Bulk-edge correspondence in graphene with/without magnetic field:
Chiral symmetry, Dirac fermions and Edge states

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There are two types of edge states in graphene with/without magnetic field. One is a quantum Hall edge state, which is topologically protected against small perturbation. The other is a chiral zero mode that is localized near the boundary with/without magnetic field. The latter is also topological but is guaranteed to be zero energy by the chiral symmetry, which is also responsible for massless Dirac like dispersion. Conceptual roles of the edge states are stressed and reviewed from a view point of the bulk-edge correspondence and the topological order.

I. INTRODUCTION

Many of physical states of matter are characterized by order parameters based on the symmetry breaking. Especially a symmetry with continuous parameters has special importance in a quantum state of matter. When the ground state of the system with continuous symmetry does not posses the symmetry, that is, the ground state is not invariant against the symmetry operation, there exists a gapless excitation as the Nambu-Goldston mode. A typical example is the Heisenberg magnet with antiferromagnetic order (Neel order). The ground state of the spherical symmetric (in spin space) hamiltonian is not invariant against the spin rotation. Then above the ground state, there is a gapless spin excitation as the spin wave. This excitation is realized by infinitesimally small spin deformation over infinitely wide range as was done by the Lieb-Schultz-Mattis.

Although it has been quite successful to characterize many of phases, it has been realized that there still exist many important physical phases that are not well described by this spontaneous symmetry breaking recipe. This class of matter includes many of quantum Hall states, Haldane spin chains (integer spin chains), Kondo insulators and much more. A ground state of graphene also belongs to this new class. In a ground state with strong quantum fluctuation, order formation is strongly suppressed and a quantum ground state without any fundamental symmetry breaking is realized. In such a case, there is no reason to expect gapless excitations, which results in a gapped quantum state. Phases of this class of matter are the quantum liquids. Then to characterize such a quantum liquid phase is one of the important problems. A novel concept as the topological order that was first proposed to discuss the quantum Hall states is now under active studies for the purpose.

Due to the absence of symmetry breaking, one needs to use something new to describe the topological order. One of such possibilities to use geometrical phases of the quantum states. It works well theoretically to describe some of quantum liquids and spin liquids. Another tool is to use edge states, which are one of the feature of the topological ordered states. There exist non trivial edge states, as the bound states near the boundaries, appear when the bulk are topologically non-trivial. Even if the quantum liquid does not posses any symmetry breaking and featureless, there exist characteristic boundary states when the system has boundaries and impurities. These generic edge states are characteristic to the topological ordered states and they themselves characterize the quantum states, which we call the bulk-edge correspondence. These kinds of non-trivial edge states appear in many different ares in condensed matter physics, such as optical lattices and photonic crystals. Further an entanglement entropy, which is also useful to characterize the quantum liquids, is also directly related to the edge states. In this short review, we have focused on non trivial edge states of graphene based on the bulk-edge correspondence and try to make clear topological aspects of graphene with and without magnetic field.

II. QUANTUM HALL EFFECT OF GRAPHENE

A. Edge states of the Quantum Hall states

As is well known, the Hall conductance of two dimensional electrons has an intrinsic topological meaning that is an origin of high accuracy of the quantization. This quantization is clearly demonstrated by Laughlin using an adiabatic process with gauge invariance where Aharonov-Bohm(AB) flux passes through the hole of the cylinder. Quantized value of the Hall conductance (in a suitable unit) is a number of electrons carried across the system when the AB flux is adiabatically increased by one flux quantum. Considering a system with edges, this quantized but ambiguous integer is uniquely specified by the number of edge modes $I_j$ in the $j$-th Landau gap where the Fermi energy lies.

$$\sigma_{xy}^\text{Edge} = \frac{e^2}{h} I_j.$$  

It implies that the edge states has essential importance for the physics of the quantum Hall effects.

Although the Hall current is dissipation less, it is natural to describe the Hall conductance as a bulk property. It is given within the linear response theory as

$$\sigma_{xy}^\text{Bulk} = \frac{e^2}{h} \sum_{\ell} C_\ell$$  

where the summation is over the filled Landau
FIG. 1: Cylinder used in the Laughlin’s argument. Edge states in this review are all discussed in this cylindrical geometry.

FIG. 2: (a) One particle energy spectrum of graphene under a magnetic field. Horizontal axis $\phi$ is a magnetic flux per hexagon in a unit of magnetic flux quantum. (b) Schematic Dirac sea without magnetic field and Landau level of the Dirac fermions

levels and $C_\ell$ is the first Chern number of the $\ell$-th Landau band, $C_\ell = \frac{1}{2\pi} \int d^2k \left( \text{rot}_k A_\ell \right)_z$, $A_\ell = \langle \psi_\ell | \nabla_k | \psi_\ell \rangle$, where $| \psi_\ell \rangle$ is a one body wave function of the $\ell$-th Landau band.

One particle spectrum of the graphene in a magnetic field is given in Fig. 2. When the Fermi energy is set around $E = 0$, one needs to fill the Dirac sea, which causes numerical difficulties. In such a case, following non Abelian formulation for the Hall conductance is useful

$$\sigma_{xy}^{\text{Bulk}} = \frac{e^2}{h} C_F, \quad C_F = \frac{1}{2\pi i} \int d\text{Tr} A \quad (1)$$

$$A = \psi^\dagger d\psi = \psi^\dagger \partial_\mu \psi dx^\mu$$

$$\psi = (| \psi_1 \rangle, \cdots, | \psi_j \rangle)$$

where $(x^1, x^2) = (k_x, k_y)$.

Especially as for the numerical evaluation of the weak field limit. By using this method with a technique invented in the lattice gauge theory, the Hall conductance of the graphene as a function of the chemical potential $\mu$ is calculated without any numerical difficulties. The results by the single band case is plotted in Fig. 3 with the density of states (DOS) without magnetic field. Three different behaviors (electron like, Dirac like and hole like) are clearly observed which are separated by the singularities of the DOS. Near $E = 0$, it reads $\sigma_{xy}^{\text{Bulk}} = \frac{e^2}{h} (2N + 1)$ with integer $N$. This is a Hall conductance of the Dirac fermions.

Although he Laughlin’s argument is enough to guarantee the integral nature of the Hall conductance, only the generic consideration can not fix this integer. It is specified by considering edge states that is implicitly assumed in the Laghlin argument. The Hall conductance is given by the number of edge modes in the energy gap

FIG. 3: Hall conductance of the graphene as a function of the chemical potential $\mu$. ($\phi = 1/31$)

FIG. 4: Energy spectrum of the graphene on a cylinder with zigzag edge via momentum along the cylindrical direction $k_y$. Red and blue lines are energies of the edge states localized at right and left edges. ($\phi = 1/21$)
that the Fermi energy lies. In Fig.4 energy spectrum of graphene on the cylinder (with zigzag boundary) is shown. The red and blue lines in the energy gap regions are the energies of the edge states localized near the right and left boundaries. Counting the number of edge mode in the energy gap region, we have obtained the Hall conductance of the graphene with edges which does coincide to that given by the Chern number, eq.(1).
\[ \sigma_{xy}^{\text{Edge}} = \sigma_{xy}^{\text{Bulk}}. \]

\[ C_j = I_j - I_{j-1}. \] (2)

This general structure is also applied for the graphene. As discussed in the previous section, the Chern number \( C_j \) is a topological quantity. Also the number of edge modes, \( I_j \) has also topological meaning. Here let us give rough idea of the topological meaning of the edge modes. When one discusses usual electrons in a magnetic field \( B \) in a Landau gauge in \( x \)-direction, two dimensional hamiltonian is decomposed into the sum of the one dimensional hamiltonian of the harmonic oscillators (with parameter \( k_y \)). When one describes the Bloch electrons as graphene on the cylinder with the Landau gauge, similar decomposition of the two dimensional hamiltonian is possible. In this case, corresponding one dimensional system with parameter \( k_y \) is not a simple harmonic oscillator but the Harper equation.

\[ H(2\text{D electrons with } B) = \sum_{k_y} H_{k_y} (\text{harmonic oscillator}) \]

\[ H(\text{graphene with } B) = \sum_{k_y} H_{k_y} (\text{harper problem}) \]

To describe the edge states (bound states) and the Bloch states (scattering states) on the same footing, we need to consider a complex energy surface. As for the Harper equation, there are multiple (\( q \)) energy bands that correspond to the Landau levels. We need to prepare two complex energy planes \( R^+ \) and \( R^- \) by making these \( q \) energy bands as branch cuts as in Fig.4(a). To discuss the problem, it is useful to make them into Riemann spheres by identifying the infinities into each single points. Then the two Riemann spheres are glued into one along the branch cuts (Fig.4(a)-(e)). In Figs.3 we have shown this procedure symbolically for \( q = 3 \) case. Finally we have Riemann surface (RS) with \( g = q - 1 \) holes (handles), which coincide to the energy gaps of the Harper equation. On this RS, generic Bloch function has several zeros which correspond to the energies of the edge states.

One can identify the edge of the cylinder where the edge states localize by the position of the zeros. When it is on the \( R^+ \) (\( R^- \)), the edge state is localized at the right (left) edge. This is for fixed \( k_y \). Then by changing \( k_y \), these zeros of the Bloch state (edge state energies) move and form loops since \( k_y = 0 \) and \( k_y = 2\pi \) to be identified. Then the winding numbers of the loops around the holes (gaps) of the RS give the numbers of edge state, \( I_j \) is defined. By using the Laughlin’s argument, the winding number \( I_j \) gives the Hall conductance when the chemical potential lies in the \( j \)-the gap. In this way, the relation eq.(2) implies a bulk-edge correspondence of the topological quantities. It is clearly demonstrated in the graphene quantum Hall effects.

III. CHIRAL SYMMETRY AND ZERO MODE EDGE STATES

A. Universality of the Dirac fermions and the chiral symmetry

As discussed in the previous section, graphene under a magnetic field has edge states, which are topologically stable and characteristic to the quantum Hall effects. Since the graphene has a chiral symmetry, there are additional edge states, which are protected not only by the topological constraint but also by the chiral symmetry. The chiral symmetry requires the edge states to have the zero energy as discussed below.

As is well known the energy dispersion of graphene is the Dirac fermions like and vanishing linearly at some momentum (Fig.5(a)). Another example of the Dirac like dispersion in two dimensions is also known in condensed matter. That is the \( d_{x^2-y^2} \) wave superconductor (Fig.5(b)) which has been discussed for the high-\( T_c \) materials. In momentum representation, the
When one change cut the origin in the complex plane even number of times
where $C$ is a two component spinor of the fermion operators. They are respectively given as $c_k = c^0_k$ and $c_k = c^1_k$, $H_k = H_{k}^g$ and $H_k = H_{k}^s$ for the graphene and the $d_{x^2-y^2}$-wave superconductor respectively where

$$H_{k}^g = \begin{pmatrix} 0 & D(k) \\ D^*(k) & 0 \end{pmatrix}, \quad c_k = \begin{pmatrix} c_0(k) \\ c_s(k) \end{pmatrix}$$

$$H_{k}^s = \begin{pmatrix} \epsilon(k) & \Delta(k) \\ \Delta^*(k) & -\epsilon(k) \end{pmatrix}, \quad c_k = \begin{pmatrix} c_1(k) \\ c_1^s(k) \end{pmatrix}$$

As for the graphene, we have assumed that the hopping is only allowed between the different sublattices $\circ$ and $\bullet$. Then the one particle hamiltonian has a chiral invariance

$$\{H_{k}^g, \Gamma^g \} = 0, \quad \Gamma^g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (\Gamma^g)^2 = 1 \quad (\text{for the graphene})$$

As for the $d_{x^2-y^2}$-wave superconductivity, when the order parameter does preserve the time reversal, the order parameter, $\Delta(k)$, is real ($\Delta(k) \in \mathbb{R}$). In this case, it also has a chiral invariance

$$\{H_{k}^s, \Gamma^s \} = 0, \quad \Gamma^s = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad (\Gamma^s)^2 = 1 \quad (\text{for the TR invariant $d$-wave})$$

Then the energy dispersion is given by

$$E(k) = \pm |Z(k)|$$

$$C \ni Z(k) = \begin{cases} D(k) & \text{for the graphene} \\ \epsilon(k) + i\Delta(k) & \text{for the TR invariant $d$-wave} \end{cases}$$

It guarantees existence of even number of Dirac fermions, since the zero of the $Z(k)$ gives the linearly vanishing energy gap (generically) and the closed curve $C(k_y) = \{Z(k_x, k_y) | k_x \in [0, 2\pi]\}$ moves on the complex $Z$ plane under the condition $C(0) = C(2\pi)$. It implies the curve cut the origin in the complex plane even number of times when one change $k_y : 0 \rightarrow 2\pi$.

From this two examples, we have realized that there are universality of the Dirac like dispersion when the system has a chiral symmetry. This universal feature further guarantees the physics of boundary states as discussed below.

B. Berry phases and the Edge states

The doubling of the generic Dirac fermion with chiral symmetry is a universal property of the bulk. This bulk property also restricts the existence of special edge states as an example of the bulk-edge correspondence. As for the chiral invariant system, generic condition for the existence of the zero mode on a cylinder (Fig. 7) are given. When one takes a momentum along the cylinder as $k_y$, the Berry phase (Zak phase) for each $k_y$, $\gamma(k_y)$, of the one dimensional hamiltonian $H_k$ ($k_x$ fixed) is defined using the Bloch state $|\psi_k\rangle$, ($H_k|\psi_k\rangle = E(k)|\psi_k\rangle$),

$$i\gamma(k_y) = \int_0^{2\pi} dk_x A(k), \quad A(k) = \langle \psi_k | \frac{\partial}{\partial k_x} | \psi_k \rangle$$

Of course, it does have an ambiguity of the gauge (phase of the Bloch state $|\psi_k\rangle$, $\gamma(k_y)$ is well defined up to modulo $2\pi \mathbb{Z}$. Generically speaking the Berry phase can take any values. However the chiral symmetry of the hamiltonian requires the Berry phase has to be quantized into 0 or $\pi$. Using this quantized Berry phases of the bulk, one can guarantee the existence of the edge states for an infinitely long (along $x$-direction) cylindrical system when the Berry phase $\gamma(k_y)$ is $\pi \mod 2\pi$ as far as the chiral symmetry is still preserved with edge superconductive.

$$\gamma(k_y) = \pi \mod 2\pi \Rightarrow$$

Two zero energy localized modes near the at the right and left boundaries of the cylinder.

To carry out concrete evaluation of the Berry phases analytically, one needs to fix the gauge. However, this gauge fixing is not necessary, at least, to obtain numerical values.

Since this condition is applied for each momentum $k_y$, the zero energy edge states form doubly degenerate flat bands when one considers the original two dimensional problem on the cylinder (Fig. 7). Generically speaking, this condition is not satisfied for all $k_y$, then the flat bands only exist for restricted momenta. Applying this generic consideration for graphene, one predicts flat band zero energy edge states for 1/3 of the total momentum along $y$ direction near the zigzag edge (Fig. 7), which was found by Fujita et al. This edge mode does not exist for armchair edges. It is also consistent with this generic condition (Fig. 7).

As for the $d_{x^2-y^2}$-wave superconductor, we have applied it and obtain the flat band zero mode edge states for (110)-direction. As for the (100)-direction, we predict absence of the zero energy edge states (There is no topological reason to have the edge states. See Fig. 7).
FIG. 7: Energy spectrum of the graphene and $d_{x^2-y^2}$-wave superconductors with different angles on cylinders.

This is consistent with the existence of the Andreev bound states only for the (110)-direction, which has been observed in the zero bias conductance measurements.27

C. Spontaneous local chiral symmetry breaking

As discussed, graphene and the $d_{x^2-y^2}$-wave superconductors have zero energy edge states protected by the chiral symmetry. It is topological in the sense that the quantized Berry phase (Zak phase) is a key (bulk) quantities to guarantee the edge states.

These zero energy edge bands are completely flat ($E = 0$) if they exist. The flatness is guaranteed by the chiral symmetry. Of course, the symmetry of the bulk can not be changed by the existence of the boundaries. However, edge potential induced by the edges may break the bulk symmetry. This symmetry breaking is allowed to exist only near the boundaries (by the edge potential). When one regards the flat band zero modes as a one-dimensional system, it is natural to expect the Peierls instability that reduces the symmetry since the flat bands have a diverging density of states. Then what would be expected is that the chiral symmetry has broken only near the edges to make the flat band dispersive or making a gap in the edge mode bands. This spontaneous symmetry reduction occurs only local near the boundaries.28 This actually occurs both in the graphene and the $d_{x^2-y^2}$-wave superconductors. In the case of graphene, it corresponds to the boundary magnetic moments near the zigzag edges. When one considers this boundary magnetism within the mean field theory, local moments induce site dependent potentials. It destroys the chiral symmetry of the graphene near the boundaries. It is confirmed, at least, numerically based on the density functional theory calculation.29

The same local symmetry breaking also occurs in the $d_{x^2-y^2}$-wave superconductors.30 In this case, the chiral operator corresponds to the time-reversal operation that implies real order parameters of the superconductors. Then what happens is that the order parameter of the superconductivity becomes complex only near the boundaries. It implies spontaneous generation of local fluxes. Topologically, the boundaries of the cylinder and point like impurities are equivalent. Therefore, the generic consideration predict that spontaneous local flux generation near the boundaries or impurities.31,32

D. Chiral zero modes under the magnetic field

When one considers the graphene under magnetic field, there are two different type of edge states. The one is topologically protected quantum Hall edge states. The other is chiral zero mode edge states, which are topological, but are protected by the chiral symmetry. The former is discussed in the previous section. Then we discuss the latter one here.

As shown in Fig. 8, there co-exist Dirac fermions' $n = 0$ Landau level and the chiral zero mode edge states for graphene with zigzag edges. Without magnetic field, there also exist chiral edge modes. However, it is degenerate with the bulk Dirac fermion at the gap closing momentum. Therefore there is no length scale for the $E = 0$ states. With the magnetic field, the situation is different and the length scale should be determined by the magnetic length scale. This additional contribution of the boundary state to the local charge occurs only near the zigzag edge. It is absent at the armchair edges (See Fig. 9). Generically speaking, the edge potential repels the charge density to make depletion layer near the boundary. Physically the length scale of the deple-
The situation is different at the zigzag edge, there occurs enhancement of the local charge density instead of the depletion as shown in Fig. 9(a). This is consistent with the existence of chiral zero modes, which also exist with-out magnetic field. However with magnetic field, there also exists a $n = 0$ Landau level of the Dirac fermion at $E = 0$. It plays fundamental role in reconstruction of the boundary charge. Local charge density of this $E = 0$ states, which has two physical origins as the chiral edge states and the $n = 0$ Landau level, has been investigated by Arikawa et al. They have calculated the local density of state. It can be experimentally observable by the scanning tunneling microscope (STM). Although there exist chiral zero modes at the zigzag edge, it is not enough to describe the edge charge reconstruction. The chiral zero modes actually show detailed structure and long tail into the bulk. However, what is realized in the total local charge density is exponentially localised structure and it becomes to the bulk value quite rapidly. It will be understood as the topological compensation (screening) of the chiral edge charge by the bulk. This is a new feature of the boundary reconstruction of the $E = 0$ states of graphene.

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