Edge states for the $n = 0$ Laudau level in graphene

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Abstract. In the anomalous quantum Hall effect (QHE), a hallmark of graphene, nature of the edge states in magnetic fields poses an important question, since the edge and bulk should be intimately related in QHE. Here we have theoretically studied the edge states, focusing on the $E = 0$ edge mode, which is unusual in that the mode is embedded right within the $n = 0$ bulk Landau level, while usual QHE edge modes reside across adjacent Landau levels. Here we show that the $n = 0$ Landau level, including the edge mode, has a wave function amplitude accumulated along zigzag edges whose width scales with the magnetic length, $l_B$. This contrasts with the usual QHE where the charge is depleted from the edge. The implications are: (i) The $E = 0$ edge states in strong magnetic fields have a topological origin in the honeycomb lattice, so that they are outside the continuum (“massless Dirac”) model. (ii) The edge-mode contribution decays only algebraically into the bulk, but this is “topologically” compensated by the bulk contribution, resulting in the accumulation over $l_B$. (iii) The real space behavior obtained here should be observable in STM experiments.

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 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[4]. For the ordinary integer QHE an important question is how the bulk and edge QHE conductions are related for finite samples. Many authors have addressed this question[5, 6], and the bulk QHE conductivity, a topological quantity, is shown to coincide with the edge QHE conductivity, itself another topological quantity. This is an example of the phenomena that, when a bulk system has a topological order[7, 8, 9, 10] that reflects the geometrical phase of the system[11], this should be reflected and become visible in the edge states in a bounded system.[12, 13] This “bulk-edge correspondence” persists in graphene, as shown both from an analytic treatment of the topological numbers and numerical results for the honeycomb lattice[14, 15].

In this paper, we reveal the features in the real-space profile of the edges states in graphene in magnetic fields $B$ in the one-body problem. A pecurier point on the graphene edge states is that the $E = 0$ edge mode, despite being embedded right within the $n = 0$ bulk Landau level in the energy spectrum, has a wave function whose charge is accumulated along zigzag edges. This 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. The physics here indicates a topological origin in a honeycomb lattice, which is in fact totally outside continuum models. In $B = 0$, 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 focus on the edge states in strong magnetic fields, which has a flat dispersion at $E = 0$.

We consider the tight-binding model on the honeycomb lattice with nearest-neighbor hopping $t$ (which is taken to be the unit of energy hereafter). The magnetic field is introduced as a Peierls phase. The flux in units of the magnetic flux quantum is $\phi \equiv BS_6/(2\pi) = 1/q$ in each hexagon with an area $S_6 = (3\sqrt{3}/2)a^2$. Since honeycomb is a non-Bravais, bipartite lattice with two sublattice sites $\bullet$ and $\circ$ per unit cell, we can define two fermion operators $c_\bullet(j)$ and $c_\circ(j)$ with $j = j_1e_1 + j_2e_2$ defined in Figs. 1(a) and (b) specifies the position of a unit cell. We assume that the spacing between the edges $L_1(j_1 = 1, 2, \cdots, L_1)$ is taken to be large enough to avoid interference. The length along the direction $(e_2)$ parallel to the edge is also assumed to be long enough, for which we apply the periodic boundary condition. Performing a Fourier transform in that direction, we obtain a $k_2$-dependent series of one-dimensional Hamiltonian, $H = \sum_{k_2} H_{1D}(k_2)$. The resultant eigenvalue problem reduces to $H_{1D}(k_2)|\psi(k_2, E)\rangle = E|\psi(k_2, E)\rangle$, with corresponding eigenstates $|\psi(k_2, E)\rangle$.

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

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

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).

Figure 1(c) shows the energy spectrum for a zigzag edge in a magnetic field $\phi = 1/41$. For this magnetic field the $n = 0$ Landau level around $E = 0$, with a narrow energy width, almost looks like a line spectrum on this plot. We calculate the local charge density defined in eq.(1) for the armchair and zigzag edges. Figure 2(a) depicts the charge density $I(x)$ normalized by the
bulk value $I_0(= \phi)$ against the distance from the edge $x$ measured by the magnetic length $l_B$ for $\phi = 1/41$, with the energy window $|E| < 0.05$ set to cover the $n = 0$ Landau level (along with the embedded $E = 0$ edge mode). The charge density for an armchair edge decreases monotonically toward the edge, where the depletion occurs on the magnetic length scale ($l_B = 3^{3/4}a/\sqrt{2\pi\phi}$), 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. When we perform this scaled plot the charge density with various magnetic fields, each of which coalesces on the common curves [17].

Outside the van Hove singularity, we recover the conventional Landau levels, so that we expect ordinary edge states. The result for the charge density for this energy region in Fig.2(b) indeed shows that the charge density of outermost Landau levels (labelled B and C in Fig.1) is depleted from the edge region over the magnetic length $l_B$ in usual fashion. As expected, there is no difference in behavior between the A, B sublattices nor between armchair and zigzag edges.

Going back to the $n = 0$ Landau level for a zigzag edge, there is an important question: since the edge mode exists with an exactly $E = 0$ flat dispersion, one might think that the charge accumulation along the edge entirely or primarily comes from this mode. We have checked this. We can use the transfer-matrix method[14] to examine the $I(x)$ contributed by the $E = 0$ flat band, for which nonzero amplitudes occur, rigorously, only on $\bullet$-sublattice, for a sample with an infinite length along the edge direction. Figure 3(a) presents $I(x(j_1))$ for $\phi = 1/21$ and 1/41, normalized by the bulk value of $n = 0$ Landau level, $I_0 = \phi$. Interestingly enough, we can immediately notice a plateau structure. In this plot where the horizontal axis $j_1$ is normalized by $q(\propto 1/B)$, where all the data points for different magnetic fields fall upon a common curve, which means that the charge density contributed by the edge mode has a series of plateau structures with a step arising every time $j_1$ increases by $q$ for a magnetic field $\phi = 1/q$. The height of the $n$-th plateau ($I(x)$ with $j_1 = n$) can be analytically given in terms of $\bullet$-sublattice for the zero magnetic field,

$$p_n \equiv I(x(n))|_{\phi = 0} = \frac{1}{\pi} \int_0^1 dt \frac{t^{2(n-1)}(1-t^2)}{\sqrt{1-t^2/4}}.$$  \hspace{1cm} (2)

Asymptotically $p_n$ has an algebraic decay as $p_n \sim n^{-2}/(\pi \sqrt{3})$. More interestingly, however, if we compare the total charge density with the contribution from the $E = 0$ flat band in Fig. 3(b) for the $n = 0$ Landau level, the above plateau structure vanishes in the total density. This implies that, although the edge-mode contribution has a slow, algebraic decay, the bulk contribution compensates this, and we end up with the charge accumulation over the magnetic length scale. Since the Landau spectrum has a topological nature, we may call this curious phenomena a “topological compensation of charge densities”, which is the final key result here.

To summarize, we have shown that the charge density of $n = 0$ Landau level in graphene in strong magnetic fields should be totally unlike ordinary QHE systems. The charge accumulation along zigzag edges only occurs for the $E = 0$ edge mode in the $n = 0$ Landau level, accompanied by a charge redistribution of the bulk states. The charge density around the edge can only be captured when bulk and edge contributions are considered simultaneously. The present result is expected to be measured by an STM imaging for graphene edges[18].

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Figure 2. (a) Scaled plot of the charge density $I(x)$ for magnetic flux $\phi = 1/41$ against $x/l_B$, the distance from the edge normalized by the magnetic length, for the $n = 0$ Landau level (marked with A in Fig. 1(c)). (b) The same plot for the outermost Landau levels (marked with B and C in Fig. 1(c)), for which $I_0 = \phi/2$.

Figure 3. Scaled plot of $I(x)$ at $E = 0$ edge mode for $\phi = 1/q = 1/21$ and $1/41$ (a) and comparison with $n = 0$ Landau Level contribution for $\phi = 1/41$.

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