Chiral Symmetry and Many-Body Effect in Multilayer Graphene

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Abstract. Influence of the chiral symmetry on the many-body problem in multilayer graphene in magnetic fields is investigated. For a spinless electron model on the honeycomb lattice the many-body ground state is shown to be a doubly-degenerate chiral condensate irrespective of the number of layers. The energy spectrum calculated numerically with the exact diagonalization method reveals for ABC-stacked multilayer graphenes that the many-body gap decreases monotonically with the number of layers.

1. Introduction
Graphene’s intriguing physics [1, 2, 3, 4] is intimately related to the chiral symmetry, a fundamental feature of the honeycomb lattice. The symmetry is defined by the anticommutation relation, \( \{ \mathcal{H}, \Gamma \} = 0 \), with the chiral operator \( \Gamma \) acts as

\[ \Gamma c_i \Gamma = +c_i (-c_i) \quad \text{for} \quad i \in \bullet \circ, \quad \Gamma^2 = 1, \]

where \( \bullet \) and \( \circ \) respectively denote the two sublattices. The symmetry guarantees [5, 6] the topological stability of the doubled Dirac cones, an example of Nielsen-Ninomiya theorem [7, 8], as well as the degeneracy of the \( n = 0 \) Landau level (LL), which accommodates Aharonov-Casher’s argument [9]. A remarkable phenomenon in the latter is the delta-function-like density of states (DOS) for the \( n = 0 \) LL even in the presence of ripples with wavelengths exceeding a few lattice constants [10]. These properties are expected to be inherited by multilayer graphene [11, 12, 13], since the leading hopping matrix elements, \( \gamma_0, \gamma_1 \) and \( \gamma_3 \), conserves the...
bipartite lattice structure, and hence the chiral symmetry. Indeed, a recent theory [14] predicts that AB-stacked bilayer graphene retains the anomaly in DOS, which even extends to the case of a perpendicular electric field that in fact breaks the chiral symmetry.

Then an interesting question is how the chiral symmetry affects the many-body problem in multilayer graphene. Many-body effects have been extensively studied [4, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40] from the beginning of the graphene research due to interests that include the gap opening in the central LL [41, 42, 43, 44] and the unconventional insulating $\nu = 0$ state [45]. So far, the role of the chiral symmetry in the many-body problem has been studied in the context of the lattice gauge theory, where monolayer graphene without magnetic fields is discussed, mainly based on the continuum model [46, 47, 48].

In the present work, we consider multilayer graphenes in magnetic fields, and investigate the many-body problem in terms of the chiral symmetry.

2. Ground states

We consider spinless electrons in multilayer graphenes in a magnetic field, for which the kinetic energy is

$$H_{\text{kin}} = -\sum_{\langle ij \rangle} \gamma_{ij} e^{i\theta_{ij}} c_i^+ c_j + \text{H.c.},\quad (2)$$

where $\gamma_{ij}$ is the electron hopping between sites $\langle ij \rangle$. For the nearest-neighbor in-plane sites $\gamma_{ij} = \gamma_0$, while for the inter-layer vertical hopping $\gamma_{ij} = \gamma_1$. The magnetic field is included as the Peierls phase $\theta_{ij}$ such that magnetic flux per elementary hexagon equals to $\phi = \frac{1}{2\pi} \sum_{ij} \theta_{ij}$ in units of the magnetic flux quantum $\hbar/e$. In the string gauge [49], the magnetic flux reads $\phi = n/N_c$ with an integer $n$ and the number of unit cells, $N_c$. Since the $\gamma_0$-$\gamma_1$ model preserves the chiral symmetry, one can construct a zero-energy multiplet, $\psi = (\psi_+, \psi_-)$ with $\psi_{\pm} = (\psi_{1\pm}, \cdots, \psi_{M_\pm})$, where $\psi_{m\pm}$’s denote $M_\pm$-fold degenerate eigenstates of $\Gamma$ corresponding to chirality $\pm 1$, i.e., $\Gamma \psi_{m\pm} = \pm \psi_{m\pm}$. For an $N_l$-layer bulk system with a magnetic flux $\phi = n/N_c$, $\nu = 0$, the degeneracy reads $M_\pm = M = nN_l$. It should be noted that the zero modes with chirality $+$ or $-$ are localized on sublattice $\bullet$ or $\circ$, respectively. Especially for ABC-stacked multilayers, the zero modes show sublattice-selective charge accumulation towards the top or bottom layer, which decays rapidly away from the surface [50, 51, 52]. The surface states are analogous to the zigzag edge states in the ribbon structure [53] and should be observed experimentally as local density of states near zero energy with a scanning tunneling microscope.

For a half-filled multilayer graphene, the interaction for spinless electrons can be written in
a particle-hole symmetric form as

\[ \mathcal{H}_{\text{int}} = \sum_{i \neq j} V_{ij} \left( n_i - \frac{1}{2} \right) \left( n_j - \frac{1}{2} \right) = \frac{1}{2} \sum_{i \neq j} V_{ij} (c_i^\dagger c_j^\dagger c_j c_i + c_i c_j c_i^\dagger c_j^\dagger) + \text{const} \] (3)

with interaction strength \( V_{ij} \). Since it is hard to treat all the many-body states exactly, we focus on the many-body problem within the zero-energy LL. Such a treatment is adequate as long as the interaction energy is sufficiently smaller than the Landau gap between the central and adjacent LLs. The projection onto the zero-energy LL is performed as \( \tilde{c} = (\psi \psi^\dagger) c \), where \( c = (c_1, \cdots, c_N)^T \) with the number of sites \( N \), and \( \psi \psi^\dagger \) denotes the projection matrix. Note that the projected creation and annihilation operators are no longer fermionic; they obey anticommutation relations \( \{ \tilde{c}_i, \tilde{c}_j^\dagger \} = (\psi \psi^\dagger)_{ij} \) and \( \{ \tilde{c}_i, \tilde{c}_j \} = \{ \tilde{c}_i^\dagger, \tilde{c}_j^\dagger \} = 0 \). In what follows, we assume that the electron-electron repulsion only acts between electrons on different sublattices \( [V_{ij} > 0 \text{ for } (i, j) = (\bullet, o)] \). The simplest example is the nearest-neighbor repulsion, which is the leading term for spinless electrons. The total Hamiltonian in the projected subspace reads, up to a constant,

\[ \tilde{\mathcal{H}} = \sum_{i \in \bullet, j \in o} \frac{V_{ij}}{2} (\tilde{c}_i^\dagger \tilde{c}_j^\dagger \tilde{c}_j \tilde{c}_i + \tilde{c}_i \tilde{c}_j \tilde{c}_i^\dagger \tilde{c}_j^\dagger) = \frac{1}{2} \sum_{klmn} (V_{klmn} d_{kl}^d d_{mn}^d - d_{kl}^d d_{mn}^d) \] (4)

where \( d_{kl}^d = c_i^\dagger \psi_{m_+} \) is the creation operator for the zero mode \( \psi_{m_+} \), while the pseudopotential appearing for \( d, d^\dagger \) is defined as \( V_{klmn} = \sum_{i \in \bullet, j \in o} V_{ij} (\psi_k)^\dagger (\psi_l)^\dagger (\psi_m) (\psi_n) \). Clearly, \( \tilde{\mathcal{H}} \) is semi-positive definite; for an arbitrary many-body state \( |\Phi\rangle \), \( \langle \Phi| \tilde{\mathcal{H}} |\Phi\rangle = \frac{1}{2} \sum_{i \in \bullet, j \in o} V_{ij} |(\tilde{c}_i \tilde{c}_j + (\tilde{c}_i^\dagger \tilde{c}_j^\dagger))| |\Phi\rangle |^2 \geq 0 \). Since \( \tilde{\mathcal{H}} \) commutes with \( G \equiv \sum_m (d_{m_+}^d d_{m_+}^d - d_{m_-}^d d_{m_-}^d) \), eigenstates of \( \tilde{\mathcal{H}} \) are classified according to the total chirality, \( \chi = (|G\rangle) \). The highest and lowest sectors in \( \chi \) correspond to chiral condensates,

\[ |G_\pm\rangle = d_{k_+}^d \cdots d_{M_+}^d |D_\lesssim\rangle, \quad \mathcal{G}|G_\pm\rangle = \pm M_\pm |G_\pm\rangle, \] (5)

where all the zero modes with chirality \( + \) (or \( - \)) are occupied, while others are empty. \( |D_\lesssim\rangle \) denotes the Dirac sea of completely filled negative energy states. The chiral condensates are in fact the many-body ground states, since they are annihilated by both of \( d_{k_+}^d d_{k_+}^d \) and \( d_{m_-}^d d_{m_-}^d \), hence \( (G_\pm)|\tilde{\mathcal{H}}|G_\pm\rangle = 0 \). Thus the chiral condensates form a ground-state doublet, \( \Psi = (|G_+\rangle, |G_-\rangle) \), so that any unitary-mixture, \( \Psi \rightarrow \Psi e^{\omega} \) with \( \omega \in U(2) \), is again an eigenstate. We expect that the chiral condensate remains the ground state for e.g. Coulomb interaction.
because its leading part is the nearest-neighbor repulsion. Since the above discussion holds irrespective of the number of layers, it is expected that $\Psi$ has properties similar to those in the monolayer case, such as vanishing Hall conductivity, or the Kekulé-type bond-order along armchair edges [54, 55]. Although the spinless model with interaction between opposite sublattices might seem rather artificial, the results obtained here should have an experimental relevance in e.g. cold atoms on an optical lattice.

As a physical property peculiar to the multilayer case, we plot in Figure 1 layer-by-layer charge distribution in $|G_{\pm}|$ for an ABC-stacked multilayer with $N_c = 15^2$ and $N_l = 10$, where only the electrons in the zero-energy LL is shown. Since an experimental cyclotron frequency $!c$ is too small to treat numerically based on our lattice model, we adopt a rather large parameter $\gamma_1/\gamma_0 = 0.5$ to access the realistic parameter region $\gamma_1 > \omega_c$. One can see charge accumulation towards the top or bottom layer, which reflects the property of the zero modes as the surface states [50, 51, 52]. Notably, a shoulder structure evolves on the intermediate layers with increasing $\phi$. Although the non-monotonic behavior disagrees with the results of the continuum model, where low-energy wave functions decays exponentially away from a surface, the discrepancy seems to be due to the finite size effect of our lattice model.

3. Excited states

Next we investigate excited states at half filling by numerically diagonalizing the projected Hamiltonian (4). For simplicity, only the nearest-neighbor repulsions in the same layer $V_0$ and those between adjacent layers $V_1$ are taken into account. Fig. 2 shows typical examples of energy spectra plotted against the total chirality, $\chi$, for AB-stacked bilayer graphene and for ABC- or ABA-stacked trilayer graphene. The spectra are symmetric with respect to $\chi$, since now we have the degeneracies of the zero modes with chirality $+\ $ and $-\ $ are equal. From this total-chirality-resolved plot one can confirm that the ground states are indeed chiral condensates, as expected from the above discussion. More importantly, these data suggest that the first excited states are obtained by flipping a single-chirality of the chiral condensates as

$$|E_{\pm}\rangle = \sum_{mn} C_{mn} a_{m\mp}^\dagger d_{n\pm}|G_{\pm}\rangle$$

(6)

with coefficients $C_{mn}$ determined numerically. Although the size of the Hilbert space blows up exponentially with the number of layers, the ansatz (6) enables us to calculate the energy gap $\Delta$ between the ground state and the first-excited state by restricting ourselves to the sector of total chirality $\chi = \pm(M_+ - 2)$. Figure 3 plots thus obtained energy gap $\Delta$ of ABC-stacked multilayer graphene composed of $N_l$ graphene sheets. The decrease in $\Delta$ as a function of $N_l$ is consistent with the fact the overlap of the opposite-chirality zero modes, which are accumulated near the opposite surfaces, becomes small with increasing $N_l$. The saturation in $\Delta$ for large $N_l$ suggests that the overlap does not completely vanish due to the finite size effect.
4. Summary
We have considered spinless fermions in multilayer graphene and investigated many-body states in the quantum Hall regime. For the electron-electron repulsion restricted to unlike sublattices, the ground state is exactly identified to be chiral condensates as in the case of monolayer graphene. Using the exact diagonalization method, we have numerically calculated the many-body gap, which decreases monotonically with increasing the number of layers.

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