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# **Topological Aspects of Graphene**

### Dirac Fermions and Bulk-Edge Correspondence in a Magnetic Field

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with T. Fukui (Ibaragi U.) H. Aoki (U. Tokyo)

> Ref. Y. Hatsugai, T. Fukui and H. Aoki, to appear in Phys. Rev. B, cond-mat/0607669

### Today's Talk

Graphene as a basic platform of Dirac Fermions **Massless** Dirac Fermions in Condensed Matter Physics Anomalous Quantum Hall Effect (QHE) in Graphene Topological Aspects of Graphene (Bulk) **Topological Stability** of the Dirac Fermions Topological Stability of the Anomalous QHE Adiabatic Principle and Topological Equivalence Quantum phase Transition by chemical potential shift Technical development for calculating Chern numbers (Lattice Gauge Theory) Topological Aspects of Graphene (Edge) 😪 Without Magnetic field \* Topological Origin of Zero Modes in Graphene (c.f. d-wave superconductors) With Magnetic field Edge States of Dirac Fermions Sulk – Edge Correspondence (Analytical & Numerical) Edge States and Bloch States ( complex energy structure )

# Massless Dirac Fermions in Condensed Matter

**Gapless Superconductor with point Nodes** 



d-wave superconductivity

### Graphene as a 2D Carbon sheet



Wallace (1946)

Fig.Zhang et al. (2005)

# **Observation of Anomalous QHE in Graphene**

Anomalous QHE of gapless Dirac Fermions



Novoselov et al. Nature 2005

### **Conventional QHE**

Landau Level and Integer QHE



# **QHE and Band Structures**

### **QHE** of electrons and holes

2D organic metal (TMTSF)<sub>2</sub>PF<sub>6</sub> (Chaikin et al)





Lab. de Physique des Solides

### **QHE of Semiconductors**

Landau Level of Conduction band (Electrons)







### × 89 Matches on Graphene in cond-mat in the past year

**Experiments** and theories

# **Motivations Here**



\* How does the Anomalous QHE persist for higher Energy? Quantum Phase Transition? \* Is it specific to the honeycomb lattice? Edge State? Laughlin 81 Halperin 82 Arr How do the edge states look like? Edge States & Topological Numbers Hatsugai 1993 \* How about the bulk-edge correspondence?

### Hofstadter diagram for the honeycomb

Tight-binding model on a honeycomb lattice



 $H = \sum t_{ij} e^{i\theta_{ij}}$  $\langle ij \rangle$  $2\pi\phi_P = \sum \theta_{ij}$  $\langle ij \rangle \in P$  $\phi_P = \phi = \frac{p}{a}$ (p,q) = 1

Rammal 1985

E=0 Landau level : outside Onsager's semiclassical quantisation scheme

### Bulk $\sigma_{xy}$ by the topological invariant

Hall conductance by Chern number

Counting vortices in the band

$$\sigma_{xy}^{j} = \frac{e^{2}}{h} \sum_{\substack{\ell=1\\\epsilon_{\ell}(k) < \mu_{F}, \ \ell = 1, \cdots, j}}^{j} C_{\ell}, \quad C_{\ell} = \frac{1}{2\pi i} \int_{BZ} dA_{\ell}, \quad A_{\ell} = \langle \psi_{\ell} | d\psi_{\ell} \rangle$$

$$\overset{\text{with randomness Aoki-Ando 1986}}{\text{Integration of the NonAbelian Berry Connection of the}}$$

$$\overset{\text{"Fermi Sea"}}{\sigma_{xy}} = \frac{e^{2}}{h} \frac{1}{2\pi i} \int_{BZ} \text{Tr}_{j} dA_{\text{FS}} \text{ Fermi Sea of } j \text{ filled bands}}$$

$$A_{\mathrm{FS}} = \Psi^{\dagger} d\Psi, \ \Psi = (\psi_1, \cdots, \psi_j)$$
 Hatsugai 2004

☆ Tolological Invariant on Discretized Lattice Lattice in k space  $\sigma_{xy} = \frac{e^2}{h} \frac{1}{2\pi i} \sum F_{1234}$ Technical Advantage for large Chern Numbers  $F_{1234} = \text{Im } \log U_{12}U_{23}U_{34}U_{41}$ Fukui-Hatsugai-Suzuki 2005  $U_{mn} = \det_{j} \Psi_{m}^{\dagger} \Psi_{n}, \quad \Psi_{n} = (\psi_{1}(k_{n}), \cdots, \psi_{j}(k_{n}))$ 

### Hall Conductace vs chemical potential

Accurate Hall conductance over the whole spectrum



# Hall Conductace vs chemical potential

Accurate Hall conductance over the whole spectrum



### Hall Conductace vs chemical potential × Accurate Hall conductance over the whole spectrum Quantum phase transition D(E) at the van Hove Energies Singularity breaks **Topological Stability** -2 Dirac behavior in this region xy10 $t \approx 1 [eV]$ for graphene $\mu/t$ , -2 -10

-20

 $\phi = 1/31$ 

 $E(k_x, k_y) = \pm \sqrt{(1 + \cos k_x + \cos k_y)^2 + (\sin k_x + \sin k_y)^2}$ 

### (Sheng et al, cond-mat/0602190)





# **Dirac Cones are Stable!**

The Dirac Cornes are not accidental
 It has topological stability

$$-3 < \frac{t'}{t} < 1 \implies \text{Doubled Dirac Cones}$$



t'/t = 1 : Square Lattice t'/t =0 :Honeycomb Lattice t'/t=-1 : π Flux State

**Density of States** 

### Vanishing DOS near the zero energy





t'/t = 1 : Square Lattice t'/t =0 :Honeycomb Lattice t'/t=-1 : π Flux State

Stability of the Dirac Cornes!

# **Dirac Cornes**

### **Adiabatic Equivalence**



t'/t = 1 : Square Lattice t'/t =0 :Honeycomb Lattice t'/t=-1 : π Flux State

# **Topological Stability of the Dirac Cornes** $H(k_x, k_y) = \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix}$ $\Delta = -t(1 + e^{ik_y} + e^{ik_x}(1 + re^{-ik_y}), \quad r = t'/t$ $E(k_x, k_y) = \pm |\Delta|$ $= \pm \sqrt{(1 + \cos k_x + \cos k_y)^2 + (\sin k_x + \sin k_y)^2}$

 $\Rightarrow$  General zeros of  $\Delta(k_x, k_y) \longrightarrow$  Dirac Cones



$$\Delta(k_x, k_y), \ k_x : 0 \to 2\pi : \text{ loop } C(k_y) \text{ in } \mathbb{C}$$
$$\text{loop } C(k_y) \text{ moves } : k_y : 0 \to 2\pi$$

# **Topological Stability of the Dirac Cornes** $H(k_x, k_y) = \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix}$ $\Delta = -t(1 + e^{ik_y} + e^{ik_x}(1 + re^{-ik_y}), \quad r = t'/t$ $E(k_x, k_y) = \pm |\Delta|$ $= \pm \sqrt{(1 + \cos k_x + \cos k_y)^2 + (\sin k_x + \sin k_y)^2}$

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 $\Delta(k_x, k_y), \ k_x : 0 \to 2\pi : \ \text{loop} \ C(k_y) \ \text{in} \ \mathbb{C}$  $\text{loop} \ C(k_y) \ \text{moves} \ : k_y : 0 \to 2\pi$  $\text{The loop cut the origin} \rightarrow \text{Dirac Cones}$ Topological Stabilityof the doubled Dirac Cones

# Hofstadter Diagrams



### ☆ Hall Conductance v.s. chemical potential



t'/t = 1 : Square Lattice t'/t =0 :Honeycomb Lattice t'/t=-1 : πFlux State

# van Hove singularity & Hall Conductance



# $\sigma_{xy}$ by Adiabatic Principle $\Rightarrow$ Hofstadter Diagram and $\sigma_{xy}$ with t'/t





t'/t = 1 : Square Lattice t'/t =0 :Honeycomb Lattice t'/t=-1 : π Flux State

# **Adiabatic Connections Near zero Field**



### $\Rightarrow$ Honeycomb Lattice $\leftrightarrow \pi$ flux

Main Gaps Preserve

Near E=0

Honeycomb System is Topologically Equivalent to  $\pi$  flux System Near E=0



### 

Main Gaps Preserve

Near Band Edges

Honeycomb System is Topologically Equivalent to Square System Near the Band Edges

# Honeycomb $\sigma_{xy}$ From Diophantine Equations

☆ As for the π flux system and square system,
 σ<sub>xy</sub> is determined by a Diophantine equation
 ☆ By the Adiabatic Equivalence, σ<sub>xy</sub> of the honeycomb is determined algebraically.

Master Eq. D

$$\Phi = \frac{P}{Q}, \quad J \equiv Pc_J, \quad (\operatorname{mod} Q), \quad |c_J| < Q/2 \quad \text{tknn1982}$$

Solution State Adiabatic Equivalence

 $\Phi = \frac{P}{Q} = \frac{1}{2} + \frac{\phi}{2} = \frac{q+1}{2q}, \quad \phi = \frac{1}{q}$   $P = q+1, \quad Q = 2q$  J = q - 1 + 2(N+1) = q + 2N + 1 Algebraicallyon Honeycomb Lattice

 $c_J = 2N + 1, \ N = 0, 1, 2, \cdots$ 

# Edge states of Graphene

### **Without magnetic field**

 YH

 with S. Ryu (now KITP)

Ref.[1] Phys. Rev. B65, 212510 (2002)
[2] Phys. Rev. Lett. 89, 077002(2002)
[3] Physics C 388-389, 78 (2003), ibid 90 (2003)
[4] Phys. Rev. B67, 165410 (2003)
[5] Physica E 22, 679 (2004)

**With magnetic field** 

**Recent works** 

# Graphene on a Cylinder



 $H_{\text{total}} = \sum H(\mathbf{k}_{\mathbf{y}})$  $k_{u}$ 

Total System as a sum of 1D system parametrized by  $k_y$  Let me remind old works without magnetic field for a while

**Topological Equivalence** between Anisotropic Superconductors and Carbon 2D Systems **From Topological Orders** Y. Hatsugai with S.Ryu **Department of Applied Physics** University of Tokyo

Ref.[1] Phys. Rev. B65, 212510 (2002) [2] Phys. Rev.Lett. 89, 077002(2002) [3] Physics C 388-389, 78 (2003), ibid 90 (2003) [4] Phys. Rev. B67, 165410 (2003)

[5] Physica E 22, 679 (2004)

### Localized Boundary State in Carbon Sheet (1) now called as Graphene





"Peculiar Localized State at Zigzag Graphite Edge" M. Fujita, K. Wakabayashi, K. Nakada and K. Kusakabe, JPSJ 65, 1920 (1996)

### **Localized Boundary State in Carbon Sheet (2)**

# Local Spin Density Functional Appr. Calculation Volume 87, NUMBER 14 PHYSICAL REVIEW LETTERS 1 OCTOBER 2001 (a) (a) (b) (b) (b) (b) (c) (c) (c) (c) (b) (c) (c)

FIG. 1. Contour plots of spin density  $n_{\dagger}(r) - n_{\downarrow}(r)$  (a) on a plane perpendicular to a graphite flake with zigzag edges and (b) on a plane including the graphite flake. In (a) the edges are perpendicular to the plane and C atoms on the plane are depicted by shaded circles. Positive and negative values of the spin density are shown by solid and dashed lines, respectively. Each contour represents twice (or half) the density of the adjacent contour lines.

B, N, and C atoms have been observed indeed [8–10]. Second, the phase separation of graphite and BN regions leading to the striped structures above is energetically favorable. In fact, we have performed the total-energy calculations for graphite, BN, BC, and NC heterosheets by DFT. The calculated bond energies of B-C and N-C are smaller than that of graphite by 1.52 and 0.81 eV, respectively. On the other hand, the bond energy of B-N is smaller than that of graphite only by 0.31 eV. Third, undulation

"Magnetic Ordering in Hexagonally Bonded Sheets with First-Row Elements", Okada, Oshiyama, Phys. Rev. Lett. 87, 146803 (2001)

### Zero Bias Conductance Peak d-wave superconductivity in Anisotropic Superconductivity



bias and magnetic field is shown. The field *H* is always applied parallel to the junction interface, and either parallel or perpendicular to the YBCO *ab* planes, as labeled. The theoretical curve (solid line) is calculated using the FRS theory [11], as described in the text. For junction 2, lowtemperature spectra for low and high applied magnetic field are shown. Note the field-induced splitting in the ZBCP is strongly anisotropic with respect to the field orientation. Data obtained on junction 1 show reproducibility between junctions for data taken at low temperature and field (T = 1.5 K, H = 0.2 T). Zero-field data taken at a temperature above the  $T_e$  of Pb is also shown for junction 1. Zero Energy Boundary States of Anisotropic Superconductivity



L. J. Buchholtz,G. Zwicknagl, Phys. Rev. B 23, 5788 (1981) (p wave ) C.-R. Hu, Phys. Rev. Lett. 72, 1526 (1994) (d wave )

S. Kashiwaya, Y. Tanaka, Phys. Rev. Lett. 72, 1526 (1994)

M. Matsumoto and H. Shiba, JPSJ, 1703 (1995)

(fig.) M. Aprili, E. Badica, and L. H. Greene, Phys. Rev. Lett. 83, 4630 (1999)

### **Edge State and Zero Modes**

1. Zero Bias Conductance Peak

2. Boundary Magnetism of the Carbon Nanotubes

These 2 systems are topologically equivalent with each other

Localized zero modes of topological ordered states

cf. Witten's SUSY QM

### Zero Energy Edge States in Various Physical Systems

Anisotropic Superconductivity (  $d_{x^2-y^2}$ -wave )



#### Zero Energy Edge States !

No Edge States !

### Zero Energy Edge States : cont.

Graphite Ribbons (zigzag, bearded, and armchair edges)


When and Why the Zero Energy Edge States Appear ?



- Bulk-Edge Correspondence
- Particle Hole Symmetry
- Topological Stability

S. Ryu and Y. Hatsugai, Phys. Rev. Lett. 89, 077002-1-4 (2002)

#### Berry's parametrization As for a1D system parametrized by ky

$$h_{k} = \begin{pmatrix} \xi_{k} & \Delta_{k} \\ \Delta_{k}^{*} & -\xi_{k} \end{pmatrix} = \mathbf{R}(\mathbf{k}) \cdot \boldsymbol{\sigma} \quad \boldsymbol{\sigma} : \text{Pauli matrices}$$

$$\boldsymbol{R}(\boldsymbol{k}) = (\operatorname{Re}\Delta_k, -\operatorname{Im}\Delta_k, \xi_k)$$

• Map from  $\boldsymbol{k}$  to  $\boldsymbol{R}$  as  $\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{k})$ .

- In 1D,  $k \in S^1$  ( $k : 0 \to 2\pi$ ), so  $\boldsymbol{R}$  forms a loop  $\ell$ 
  - This map is one to one

A loop in R space characterize the hamiltonian

$$H^{bulk}[\ell]$$



• The system with edges is also constructed by cutting all the matrix elements between the sites 1 and N in real space.

$$H^{edge}[\ell]$$



## When the Zero Mode Edge States Exist ?

(Sufficient Condition)

S.Ryu & Y.Hatsugai, Phys. Rev. Lett. 89, 077002 (2002)

I. The loop  $\ell$  is on the plane cutting the origin  $\mathcal{O}$ .

II. The loop  $\ell$  is continuously deformed to the circle whose

... origin is at  $\mathcal{O}$  without passing through  $\mathcal{O}$ 



**Check for the Anisotropic Superconductivity** ( $d_{x^2-y^2}$ -wave) (110) surface: the unit cells, loops, and the dispersion



#### The origin $\mathcal{O}$ is always inside the loop.

#### **Check for the Anisotropic Superconductivity : cont.**

(100) surface: the unit cells, loops, and the dispersion



The origin  $\mathcal{O}$  is never inside the loop except at  $k_y = \pm \pi$ .

#### **Check for the Graphite Ribbons**

Zigzag edge : the unit cells, loops, and the dispersion



The origin  $\mathcal{O}$  is inside the loop when  $|k_y| > 2\pi/3$ .

#### **Check for the Graphite Ribbons : cont.**

Bearded edge : the unit cells, loops, and the dispersion



The origin  $\mathcal{O}$  is inside the loop when  $|k_y| < 2\pi/3$ .

#### **Check for the Graphite Ribbons : cont.**

Armchair edges : the unit cells, loops, and the dispersion



The origin  $\mathcal{O}$  is always outside the loop.

## Now go back to the present work

# Edge States of Graphene with magnetic field & Edge States and their local charges (Zigzag edges)





# How the Edge states look like ?

#### **Field dependence**





### Adiabatic Equivalences of Edge States



How the edge states determine ? How to calculate  $\sigma_{xy}$  by the edge states?



Quantization of  $\sigma_{xy}$  by Edge states





# Bulk – Edge Correspondence ?



## Bulk – Edge Correspondence ? $\Rightarrow$ Numerically $\sigma_{xy}^{bulk} = \sigma_{xy}^{edge}$ Near Zero



k<sub>v</sub>





Followed by the discussion on a square lattice Y.H., Phys. Rev. B 48, 11851 (1993)

Phys. Rev. Lett. 71, 3697 (1993)





## Edge State and Bloch State \$\approx reduced 1D system and transfer matrix

$$H = \sum_{k_y} H_{1D}(k_y)$$

$$Y.H., Phys. Rev. B 48, 11851 (1993)$$

$$Phys. Rev. Lett. 71, 3697 (1993)$$

$$|E, k_y\rangle = \sum_{j_x} \left[ \psi_{\bullet}(E, j_x, k_y) c_{\bullet}^{\dagger}(j_x, k_y) | 0 \right] + \psi_{\circ}(E, j_x, k_y) c_{\circ}^{\dagger}(j_x, k_y) | 0 \right],$$

$$H_{1D}(k_y) | z, k_y\rangle = z | z, k_y\rangle, z = E$$

$$M_{\circ \bullet}(j_x) = \begin{pmatrix} \frac{w}{t_{\circ}(j_x)} & -\frac{t_{\circ \circ}(j_x-1)}{0} \\ 1 & 0 \end{pmatrix}$$

$$M_{\circ \circ}(j_x) = \begin{pmatrix} \frac{\psi_{\bullet}(j_x)}{1} & M_{t}(j_x) = M_{\bullet \circ}(j_x)M_{\circ \bullet}(j_x) \\ \psi_{\circ}(j_x-1) & M_{t}(j_x) = M_{\bullet \circ}(j_x)M_{\circ \bullet}(j_x) \\ How these two are related ??$$

$$How these two are related ??$$

$$W_B(q) = M\psi_B(0) = \rho\psi_B(0)$$

$$|\rho| = 1$$

$$\psi_E(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_E(q) = \begin{pmatrix} * \\ 0 \end{pmatrix}$$

 $M = M_{\rm t}(q-1)M_{\rm t}(q-2)\cdots M_{\rm t}(0)$ 

# Analytic Continuation of the Bloch State

- The Edge State is obtained from the Bloch State by Analytical continuation
  Y.H., Phys. Rev. B 48, 11851 (1993)
  Phys. Rev. Lett. 71, 3697 (1993)
  - st Energy of the Bloch state  $\psi_{B}$  is in the band
  - symp lpha Energy of the edge state  $\psi_{E}$  is in the gap
- Complex energy surface is required
  - $oldsymbol{\psi}_B$  &  $oldsymbol{\psi}_E$  :Unified on Complex Energy surface
  - Energy bands : branch cuts, 2 Riemann sheets required
     Q branch cuts
  - genus (number of holes) g=Q-1 Riemann surface
  - 🛱 g : number of the energy gaps



## **Construction of the Riemann surface** $\Phi = P/Q, \quad Q = 3$ $P = P/Q, \quad Q = 3$ $\Rightarrow Glue \ 2 \ complex \ planes \ with \ Q \ branch \ cuts$

Q=3 energy bands: Q=3 branch cuts



Q-1 holes

# **Construction of the Riemann surface** $$\begin{split} \Phi &= P/Q, \quad Q = 3 \\ & \bigstar \ \text{Glue 2 complex planes} \ \text{vith} \ \begin{array}{l} Q \ \text{branch cuts} \\ Q = 3 \ \text{energy bands: } Q = 3 \ \text{branch cuts} \\ \end{array} \end{split}$$



#### Construction of the Riemann surface $\Phi = P/Q, \quad Q = 3$ $\Rightarrow$ Glue 2 complex planes with Q branch cuts Q=3 energy bands: Q=3 branch cuts



g=Q-1 holes





g=Q-1 holes





# **Construction of the Riemann surface** $$\begin{split} \Phi &= P/Q, \quad Q = 3 \\ & \bigstar \ \text{Glue 2 complex planes} \ \text{vith} \ \begin{array}{l} Q \ \text{branch cuts} \\ Q \ \text{energy bands: } Q = 3 \ \text{branch cuts} \\ \end{array} \end{split}$$



g=Q-1 holes



 $\thickapprox$  Changing  $k_y \in [0, 2\pi]$  , the zero in the j-th gap makes a closed loop



A Changing  $k_y \in [0, 2\pi]$  , the zero in the j-th gap matrix a closed loop

## Riemann surface & Laughlin's Argument R $\alpha_1$ $E_F$ R R R R $I(\alpha_j, L^{\mathcal{I}}_{\text{edge}}) = +1, \ j = 1$ Winding number or $k_{\eta}$ Intersection number with j,Edge $= rac{e^2}{b} \cdot I(\alpha_j, C_{edge}^j)$ canonical loop Y.H., Phys. Rev. B 48, 11851 (1993)

Edge State make a vortex when it touches to the bands



Bulk – Edge Correspondence pprox Hall Conductance of the Bulk States  $\sigma_{xu}^{
m bulk}$ lpha Chern Number,  $C_{\rm FS}^{\jmath}$ lpha Hall Conductance of the Edge States  $\sigma_{xu}^{
m edge}$  $\approx$  Intersection number,  $I(\alpha_j, C_{edge}^j)$ Their relation: Edge State make a vortex when it touches to the bands As for topological quantities  $C_{\rm FS}^j = I(\alpha_j, C_{\rm edge}^j)$ Its physical outcome Y.H., Phys. Rev. Lett. 71, 3697 (1993)  $\sigma_{xy}^{\text{ bulk}} = \sigma_{xy}^{\text{ edge}}$ Justified in Graphene as well


Imagine loops on the Riemann surrface





## Summary

Topological Aspects of Graphene (Bulk) \* Topological Stability of the Dirac Fermions **Topological Stability** of the Anomalous QHE **Adiabatic Principle** and Topological Equivalence Quantum phase Transition by chemical potential shift 🛿 Technical development for calculating Chern numbers (Lattice Gauge Theo Topological Aspects of Graphene (Edge) Without Magnetic field (old work) Topological Origin of Zero Modes With Magnetic field Edge States of Dirac Fermions Sulk – Edge Correspondence × Analytially and numerically