The recent realization of graphene in laboratories has attracted extensive interests to this 2D lattice [13, 14, 15]. Its bulk band structure has two degenerate and inequivalent valleys centered at the corners of the first Brillouin zone (known as the Dirac points). The free standing graphene crystallite is a zero-gap semiconductor where the conduction and valance band touch each other at the Dirac points. A bulk energy gap can be opened by breaking the inversion symmetry, e.g. by a staggered sublattice potential in single layer graphene, or by an interlayer bias in graphene bilayer. The neutral graphene system then becomes a normal insulator, with vanishing Hall conductance and spin Hall conductance. Nevertheless, it does acquire a nontrivial bulk topological property: the two inequivalent valleys each carry a non-zero topological charge with opposite signs, giving rise to the valley-dependent Hall effect [16, 17]. Not by coincidence, edge-states also exist in such graphene systems with peculiar behaviors [18, 19, 20, 21, 22, 23, 24]. For graphene sheet terminated with zigzag edges, edge-states form a one dimensional band which connects the two Dirac points with completely flat dispersion. Because of its unusual dispersion relation, the edge-bands in graphene have been exploited for a number of interesting phenomena including valley-filtered transport [25], magnetism [26, 27, 28, 29], and superconductivity [30].

In this work, we study edge-state behaviors in graphene systems where a bulk energy gap is opened by inversion symmetry breaking. We find that the edge-bands dispersion can be controlled by potentials applied on the boundary with unit cell length scale. Under certain boundary potentials, gapless edge-states with valley-dependent velocity are found, exactly analogous to the spin-dependent gapless chiral edge-states in quantum spin Hall systems. The connection of the edge-states to bulk topological properties is revealed.

FIG. 1: (Color online) (a) Schematic illustration of a single layer graphene with zigzag edge on the left boundary. The two triangular sublattices are denoted by solid and dotted respectively. A unit cell contains one atom from each sublattice (denoted by the oval). (b) and (c), only the edge-states on the left boundary are shown (red curves). A staggered sublattice potential $\Delta_1/2 = 0.1$ is universally applied in the bulk and on the boundary (see text).
systems do not have nontrivial $Z_2$ topological order in the bulk \cite{Chen2014, Zeng2015, Zeng2016}, the edge-states can nevertheless have the same features as those edge-states in QSHE, with the valley index playing the role of the spin. We further prove that these gapless edge-states are equivalent to the gapless chiral modes confined by topological domain wall in graphene, whose existence and chiral nature have been related to the valley-dependent bulk topological charge \cite{Zhang2019, Zhang2020}. Therefore, the peculiar edge-states on the boundary indeed share the same topological origin as the valley-dependent Hall effect in the bulk. This also opens up a new perspective to the existence of gapless chiral edge-states by contrasted topological charges in different regions of the Brillouin zone.

In the tight binding approximation with nearest neighbor hopping energy $t$, a single layer of graphene can be described by the following Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_i U_i c_i^\dagger c_i, \quad (1)$$

where $\sum_{\langle i,j \rangle}$ sums over only nearest neighbor pairs. We consider a general situation where the bulk lattice can be subject to a staggered sublattice potential: $U_i = \Delta/2$ for sublattice $\bullet$, and $U_i = -\Delta/2$ for sublattice $\circ$ (see Fig. 1(a)). On the boundary, graphene sheet terminated with the zigzag or the bearded edge preserves the two-valley band structure, and the edge-states form well known flat 1D bands which connect the two Dirac points \cite{Zhang2015, Zhang2016, Zhang2017}. We find that the edge-states are also gapped when the staggered sublattice potential is universally applied to all sites including those on the boundary. In Fig. 1(b) and (c), for clarity, only the edge-states on the left boundary are shown, while we note that an edge-state near the two Dirac points respectively (see Fig. 1(a)) are tuned to different values from positive to negative. (e) with $U(L_1) = \Delta/2 = 0.1$ is the same plot as Fig. 1(b). The inset in (g) is a blow up of the bulk gap region near $k_y = \frac{\pi}{2}$. Only the edge-states on the left boundary are shown (red curves).

![FIG. 2: (Color online) Band structure of single layer graphene with zigzag edges. A staggered sublattice potential $\Delta/2 = 0.1$ is applied throughout the sheet, while the on-site energies $U(L_i)$ of the outermost column $L_1$ (Fig. 1(a)) are tuned to different values from positive to negative. (e) with $U(L_1) = \Delta/2 = 0.1$ is the same plot as Fig. 1(b). The inset in (g) is a blow up of the bulk gap region near $k_y = \frac{\pi}{2}$. Only the edge-states on the left boundary are shown (red curves).](image-url)

The gapless edge-states usually reflect non-trivial topological orders in the bulk. In QHE, it is well known that the number of gapless chiral edge-states is given by the bulk Chern invariant $\mathcal{C}_i$. This connection has been generalized to QSHE recently \cite{Chen2014, Zeng2015, Zeng2016}, where the existence of gapless chiral edge-states are dicted by a generalized definition of bulk Chern invariant $\mathcal{C}_i$, also known as the $Z_2$ topological invariant \cite{Chen2014, Zeng2015, Zeng2016}. To understand the edge-states in the present graphene system, we shall look into its bulk properties.

In the bulk, we can make a Fourier transform $c_{i,\bullet/\circ} \equiv \sum_k c_{k,\bullet/\circ} e^{ikR_i}$ with $R_i$, being the lattice vector, and the
Hamiltonian in Eq. (1) becomes

\[ H_{\text{bulk}} = \sum_k \left[ \frac{\Delta}{2} \left( \begin{array}{c} V(k) \ V^*(k) \end{array} \right) - \Delta/2 \right] \left( \begin{array}{c} c_{k,\sigma}^\dagger \ c_{k,\sigma} \end{array} \right) \]  

where \( V(k) = -(1 + e^{-ik \cdot a_1} + e^{-ik \cdot a_2}) \), and \( a_{1,2} \) are the two primitive translation vectors (see Fig. 1(a)). Eq. (2) has the solutions of a conduction band \( |u_{c,k}\rangle \) and a valence band \( |e_{v,k}\rangle \). In order to describe the bulk topological property for the graphene system as an insulator, it is convenient to introduce a gauge potential and a gauge field in the valence band, defined as \( A(k) = \langle u_{c,k}| \nabla_k |u_{c,k}\rangle \) and \( \Omega(k) = \nabla_k \times A \) respectively. This gauge field, known as the Berry curvature, is analogous to a magnetic field in the crystal momentum space. Its integral over a \( k \)-space area yields the Berry phase of an electron adiabatically going around the boundary of the area, which is similar to the relationship between a magnetic field and the Aharonov-Bohm phase. In 2D system, the Berry curvature vector is pointing out-of-plane and the Chern invariant is given by the flux of the Berry curvature threading the entire Brillouin zone \( C = \frac{1}{2\pi} \int_{BZ} d^2k \Omega(k) \). For the graphene system described by Eq. (2), one finds the Berry curvature has a distribution sharply centered at the two Dirac points, \( \Omega(q) = \tau_z \frac{\Delta}{2(\sqrt{3}q^2+q^2)^{1/2}} \), where \( \tau_z = \pm \) is the index for the two valleys and \( q \) is the wavevector measured from the Dirac points \([16, 17]\). We find the two valleys each carry a topological charge of \( \tilde{N}_3 = \frac{1}{2\pi} \int d^2q \Omega(q) = \frac{1}{2} \tau_z \text{sgn}(\Delta) \), corresponding to a half-quantized valley Hall conductivity in the bulk \([16, 17]\). However, the Chern invariant is zero because of the time reversal symmetry in the system. It can be further shown that the \( Z_2 \) topological invariant also vanishes when the gap is from inversion symmetry breaking only. Clearly, the gapless edge-states we found here do not have the same origin as those in the QHE and QSHE.

In searching for the topological origin of these edge-states, we notice that similar gapless valley-dependent chiral zero-modes also exist at topological domain walls in biased graphene bilayer, and the number and chiral nature of these modes have been related to the valley-dependent topological charge \( \tilde{N}_3 \) in the bulk \([34]\). More specifically, in each valley, the topological charge \( \nu \) of the zero-modes, i.e. the number of zero-modes moving in \(+y\) direction minus the number of zero-modes moving in \(-y\) direction, is equal to the difference of the bulk topological charges \( \tilde{N}_3 \) of the vacuum on the two sides of the interface, \( \nu = \tilde{N}_3(\text{right}) - \tilde{N}_3(\text{left}) \) \([34, 35]\). For the single layer graphene under staggered sublattice potential, we can similarly consider a topological domain wall represented by a sharp kink in the order parameter \( \Delta \) as shown in Fig. 3. Gapless chiral modes with topological charge \( \nu = \tau_z \) is thus expected in the domain wall region \([36]\). Interestingly, \( \nu = \tau_z \) is exactly the topological charge of the gapless edge-states shown in Fig. 2(g), when the on-site energy of the atoms on the outermost column is equal to the nearest neighbor hopping energy. Below, we show the intrinsic connection between the gapless zero-modes in the domain wall and the gapless edge-states on the boundary.

Graphene with the above mentioned topological domain wall can be described by the following Hamiltonian

\[ H = -\sum_{\langle i,j \rangle} c_{i,S}^\dagger c_{j,S} + \sum_i U_i, c_{i,S}^\dagger c_{i,S} \]

\[ -\sum_{\langle i,j \rangle} c_{i,A}^\dagger c_{j,A} + \sum_i U_i, c_{i,A}^\dagger c_{i,A} \]

where the index \( i,j \) here run over lattice sites on one side of the domain wall. \( c_{j,A} = \frac{1}{\sqrt{2}} (c_{j,\mathcal{R}} - c_{j,\mathcal{L}}) \) and \( c_{j,S} = \frac{1}{\sqrt{2}} (c_{j,\mathcal{R}} + c_{j,\mathcal{L}}) \) describe respectively the antisymmetric and symmetric combination of wavefunction on the two sites \( i \) and \( j \) located symmetrically on the two sides of the domain wall (see Fig. 3). For \( i \) in the nearest column to the domain wall \( L_1 \) in Fig. 3, we have \( U_i,S = -1 + \frac{|\Delta|}{2} \) and \( U_i,A = 1 + \frac{|\Delta|}{2} \) respectively, while for all other lattice sites, both \( U_i,A \) and \( U_i,S \) are equal to \( \frac{|\Delta|}{2} \) on sublattice \( \bullet \) and equal to \( -\frac{|\Delta|}{2} \) on sublattice \( \circ \). In this way, we establish the equivalence between an extended graphene with a domain wall and a semi-infinite graphene with one zigzag edge subjected to certain boundary potential. In particular, the gapless chiral zero-modes in the domain wall are of symmetric wavefunction and are equivalent to the gapless edge-states on the boundary when on-site energy of the outermost column is \( -1 + \frac{|\Delta|}{2} \) (cf. Fig. 2(g)). Therefore, the number of gapless edge-states in the latter situation is also determined by the bulk topological charge \( \tilde{N}_3 \) in the two valleys.

We note that the edge-states can evolve continuously from the gapless chiral modes near the Dirac points to the flat dispersion band connecting the two Dirac points by tuning the magnitude of the boundary potential only, during which the bulk property is unchanged. Therefore, these edge-states spectra shall all have the same origin from the valley-dependent bulk topological charge, and in particular, the number of edge-band is determined by the value of \( \tilde{N}_3 \).

Finally, we turn our attention to a different graphene system, the bilayer graphene with Bernal stacking. By applying
a bias $\Delta$ between the two layers, a bulk gap can be induced and it has been shown that, in the insulating states, the two valleys carry the topological charge of $\tau_s \text{sgn}(\Delta)$ in the highest valance band $|16, 17, 34\rangle$. By the above topological argument, similar edge-states behaviors to those in the single layer shall be expected. In Fig. 4 we show the edge-states spectrum when the on-site energy is universally $-0.015$ in the upper layer and $0.015$ in the bottom layer. As expected, each boundary now carry two bands $|23\rangle$. Edge band 1 has a flat dispersion in the region $k_y \in \left[ \frac{2\pi}{3}, \frac{4\pi}{3} \right]$, similar to the edge-band in the single layer case, and we find that the states near $k_y = \pi$ are completely localized on the outermost column ($R_d$) of the upper layer. Edge band 2 also has a flat dispersion near $k_y = \pi$, but acquires finite valley-dependent velocity near the Dirac points $|23\rangle$. The two edge-bands have an energy difference equal to $\Delta = -0.03$ in the flat region, which is due to the fact that, in edge-band 2, the states near $k_y = \pi$ are localized on the outermost column ($R_d$) in the lower layer. Thereby, the dispersion of the two edge-bands can be individually controlled by tuning on-site energies of $R_u$ and $R_d$ columns respectively. In particular, depending on the boundary potential, we can have either one or two valley-dependent gapless chiral modes per valley per boundary, as shown in Fig. 4(c) and (d). In fact, the gapless edge-states when $U(R_u) = U(R_d) = 1$ are equivalent to the symmetric modes confined by a line dislocation so that the bilayer is of AB stacking to the left of this topological line defect and is of BA stacking to the right of the defect $|37\rangle$. The topological charge of these gapless modes $\nu = -2\tau_z$ in each valley, which is found consistent with the bulk topological charge $N_3 = -\tau_z$. Indeed, in bilayer graphene, the behaviors of the edge-states are also determined by the valley-dependent topological charges in the bulk.

The work was supported by NSF, DOE, the Welch Foundation, and NSFC.

[1] R. B. Laughlin, Phys. Rev. B 23, 5632 (1981).
[2] B. I. Halperin, Phys. Rev. B 25, 2185 (1982).
[3] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[4] C. Wu, B. A. Bernevig, and S.-C. Zhang, Phys. Rev. Lett. 96, 106401 (2006).
[5] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science 314, 1757 (2006).
[6] M. Onoda and N. Nagaosa, Phys. Rev. Lett. 95, 106601 (2005).
[7] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
[8] Y. Hatsugai, Phys. Rev. Lett. 71, 3697 (1993).
[9] X.-L. Qi, Y.-S. Wu, and S.-C. Zhang, Phys. Rev. B 74, 045125 (2006).
[10] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
[11] L. Fu and C. L. Kane, Phys. Rev. B 74, 195312 (2006).
[12] J. E. Moore and L. Balents, Phys. Rev. B 75, 121306 (2007).
[13] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Nature 438, 197 (2005).
[14] Y. Zhang, Y.-W. Tan, H. L. Stormer, and P. Kim, Nature 438, 201 (2005).
[15] A. K. Geim and K. S. Novoselov, Nature Mater. 6, 183 (2007).
[16] D. Xiao, W. Yao, and Q. Niu, Phys. Rev. Lett. 99, 236809 (2007).
[17] W. Yao, D. Xiao, and Q. Niu, Phys. Rev. B 77, 235406 (2008).
[18] K. Nakada, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. B 54, 17954 (1996).
[19] S. Ryu and Y. Hatsugai, Phys. Rev. Lett. 89, 077002 (2002).
[20] L. Brey and H. A. Fertig, Phys. Rev. B 73, 235411 (2006).
[21] N. M. R. Peres, A. H. Castro Neto and F. Guinea, Phys. Rev. B 73, 195411 (2006).
[22] N. M. R. Peres, F. Guinea and A. H. Castro Neto, Phys. Rev. B 73, 125411 (2006).
[23] E. V. Castro, N. M. R. Peres, J. M. B. Lopes dos Santos, A. H. Castro Neto and F. Guinea, Phys. Rev. Lett. 100, 026802 (2008).
[24] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, arXiv:0709.1163, (2008).
[25] A. Rycerz, J. Tworzydlo, and C. W. J. Beenakker, Nature Phys. 3, 172 (2007).
[26] B. Wunsch, T. Stauber, F. Solis, and F. Guinea, Phys. Rev. Lett. 101, 036803 (2008).
[27] K. Sawada, F. Ishii, and M. Saito, Appl. Phys. Express 1, 064004 (2008).
[28] O. V. Yazyev and M. I. Katsnelson, Phys. Rev. Lett. 100, 047209 (2008).
[29] S. Bhowmick and V. B. Shenoy, J. Chem. Phys. 128, 244717 (2008).
[30] K. Sasaki, J. Jiang, R. Saito, S. Onari, and Y. Tanaka, J. Phys. Soc. Jpn. 76, 033702 (2007).
[31] S. V. Morozov, K. S. Novoselov, M. I. Katsnelson, F. Schedin, L. A. Ponomarenko, D. Jiang, and A. K. Geim, Phys. Rev. Lett. 97, 016801 (2006).
[32] A. F. Morpurgo and F. Guinea, Phys. Rev. Lett. 97, 196804 (2006).
[33] R. V. Gorbachev, F. V. Tikhonenko, A. S. Mayorov, D. W. Horsell, and A. K. Savchenko, Phys. Rev. Lett. 98, 176805 (2007).
[34] I. Martin, Y. M. Blanter, and A. F. Morpurgo, Phys. Rev. Lett. 100, 036804 (2008).
[35] G. E. Volovik, The Universe in a Helium Droplet (Oxford University Press, 2003).
[36] G. W. Semenoff V. Semenoff, and Fei Zhou Phys. Rev. Lett. 101, 087204 (2008).
[37] Note that this is a different type of topological domain wall from the one explored in Ref. [34].