtained from the eigenstates only in a single valley.

### TABLE I: Parameters for the 4BCM.

| & t (eV) & \( t_{1} \) (eV) & \( a \) (Å) & \( d \) (Å) & \( \alpha \) (a⁻¹) & \( \epsilon \) |
|---|---|---|---|---|---|---|
| & 2.8 & 0.39 & 2.4 & 3.34 & 0.675 & 3 |

### A. The OCS at \( B = 0 \)

Under the MFA and with the wave functions \( \psi_{k}^{\mu} \)'s, the order parameters \( \Delta_{1} \) and \( \Delta_{2} \) are determined by

\[
\Delta_{1} = \frac{\sqrt{3}v_{s}}{2V} \sum_{k\mu} f(E_{k}^{\mu})(|\psi_{k}^{1\mu}|^{2} - |\psi_{k}^{2\mu}|^{2}),
\]

\[
\Delta_{2} = \frac{\sqrt{3}v_{s}}{2V} \sum_{k\mu} f(E_{k}^{\mu})(|\psi_{k}^{3\mu}|^{2} - |\psi_{k}^{2\mu}|^{2}),
\]

where \( f \) is the Fermi distribution function, \( \psi_{k}^{\mu} \) is the \( \nu \)th component of the eigenfunction \( \psi_{k} \), and \( V = \sqrt{3}N/2 \) is the total area of one layer. From the 2BCM, we know that the valence and conduction bands are connected to the electronic motions in the a₁ and b₂ sublattices. Therefore, the energy gap between the valence and conduction bands is determined by \( 2\Delta_{1} \). To reproduce the experimental data \( |\Delta_{1}| = 1 \text{ meV} \) at the CNP, \( v_{s} \) needs to be 5.8e₀ = 14.06 eV. Supposing the effective interaction

\[
v(r) \approx e^{2}/er[1 + (\alpha r)^{2}]
\]

(decaying as \( r^{-3} \), a typical behavior in the two-dimensional electron liquid(22)) with \( \varepsilon \approx 3 \) as the screening constant of high frequency limit of BLG, we obtain the desired value \( v_{s} = 5.8e_{0} \) with \( \alpha = 0.675 \). Another coupling constant is obtained as \( v_{s} = 4.7e_{0} \). Table I summaries all the parameters for the 4BCM.

### B. The OCS at finite \( B \)

In the presence of the magnetic field \( B \) applied perpendicularly to the sample plane, we take the Landau gauge for the vector potential, \( A = (0, Bx) \). With this gauge, the \( y \) component momentum \( k_{y} \) is a good quantum number. Replacing the variable \( x \) and the operator \( k_{x} = -i\nabla_{x} \) with the raising and lowering operators \( a \) and \( a \), \( k_{x} + Bx = \sqrt{B^{2}/2(a^{\dagger} + a)} \) and \( k_{x} = i\sqrt{B^{2}/2(a^{\dagger} - a)} \), we can rewrite the effective Hamiltonian in real space. At the \( K \) valley, the Hamiltonian is

\[
H_{Kx} = \begin{pmatrix}
-\Delta_{1} & i\sqrt{2Ba^{\dagger}} & 0 & 0 \\
i\sqrt{2Ba} & \Delta_{2} & -t_{1} & 0 \\
0 & -t_{1} & -\Delta_{2} & i\sqrt{2Ba^{\dagger}} \\
0 & 0 & -i\sqrt{2Ba} & \Delta_{1}
\end{pmatrix}.
\]

Here \( B \) is in the unit of \( B_{0} = \hbar c/ea^{2} = 1.105 \times 10^{4} \text{T} \). The \( K \)-valley eigenfunction \( \psi_{K}^{\mu} \) is expressed as

\[
\psi_{K}^{\mu} = (ix_{n}^{\mu}\phi_{n}, x_{n}^{2\mu}\phi_{n-1}, x_{n}^{3\mu}\phi_{n-1}, -ix_{n}^{2\mu}\phi_{n-2})^{t}.
\]
for \( n \geq 2 \), where \( \phi_n \) is the \( n \)th level wave function of a harmonic oscillator of frequency \( 2B \) and mass \( 1/2 \) centered at \( x_c = -k_y/B \), and the superscript \( t \) means the transpose of the vector. The vector \( X^\mu_{Kn} = (x^\mu_{1n}, x^\mu_{2n}, x^\mu_{3n}, x^\mu_{4n})^t \) and the eigenenergy \( E_{Kn} \) are determined by

\[
H_{Kn} X^\mu_{Kn} = E^\mu_{Kn} X^\mu_{Kn}
\]

with

\[
H_{Kn} = \begin{pmatrix}
-\Delta_1 & \sqrt{2Bn} & 0 & 0 \\
\sqrt{2Bn} & \Delta_2 & -t_1 & 0 \\
0 & -t_1 & -\Delta_2 & \sqrt{2B(n-1)} \\
0 & 0 & \sqrt{2B(n-1)} & \Delta_1
\end{pmatrix}.
\]

The vector \( X^\mu_{Kn} \) is normalized to unity. For each \( n \geq 2 \), the four energy levels appear at the valence, conduction, and other two bands about \( \pm t_1 \) far from the zero energy, respectively. For \( n = 1 \), there are only three states with \( x^\mu_{1n} = 0 \) and the other three components and eigenvalues are determined by the upper left 3x3 matrix of \( H_{K1} \).

For \( n = 0 \), we have only one state \( X^\mu_{K0} = (1,0,0,0) \) and \( E^\mu_{K0} = -\Delta_1 \).

At the \( K' \) valley, the Hamiltonian is

\[
H_{K'x} = \begin{pmatrix}
\Delta_1 & i\sqrt{2Ba} & 0 & 0 \\
-i\sqrt{2Ba} & -\Delta_2 & -t_1 & 0 \\
0 & -t_1 & \Delta_2 & i\sqrt{2Ba} \\
0 & 0 & -i\sqrt{2Ba} & -\Delta_1
\end{pmatrix}.
\]

Since the Hamiltonian has the symmetry \( H_{K'x} = SH_{Kx}S^{-1} \), the eigenfunction \( \psi^\mu_{K'n} \) is therefore given as \( S\psi^\mu_{Kn} \) with the same eigen value \( E^\mu_{Kn} \).

In the presence of the magnetic field \( B \), the formulas determining the order parameters \( \Delta_{1,2} \) are different from Eqs. (13) and (14). The \( k_y \) summations in Eqs. (13) and (14) are now replaced with the summations over \( k_y \) and the Landau index \( n \). Correspondingly, the wavefunction \( \psi^\mu_{Kn} / \sqrt{L_x} \) is replaced with \( \psi^\mu_{Kn} \) with \( L_x \) as the length of the BLG in \( x \) direction. By denoting the length in \( y \) direction as \( L_y \), we have \( V = L_x L_y \). The \( k_y \) summation is performed as

\[
\frac{1}{L_y} \sum_{k_y} |\psi^\mu_{Kn}|^2 = \frac{1}{2\pi} \int dk_y |\psi^\mu_{Kn}|^2 = \frac{B}{2\pi} \int dx_c |\psi^\mu_{Kn}|^2 = \frac{B}{2\pi} |x^\mu_{Kn}|^2,
\]

where \( x_c \)-integral has been carried out using the normalization condition for the wave functions of the harmonic oscillator. The equations for determining the order parameters are obtained as

\[
\Delta_1 = \frac{\sqrt{3}v_s B}{4\pi} \sum_{n \mu} f(E^\mu_{Kn})(|x^\mu_{1n}|^2 - |x^\mu_{2n}|^2),
\]

\[
\Delta_2 = \frac{\sqrt{3}v_s B}{4\pi} \sum_{n \mu} f(E^\mu_{Kn})(|x^\mu_{3n}|^2 - |x^\mu_{2n}|^2).
\]

The solution to the Landau levels at \( B = 1 \) T is shown in Fig. 6(a). Only the levels in the conduction and valence bands are depicted. For \( n = 1 \), there is a level \( E^\mu_{K1} \) slightly above \(-\Delta_1(B)\) in the valence band. There is no state in the conduction band for \( n = 0 \) and 1. Only when \( n \geq 2 \), the level \( E^\mu_{Kn} \) in the conduction band appears. The energy gap is

\[
E_{\text{gap}} = E^\mu_{K2} - E^\mu_{K1}.
\]

Clearly, the particle-hole symmetry is no longer valid at finite \( B \), in agreement with the experiment. Figure 6(b) shows \( E_{\text{gap}} \) of the OCS as function of \( B \). The AF calculation of the same 4BCM (see Sec. IV) and experimental results for \( E_{\text{gap}} \) are also plotted for comparison. Here, the only fitting parameter is \( v_s \) for reproducing \( \Delta_1(0) = \Delta_0 \) at \( B = 0 \). The theoretical result for \( E_{\text{gap}} \) of the OCS as a function of \( B \) is in surprisingly good agreement with the experiment.
V. THE AF STATE

In the AF state, the magnetization at site $j$ is defined as

$$m_j = \langle n_{j\uparrow} - n_{j\downarrow} \rangle / 2 = -\langle \delta n_{j\downarrow} \rangle$$  \hspace{1cm} (21)

where in the second equality we have used the facts that $\langle \delta (n_{j\uparrow} + n_{j\downarrow}) \rangle = 0$ and the total number of up-spin electrons coincides with that of down-spin electrons. The magnetizations in an unit cell are given by $(m_a, m_b, m_c, m_d) \equiv (m_1, -m_2, m_2, -m_1)$. The order parameters are defined as $-U(m_a, m_b, m_c, m_d) \equiv (-\Delta_1, \Delta_2, -\Delta_2, \Delta_1)$.

Under the MFA, the interaction Hamiltonian reads

$$H' = U \sum_{lj} (\langle n_{lj\uparrow} \rangle \langle \delta n_{lj\downarrow} \rangle + \langle \delta n_{lj\uparrow} \rangle \langle n_{lj\downarrow} \rangle) + \sum_{l \neq i \in \nu} v_{li\nu} \langle c_{li\sigma} \gamma_{lj\sigma} \rangle \langle c_{li\sigma} \gamma_{lj\sigma} \rangle$$  \hspace{1cm} (22)

By supposing $\langle c_{li\sigma} \gamma_{lj\sigma} \rangle$ is real, the second term in right hand side of Eq. (22) then describes the electron hopping and is a renormalization of the noninteracting Hamiltonian. As aforementioned, we suppose such a renormalization has already been included in the noninteracting Hamiltonian; we will not take into account this exchange effect again.

With the MFA, we obtain an effective Hamiltonian as

$$H_{k\sigma} = \begin{pmatrix} -\sigma \Delta_1 & e_k & 0 & 0 \\ e_k^* & \sigma \Delta_2 & -t_1 & 0 \\ 0 & -t_1 & -\sigma \Delta_2 & e_k \\ 0 & 0 & e_k^* & \sigma \Delta_1 \end{pmatrix}$$  \hspace{1cm} (23)

where $\sigma = +1 (-1)$ for spin-up (down) electrons. Note the matrices $H_{k\sigma}$ and $H_{k\sigma}$ are related by

$$H_{k\sigma} =SH_{k\sigma}^*S.$$

If $\psi_k^\mu$ is an eigenfunction of $H_{k\uparrow}$ with eigenvalue $E_k^\mu$ ($\mu = 1, 2, 3, 4$), then $S\psi_k^{\mu*}$ is an eigenfunction of $H_{k\downarrow}$ with the same eigenvalue. Therefore, we need to find out only the eigenstates of up-spin electrons.

A. The AF state at $B = 0$

Using the property of the wave functions, we can obtain the equations for determining the order parameters. For $\Delta_1$, for example, we get

$$\Delta_1 = \frac{U}{2N} \sum_{k\mu} f(E_k^\mu)(|\psi_k^{1\mu}|^2 - |\psi_k^{2\mu}|^2)$$

$$\approx \sqrt{3U} \sum_{k\mu} f(E_k^\mu)(|\psi_k^{3\mu}|^2 - |\psi_k^{4\mu}|^2).$$  \hspace{1cm} (24)

Here, the $k$ summation in the first line runs over the first Brillouin zone, while it runs over a single valley in the second line (because both valleys give the same contribution). Similarly, we obtain for $\Delta_2$,

$$\Delta_2 \approx \sqrt{3U} \sum_{k\mu} f(E_k^\mu)(|\psi_k^{3\mu}|^2 - |\psi_k^{2\mu}|^2).$$  \hspace{1cm} (25)

Equations (24) and (25) for determining the AF order parameters happen to be the same as Eqs. (13) and (14) for the OCS order parameters by setting $U = v_0$. Since the valence and conduction bands are connected to the electronic motions in the $a_1$ and $b_2$ sublattices, the energy gap between the valence and conduction bands is determined by $2\Delta_1$. To reproduce the experimental data $|\Delta_1| = 1$ meV at the CNP, $U$ needs to be $5.8e_0 \approx 14.06$ eV. This value of $U$ is larger than 9.3 eV of the recent ab initio calculation, which means the AF state of $U = 9.3$ eV cannot reproduce the experimental data $\Delta_0$.

B. The AF state at finite $B$

We now consider the behavior of the order parameters in the presence of the magnetic field $B$ applied perpendicularly to the BLG plane. Since the system under the magnetic field is not homogeneous, the Hamiltonian cannot be written in momentum space. For low energy electrons, however, their overall momenta are close to the Dirac points $K$ and $K'$. We here formulate the problem by a different way. From the beginning, we write the electron operator $c_{ij\sigma}$ as

$$c_{ij\sigma} = a_{ij\sigma}^Ke_i^K\gamma_j + a_{ij\sigma}^{K'}e_i^{K'}\gamma_j$$  \hspace{1cm} (26)

where $a_{ij\sigma}^{K(K')}$ is a fermion operator in valley $K(K')$ separated from the fast phase factor $\exp[i\lambda_\sigma^K(K')j]$. $\gamma$ annihilates electrons of valley $K(K')$ and spin $\sigma$ at site $j$ of $l$ sublattice. The operator $a_{ij\sigma}^{K(K')}$ weakly depends on coordinate $j$. For later use, we here define the operator

$$A_{ij\sigma}^l = (a_{a_1j\sigma}^{v\downarrow}, a_{b_1j\sigma}^{v\downarrow}, a_{a_2j\sigma}^{v\downarrow}, a_{b_2j\sigma}^{v\downarrow})$$  \hspace{1cm} (27)

where $v = K$ or $K'$ is the valley index. In the presence of $B$, as did in Sec. III, we take the Landau gauge for
the vector potential $\vec{A} = (0, Bx)$ and use the raising and lowering operators $a^\dagger$ and $a$. We get the effective Hamiltonian for the AF state as

$$H_{\text{eff}} = \sum_{ij\sigma} A_{i,j\sigma} H_{ij\sigma} A_{i,j\sigma}$$

with

$$H_{K,j\sigma} = \begin{pmatrix} -\sigma \Delta_1 & i\sqrt{2B}a_1 & 0 & 0 \\ -i\sqrt{2B}a_1 & -\Delta_2 - t_1 & 0 \\ 0 & -t_1 & 0 & -\sqrt{2B}a_1 \\ 0 & 0 & -i\sqrt{2B}a_1 & \sigma \Delta_1 \end{pmatrix}$$

for electrons at $K$ valley, and

$$H_{K',j\sigma} = \begin{pmatrix} -\sigma \Delta_1 & i\sqrt{2B}a_1 & 0 & 0 \\ -i\sqrt{2B}a_1 & -\Delta_2 - t_1 & 0 \\ 0 & -t_1 & 0 & -\sqrt{2B}a_1 \\ 0 & 0 & -i\sqrt{2B}a_1 & \sigma \Delta_1 \end{pmatrix}$$

for electrons at $K'$ valley. The Hamiltonian satisfies the transformation $H_{K',j\sigma} = S H_{K,j\sigma} S_{j\sigma}$.

As mentioned above, we need to find out the eigenstates of up-spin electrons,

$$H_{\text{eff}} \psi_{v\mu}^\alpha(j) = E_{K,j\sigma}^\mu \psi_{v\mu}^\alpha(j)$$

for $\mu = 1, 2, 3, 4$, and $n = 0, 1, \ldots$. For each index $n$, the four energy levels (if they exist) appear at the valence, conduction, and other two bands about $\pm t_1$ far from the zero energy, respectively. At $K$ valley, the eigenfunction is given by

$$\psi_{K,n}^\mu(j) = \begin{pmatrix} i x_{K,n}^{1\mu} \phi_n(j) \\ x_{K,n}^{2\mu} \phi_{n-1}(j) \\ x_{K,n}^{3\mu} \phi_{n-1}(j) \\ -i x_{K,n}^{4\mu} \phi_{n-2}(j) \end{pmatrix}$$

for $n \geq 2$. The vector $X_{K,n}^\mu = (x_{K,n}^{1\mu}, x_{K,n}^{2\mu}, x_{K,n}^{3\mu}, x_{K,n}^{4\mu})^t$ and the eigenenergy are determined by

$$H_{K,n} X_{K,n}^\mu = E_{K,n}^\mu X_{K,n}^\mu$$

with

$$H_{K,n} = \begin{pmatrix} -\Delta_1 & \sqrt{2Bn} & 0 & 0 \\ \sqrt{2Bn} & 2B(n-1) & -t_1 & 0 \\ 0 & -t_1 & 0 & \sqrt{2B(n-1)} \\ 0 & 0 & \sqrt{2B(n-1)} & \Delta_1 \end{pmatrix}$$

The vector $X_{K,n}^\mu$ is normalized to unity. For $n = 1$, there are only three states with $x_{K,1}^{4\mu} = 0$ and the other three components and eigenvalues are determined by the upper left $3 \times 3$ matrix of $H_{K,1}$. For $n = 0$, we have only $X_{K,0}^{1\mu} = (1, 0, 0, 0)$ and $E_{K,0}^\mu = -\Delta_1$. Note that this energy level is close to a level of $n = 1$. On the other hand, at valley $K'$, the eigenfunction is given by

$$\psi_{K',n}^\mu = (ix_{K',n}^{1\mu} \phi_{n-2}, x_{K',n}^{2\mu} \phi_{n-1}, x_{K',n}^{3\mu} \phi_{n-1}, -ix_{K',n}^{4\mu} \phi_n)^t$$

for $n \geq 2$. The eigen equation reads

$$H_{K',n} X_{K',n}^\mu = E_{K',n}^\mu X_{K',n}^\mu$$

with

$$H_{K',n} = \begin{pmatrix} -\Delta_1 & \sqrt{2B(n-1)} & 0 & 0 \\ \sqrt{2B(n-1)} & 2B(n-1) & -t_1 & 0 \\ 0 & -t_1 & 0 & \sqrt{2B(n-1)} \\ 0 & 0 & \sqrt{2B(n-1)} & \Delta_1 \end{pmatrix}$$

For $n = 1$, we have three states with $x_{K',1}^{1\mu} = 0$ and the other three components and eigenvalues are determined by the lower right $3 \times 3$ matrix of $H_{K,1}$. For $n = 0$, we have only $X_{K',0}^{1\mu} = (0, 0, 0, 1)$ and $E_{K',0}^\mu = \Delta_1$ (close to a level of $n = 1$).

The order parameter $\Delta_1$ is determined by

$$\Delta_1 = \frac{U}{2} \sum_v (a_{v,1\mu}^1 a_{v,1\mu}^\dagger - a_{v,1\mu}^\dagger a_{v,1\mu}^1)$$

$$= \frac{\sqrt{3}U}{4L_y} \sum_{v,n\mu} f(E_{v,n}^\mu)(|\psi_{v,n}^{1\mu}(j)|^2 - |\psi_{v,n}^{4\mu}(j)|^2)$$

$$= \frac{\sqrt{3}UB}{8\pi} \sum_{v,n\mu} f(E_{v,n}^\mu)(|x_{v,n}^{1\mu}|^2 - |x_{v,n}^{4\mu}|^2)$$

where the first line is the definition; the second line represents the averages in terms of the wave functions with $\psi_{v,n}^{1\mu}$ as the $v$th component of $\psi_{v,n}^\mu$, $S_{v,n}^{1\mu}$ has been used for spin down electrons, and a factor $\sqrt{3}/2$, the area of the unit cell of one layer graphene, comes from the fact that $|\psi_{v,n}^{2\mu}(j)|^2/L_y$ is the probability density of electrons around site $j$ and the multiplication with $\sqrt{3}/2$ gives rise to the probability of electrons in the cell at site $j$; in the last line, the $k_y$ summation is carried out according to

FIG. 8: (Color online) The AF order parameters $\Delta_1$ and $\Delta_2$ as functions of the magnetic field $B$. The blue solid line is the experimental result $\Delta(B)/\Delta_0$ for $E_{gap}/2\Delta_0$.\[ $U/\epsilon_0 = 5.8$ \]
Eq. (17). Analogously, the order parameter $\Delta_2$ is determined by

$$
\Delta_2 = \frac{\sqrt{3} U B}{8\pi} \sum_{\nu m} f(E^{\mu}_{vn}) |(x^{3\mu}_v)^2 - (x^{2\mu}_v)^2|. \tag{33}
$$

At the CNP and zero temperature, the order parameters $\Delta_1$ and $\Delta_2$ are self-consistently determined by Eqs. (30)-(33). In Fig. 8, we show the results for $\Delta_1$ and $\Delta_2$ at zero temperature as functions of the magnetic field $B$ and compare them with the experimental data for $E_{\text{gap}}/2\Delta_0$. Clearly, even though $\Delta_1$ and $\Delta_2$ grow with increasing $B$, their dependence of $B$ is not strong enough to match the experimental result. Therefore we cannot expect the AF state as the candidate for the ground state of electrons in BLG.

The Landau levels $E^{\mu}_{vn}$ of the AF state at $B = 1$ T are shown in Fig. 9. In different from the OCS, the distributions of the levels in the two valleys are now different. Especially, in the $K$ valley, there are no levels of $n = 0$ and 1 in the conduction band (for positive $\Delta_1$), while they appear in the conduction band but disappear in the valence band in the $K'$ valley. The energy gap is therefore the indirect gap $E_{\text{gap}} \approx E^{1}_{vK0} - E^{1}_{vK0} = 2\Delta_1$.

As known, there is a momentum cutoff $k_c \approx a^{-1}$ for the 4BCM. The corresponding cutoff for the Landau levels is given by $n_c \approx B_0/2B$. At small $B$, $n_c$ is very large. For accelerating the numerical computation, we have used the super-high efficiency algorithm for sum of series. According to the algorithm, one needs to compute only a number of selected Landau levels.

V. THE OCS UNDER EXTERNAL ELECTRIC FIELD

When an external electric field $E$ is applied perpendicularly to the BLG plane, there is an effective potential difference $2u = Ecd/e$ between the two layers. The Hamiltonian $H_{vk}$ for the OCS now is obtained by adding the diagonal matrix $\text{Diag}(u + r_1 v_c - s_0 \Delta_1, u + r_2 v_c + s_0 \Delta_2, -u - r_2 v_c + s_0 \Delta_2, -u + r_1 v_c + s_0 \Delta_1)$ to $H_{vk}$. Here the terms $r_1 v_c$ appear because of the electric polarization by $E$. Note that $r_1$ has the same sign of $u$, and thereby $H_{vk}(u) = S H_{-u,-k}(-u) S'$, which means that the order parameters are even functions of $u$. The model shows that if $E$ closes the energy gap, then $-E$ does it either. For the sake of illustration, we here consider the case of $B \geq 0$ and $u > 0$. The results for other cases can be deduced by the symmetry of the Hamiltonian. For $B \geq 0$ and $u > 0$, we still have two cases: $\Delta_1 > 0$ and $\Delta_1 < 0$. Here, we consider the case of $\Delta_1 > 0$. The discussion can be extended to the case of $\Delta_1 < 0$. At $B = 0$, the effective gap parameter is $u + r_1 v_c - \Delta_1 \equiv E_{K0}$. The positive voltage $u$ pushes this level from the valence band toward the conduction band. The critical potential $u_c$ closing the effective gap is obtained as $u_c \approx 0.253 \Delta_0 \approx 0.253$ meV. The critical field of the experimental data is $E \approx 1.25$ mV\text{A}^{-1}$, which corresponds to $u_c \approx 0.69$ meV (using $\epsilon \approx 3$).

Since the system satisfies the particle-hole symmetry at $B = 0$, we can take the chemical potential as zero for the system at the CNP. Then, the level $E_{K0}$ is occupied if it is negative, otherwise it is empty. Therefore, with increasing $u$ from 0, the system undergoes a phase transition at $u = u_0$ from the state with the level $E_{K0}$ occupied to the state with the level empty. Thus, to search the critical $u_0$ where the gap closes at finite $B$, we study the phase transition.

At finite $B$, a state at $(B, u)$ can be obtained by continuously changing the parameters $B$ and $u$ from the state at $(0, u_0)$. If $u > u_0(0)$, then the level $E_{K0}$ is empty. Note that $E_{K0}$ is the only Landau level of $n = 0$ at finite $B$ and there is another level of $n = 1$ close to it similarly as the case of $u = 0$. So the two levels of $n = 0$ and 1 in the $K$ valley keep empty on the path from $(0, u_0)$ to $(B, u)$. On the other hand, if one starts from an initial state with $u_i < u_0(0)$, then the two levels of $n = 0$ and 1 keep filled. (We denote the filling number as $f_K = 0$ and 1 for the two levels empty and filled, respectively.) We thus have two states at $(B, u)$. By comparing their energies, the ground state at $(B, u)$ is uniquely determined. At the critical potential $u_0(B)$, the two states have the same ground-state energy. The ground-state energy per unit cell, $E_0$, is given by

$$
E_0 = \frac{\sqrt{3} B}{4\pi} \sum_{\nu m} f(E^{\mu}_{vn}) [2E^{\mu}_{vn} - x^{\mu\nu}_v \Sigma(v) x^{\nu\mu}_v] \tag{34}
$$

where $\Sigma(v)$ is the self-energy matrix given by $\Sigma(v) = \text{Diag}(r_1 v_c - s_0 \Delta_1, r_2 v_c + s_0 \Delta_2, -r_2 v_c - s_0 \Delta_2, -r_1 v_c + s_0 \Delta_1)$. 

FIG. 9: (Color online) Landau levels $E^{\mu}_{vn}$ of the AF state in the valence and conduction bands at $B = 1$ T. The circles and solid circles represent the levels in the $K$ and $K'$ valleys, respectively. The lines represent the continuum conduction (solid) and valence (dashed) bands at $B = 0$ with momentum $k$ as the abscissa.
by the theoretical calculation is in fairly good agreement with the experimental data. As seen from Fig. 10, the behavior of \( u \) given by the formula (34) can be derived according to many-particle theory. The solid points and the diamonds (connected by the dashed line) are converted from the critical \( E \) of the experimental data (see Ref. 7) using \( \epsilon \approx 3.4 \) and 3, respectively. The inset shows the result for \( \Delta_1 < 0 \) in the range \( 0 < B < 0.15 \) T.

Note that the energy levels of the OCS at finite \( u \) are not degenerate for interchanging the indices of the two valleys. Especially, the Landau levels \( E_{K'0} \) and \( E_{K0} \) are given by \( u + r_1 v_c - \Delta_1 \) and \( -u - r_1 v_c - \Delta_1 \), respectively. For positive \( u \) and \( \Delta_1 \), the level \( E_{K'0} \) is always occupied.

In Fig. 10, we exhibit the result for \( u_0(B) \) as function of \( B \) and compare it with the experimental data. The experimental data are obtained by converting the critical electric field \( E \) to \( u_0 \) according to \( u_0 = E \text{ed}/2\kappa \) with the dielectric constant \( \epsilon \approx 3.4 \) (solid points) and 3 (diamonds). As seen from Fig. 10, the behavior of \( u_0(B) \) by the theoretical calculation is in fairly good agreement with the experimental data with \( \epsilon \approx 3.4 \) in the converting from \( E \) to \( u_0(B) \).

As already seen, there is another solution of \( \Delta_1 < 0 \) in the range \( 0 < B < 0.18 \) T. We show in the inset in Fig. 10 the phase boundary for this case. We see that the state of \( \Delta_1 < 0 \) in \( B > 0.07 \) T is unstable with respect to a small \( E \). The range for the stable state of \( \Delta_1 < 0 \) is reduced to \( |B| < 0.07 \) T, with \( |B_{\text{max}}| = 0.07 \) T close toward to the experimental data.

VI. SUMMARY

With the MFA to the 4BCM, we have studied the OCS and the AF state of the electrons with finite-range repulsive interactions in BLG at the CNP. We have shown that the result of AF state is not in agreement with the experimental observation on the energy gap behavior that grows with increasing the magnetic field \( B \). However, for the OCS with only one coupling constant \( v_s \) fitting the experimental gap at \( B = 0 \), the obtained energy gap at finite \( B \) is in surprisingly good agreement with experimental data. The results for the phase transition in the system in the presence of external electric and magnetic fields, and the particle-hole asymmetry spectra in the presence of \( B \) are in qualitative agreements with the experimental observations. There is also the intermediate experimental support to the prediction for the hysteresis energy gap behavior with varying \( B \). These facts show that the OCS is a possible ground state of electrons in BLG. The model explored here can be useful for understanding the physics of the electrons in BLG that is expected as a new generation of semiconductor.

This work was supported by the National Basic Research 973 Program of China under Grants No. 2011CB932702 and No. 2012CB932302, NSFC under Grant No. 10834011, and the Robert A. Welch Foundation under Grant No. E-1146.

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