Edge states in graphene in magnetic fields
— a speciality of the edge mode embedded in the $n = 0$ Landau band

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While usual edge states in the quantum Hall effect (QHE) reside between adjacent Landau levels, QHE in graphene has a peculiar edge mode at $E = 0$ that reside right within the $n = 0$ Landau level as protected by the chiral symmetry. We have theoretically studied the edge states to show that the $E = 0$ edge mode, despite being embedded in the bulk Landau level, does give rise to a wave function whose charge is accumulated along zigzag edges. This property, totally outside continuum models, implies that the graphene QHE harbors edges distinct from ordinary QHE edges with their topological origin. In the charge accumulation the bulk states re-distribute their charge significantly, which may be called a topological compensation of charge density. The real space behavior obtained here should be observable in an STM imaging.

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Introduction — Ever since the anomalous quantum Hall effect (QHE) was experimentally observed[1,2] fascination with graphene is mounting. The interests have been focused on the “massless Dirac” dispersions around Brillouin zone corners (K, K') in graphene, where the Dirac cone is topologically protected due to the chiral symmetry[3]. The peculiar dispersion is responsible for the appearance of the $n = 0$ Landau level ($n$: Landau index) precisely around energy $E = 0$ in magnetic fields. For the ordinary integer QHE an important general question is how the bulk and edge QHE conductivities are related for finite samples. Many authors have addressed this question,[4, 5] where one of the present authors has shown that the bulk QHE conductivity, a topological quantity, coincides with the edge QHE conductivity, itself another topological quantity. This constitutes a typical example of phenomena that, when a bulk system has a topological order[6, 7, 8, 9] that reflects the geometrical phase of the system[10], this should be reflected and become visible in the edge states in a bounded system.[11, 12]

For graphene, two of the present authors and Fukui have shown that this “bulk-edge correspondence” persists in graphene, with both an analytic treatment of the topological numbers and numerical results for the honeycomb lattice[13, 14].

Now, in the physics of graphene, it is important to distinguish between the properties that arise from the continuum theory (i.e., the massless Dirac dispersion that comes from the $k \cdot p$ perturbation in the effective-mass formalism) from the properties that can only be captured by going back to the honeycomb lattice. In ref.[12, 13], we have already recognized this in a change from the Dirac to fermionic behaviors at van Hove singularities of the honeycomb lattice, and in the QHE edge modes that depend on whether the edge is zigzag of armchair.

The purpose of the present paper is to reveal the features in the real-space profile of the edges states in graphene in magnetic fields $B$ in the one-body problem. The graphene edge states in fact turn out to behave unusually. A crucial point is that we find, from numerically obtained dispersion and wave functions, that the $E = 0$ edge mode, despite being embedded in the $n = 0$ Landau level in the energy spectrum, has a wave function whose charge is accumulated along zigzag edges. This situation is drastically different from the ordinary QHE where edge modes reside, in energy, between adjacent Landau levels, and their charge is depleted toward an edge. We can indeed realize in Fig. 1(Landau spectrum vs position) that $E = 0$ mode in graphene is special. The physics here points to a topological origin in a honeycomb lattice, which is in fact totally outside continuum models. In the absence of magnetic fields, a zigzag edge in graphene has been known to have a flat dispersion at $E = 0$,[16] which is protected by the bipartite symmetry of the honeycomb lattice. Here we are talking about the edge states in strong magnetic fields, which has a flat dispersion at $E = 0$. The charge accumulation along zigzag edges only occurs for the $E = 0$ edge mode in the $n = 0$ Landau level. To be more precise, the bulk states re-distribute their charge significantly on top of the zero-mode contribution, which may be called a topological compensation of charge density. On a practical side the present result predicts how an STM imaging should look like for graphene edges.[17] For comparison we have also examined edges in a bilayer graphene.[20, 21]

Single Layer — We consider the standard tight-binding model on the honeycomb lattice with nearest-neighbor hopping, where the magnetic field is introduced as a Peierls phase in the Landau gauge. The magnetic field is characterized by the flux in units of the magnetic flux quantum, $\phi \equiv BS_6/(2\pi) = 1/q$ in each hexagon with area $S_6 = (3\sqrt{3}/2)a^2$. Since we want to look at edges, we should be more explicit about the Hamiltonian. Since honeycomb is a non-Bravais, bipartite lattice with two sublattice sites \(\bullet\) and \(\circ\) per unit cell, we can define two fermion operators $c_\bullet$ and $c_\circ$. For an armchair
specifies the position of a unit cell. For a zigzag edge (Fig. 2(a)) the Hamiltonian then reads

\[ H_A = t \sum_j \left[ c_j^\dagger (j) c_{j+1} \right] + \text{H.c.} \]

Here \( j = j_1 e_1 + j_2 e_2 \) with \( e_1, e_2 \) defined in Fig. 2(b) specifies the position of a unit cell. For a zigzag edge (Fig. 2(b)) the Hamiltonian reads

\[ H_Z = t \sum_j \left[ c_j^\dagger (j) c_{j+1} + e^{i2\pi j x} c_j^\dagger (j) c_{j+1} - j e_2 \right] + \text{H.c.} \]

with \( e_1, e_2 \) as defined in Fig. 2(b). Hereafter we take \( t \) as a unit of energy and \( a \) as a unit of length.

We assume that the system has left and right edges with a spacing \( L_1 \), taken to be large enough (\( L_1 = 5q \)) here to avoid interference. The length along the direction \( (e_2) \) parallel to the edge is also assumed to be long enough (\( L_2 \)), for which we apply the periodic boundary condition. We can then make a Fourier transform in that direction, \( c_\alpha (j) = L_2^{-1/2} \sum_{k_2} e^{ik_2 j} c_\alpha (j_1, k_2) \), for \( j_2 = 1, 2, \cdots, L_2 \) and \( \alpha = \bullet, \circ \). This yields a \( k_2 \)-dependent series of one-dimensional Hamiltonian, \( H = \sum_{k_2} H_{1D}(k_2) \). The resultant eigenvalue problem reduces to \( H_{1D}(k_2) \psi(k_2, E) = E \psi(k_2, E) \), with corresponding eigenstates \( \psi(k_2, E) \).

Having STM images in mind, we define the local charge density,

\[ I(x(j_1)) = \frac{1}{2\pi} \int_{E_1}^{E_2} dE \int dk_2 |\psi_\alpha(E, j_1, k_2)|^2. \]

Here \( x \) is the distance from the edge (as related to \( j_1 \) via \( e_1 \) which is not normal to the edge), and \( E_1 < E < E_2 \) is the energy window to be included in the charge density (which is normalized to unity when the window covers the whole spectrum).

We have stressed that the \( E = 0 \) edge mode is embedded within the \( n = 0 \) Landau level, which is depicted in Fig. 3 a blowup of the energy spectrum (for a relatively high \( \phi = 1/5 \) for clarity). The shaded regions represent the \( n = 0 \) Landau band, while the red curves the edge modes localized along the zigzag edge. We can see that, despite the presence of a strong magnetic field, there exists an exactly \( E = 0 \) edge mode piercing the \( n = 0 \) bulk Landau band. We can realize its topological origin by noting that there are an odd number \((2q - 1)\) of edge modes with zig-zag edges, so that the bipartite...
symmetry (that forces an electron-hole symmetric energy spectrum) precisely dictates that the central edge mode has to be flat and at $E = 0$.\[13\]

Figure 4 shows the energy spectrum in a magnetic field $\phi = 1/21$ adopted hereafter for the armchair and zigzag edges. For this more moderate field the $n = 0$ Landau level around $E = 0$, with a narrow energy width ($\sim 0.05$), almost looks like a line spectrum on this energy resolution. We calculate the local charge density defined in eq.(1) for the armchair and zigzag edges with the energy window $-0.05 < E < 0.05$ set to cover the $n = 0$ Landau level (along with the embedded $E = 0$ edge mode).\[19\] In the result in Fig. 5 the charge density for an armchair edge decreases monotonically toward the edge, where the depletion occurs on the magnetic length scale ($l_B = \frac{3^{3/4}a}{\sqrt{2\pi\phi}}$), as in ordinary QHE systems. In sharp contrast, a zigzag edge has the charge density for the $\bullet$-sublattice that is accumulated toward the edge while the charge density for the $\circ$-sublattice is depleted.

The question then is how the accumulation of the charge around the zigzag edge scale with the magnetic field. We plot in Fig.6 the charge density $I(x)$ normalized by the bulk value $I_0$ (which is $\phi$, when each Landau level of massless Dirac particles is fully occupied)\[18\] against the distance from the edge normalized by the magnetic length $l_B$ for various values of magnetic field $\phi = 1/41$ for armchair(a) or zigzag(b) edges. In this scaled plot the profile of the zigzag edge states for various values of magnetic fields fall upon common lines, where the accumulation of the charge on $\bullet$ sublattice as well as the depletion on $\circ$ sublattice are seen to occur, respectively, on the magnetic length scale toward the edge. We have seen in Fig.3 that the flat dispersion for $B \neq 0$ on a zigzag edge only exists over $1/3$ of the $k_2$ Brillouin zone (that satisfies $1 + (-1)^n e^{i\phi k_2} \leq 1$). We indeed observe that the accumulated $\bullet$ charge over the depleted $\circ$ charge, estimated by integrating the density over one half the sample width is $(1 - \phi)/3$ within the numerical accuracy.

In order to confirm that the charge accumulation around zigzag edges is specific to the $n = 0$ Landau level which embeds the edge mode, we can look at the charge density for $n = 1$ Landau level. The result in Fig.7 has $I(x)$ monotonically decreases toward the edge for both armchair and zigzag edges, although we can notice that the charge density exhibits plateaus for each of $\bullet$ and $\circ$ sublattices in a zigzag edge.

**Double Layer** — We finally examine the bilayer...
FIG. 9: (Color online) Local charge density ($\pi$ area of each circle) for a bilayer graphene with $t_1 = t_2 = 0.1t$ for armchair(a) or zigzag(b) edges (indicated by arrows) in a magnetic field $\phi = 1/21$ for the energy window $-0.05 < E < 0.05$. Red (blue) circles represent top (bottom) layer.

graphene (Fig. 8(a)), which is interesting in its own right as many papers have pointed out, but the system is practically interesting as well, since, experimentally, the STM imaging may be easier for the edge of the top layer residing on a wider bottom layer. We consider the bilayer graphene with the AB (Bernal) stacking in the standard Slonczewski-Weiss-McClure model[22, 23], where there are two types of interlayer transfers, $t_1$ and $t_2$. For simplicity we have taken $t_1 = t_2 = 0.1t$, which are roughly the estimated values $0.2, 0.25, 0.26$. As in the single layer, the periodic boundary condition is applied in $e_2$-direction, while a wider width ($L_1 = 7q$) is taken for the bottom layer (with $L_1 = 5q$ for the top layer). Despite the interlayer coupling, the Landau-quantized energy spectrum (Fig. 8(b)) is similar to those for the $n = 0$ Landau level on this energy scale. Figure 9 displays the charge density for armchair and zigzag edges with an energy window that covers the bilayer $n = 0$ Landau level. We can see that the edge states in the top layer are similar to those in the single layer, namely, the charge density is accumulated toward the zigzag edge on one sublattice. So we can predict that a bright edge should be observed when an STM study is done for a zigzag edge of the top layer in a bilayer graphene.

To summarize, we have shown that the charge density in graphene in strong magnetic fields should be totally unlike ordinary QHE systems, where the charge is accumulated toward zigzag edges. We wish to thank Hiroshi Fukuyama and Tomohiro Matsui for illuminating discussions, and for pointing out that bilayer graphene may be suitable for STM imaging. This work has been supported in part by Grants-in-Aid for Scientific Research, No.20340098, 20654034 from JSPS and No. 220029004 on Priority Areas from MEXT for MA, No.20340098, 20654034 from JSPS and No. 220029004, 20046002 on Priority Areas from MEXT for YH, No.20340098 from JSPS for HA.

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[17] We assume that when the left edge is armchair (zigzag), the right edge is armchair (bearded). Although the structure of the opposite edge does not affect the discussion here, this convention makes the edge spectrum simpler.
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