Edge states in graphene in magnetic fields: A specialty 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 resides 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 redistribute their charge significantly, which may be called a *topological compensation* of charge density. The real-space behavior obtained here should be observable in a scanning tunnel microscope imaging.

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I. 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 conductions 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. The bulk-edge correspondence constitutes a typical example of phenomena that, when a gapped quantum liquid reflects a geometrical phase[6] characteristic of the quantum ground state and thus possess a hidden nontrivial topological structure,[7–10] this becomes visible when the system is geometrically perturbed such as the introduction of edges.[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[15]) from the properties that can only be captured by going back to the honeycomb lattice. In Refs. 13 and 14, 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 edge 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 that the $E=0$ edge mode has a wave function whose charge is accumulated along zigzag edges, despite being *embedded* right within the $n=0$ bulk Landau level in the energy spectrum. 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 have 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 redistribute their charge significantly on top of the zero-mode contribution, which may be called a *topological compensation of charge density*. While disorder can affect the physics of the $n=0$ Landau level[17] including a possible splitting of the level, an interesting problem in its own right, here we focus on the clean case. Experimentally the present result on the real-space wave functions predicts how an scanning tunneling microscope (STM) imaging should look like for graphene edges.[18] For comparison we

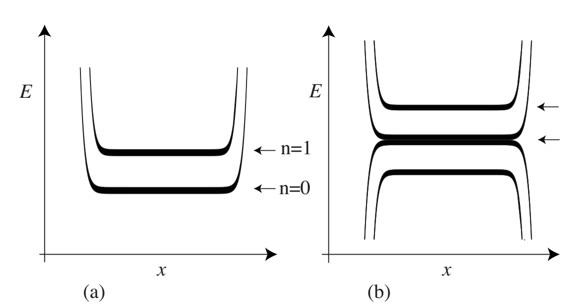

FIG. 1. Schematic Landau-quantized spectra against real-space position (x) for finite systems for ordinary (a) QHE systems and (b) graphene QHE.

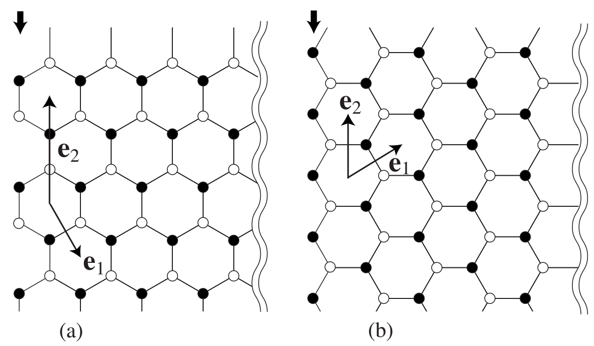

FIG. 2. Honeycomb lattice with (a) armchair or (b) zigzag edges (indicated by arrows) with $\mathbf{e}_1,\mathbf{e}_2$ being respective unit translation vectors.

have also examined edges in a bilayer graphene[19,20] in Sec. III.

II. SINGLE LAYER

We first examine the single-layer graphene in strong magnetic fields. 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. We specify the magnetic field as the flux in each hexagon with area $S_6=(3\sqrt{3}/2)a^2$ in units of the magnetic-flux quantum, $\phi \equiv BS_6/(2\pi)=1/q$. 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 • and ◦ per unit cell, we can define two fermion operators $c_\bullet$ and $c_\circ$. For an armchair edge [Fig. 2(a)], the Hamiltonian reads

$$\mathcal{H}_A = t\sum_{\mathbf{j}} [c_\bullet^\dagger(\mathbf{j})c_\circ(\mathbf{j}) + c_\bullet^\dagger(\mathbf{j}+\mathbf{e}_1)c_\circ(\mathbf{j}) + e^{i2\pi\phi j_1}c_\circ^\dagger(\mathbf{j}+\mathbf{e}_1+\mathbf{e}_2)c_\bullet(\mathbf{j})] + \text{H.c.}.$$

Here $\mathbf{j}=j_1\mathbf{e}_1+j_2\mathbf{e}_2$ with $\mathbf{e}_1,\mathbf{e}_2$ defined in Fig. 2(a) specifying the position of a unit cell. For a zigzag edge [Fig. 2(b)] the Hamiltonian reads

$$\mathcal{H}_Z = t\sum_{\mathbf{j}} [c_\bullet^\dagger(\mathbf{j})c_\circ(\mathbf{j}) + e^{i2\pi\phi j_1}c_\bullet^\dagger(\mathbf{j})c_\circ(\mathbf{j}-\mathbf{e}_2) + c_\bullet^\dagger(\mathbf{j}+\mathbf{e}_1)c_\circ(\mathbf{j})] + \text{H.c.},$$

with $\mathbf{e}_1,\mathbf{e}_2$ 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.[21] The length along the direction ($\mathbf{e}_2$) 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, $c_\alpha(\mathbf{j}) = L_2^{-1/2}\Sigma_{k_2}e^{ik_2j_2}c_\alpha(j_1,k_2)$, for $j_2=1,2,\cdots,L_2$ and $\alpha=\bullet,\circ$. This yields a k_2-dependent series of one-dimensional Hamiltonian, $\mathcal{H}=\Sigma_{k_2}\mathcal{H}_{1\text{D}}(k_2)$. The resultant eigenvalue problem reduces to $\mathcal{H}_{1\text{D}}(k_2)|\psi(k_2,E)\rangle = E|\psi(k_2,E)\rangle$, with corresponding eigenstates $|\psi(k_2,E)\rangle$.

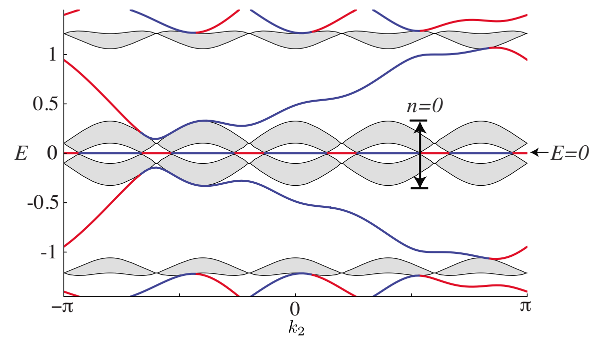

FIG. 3. (Color online) Energy spectra against k_2 (momentum along the edge) for a single-layer graphene in a magnetic field of $\phi=1/5$ with zigzag edges. Shaded regions are the bulk energy spectra while red (blue) lines are the modes localized on the zigzag (bearded) edge.

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

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

Here x is the distance from the edge (as related to j_1 via $\mathbf{e}_1$ 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).[13] The shaded regions represent the $n=0$ Landau band while the red curves represent 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 zigzag 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

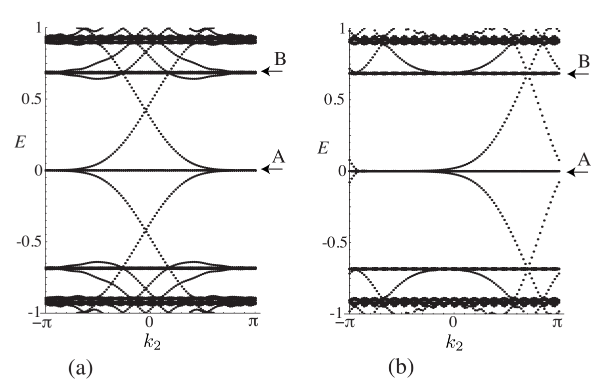

FIG. 4. Energy spectra against k_2 (momentum along the edge) for a single-layer graphene in a magnetic field of $\phi=1/21$ for (a) armchair or (b) zigzag edges.

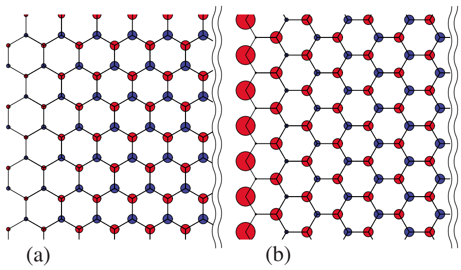

FIG. 5. (Color online) Local charge density ($\propto$ area of each circle; red and blue indicate two sublattices) for a single-layer graphene with (a) armchair or (b) zigzag edges in a magnetic field $\phi=1/21$ for the energy window $-0.05<E<0.05$ around $n=0$ Landau level (see Fig. 4).

$\phi=1/21$ 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 (~ 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).[22] 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 ($l_B=3^{3/4}a/\sqrt{2\pi\phi}$), 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. This is the first key result here.

The question then is how the accumulation of the charge around the zigzag edge scales with the magnetic field. We plot in Fig. 6 the charge density $I(x)$ normalized by the bulk value I_0 (which is ϕ, when each Landau level of massless Dirac particles is fully occupied[23]) against the distance from the edge x measured in units of the magnetic length l_B for various values of the magnetic field with the energy window fixed at $-0.05<E<0.05$. In this scaled plot the profile of the zigzag edge states for various values of the magnetic field 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.

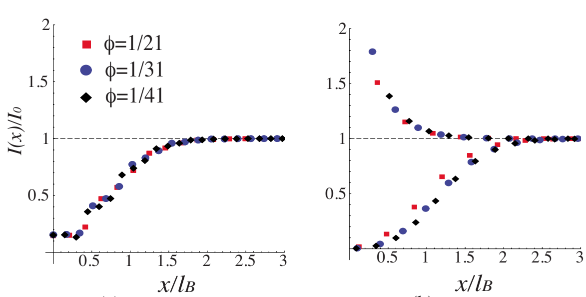

FIG. 6. (Color online) Scaled plot of the charge density $I(x)$ against x/l_B, the distance from the edge normalized by the magnetic length, for the $n=0$ Landau level (marked with A in Fig. 4) with various values of magnetic field ϕ for (a) armchair or (b) zigzag edges.

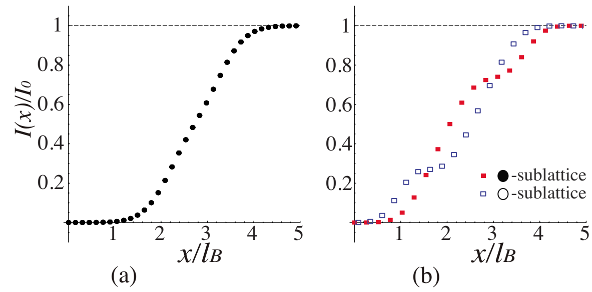

FIG. 7. (Color online) Scaled plot of the charge density $I(x)$ against x/l_B for the $n=1$ Landau level (marked with B in Fig. 4) with magnetic field $\phi=1/41$ for (a) armchair or (b) zigzag edges.

We have seen in Fig. 3 that the flat dispersion for $B\neq 0$ on a zigzag edge only exists over one third of the k_2 Brillouin zone (that satisfies $|1-(-1)^q e^{iqk_2}|\leq 1$, see Appendix). We indeed observe that the accumulated $\bullet$ charge over the depleted $\circ$ charge, estimated by integrating the density around the edge, is

$$\int I^{\bullet}(x)-I^{\circ}(x)dx=\frac{1}{3}(1-\phi)$$

within the numerical accuracy. Effects of disorder or electron-electron interaction can cause splitting and broadening of the $n=0$ Landau level[17,24–29] but we expect a small splitting will not change the charge density $I(x)$ significantly as far as the energy window covers the split Landau levels.

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. We can see in Fig. 7 that $I(x)$ 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.

III. DOUBLE LAYER

Next we examine the bilayer graphene [Fig. 8(a)], which

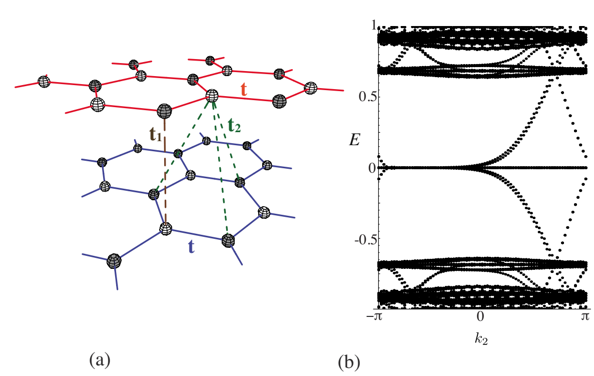

FIG. 8. (Color online) (a) A bilayer graphene with Bernal stacking with the top layer having a zigzag edge. The transfer energies considered in the Slonczewski-Weiss-McClure model are displayed. (b) Energy spectrum for a bilayer graphene having a zigzag edge in the top layer with interlayer couplings $t_1=t_2=0.1t$ in a magnetic field of $\phi=1/21$.

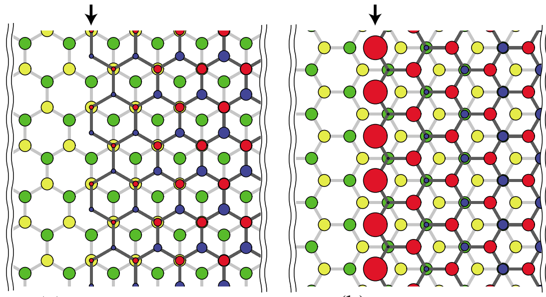

FIG. 9. (Color online) Local charge density ($\propto$ area of each circle) for a bilayer graphene with $t_1 = t_2 = 0.1t$ (a) armchair or (b) zigzag edges (indicated by arrows) in a magnetic field $\phi = 1/21$ for the energy window $-0.05 < E < 0.05$. Red/gray and blue/dark gray (green/light gray and yellow/very light yellow) circles represent top (bottom) layer.

is interesting in its own right as studied by many papers 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,[30,31] 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.[32–34] As in the single layer, the periodic boundary condition is applied in $\mathbf{e}_2$ 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.[35] 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.

IV. SUMMARY

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, in which a topological compensation of the charge occurs in the bulk states as well. 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.

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APPENDIX: ZERO-ENERGY EDGE-MODE CONTRIBUTION TO THE CHARGE ACCUMULATION

Here we consider the charge density along the edge contributed from the zero-energy edge mode. If we follow Ref. 13 for the honeycomb lattice with zigzag edges, we have a relation between the wave functions at • and ◦ sites as

$$E\psi_\circ(j_1,k_2) = t_{\circ\bullet}(j_1,k_2)\psi_\bullet(j_1,k_2) + \overline{t_{\bullet\circ}}(j_1,k_2)\psi_\bullet(j_1+1,k_2),$$

$$E\psi_\bullet(j_1,k_2) = t_{\bullet\circ}(j_1-1,k_2)\psi_\circ(j_1-1,k_2) + \overline{t_{\circ\bullet}}(j_1,k_2)\psi_\circ(j_1,k_2),$$

where $t_{\circ\bullet}(j_1,k_2) = t(1+e^{ik_2 - i2\pi g\phi j_1})$ and $t_{\bullet\circ}(j_1,k_2) = t$, $\bar{x}$ denotes the complex conjugate of x. As for the • sublattice of $E=0$ mode, we have a recursion relation,

$$\psi_\bullet(j_1+1,k_2) = -(1+e^{ik_2 - i2\pi\phi j_1})\psi_\bullet(j_1,k_2).$$

For $\phi = 1/q$ (with q: an odd integer) we have an identity,

$$\prod_{m=1}^{q-1} |1+e^{ik_2 - i2\pi\phi m}|^2 = |1+e^{iqk_2}|^2 = 4\cos^2\frac{qk_2}{2},$$

so that we have a recursion relation $|\psi_\bullet(j_1+q,k_2)|^2 = (4\cos^2\frac{qk_2}{2}) \times |\psi_\bullet(j_1,k_2)|^2$. For the charge density to decay for large j_1, we need the relation $4\cos^2\frac{qk_2}{2} < 1$, which is satisfied over one third of the k_2 Brillouin zone. Therefore the charge density of the jth • sublattice is obtained as

$$I_j = \frac{1}{2\pi}\int dk_2 \frac{\prod_{m=1}^{j-1}|1+e^{ik_2 - i2\pi m\phi}|^2}{\sum_{l=1}^{\infty}\prod_{m=1}^{l}|1+e^{ik_2 - i2\pi m\phi}|^2}$$

$$= \frac{1}{2\pi}\int dk_2 \frac{\prod_{m=1}^{j-1}|1+e^{ik_2 - i2\pi m\phi}|^2}{\sum_{l=1}^{q}\dfrac{\prod_{m=1}^{l-1}|1+e^{ik_2 - i2\pi m\phi}|^2}{1-4\cos^2\dfrac{qk_2}{2}}},$$

where the integral is performed over k_2 that satisfies the condition $4\cos^2\frac{qk_2}{2} < 1$. We can then readily show the relation $\sum_{j=1}^{\infty} I_j = 1/3$. A numerical study[36] indicates that the charge density contributed by the edge mode I_j/I_0 (scaled by the bulk intensity $I_0 = \phi$) exhibits a series of plateaus with a step arising every time j increases by q and the height of the nth plateau p_n is given in terms of the intensity I_n of the • sublattice for *zero* magnetic field. The intensity I_n for zero magnetic field can be obtained by our substituting $q=1$ into the above integral, which can be simplified into

$$I_n = \frac{1}{\pi}\int_0^1 dt \frac{t^{2(n-1)}(1-t^2)}{\sqrt{1-t^2/4}}.$$

For large n's the plateau p_n decays like $p_n \simeq n^{-2}/(\pi\sqrt{3})$. This implies that, although the zero-energy mode contribution has an algebraic decay with no characteristic decay length present, the bulk contribution compensates this in such a way that the charge accumulation occurs over a definite length scale (which is the magnetic length). Since the Landau spectrum has a topological nature, we may call the curious phenomena a "topological compensation of charge densities."[36]

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