Chiral condensate with topological degeneracy in graphene and its manifestation in edge states

Yuji Hamamoto, Hideo Aoki, and Yasuhiro Hatsugai

1Institute of Physics, University of Tsukuba, Tsukuba 305-8571, Japan
2Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan
3Tsukuba Research Center for Interdisciplinary Material Science, University of Tsukuba, Tsukuba 305-8571, Japan

(Dated: May 1, 2014)

Role of chiral symmetry in many-body states of graphene in strong magnetic fields is theoretically studied with the honeycomb lattice model. For a spin-split Landau level where the leading electron-electron interaction is the nearest-neighbor repulsion, a chiral condensate is shown to be, within the subspace of \( n = 0 \) Landau level, an exact many-body ground state with a finite gap, for which calculation of Chern numbers reveals that the ground state is a Hall insulator with a topological degeneracy of two. The topological nature of the ground state is shown to manifest itself as a Kekuléan bond order along armchair edges, while the pattern melts in the bulk due to quantum fluctuations. The whole story can be regarded as a realization of the bulk-edge correspondence peculiar to the chiral symmetry.

PACS numbers: 73.22.Pr, 71.10.Fd, 73.43.-f

Introduction.—While the physics of graphene started from the one-body electronic structure as a Dirac fermion, a possible relevance of electron correlation in graphene has been intensively studied after a gap opening in the \( n = 0 \) Landau level (LL) was experimentally observed in strong magnetic fields. Since it is difficult to explain the gap within a simple one-body problem, considerable theoretical efforts have ensued to clarify many-body effects in graphene quantum Hall (QH) systems. However, little attention has been paid on how many-body effects should reflect the chiral symmetry in the graphene QH regime, which is after all a fundamental symmetry inherent in graphene’s honeycomb lattice. On the one-body level, the effects of chiral symmetry in graphene is well understood: To start with, the symmetry guarantees the emergence of doubled Dirac cones in the Brillouin zone, which can be interpreted as a two-dimensional analogue of the Nielsen-Ninomiya theorem well-known in the four-dimensional lattice gauge theory. We can even examine the wave functions in terms of Aharonov-Casher argument, which states that chiral symmetry topologically protects the degeneracy of the \( n = 0 \) LL against random gauge fields. A similar situation occurs for ripples in a graphene sheet, which can be modelled by random hopping amplitudes. Kawarabayashi et al. have shown that the \( n = 0 \) LL exhibits an anomalously sharp (delta-function-like) density of states (DOS) as soon as the spatial wavelength of the ripple exceed a few lattice constants.

In the presence of electron-electron interactions, on the other hand, the role of chiral symmetry has primarily been investigated in zero magnetic fields in the context of spontaneous symmetry breaking. While these studies mainly employ a Dirac field model in a continuum space to discuss many-body gap formation, such an effective treatment may well overlook the essence of graphene’s chiral symmetry, which is intimately related to the underlying honeycomb lattice.

With this background, we shed light in the present work on how the chiral symmetry influences the many-body problem in graphene QH effect, by fully taking account of the lattice structure. We first examine the many-body problem with exact diagonalization in a subspace projected onto the \( n = 0 \) LL. Working on the subspace enables us to classify many-body states according to a notion of the total chirality of the filled zero modes. In terms of this, for a “bipartite” electron-electron interaction such as the nearest neighbor repulsion, which is the dominant interaction for a spin-split LL, we show that the many-body ground state is exactly identified to be a chiral condensate with a topological degeneracy of two. We confirm numerically that there exists a finite energy gap to the first-excited state, which makes the Chern number of the ground state well-defined. The total Chern number contributed by the filled zero modes along with the negative energy states (“Dirac sea”) turns out to be zero, which implies the system is a Hall insulator with vanishing Hall conductance.

Despite the cancellation of the Chern number in the bulk, however, we move on to show that the topological nature of the chiral condensate is in fact made manifest as an emergence of a Kekuléan bond order in the edge state along armchair edges of the honeycomb lattice, which is defined as a phase transition driven by a Zeeman splitting, so that the leading Coulomb interaction acts diagonal in a subspace projected onto the \( n = 0 \) LL.

Chiral symmetry,—To model interacting electrons on a honeycomb lattice, we assume that spin degeneracy is lifted by a Zeeman splitting, so that the leading Coulomb interaction reduces to the nearest-neighbor repulsion. The Hamiltonian then reads

\[
\mathcal{H} = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{int}},
\]

where the kinetic term

\[
\mathcal{H}_{\text{kin}} = -t \sum_{\langle ij \rangle} (c_{i \uparrow}^\dagger c_{j \uparrow} + H.c.)
\]

describes electron hopping between adjacent sites \( \langle ij \rangle \) with strength \( t > 0 \). The magnetic field is included as the Peierls phase \( \theta_{ij} \) such that magnetic flux per elementary hexagon equals

\[
\sum_{\text{hexagon}} \theta_{ij} = 2\pi \phi.
\]
in units of a magnetic flux quantum $h/e$. For a honeycomb lattice with $N_{\text{sites}}$ sites in sublattice $\bullet \circ$, $c_i^\dagger = (c_i^+ \leftarrow c_i^\pm)$ with $c_i^\pm$ a row of creation operators for sublattice $\bullet \circ$ and $H_{\text{kin}}$ is a square matrix of dimension $N_+ + N_-$. If we introduce $\Gamma = \text{diag}(\Gamma_+, -\Gamma_-)$ with an identity matrix $I_{\circ\circ}$ of dimension $N_{\text{sites}}$, the kinetic term satisfies an anticommutation relation \{ $H_{\text{kin}}, \Gamma$ \} = 0, which defines the chiral symmetry. The symmetry implies that, if $\psi_k$ is the $k$-th eigenvector with energy $\varepsilon_k$, a chiral partner $\Gamma \psi_k$ exists with an energy $-\varepsilon_k$. This makes the $n = 0$ LL special in that we can take $\psi_k$ as an eigenstate of $\Gamma$ as $\Gamma \psi_k = \pm \psi_k$. The interaction between spin-polarized electrons is expressed in a particle-hole symmetric form as $\mathcal{H}_{\text{int}} = \sum_{ij} V_{ij} \psi_i^\dagger \psi_j$ with $V_{ij} = \frac{1}{2} \sum_{\sigma} (c_i^{\sigma} c_j^{\sigma} + c_j^{\sigma} c_i^{\sigma} + \text{const} \cdot)$, where $V_{ij}$ is the strength of electron-electron interaction. $n_i = c_i^\dagger c_i$ the number operator at site $i$.

Chiral condensate.—We start with an investigation of the many-body problem at half filling. It is difficult to treat all the many-body states in this space, we shrink the Hilbert space by projecting onto the $n = 0$ LL. Such a treatment is valid as long as $|V_{ij}|$ is perturbatively small compared with the Landau gaps around the $n = 0$ LL. In the $n = 0$ LL, we take a zero mode multiplet $\psi = (\psi_{\bullet}, \psi_\circ)$ we have decomposed it into eigenstates of the chiral operator, $\psi_k = (\psi_{\bullet k}, \cdots, \psi_{\bullet M_k})$ with degeneracy $M_k$. Note that the zero modes are localized on each of the sublattices as $\psi_{\bullet k}$ perturbatively small compared with the Landau gaps around the $n = 0$ LL. In the $n = 0$ LL, we take a zero mode multiplet $\psi = (\psi_{\bullet}, \psi_\circ)$ we have decomposed it into eigenstates of the chiral operator, $\psi_{\bullet k} = (\psi_{\bullet k}, \cdots, \psi_{\bullet M_k})$ with degeneracy $M_k$. Note that the zero modes are localized on each of the sublattices as $\psi_{\bullet k}$ perturbatively small compared with the Landau gaps around the $n = 0$ LL.

We call this a topological degeneracy of two. Unperturbatively small compared with the Landau gaps around the $n = 0$ LL. In the $n = 0$ LL, we take a zero mode multiplet $\psi = (\psi_{\bullet}, \psi_\circ)$ we have decomposed it into eigenstates of the chiral operator, $\psi_{\bullet k} = (\psi_{\bullet k}, \cdots, \psi_{\bullet M_k})$ with degeneracy $M_k$. Note that the zero modes are localized on each of the sublattices as $\psi_{\bullet k}$ perturbatively small compared with the Landau gaps around the $n = 0$ LL. Since it is difficult to treat all the many-body states in this space, we shrink the Hilbert space by projecting onto the $n = 0$ LL. Such a treatment is valid as long as $|V_{ij}|$ is perturbatively small compared with the Landau gaps around the $n = 0$ LL. In the $n = 0$ LL, we take a zero mode multiplet $\psi = (\psi_{\bullet}, \psi_\circ)$ we have decomposed it into eigenstates of the chiral operator, $\psi_{\bullet k} = (\psi_{\bullet k}, \cdots, \psi_{\bullet M_k})$ with degeneracy $M_k$. Note that the zero modes are localized on each of the sublattices as $\psi_{\bullet k}$ perturbatively small compared with the Landau gaps around the $n = 0$ LL.

Many-body gap.—We next calculate excitation energies numerically with the exact diagonalization method. In the projected subspace, the strength of the nearest-neighbor repulsion $V > 0$ is the only energy scale, which acts as the unit of energy. Full energy spectra of $\mathcal{H}$ for finite systems suggest that the first excited state appears in the sector of $\chi_{\text{tot}} = \pm (M_k - 2)$, which is created from a chiral condensate $|G\rangle$ by single chirality-flippings analogous to the projected single-mode approximation. Noticing this, we further shrink the Hilbert space by focusing on the sector of $\chi_{\text{tot}} = \pm (M_k - 2)$. This enables us to obtain the energy of the first excited state, or the energy gap $\Delta$, with calculation cost of the order of $O(M_k^2)$. We consider a system on a torus composed of $2L^2$ lattice sites with a linear dimension $L$. For investigating a weak-field regime, we adopt the string gauge where a magnetic flux is given by $\phi = m/L^2$ with an integer $m > 0$ and $M_k = m$ zero modes are obtained for each chirality.

In Fig. 1 we plot $\Delta$ for 30 electrons as a function of $\phi$ with $L$ changed consecutively. We immediately notice that the result exhibits a marked periodicity of three, where the values for $L \equiv 3$ (mod 3) form a clear lower envelope with a scaling $\Delta \propto \phi^2$. While those for $L \neq 3l$ deviates from this. The latter behavior is considered to be a finite-size effect, since the deviation diminishes with the sample size. To confirm the scaling, the inset plots $\Delta/\phi^2$ at $L = 3l$ against $1/L$ for various values of $\phi$, which indicates the scaling law $\Delta \propto \phi^2$ is very accurately obeyed.

Hall conductance.—Let us now consider Hall conductance of the chiral condensate. By the Niu-Thouless-Wu formula the Hall conductance is written with the Chern number as

$$\sigma_{xy} = \frac{e^2}{h} \frac{1}{N_D} C, \quad C = \frac{1}{2\pi} \int \text{Tr}N_0 dA, \quad A = \Psi^\dagger d\Psi$$

where $N_D$ is the degeneracy and $A$ is the non-Abelian Berry connection that describes multiplets. In terms of the basis that diagonalizes $G$, we have $C = C_+ + C_-$. With $C_\pm = \frac{1}{2\pi} \int (dG_{\pm} dG_{\pm})$. Each term is further decomposed
as \( C_{\pm} = C_{\psi_{+}} + C_{D_{\pm}} \) with \( C_{\psi_{+}} = \frac{1}{2a^2} \int \text{Tr}(M \phi) d\phi \) and \( C_{D_{\pm}} = \frac{1}{2a^2} \int \text{Tr}d\phi \). By the charge conjugation, we have \( C_{\psi_{-}} = -C_{\psi_{+}} = C_{D_{\pm}} \) with \( C_{D_{\pm}} = \frac{1}{2a^2} \int \text{Tr}(\Gamma d\phi) \). Thus the total Chern number of the ground-state doublet vanishes as \( C = C_{\psi_{+}} + C_{\psi_{-}} + 2C_{D_{\pm}} = 0 \), which may be called a topological cancellation. This implies that the chiral condensate is a Hall insulator with a nontrivial topological degeneracy \( N_{D} = 2 \).

**Bond order.**—As have been confirmed in various systems, while topological phases are featureless in a bulk, they show characteristic boundary states. So a natural question we can pose here is: do the edge states in the present system exhibit special features despite the bulk Chern number being zero? Before presenting the result, however, let us first have a look at the mean-field state in the present system in the bulk, which will turn out to be instructive. One virtue of a mean-field picture is that we can introduce a bond order, \( \Delta_{ij} \equiv \langle V_i^\dagger c_j^\dagger \rangle \), for adjacent sites \((i,j)\). The dominant part of the MF Hamiltonian is given by \( \mathcal{H}_{MF} = -\sum_{ij}[(r_{ij}^\mu + \Delta_{ij}) c_i^\dagger c_j^\dagger + \text{H.c.}] \), where \( \Delta_{ij} \) is determined self-consistently by diagonalizing \( \mathcal{H}_{MF} \). A spontaneous symmetry breaking is induced by the many-body effect for weak magnetic fields, where the density of states has a sharp peak at the Fermi energy. In Fig. 3, we show a typical MF result for the ordered phase. The energy spectrum is plotted in panel (a), where the qualitative structure of the LLs is preserved. This comes from the fact that the convergent order parameters turn out to retain the initial Peierls phase as \( \Delta_{ij} = |\Delta_{ij}| e^{i\phi_{ij}} \). The influence of the electron-electron interaction appears most prominently in the \( n = 0 \) LL, where a finite gap of the order of \( \phi \) opens as shown in the blowup Fig. 3(b).

To see how the symmetry is broken in the mean field, we show in panel (c) a real-space image of the bond order \( |\Delta_{ij}| \), which is seen to exhibit a Kekulé pattern. This makes the unit cell enlarged, which causes \( K \) and \( K' \) points to be coupled, and this in turn opens a finite gap. In this sense we can regard this a Peierls transition in the honeycomb lattice.

On the other hand, the chiral condensate with its topological degeneracy of two exhibits in the bulk no bond order as we have seen in Fig. 2. Due to the quantum fluctuation, the bond order of the mean field is destroyed and the quantum liquid ground state is realized.

**Edge and defect states.**—We are now in a position to ask the question: what kind of edge states does the chiral condensate accommodate? Based on the bulk-edge correspondence, we may expect a non-trivial behavior of the many-body states near edges. A prime example is the fractional QH states in a 2DEG, where a CDW-like behavior emerges along edges of a ribbon while in the bulk it melts into the Laughlin liquid with no long-range order, which has a \( q \)-fold degeneracy of the fractional QH states at filling \( \nu = 1/q \). Note that a honeycomb lattice with edges has QH edge states whose mode lies in a LL gap. To perform the projection onto the \( n = 0 \) LL we set an energy cutoff, the choice of which is shown to have little influence on the edge states shown below.

In Fig. 3 we show \( |\Delta_{ij}| \) for the chiral condensate plotted in a real space near armchair and zigzag edges. In panel (a), we can see that a Kekulé-type bond order reminiscent of the mean-field result in Fig. 2 emerges along the armchair edge. This is the key result in the present work. The enhancement in bonds rapidly decays away from the edge in a few lattice constants, and \( |\Delta_{ij}| \) slightly oscillates with a length scale of the order of the magnetic length \( l_B \sim a/\sqrt{B} \) with \( a \) being the interatomic spacing. This may naively seem to be analogous to the fractional QH edge states in a 2DEG, but here the honeycomb lattice structure is essential in the ground state. Indeed, the ring pattern is locked along the armchair edge in a Kekulé pattern, while this is not the case with zigzag edges [see panel (b)]. In the latter case, the ring pattern is blurred by the translational symmetry along a zigzag edge, and a very weak stripe pattern parallel to the edge appears. These patterns related with the three-fold degeneracy of the Kekulé pattern are washed out in the bulk chiral condensate. All these are a specific property of a honeycomb lattice model.

We can further endorse that the lattice structure is at the core by looking at the states around lattice defects. When a single atom is removed from the bulk honeycomb lattice, one-body localized zero modes appear that are protected by the
FIG. 4: (color online) Bond strength of the chiral condensate near a divacancy composed of two adjacent sites missing. Magnetic flux is \( \phi = 1/1200 \) for which the magnetic length is \( l_B \approx 22.3a \). The bond order reflects twofold axial symmetry of the divacancy.

In the presence of the electron-electron interactions, however, local chiral symmetry breaking occurs spontaneously to lower the energy by inducing effective hopping in the same sublattice. Then what if two point defects come close to each other? Such a divacancy consists of two adjacent missing atoms, and is recently observed experimentally in ion-irradiated carbon samples. We expect that the chiral symmetry may be partially recovered with a reconfiguration of the two symmetry-breaking bonds. We plot in Fig. 4 the bond order for the chiral condensate near the divacancy. We do confirm that enhancement of the bond order near the divacancy which can be considered due to the revival of the chiral symmetry.

We have thus shown that the bond order emerges along edges and around vacancies, despite the topological cancellation \( C = 0 \) that might first seem to wipe out any signature of the chiral condensate. Indeed, the charge density itself is uniform for the chiral condensate even along edges, which is due to the invariance of the chiral condensate for the charge conjugation. Thus it is the bond order \( |\Delta ij| \) that we have to look at as a probe for the chiral condensate. Thus the bond order provides a new probe for the many-body effect in half-filled graphene applied a magnetic field. The bond order near edges should be observable experimentally with some imaging techniques such as Green’s function scanning tunneling microscopes. Since the amplitude of \( |\Delta ij|/V = |\langle c_i \dagger c_j \rangle| \) is of the order of the magnetic flux \( \phi \), the magnetic field should have significant magnitudes.

Summary.—The many-body ground state at half filling in the honeycomb lattice is identified as a doubly-degenerate chiral condensate for a spin-split Landau level. The many-body effect opens a finite energy gap, which makes the chiral condensate a generic topological insulator. However, the system has a peculiar manifestation of the bulk-edge correspondence in topological systems as an emergence of a bond order with a Kekulé pattern along armchair edges in an exact ground state, while the pattern is dissolved in the bulk.

Acknowledgement.—The computation in this work has been done with the facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. This work was supported in part by Grants-in-Aid for Scientific Research No. 23340112 and No. 23654128 from the JSPS.

---

* Electronic address: hatsugai@sakura.cc.tsukuba.ac.jp

---

1. Y. Zhang, Z. Jiang, J. P. Small, M. S. Purewal, Y.-W. Tan, M. Fazlollahi, J. D. Chudow, J. A. Jaszczak, H. L. Stormer, and P. Kim, Phys. Rev. Lett. 96, 136806 (2006).
2. Z. Jiang, Y. Zhang, H. L. Stormer, and P. Kim, Phys. Rev. Lett. 99, 106802 (2007).
3. K. Nomura and A. H. MacDonald, Phys. Rev. Lett. 96, 256602 (2006).
4. J. Alicea and M. P. A. Fisher, Phys. Rev. B 74, 075422 (2006).
5. M. O. Goerbig, R. Moessner, and B. Douçot, Phys. Rev. B 74, 161407 (2006).
6. V. P. Gusynin, V. A. Miransky, S. G. Sharapov, and I. A. Shovkovy, Phys. Rev. B 74, 195429 (2006).
7. I. F. Herbut, Phys. Rev. B 75, 165411 (2007).
8. J. Alicea and M. P. A. Fisher, Sol. Stat. Comm. 143, 504 (2007).
9. L. Sheng, D. N. Sheng, F. D. M. Haldane, and L. Balents, Phys. Rev. Lett. 99, 196802 (2007).
10. Y. Aharonov and A. Casher, Phys. Rev. A 19, 2461 (1979).
11. T. Kawarabayashi, Y. Hatsugai, and H. Aoki, Phys. Rev. Lett. 103, 156804 (2009).
12. J. E. Drut and T. A. Lähde, Phys. Rev. Lett. 102, 026802 (2009).
13. J. E. Drut and T. A. Lähde, Phys. Rev. B 79, 165425 (2009).
14. Y. Araki and T. Hatsuda, Phys. Rev. B 82, 121403 (2010).
15. Y. Hatsugai, Phys. Rev. Lett. 71, 3697 (1993).
16. The detail will be given elsewhere.
17. Y. Hamamoto, Y. Hatsugai, and H. Aoki, arXiv:1108.1638.
M. M. Ugeda, I. Brihuega, F. Hiebel, P. Mallet, J.-Y. Veuillen, J. M. Gómez-Rodríguez, and F. Ynduráin, Phys. Rev. B 85, 121402 (2012). To be precise, they have detected five-membered rings adjacent to an eight-membered one, where odd-membered rings are expected to have significant effects on the chiral states.

J. M. Byers and M. E. Flatté, Phys. Rev. Lett. 74, 306 (1995).

Q. Niu, M. C. Chang, and C. K. Shih, Phys. Rev. B 51, 5502 (1995).