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ICTP Conference Graphene Week 2008

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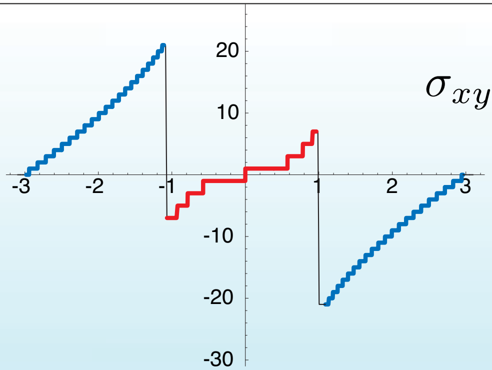
Bulk--edge correspondence in graphene with/without magnetic field Topological aspects of Dirac fermions in real materials

Y. Hatsugai

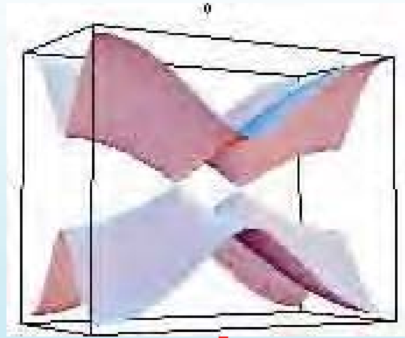
Institute of Physics, University of Tsukuba, Japan

Strada Costiera 11, 34014 Trieste, Italy - Tel. +39 040 2240 111; Fax +39 040 224 163 - sci_info@ictp.it, www.ictp.it

Graphene Week08 ICTP Trieste, Aug. 28, 2008

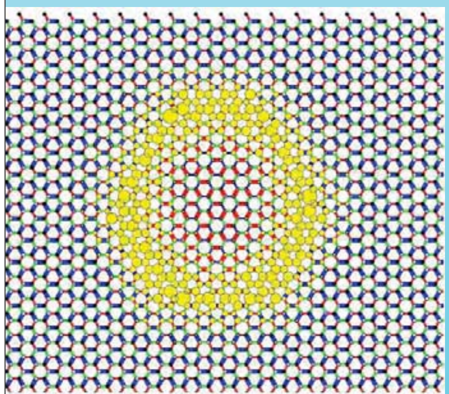


$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\int \mathrm{Tr}\, dA$$



Bulk–edge correspondence in graphene with/without magnetic field

Topological aspects of Dirac fermions in real materials



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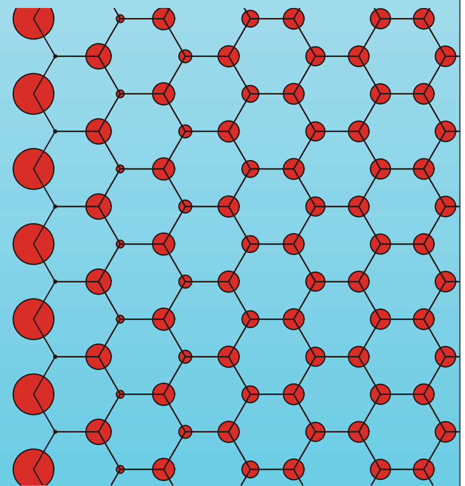
Y. Hatsugai



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Edge States in Condensed Matter Physics

- ☆ Bound states in quantum mechanics
  Levinson's theorem, Friedel's sum rule
- ☆ Surface states in Semiconductors
- ☆ Solitons in polyacetylene — Su-Schriefer-Heeger '79
- ☆ Edge states in quantum Hall effects — Halperin '82 Hatsugai '93
- ☆ Local moments in integer spin chains near the impurities
  Kennedy '90 Hagiwara-Katsumata-Affleck-Halperin-Renard '90
- ☆ Zero bias conductance peaks of the d-wave superconductors
  Hu, '94
- ☆ Zero energy localized states of graphene
  Fujita et al.'96 Ryu-Hatsugai'02
- ☆ Quantum Spin Hall Edge states
  Kane-Mele'05
  Bernevig-Hughes-Zhang '06

more possibilities

- ☆ Edge states in 2D cold atoms in optical lattice
  Scarola-Das Sarma., PRL 98, 210403 '07
- ☆ One-way edge modes in gyromagnetic photonic crystals
  Wang et al., PRL 100, 013905 '08

Why the Edge States are there??

Accidental ?

NO !

Inevitable reasons

Universal Structures behind:

Bulk determines the edges : Bulk-Edge Correspondence

Protected by

Topological constraints

and also additional Symmetry

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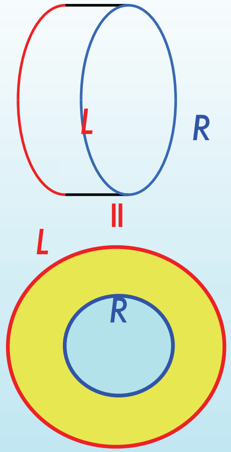
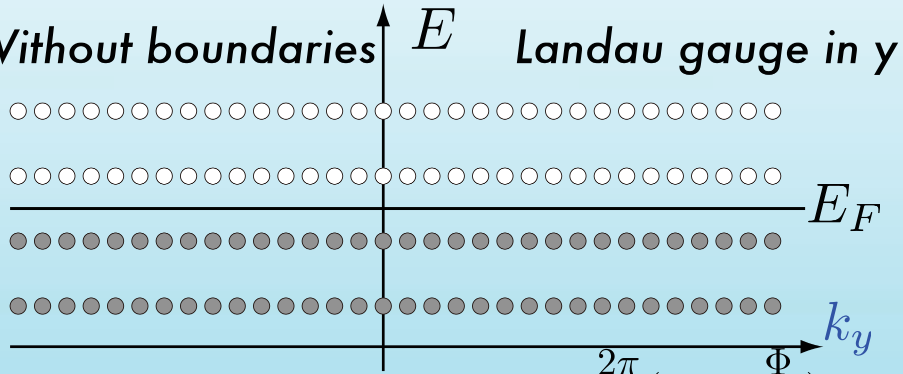
Revisit the past and discuss graphene Quantum Hall effects
Several New results
They Can Be detected by STM experiments !

Quantum Hall Effects by edge states



☆ Edge states and Hall conductance σ_{xy} Halperin '82

Without boundaries



Landau gauge in y

$$H_{2D} = \sum_{k_y} H_{1D}(k_y)$$

$H_{1D}(k_y)$: harmonic osc. centered at

$$\langle x \rangle \sim \ell_B^2 k_y$$

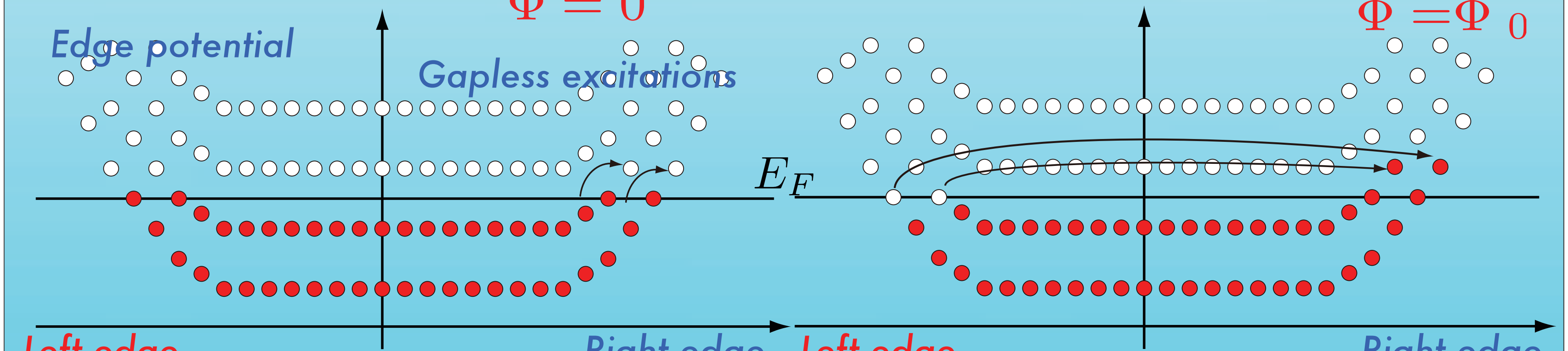
$$k_y = \frac{2\pi}{L_y}\left(n_y + \frac{\Phi}{\Phi_0}\right) \quad n_y = 0, \pm 1, \pm 2, \cdots$$

With boundaries

$\Phi = 0$

2 states are carried from L to R

$\Phi = \Phi_0$



Laughlin's undetermined n : # of Landau Levels below E_F

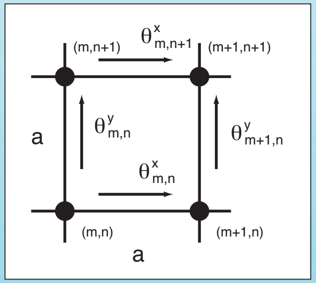
Edge states are essential in the QHE !

Hall Conductance has a Topological meaning

- Discussion by the Bloch electrons (Peierls substitution)
  - preserve U(1) gauge symmetry
  - without cutoff ambiguity
  - recover continuum theory by scaling limit (weak field limit)

$$H = \sum_{\langle ij \rangle} c_i^\dagger e^{i\theta_{ij}} c_j \qquad 2\pi\phi = \sum_{\langle ij \rangle \in P} \theta_{ij} \qquad \phi = \frac{Ba^2}{\Phi_0}$$

P : plaquette



When E_F is in the j-th gap

Two topological quantities

$$\sigma_{xy}^{\text{bulk}} = \frac{e^2}{h} \sum_{\ell:\epsilon_\ell(k)<E_F} C_\ell$$

Sum of the First Chern numbers below E_F
Thouless-Kohmoto-Nightingale-den Nijs '82

$$\sigma_{xy}^{\text{edge}} = \frac{e^2}{h} I(\alpha_j, C^j)$$

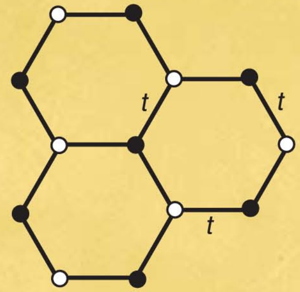
Winding number of the edge state in the complex energy surface
Hatsugai '93a

Bulk — Edge Correspondence Hatsugai '93b

$$\boxed{\sigma_{xy}^{\text{bulk}} = \sigma_{xy}^{\text{edge}}}$$

Hall Conductance has a Topological meaning

Graphene :
Lattice effects are crucial to have the Dirac dispersion



$$2\pi\phi = \sum_{\langle ij\rangle \in H} \theta_{ij}$$

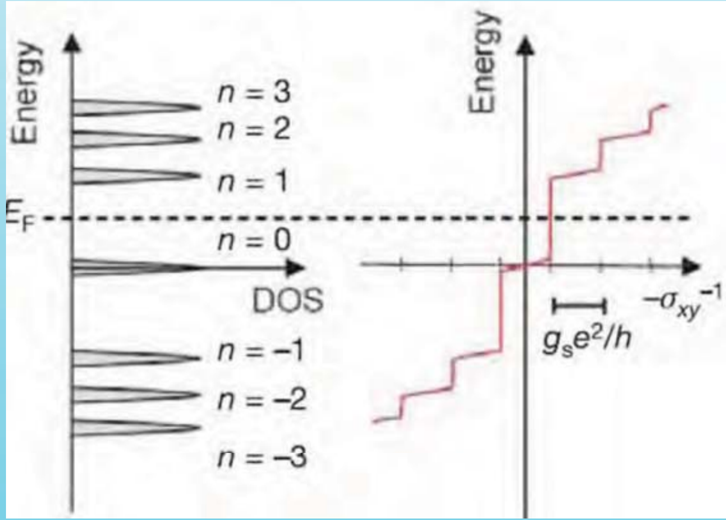
Rammal 1985

Direct application
for the Graphene

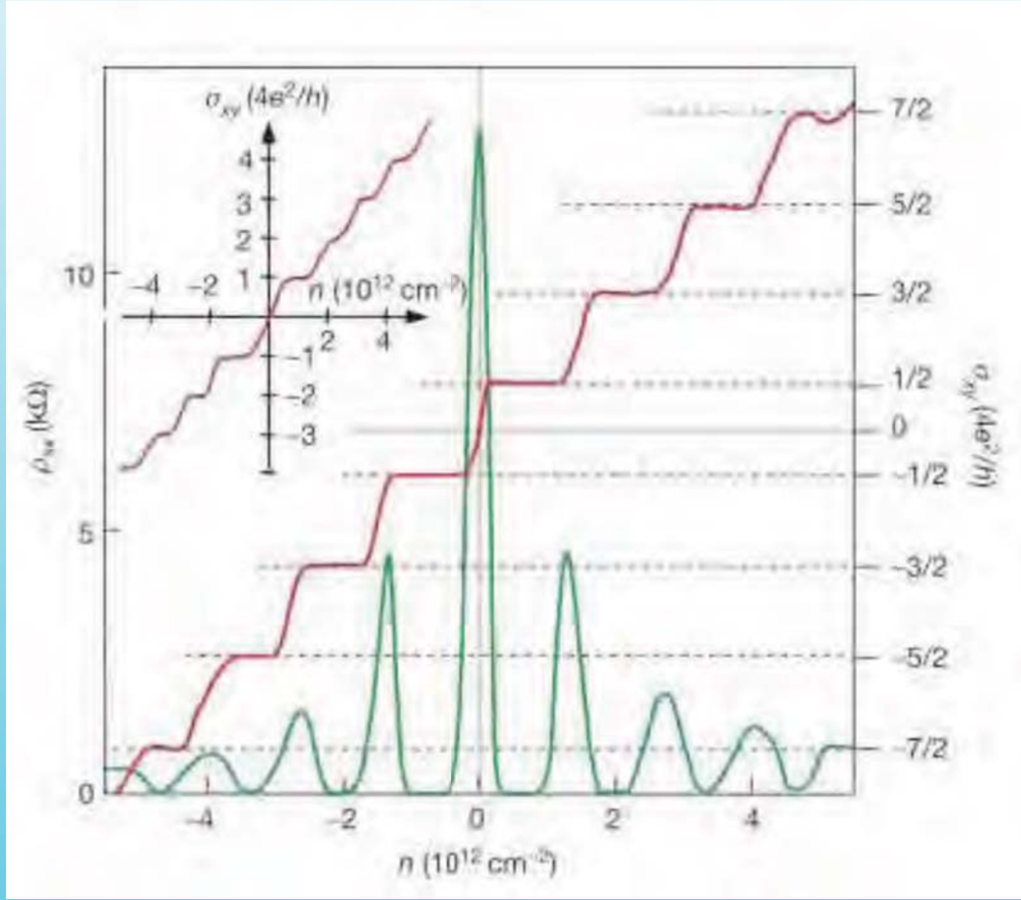
Observation of Anomalous QHE in Graphene

- *Anomalous QHE of gapless Dirac Fermions*

$$\sigma_{xy} = \frac{e^2}{h}(2n+1),\ \ n = 0, \pm 1, \pm 2, \cdots$$
$$= 2\frac{e^2}{h}(n+\frac{1}{2})$$



Zhang et al. Nature 2005



Novoselov et al. Nature 2005

Graphene under magnetic field

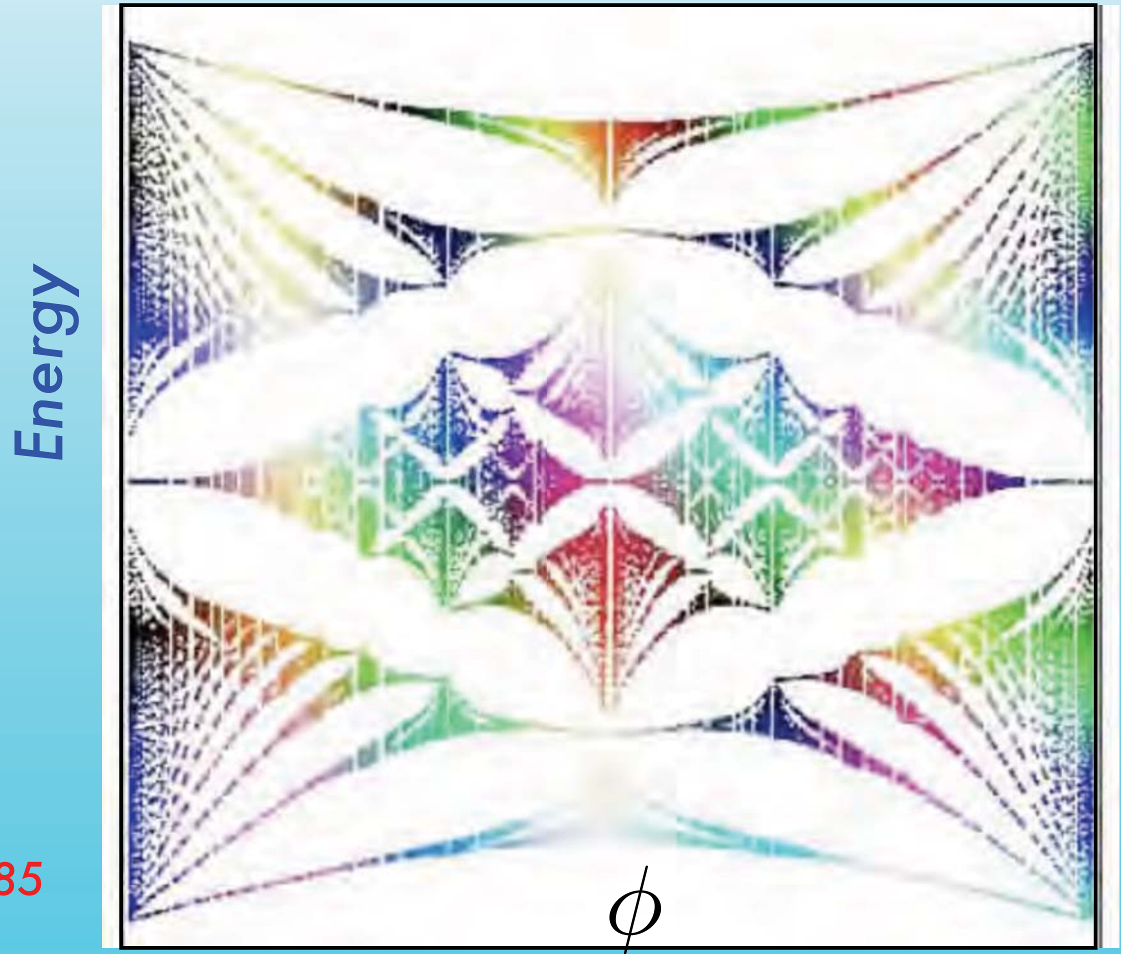
Landau gauge

- In continuum, 2D = $\sum_{k_y}$(1D harmonic oscillators with parameter k_y)
- Bloch electrons, 2D =$\sum_{k_y}$(1D Harper problem with parameter k_y)

Hofstadter diagram for the honeycomb

One particle Energy vs flux/hexagon ϕ (in flux quantum)

Rammal 1985



Topological meaning of the Hall Conductance

☆ TKNN formula: σ_{xy} as a topological invariant

Kubo formula

Thouless-Kohmoto-Nightingale-den Nijs '82

$$\sigma_{xy} = \frac{e^2}{h} \sum_{\ell:\epsilon_\ell(k)<E_F} C_\ell$$

Sum over the bands below E_F

$$C_\ell = \frac{1}{2\pi i} \int_{T^2:\mathrm{BZ}} F_\ell$$

:First Chern number of the ℓ-th Band

intrinsically integer

unless the energy gap collapses

$$\forall k,\ \epsilon_\ell(k) \neq \epsilon_{\ell\pm1}(k)$$

regularity of the Berry connection

$$F_\ell = dA_\ell = \langle d\psi_\ell | d\psi_\ell \rangle$$

$$A_\ell = \langle \psi_\ell | d\psi_\ell \rangle$$

$$H(k)|\psi_\ell(k)\rangle = \epsilon(k)|\psi_\ell(k)\rangle$$

$$k \in T^2_{\mathrm{BZ}} = \{k = (k_x, k_y) |\ 0 \leq k_x, k_y \leq 2\pi\}$$

$$d = dk_\mu \frac{\partial}{\partial k_\mu}$$

Bulk Hall conductance of graphene

☆ Hall conductance by Chern number

Counting vortices in the band

$$\sigma_{xy}^{j} = \frac{e^2}{h}\sum_{\ell=1}^{j} C_\ell, \quad C_\ell = \frac{1}{2\pi i}\int_{BZ} dA_\ell, \quad A_\ell = \langle \psi_\ell | d\psi_\ell \rangle$$

$\epsilon_\ell(k) < \mu_F,\ \ell = 1, \cdots, j$

Thouless-Kohmoto-Nightingale-den Nijs 1982

with randomness Aoki-Ando 1986

graphene

E=0

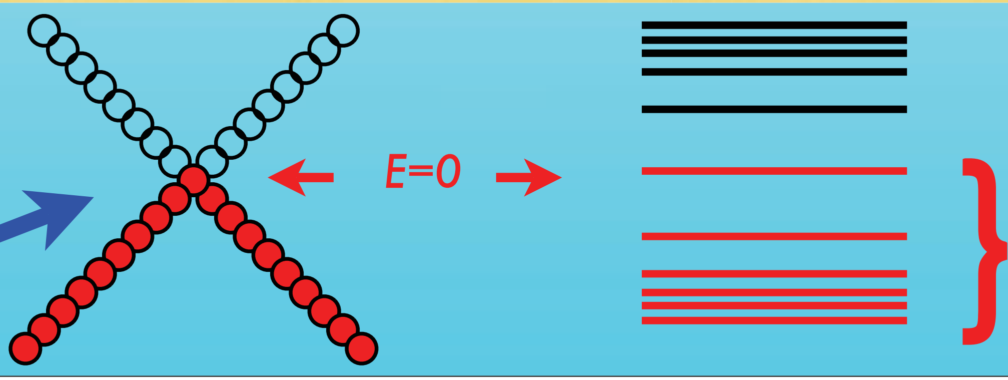
Need to sum over them

Sum over the filled bands

Need to sum many bands until E=0

Numerical difficulty for the weak field (experimental situation)

Need to fill negative energy Dirac sea



Bulk σ_{xy} of the Filled Fermi sea & Dirac Sea

- Integration of the NonAbelian Berry Connection of the filled "Fermi Sea" & "Dirac Sea"

Technical advantage for graphene

$$H_j(k)|\psi_j(k)\rangle = \epsilon_j(k)|\psi_j(k)\rangle$$

$$\Psi = (\,|\psi_1\rangle, \cdots, |\psi_M\rangle)$$

Collect M states below the Fermi level

$$A_{FS} \equiv \Psi^\dagger d\Psi = \begin{pmatrix} \langle\psi_1^\dagger|d\psi_1\rangle & \cdots & \langle\psi_1^\dagger|d\psi_M\rangle \\ \vdots & \ddots & \vdots \\ \langle\psi_M^\dagger|d\psi_1\rangle & \cdots & \langle\psi_M^\dagger|d\psi_M\rangle \end{pmatrix}$$

Matrix vector potential of the Fermi (Dirac) Sea

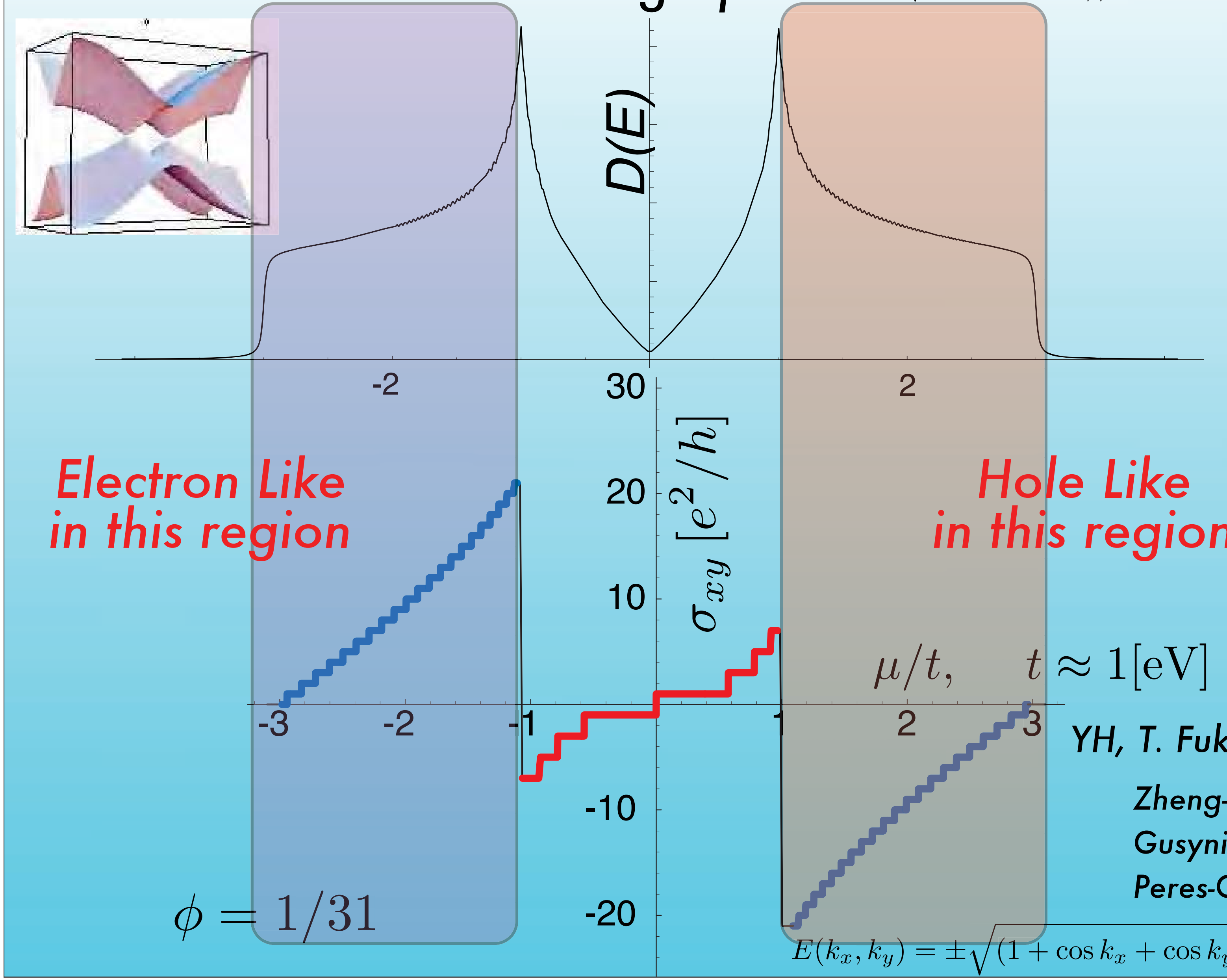
Non Abelian extension for the Chern numbers

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\int_{T^2} \mathrm{Tr}_M dA_{FS}$$

Hatsugai 2004

Hall Conductace vs chemical potential

☆ Hall conductance of graphene over the whole spectrum



YH, T. Fukui & H. Aoki, '06

Zheng-Ando 2002

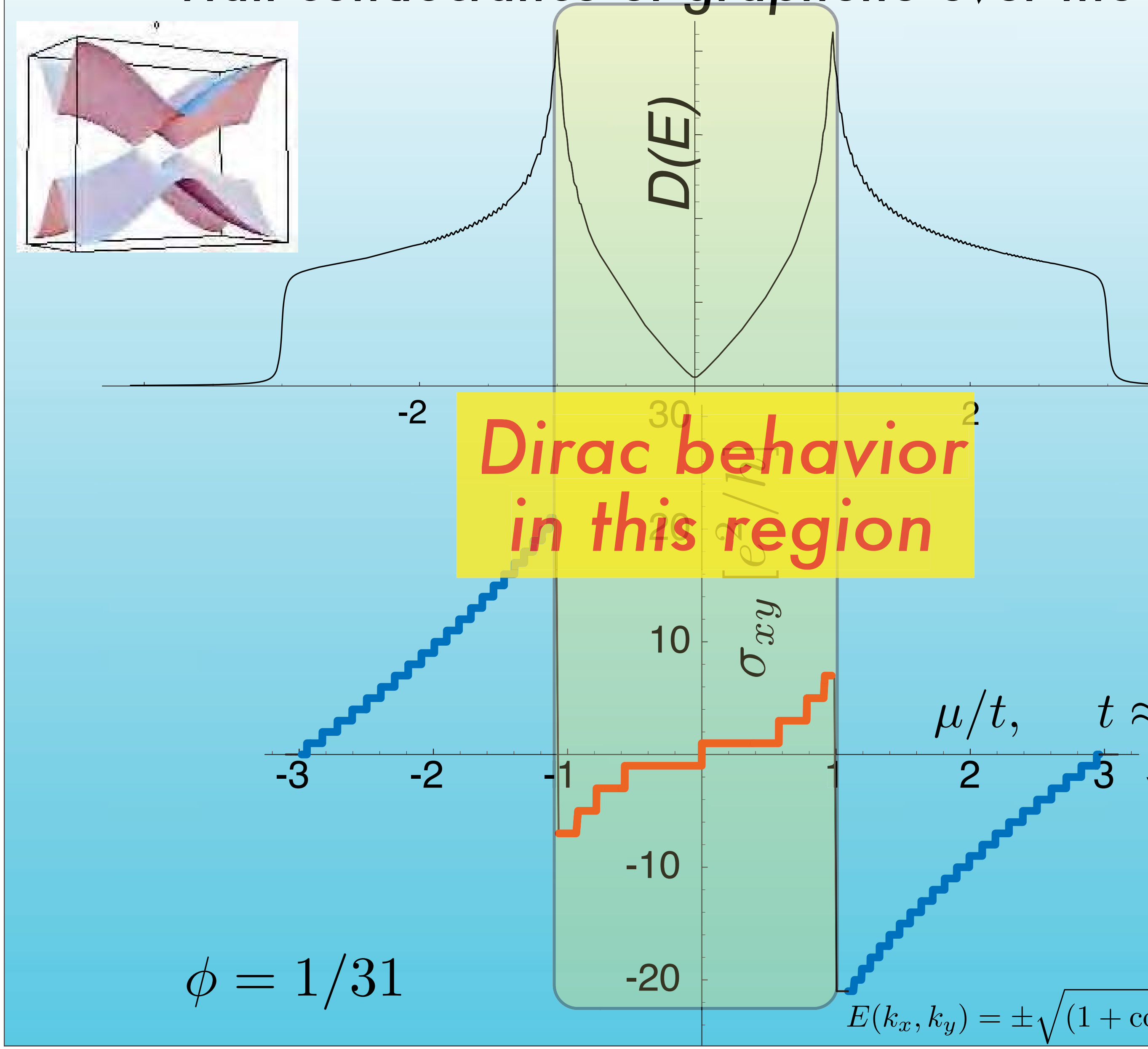
Gusynin-Sharapov, 2005

Peres-Guinea-Neto 2006

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

Hall Conductace vs chemical potential

☆ Hall conductance of graphene over the whole spectrum



$\mu/t, \quad t \approx 1[\mathrm{eV}]$ for graphene

YH, T. Fukui & H. Aoki, '06

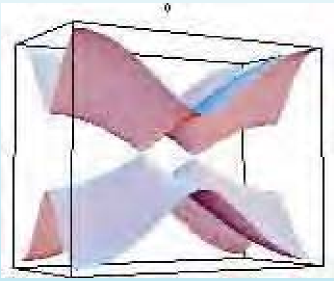
Zheng-Ando 2002
Gusynin-Sharapov, 2005
Peres-Guinea-Neto 2006

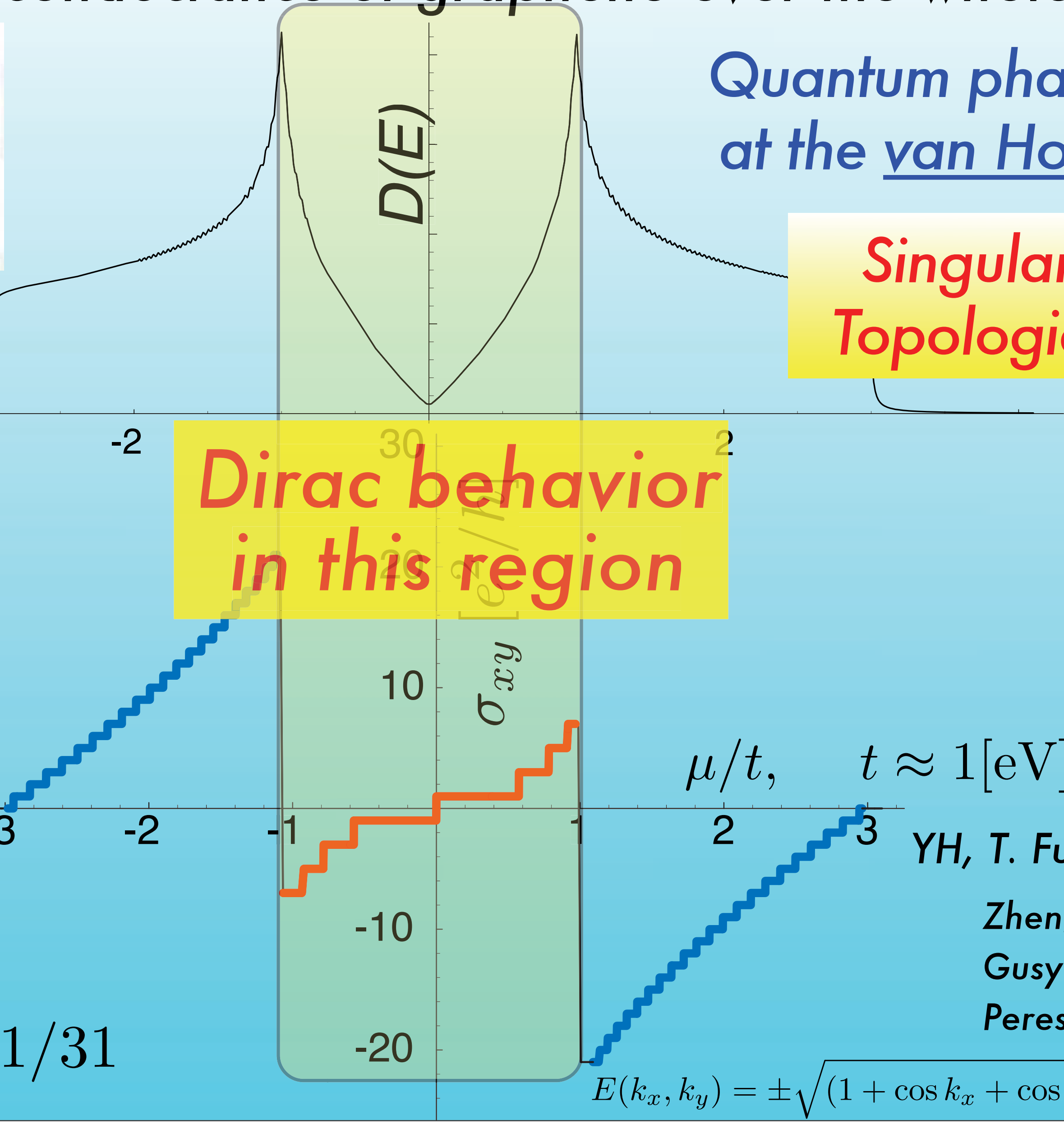
$\phi = 1/31$

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

Hall Conductace vs chemical potential

☆ Hall conductance of graphene over the whole spectrum





Quantum phase transition at the van Hove Energies

Singularity breaks Topological Stability

$\mu/t, \quad t \approx 1[\mathrm{eV}]$ for graphene

YH, T. Fukui & H. Aoki, ‘06

Zheng-Ando 2002

Gusynin-Sharapov, 2005

Peres-Guinea-Neto 2006

$\phi = 1/31$

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

3 types of Edge states in Graphene

I. QH edge states in graphene

YH, T. Fukui & H. Aoki, '06

See also, L. Brey, H. A. Fertig, '06

Edge transport : D. A. Abanin, P. A. Lee, L. S. Levitov '07

II. Zero modes edge state without magnetic field

Fujita et al., '96

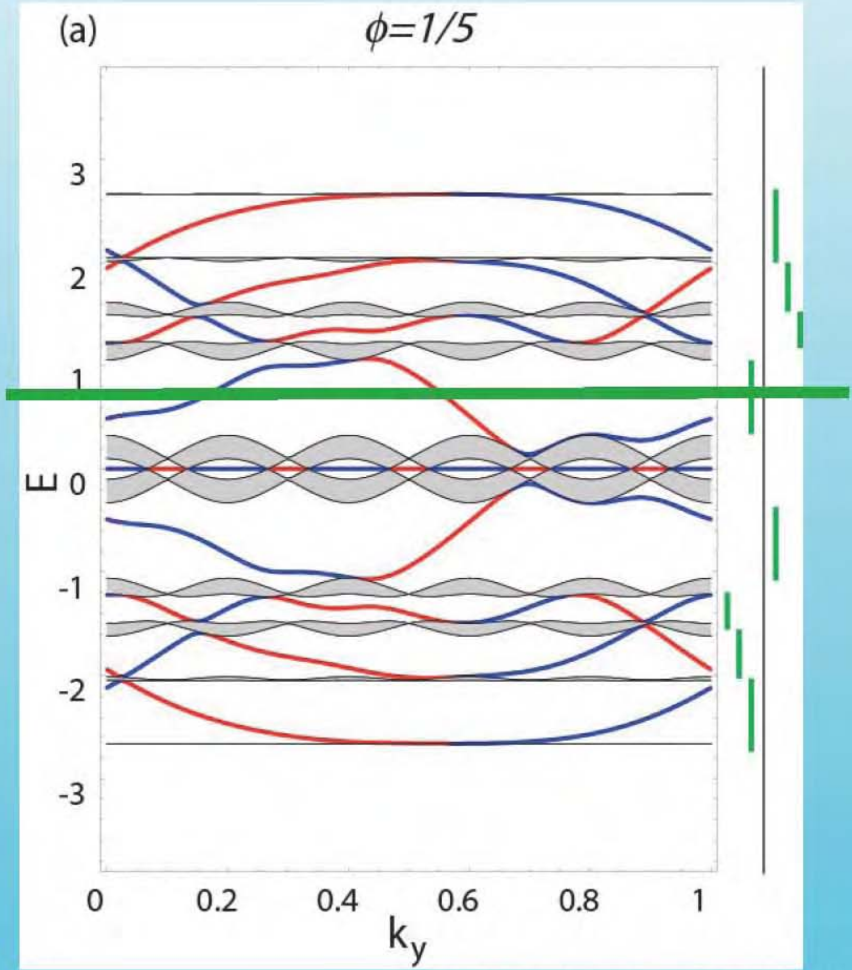
S. Ryu & YH, '02

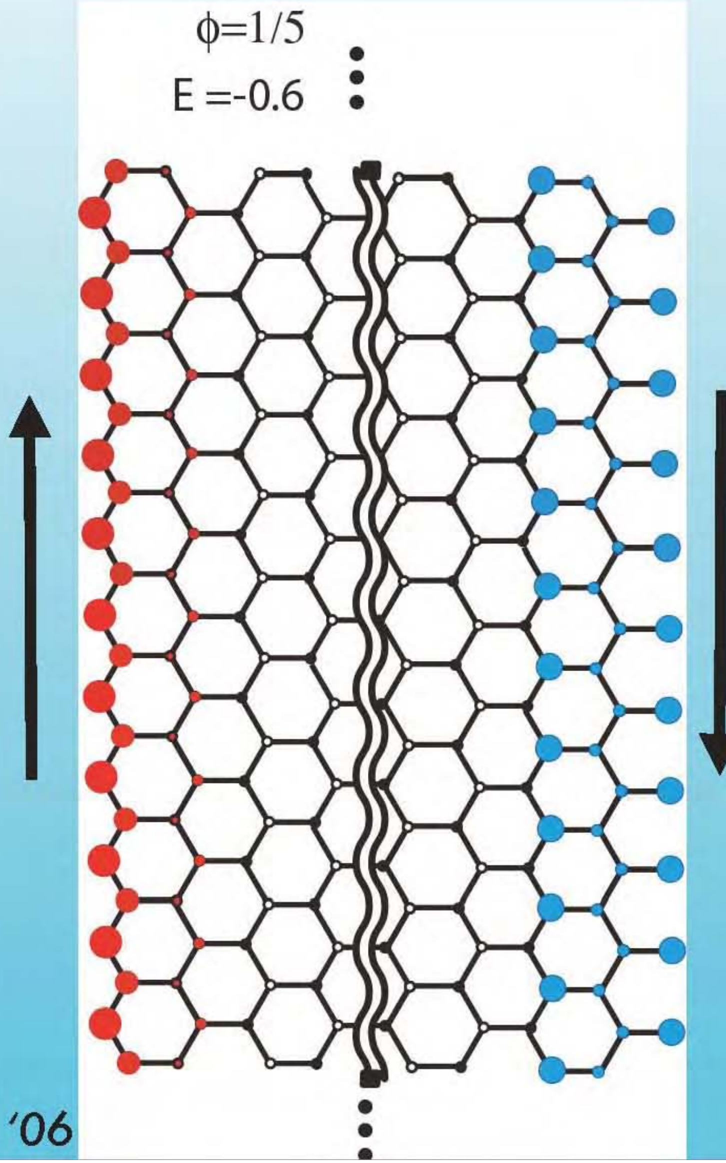
III. Zero modes with magnetic field

M. Arikawa, H. Aoki & YH *arXiv:0805.3240 & 0806.2429*

QH Edge States of Graphene

☆ *Edge States and their local charges : nothing special*





YH, T. Fukui & H. Aoki, '06

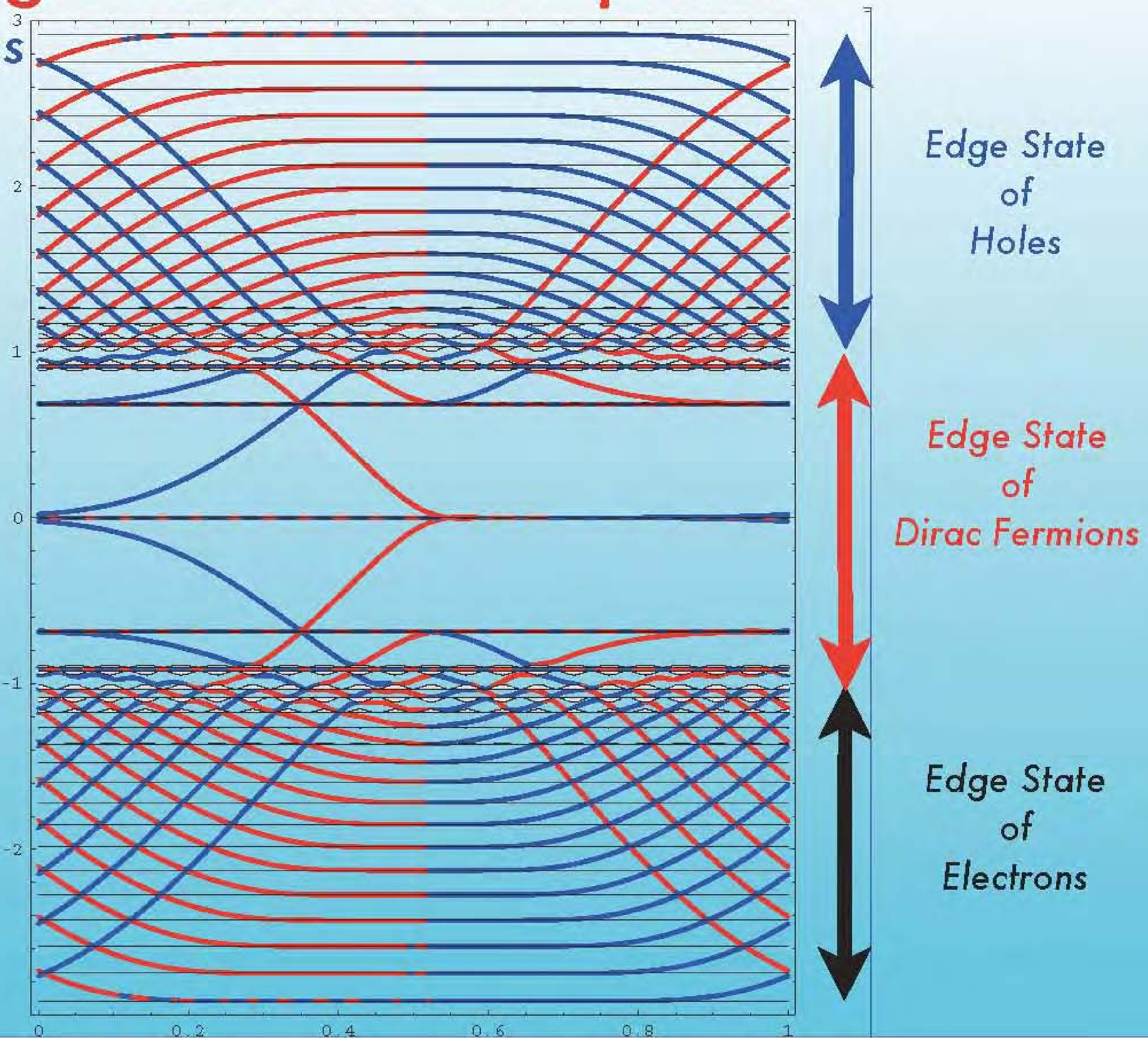
Edge States of Graphene

☆ Zigzag Edges

Full Spectrum

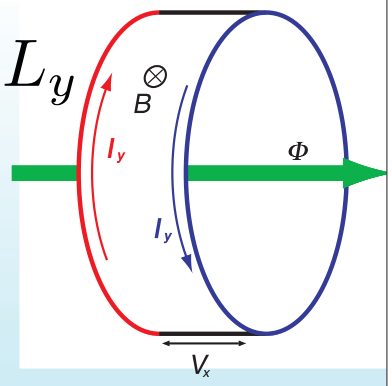
$$\phi = 1/21$$

Weak Field



Laughlin's Argument & Edge States

☆ Adiabatic Charge Transfer

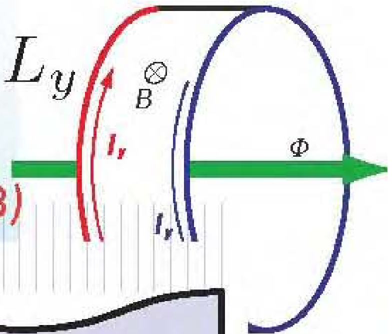


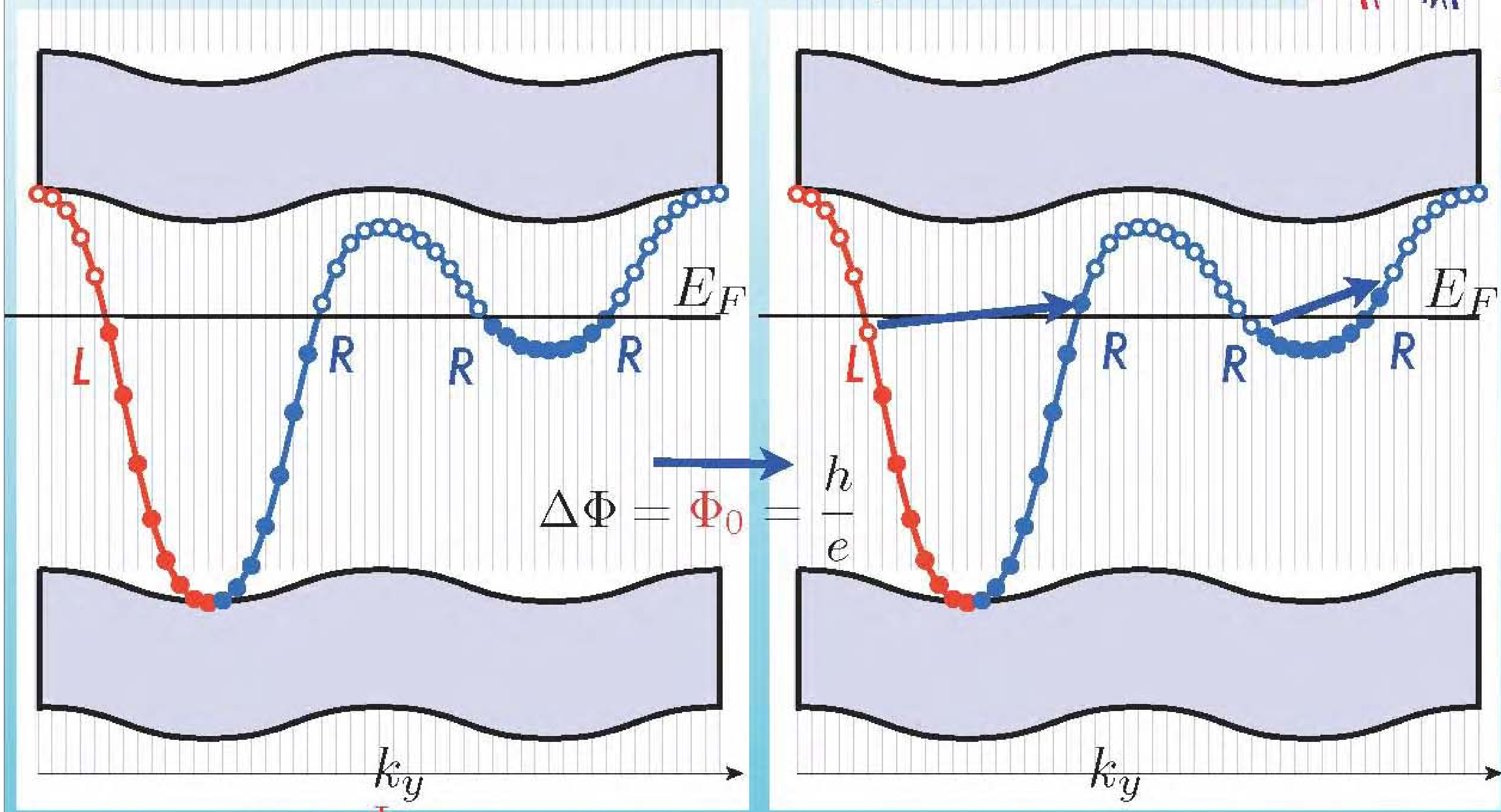
Edge States determine the Hall Conductance

Laughlin's Argument & Edge States

☆ Adiabatic Charge Transfer

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





$$k_y = 2\pi \frac{n + \frac{\Phi}{\Phi_0}}{L_y}, \; n: \text{ integers}$$

1 Electron is carried from the Left to the right in this case

$$\sigma_{xy} = \frac{e^2}{h} \cdot 1$$

Analytic Continuation of the Bloch State to the complex energy (Riemann surface)

$$C_j = I_j - I_{j-1}$$

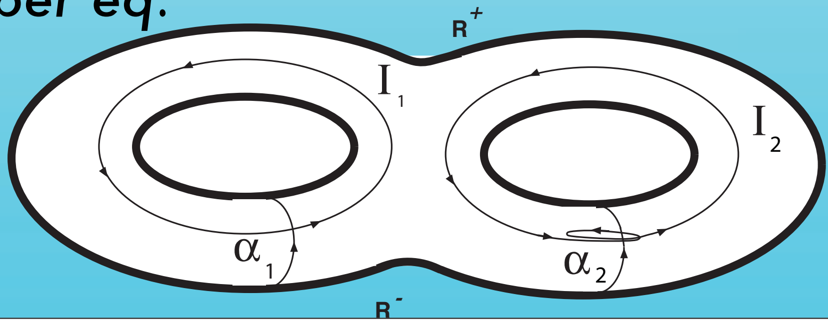
Chern # = winding # Difference between the neighboring gaps

Bulk-Edge Correspondence of the topological numbers

$$\boxed{\sigma_{xy}^{\text{bulk}} = \sigma_{xy}^{\text{edge}}}$$

$\phi = P/Q$

Complex Energy surface of Harper eq.



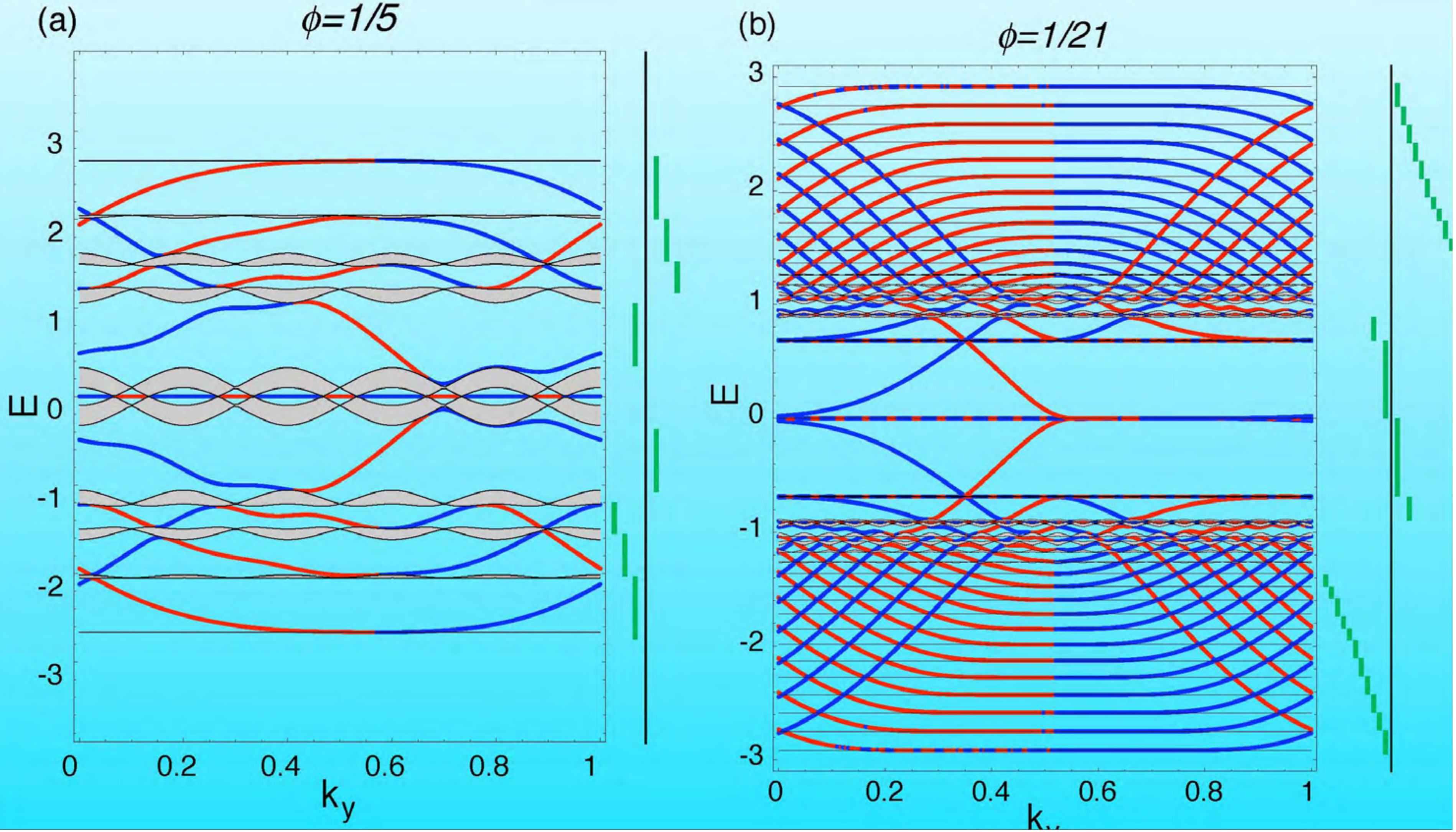
YH, T. Fukui & H. Aoki, '06

genus g=q – 1: number of the gaps

$$\phi = p/q$$

Bulk – Edge Correspondence

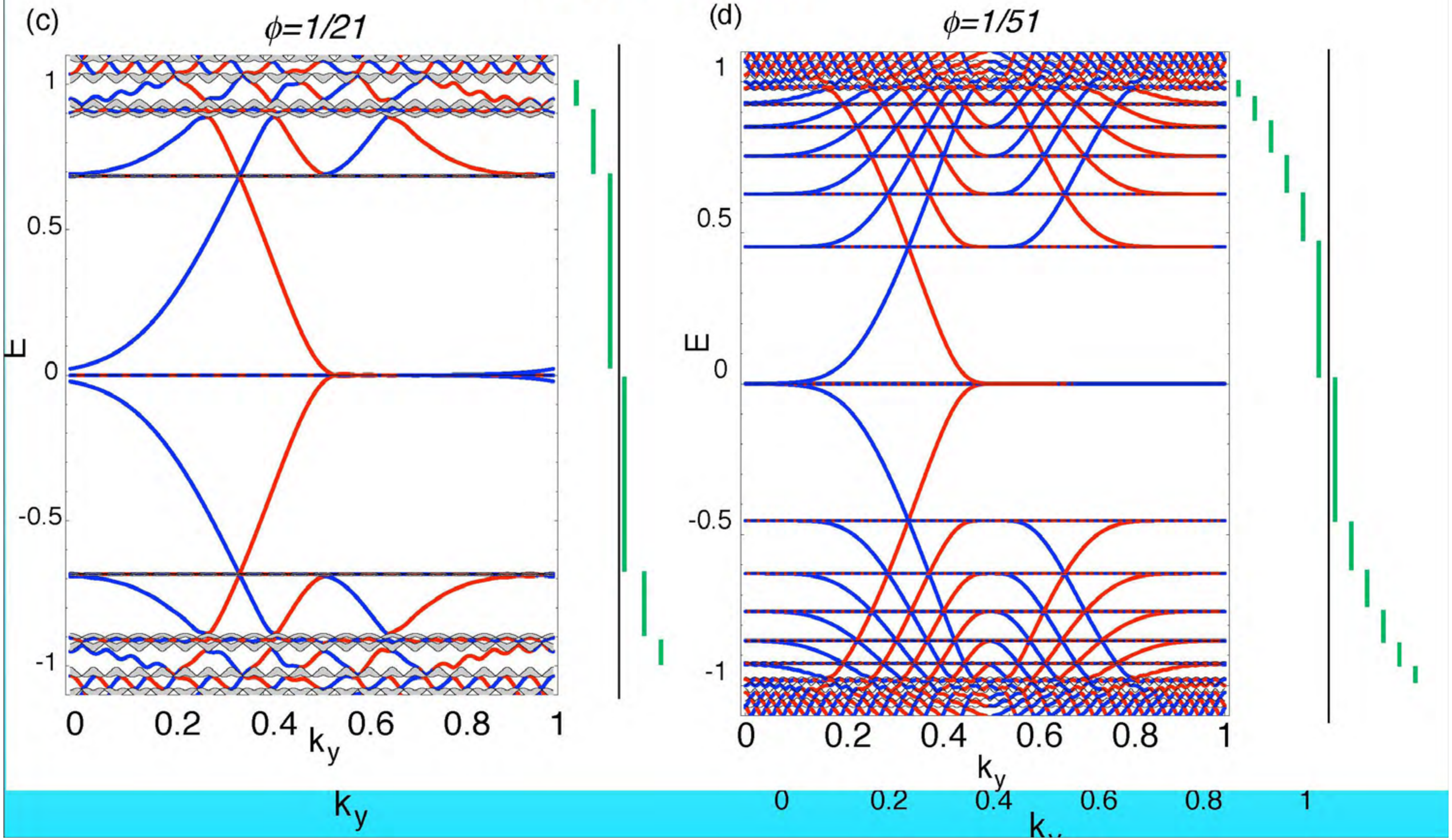
$$\sigma_{xy}^{\text{bulk}} = \sigma_{xy}^{\text{edge}}$$



Bulk – Edge Correspondence

$$\sigma_{xy}{}^{\text{bulk}} = \sigma_{xy}{}^{\text{edge}}$$

Near Zero



Another type of Edge states in Graphene

- ☆ Quantum Hall edge states
  - ☆ Topologically protected edge states
- ☆ Symmetry protected edge states: zero modes
  (topological origin & stability)

without magnetic field

Fujita et al. '96 : discovery

S. Ryu & YH '02 : topological reason

with magnetic field

M. Arikawa, H. Aoki & YH arXiv:0805.3240 & 0806.2429

New feature : topological compensation

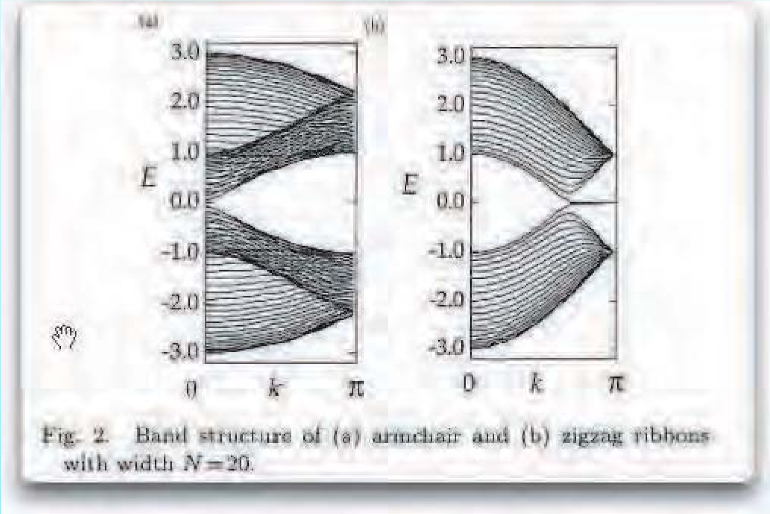
It can be observed by STM experiments under magnetic field

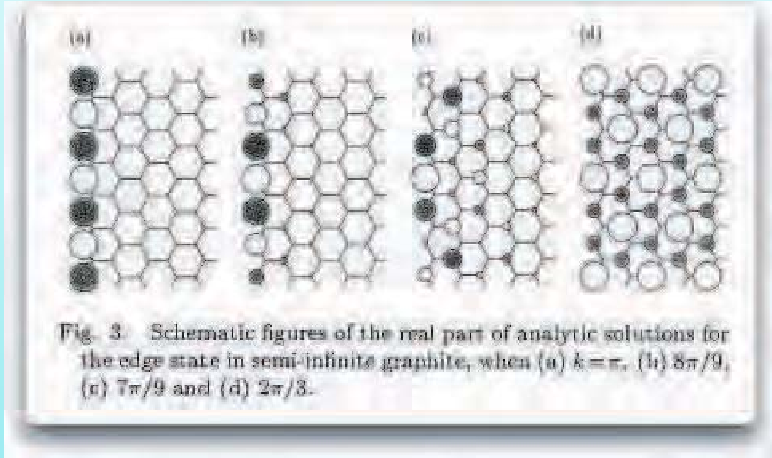
Without magnetic field

Localized Boundary State in Carbon Sheet (1)

now called as Graphene

Tight-binding Model Calculation





“ 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

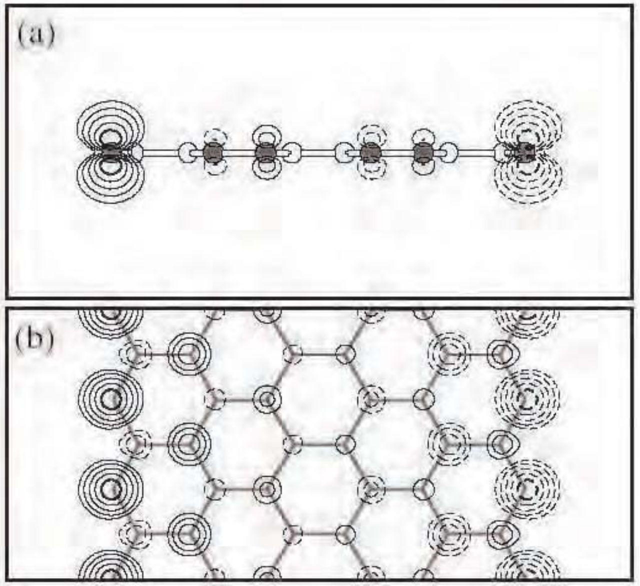


FIG. 1. Contour plots of spin density $n_{\uparrow}(r) - n_{\downarrow}(r)$ (a) on a plane perpendicular to a graphite flake with zigzag edges and (b) on a plane including the graphite flake. In (a) the edges are perpendicular to the plane and C atoms on the plane are depicted by shaded circles. Positive 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.

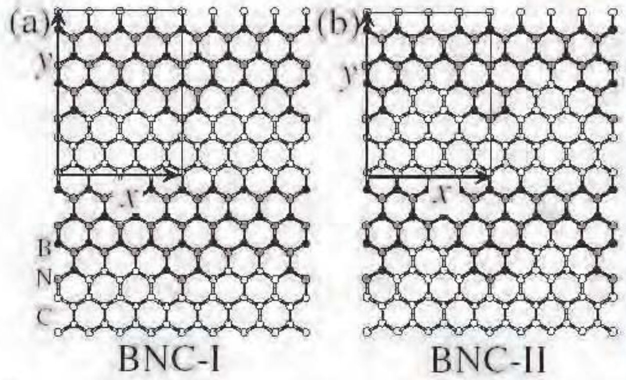


FIG. 2. Top views of fully optimized BNC heterosheets. (a) BNC-I and (b) BNC-II. White, shaded, and black circles denote C, B, and N atoms, respectively. The rectangle in each figure denotes the unit cell.

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 in Anisotropic Superconductivity

d-wave superconductivity

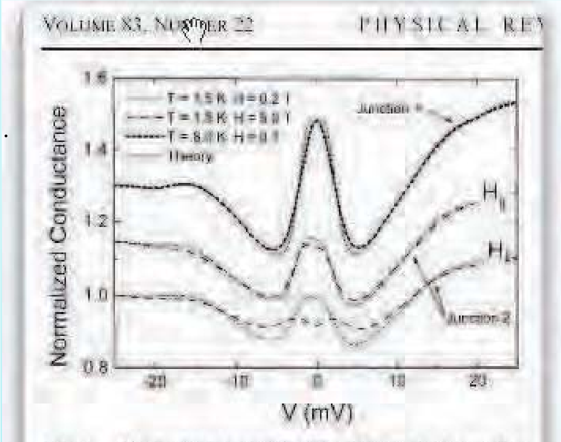


FIG. 1. The temperature dependence of the in-plane tunneling conductance of (110)-YBCO/Pb junctions as function of bias and magnetic field is shown. The field H is always applied parallel to the junction interface, and either parallel or perpendicular to the YBCO ab planes, as labeled. The theoretical curve (solid line) is calculated using the FRS theory [11], as described in the text. For junction 2, low-temperature 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_c of Pb is also shown for junction 1.

Zero Energy Boundary States of Anisotropic Superconductivity

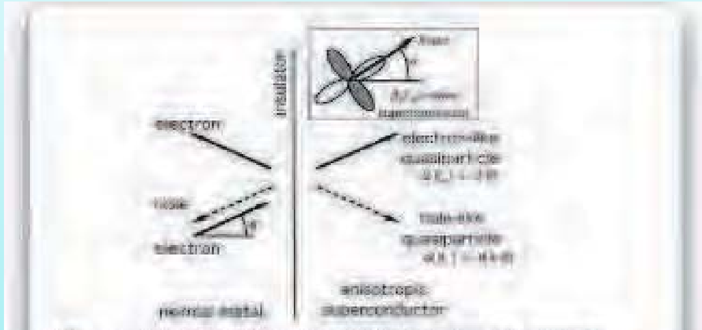


FIG. 1. Schematic illustration of the reflection and transmission processes at the interface. In this figure the quantities θ and α express the injection angle of the electron and the angle between the normal vector of the interface and the x axis of the $d_{x^2-y^2}$-wave superconductor, respectively.

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)

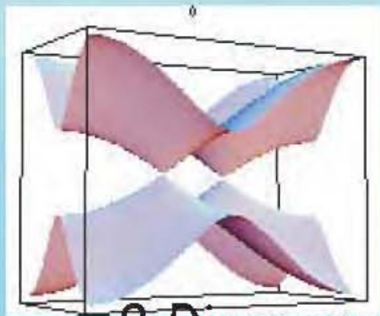
(fig.) M. Aprili, E. Badica, and L. H. Greene,Phys. Rev. Lett. 83, 4630 (1999)

Universality of Zero Energy Edge States

'02--'04 S. Ryu & YH

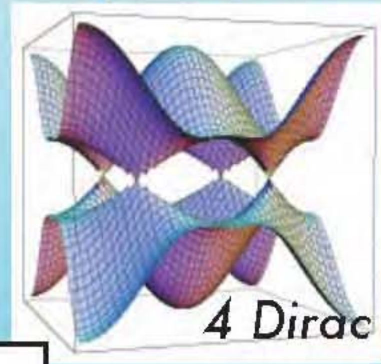
1. Zero energy edge states of graphene
   - Boundary Magnetic moments of graphene
2. Andreev bound states of d-wave superconductors
   - Zero bias conductance peak

graphene



2 Dirac cones

d-wave superconductor



4 Dirac cones

These 2 systems are topologically equivalent

Γ :Bipartite (A-B sublattice symmetry)

Symmetry protected Zero modes of Dirac fermions :1D Flat Band of edge states

Γ :Time Reversal (Real Order parameter)

$^{\exists}\Gamma$ chiral symmetry

$$\{\Gamma, H\} = \Gamma H + H\Gamma = 0\ ,\ \Gamma^2 = 1$$

Universality of Zero Energy Edge States

'02–'04 S. Ryu & YH

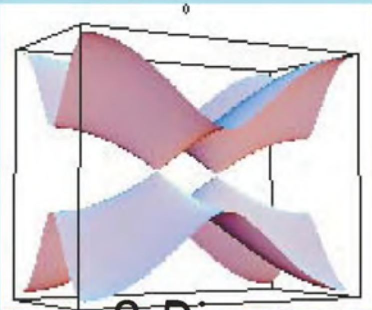
Boundary magnetic moments

Spontaneous breaking of these chiral symmetries : Peierls instabilities of Flat (edge) bands

Spontaneous local flux generation near defects

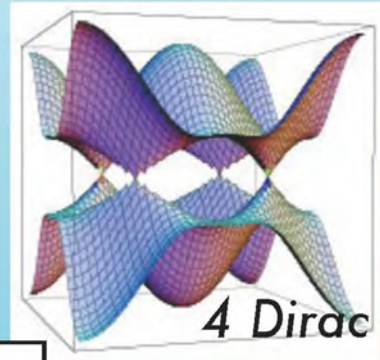
graphene

d-wave superconductor



2 Dirac cones

These 2 systems are topologically equivalent



4 Dirac cones

Γ :Bipartite

(A-B sublattice symmetry)

Symmetry protected
Zero modes of Dirac fermions
:1D Flat Band of edge states

Γ :Time Reversal

(Real Order parameter)

$^{\exists}\Gamma$ chiral symmetry

$$\{\Gamma, H\} = \Gamma H + H\Gamma = 0\ ,\ \Gamma^2 = 1$$

When the zero modes exist (1D) ?

Lattice analogue of
Witten's SUSY QM

S.Ryu & Y.Hatsugai, Phys. Rev. Lett. 89, 077002 (2002)
Y.Hatsugai., J. Phys. Soc. Jpn. 75 123601 (2006)
Kuge, Maruyama, Y. Hatsugai, arXiv:0802.2425

Edge states <u>with</u> boundaries
Determined by the Berry phase of the bulk (<u>without</u> boundaries)

Zak $\gamma = \int A = \int d\vec{k} \cdot \vec{A}$ $\quad \vec{A} = \langle \psi(k) | \vec{\nabla}_k \psi(k) \rangle$

Require Local Chiral Symmetry
(ex. bipartite)
$\{\Gamma, H\} = \Gamma H + H\Gamma = 0$

Quantized
$$\gamma = \int A = \begin{cases} \pi \\ 0 \end{cases}$$

$\boxed{\gamma = \pi}$ $\Rightarrow$ **Zero energy localized states EXIST**

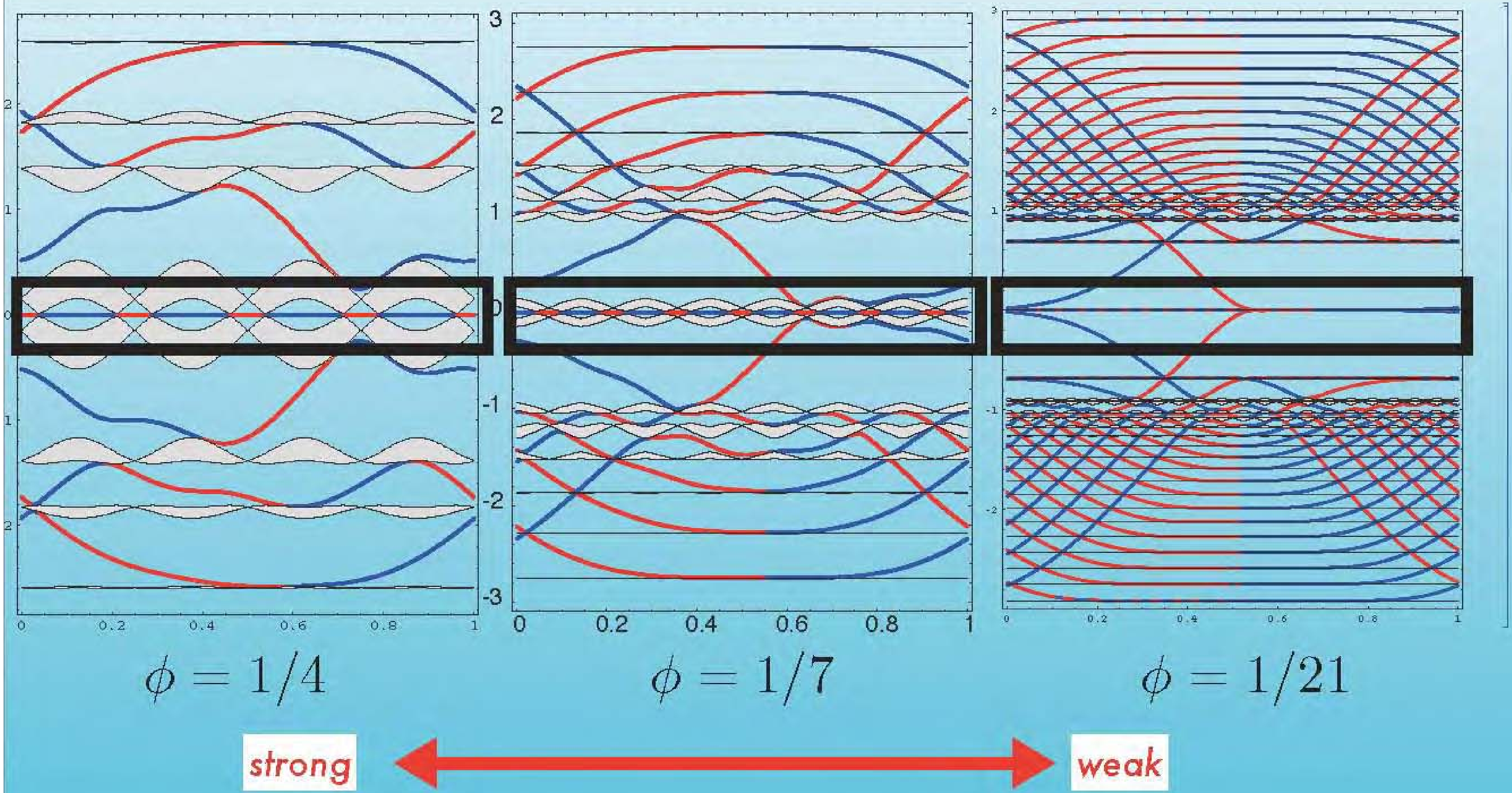
: There exists odd number of zero modes

Bulk-edge correspondence: "Bulk determines the edges"

With magnetic field

Close look at E=0

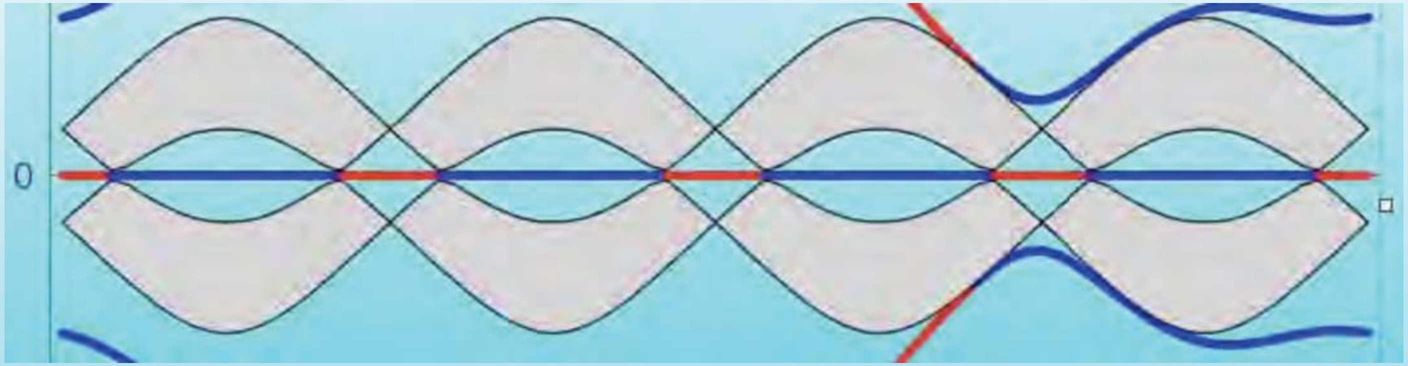
☆ *n=0 Landau Level*



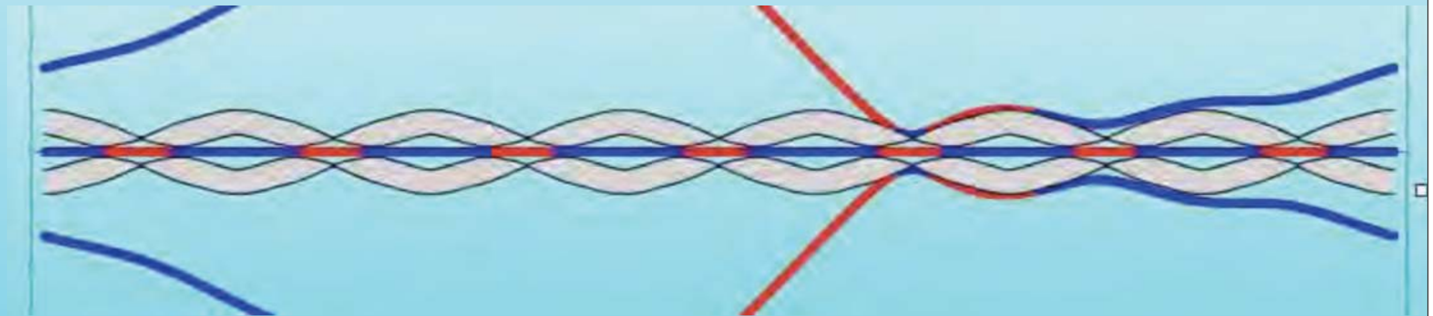
Close look at E=0

☆ *n=0 Landau Level*

$\phi = 1/4$



$\phi = 1/7$

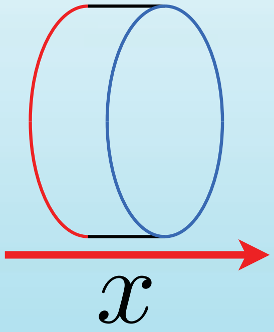


$\phi = 1/21$

Bulk Landau Level and the zero mode edge states coexist

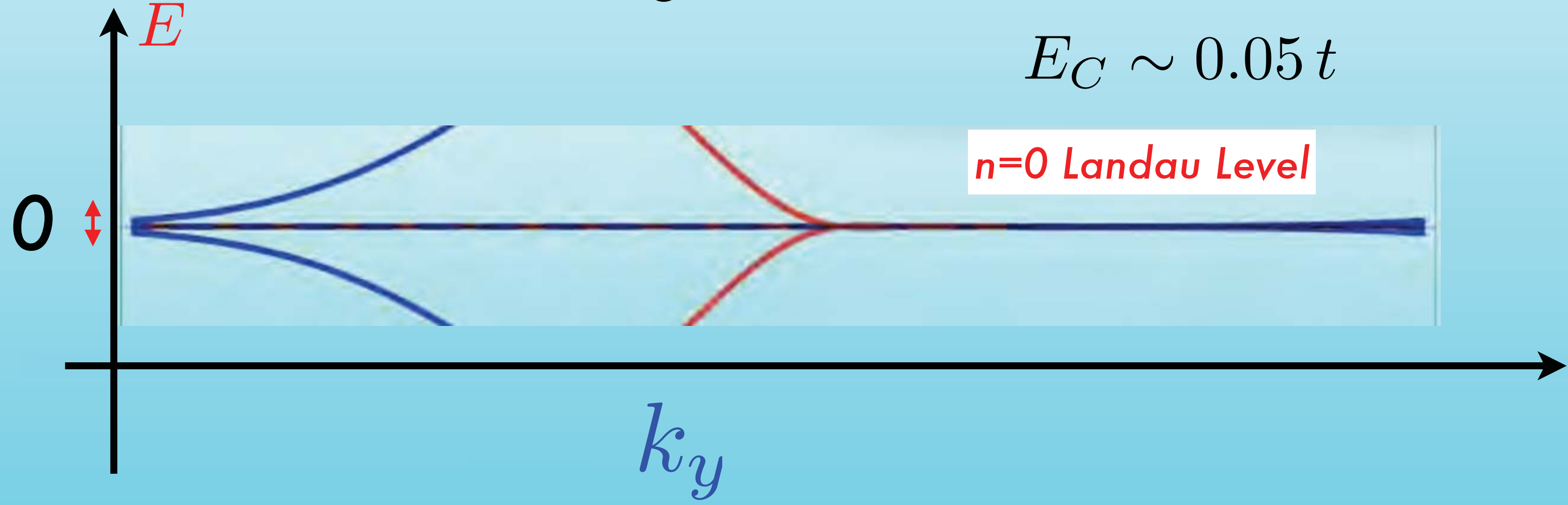
Charge density around E=0

Integrated local density of state over the n=0 LL



$$I(x) = \frac{1}{2\pi}\int_{-E_C}^{E_C} dE \int_{-\pi}^{\pi} dk_y \, |\Psi(x, k_y, E)|^2$$

$E_C \sim 0.05\,t$

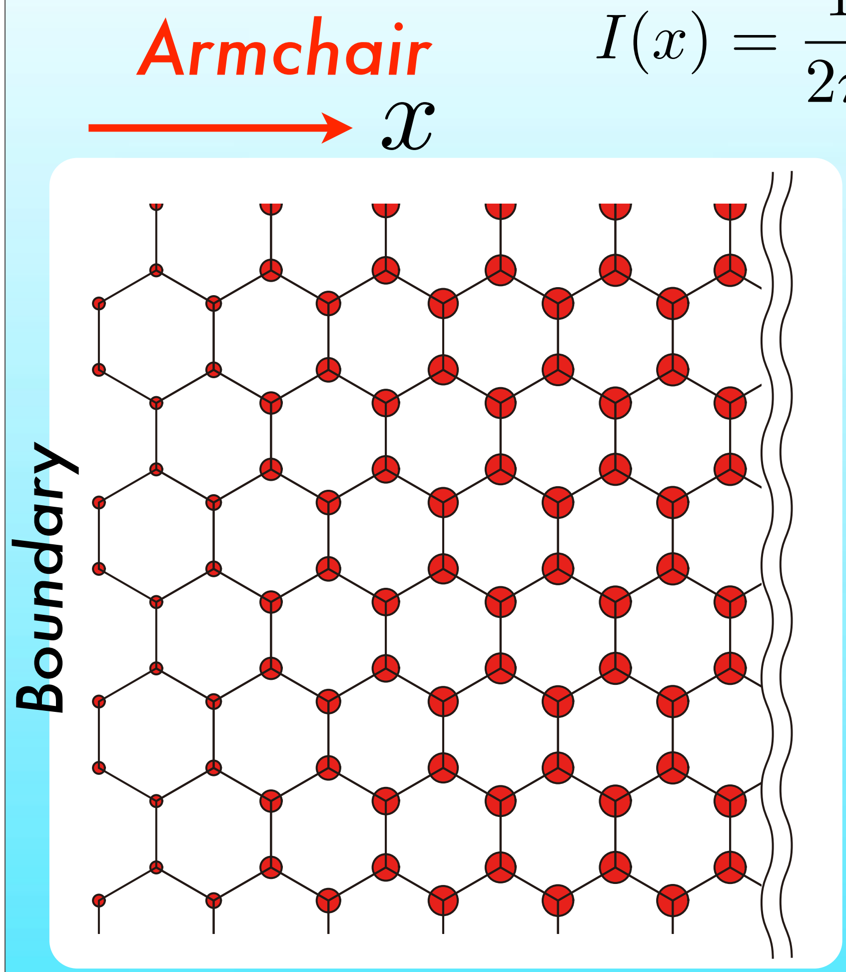


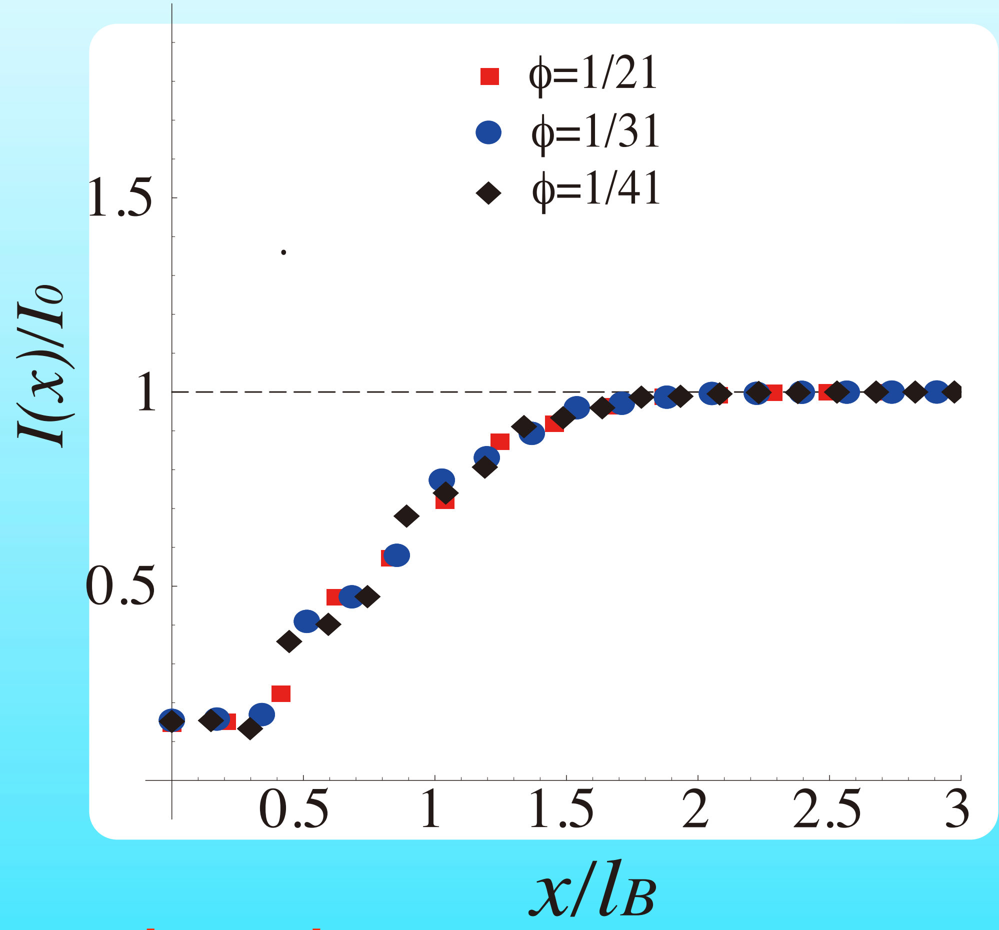
This can be observed by the STM image

M. Arikawa, H. Aoki & YH arXiv:0805.3240 & 0806.2429

LDOS around E=0 with Landau Level

$$I(x) = \frac{1}{2\pi}\int_{-E_C}^{E_C} dE \int_{-\pi}^{\pi} dk_y \, |\Psi(x, k_y, E)|^2$$





Suppression near the edge

Standard behavior due to edge potential

LDOS around E=0 with Landau Level

$$I(x) = \frac{1}{2\pi}\int_{-E_C}^{E_C} dE \int_{-\pi}^{\pi} dk_y \, |\Psi(x, k_y, E)|^2$$

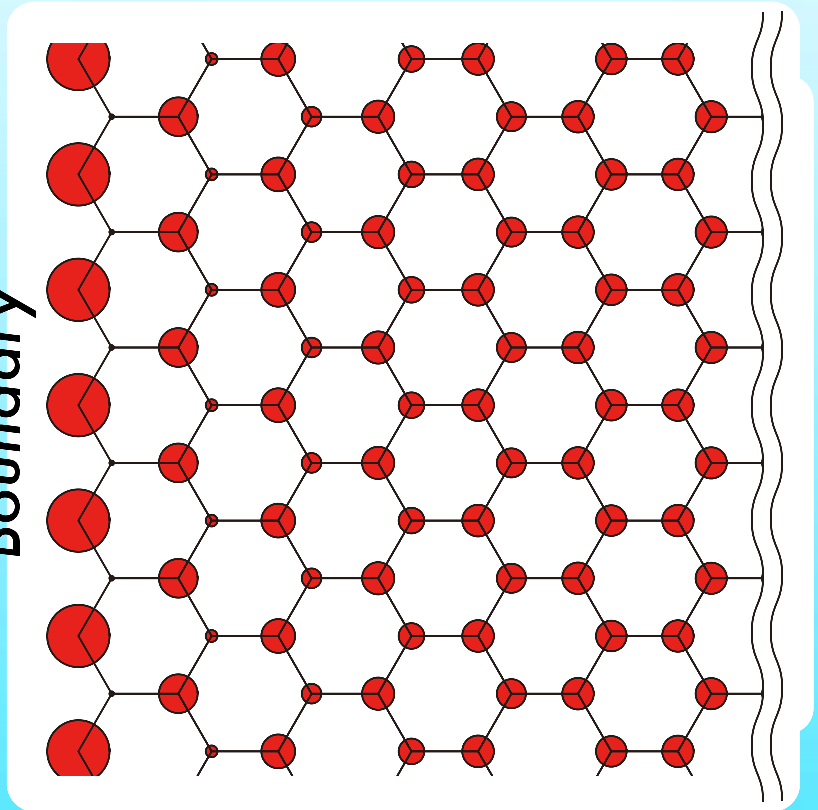
M. Arikawa, H. Aoki & YH

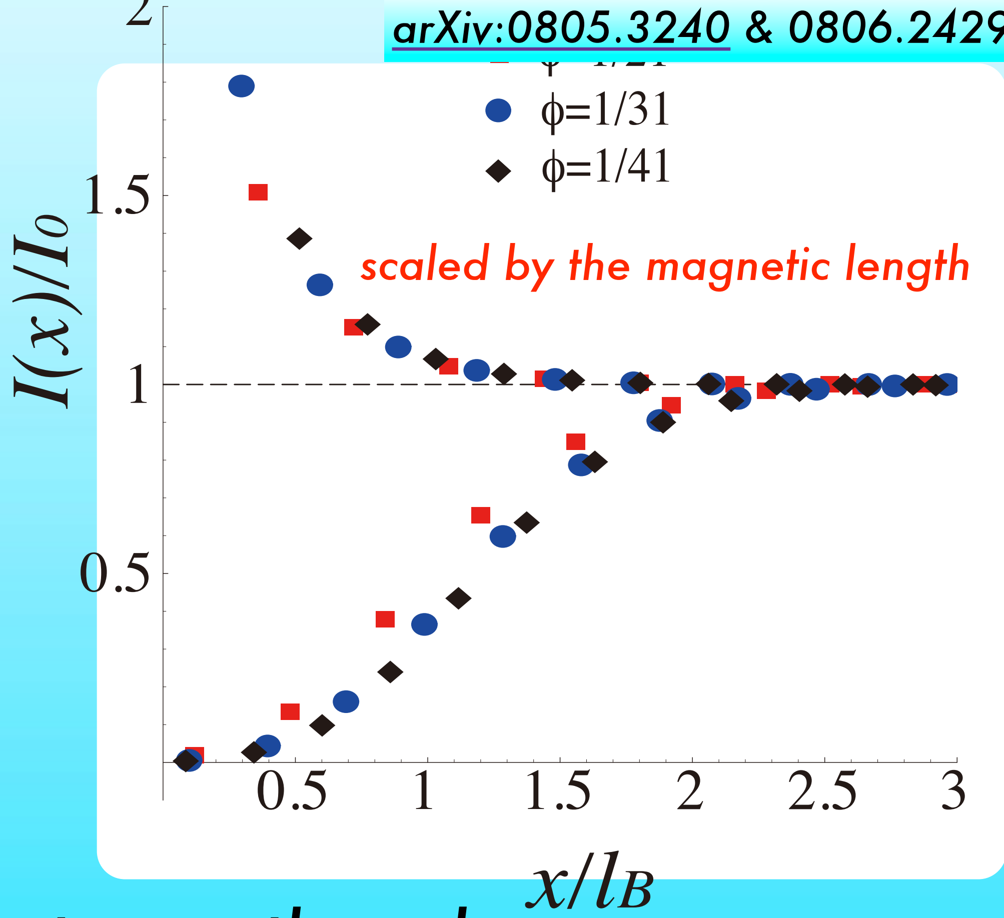
arXiv:0805.3240 & 0806.2429

Zigzag

x

Boundary





STM observable

Strong enhancement near the edge

Characteristic feature of the Graphene Zigzag edges!

Zero mode contribution ?

Not exactly true !

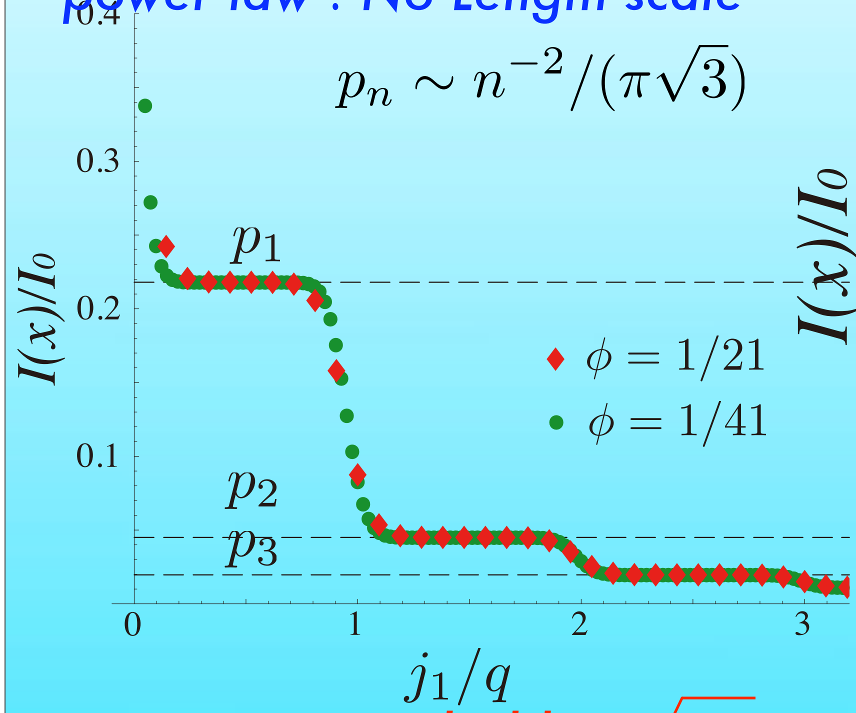
Topological Compensation by the Bulk !

Topological Compensation by Bulk

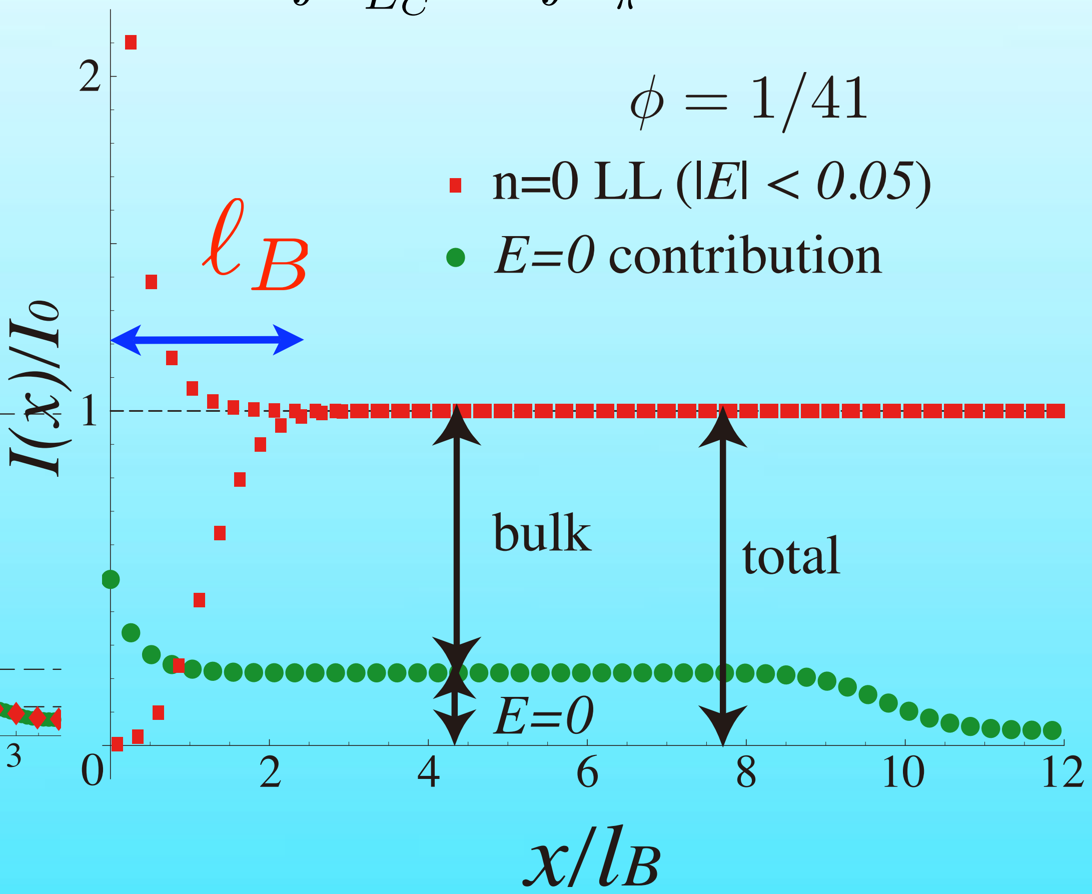
Only the Zero mode

$$I(x) = \frac{1}{2\pi}\int_{-E_C}^{E_C} dE \int_{-\pi}^{\pi} dk_y \,|\Psi(x,k_y,E)|^2$$

power law : No Length scale



scaled by $\sqrt{\ell_B}$



Bulk does give substantial contribution

Characteristic feature of the Graphene Zigzag edges!

Possible quantum liquid in Graphene

many body effects

edge states as basic objects to condense

edge states as 2D analogue of the solitons in 1D

Y. Hatsugai, T. Fukui, H. Aoki,
"Topological low-energy modes in N=,0 Landau levels of graphene: a possibility of a quantum-liquid ground state", arXiv:0804.4762, Physica E 40, 1530 (2008).

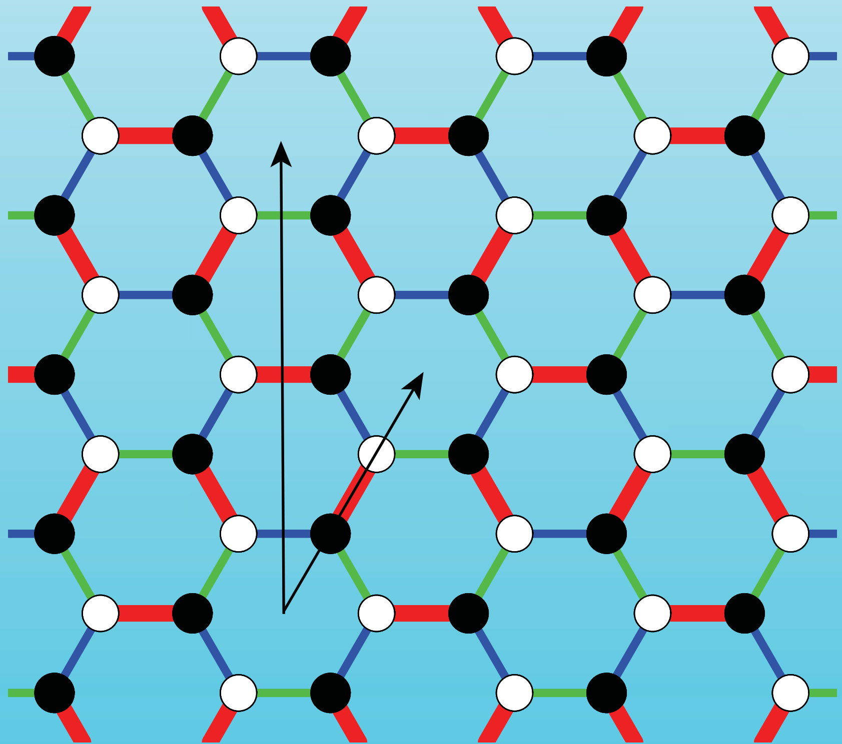
Can the E=0 Landau level be split in graphene??

A possible candidate = Bond-ordering

bond-order parameter! $\langle c_a^\dagger c_b \rangle$

Affleck-Marston '88
Voit '92
Nakamura '99

- Origin ? (with Magnetic field)
  - Electron-Electron interaction
  - (Jahn-Teller?)



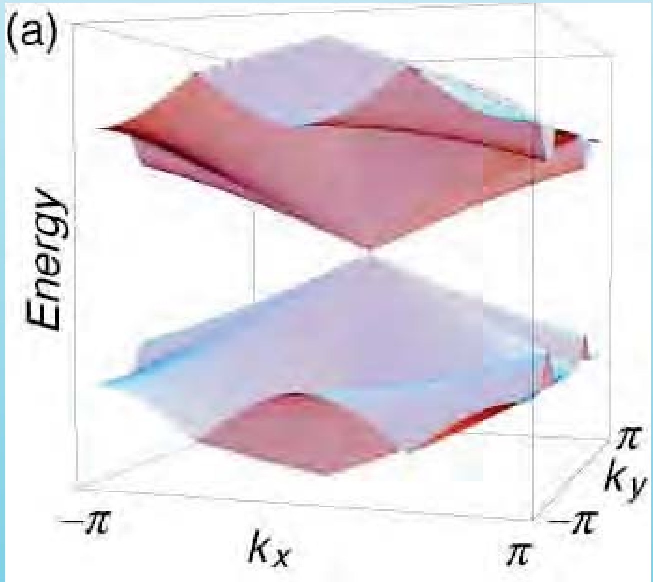
- Breaking the equivalence among 3 kinds of bonds in a Kekule pattern

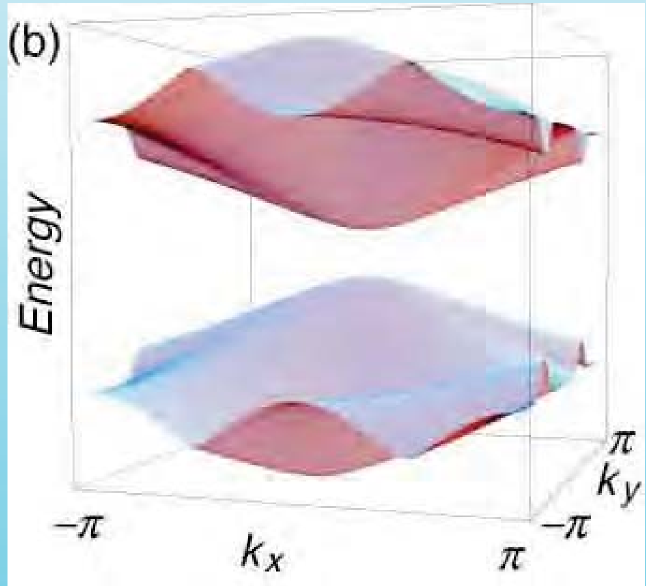
- Preserve Chiral Symmetry
- Three Fold Degeneracy
- Local Kekule pattern
- Enlarged unit cell (3times)

Energy Dispersion (without Magnetic Field)

- Enlarged Unit cell
- Chiral Symmetry is preserved
- Dirac Fermions get masses
  - The energy gap opens up

With bond-ordering





Particle-Hole Symmetric

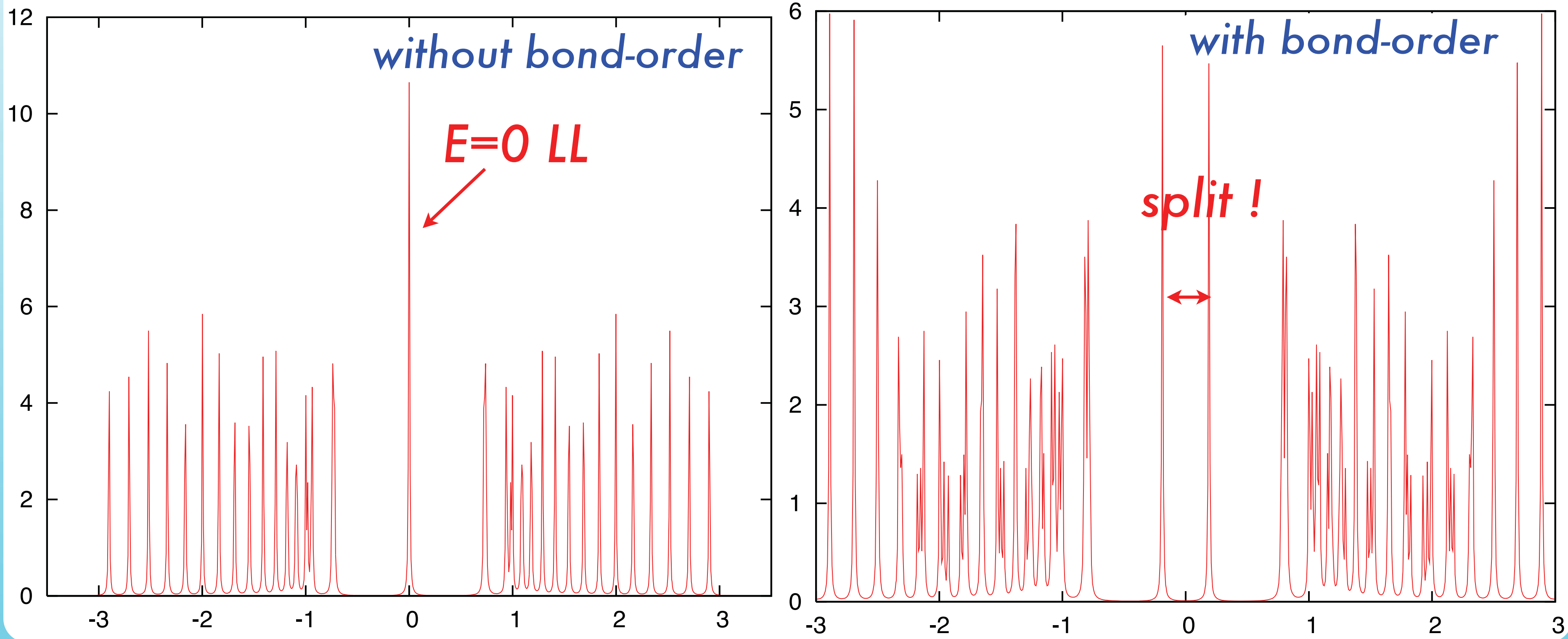
$$E(\boldsymbol{k}) \approx \pm|\det \boldsymbol{D}(\boldsymbol{k})|$$ (small gap & near E=0)

$$\boldsymbol{D} = \begin{pmatrix} t_R e^{-i(2k_1-k_2))} & t_G & t_B \\ t_B & t_R e^{-i(-k_1+k_2))} & t_G \\ t_G & t_B & t_R e^{ik_1} \end{pmatrix}$$

Landau level Structures with bond-orders

☆ Characteristic E=0 Landau Level of the Dirac Fermion splits !

One particle Density of states



<u>Bond-Order Formaion</u> *(in a mean field level)*

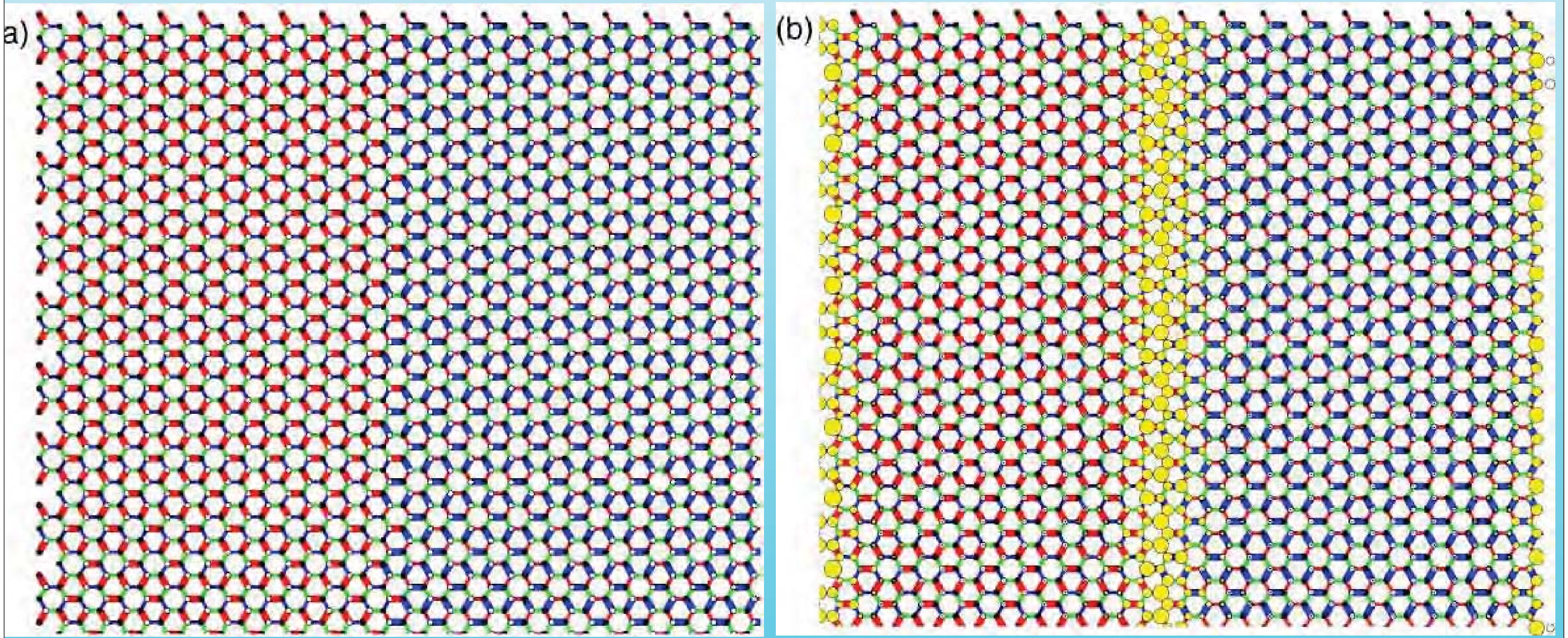
Peierls Instability of the Flat band as of the E=0 Landau Level

Bond-Ordering with Domains (Strip domain)

- ☆Straight line domain boundaries
  - ☆A possible snap shot configuration of the dynamical bond-order

Domain shape (strip)

Charge Density of the in-gap states

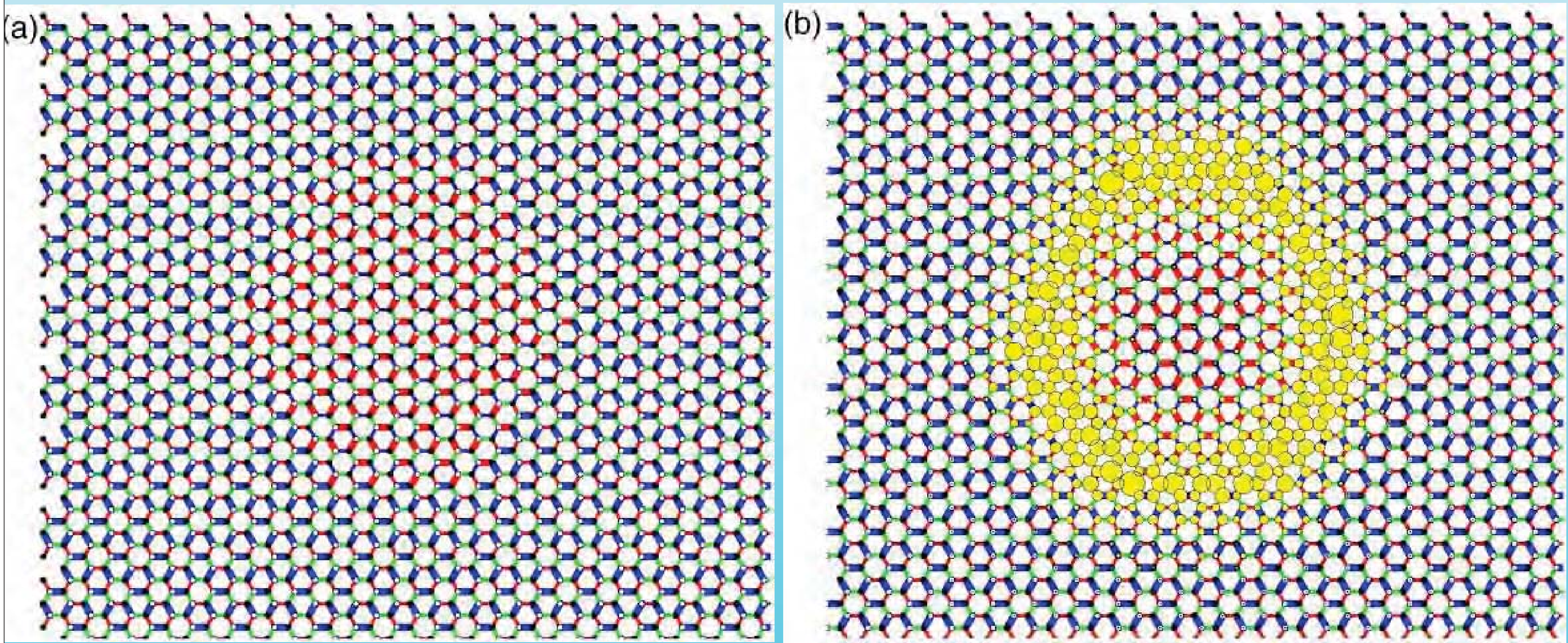


Bond-Ordering with Domains (circular domain)

- Closed loop domain boundaries
  - A possible snap shot configuration of the dynamical bond-order

Domain shape (closed loop)

Charge Density of the in-gap states

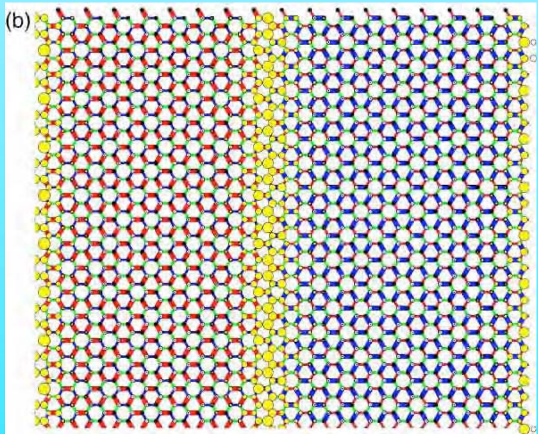


True ground state of graphene
with interaction

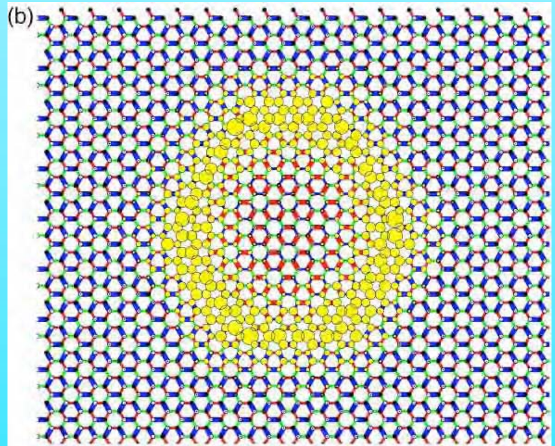
edge states as 2D analogue of the solitons in 1D

edge states as basic objects to condense

Quantum liquid
by the condensation of the edge states?

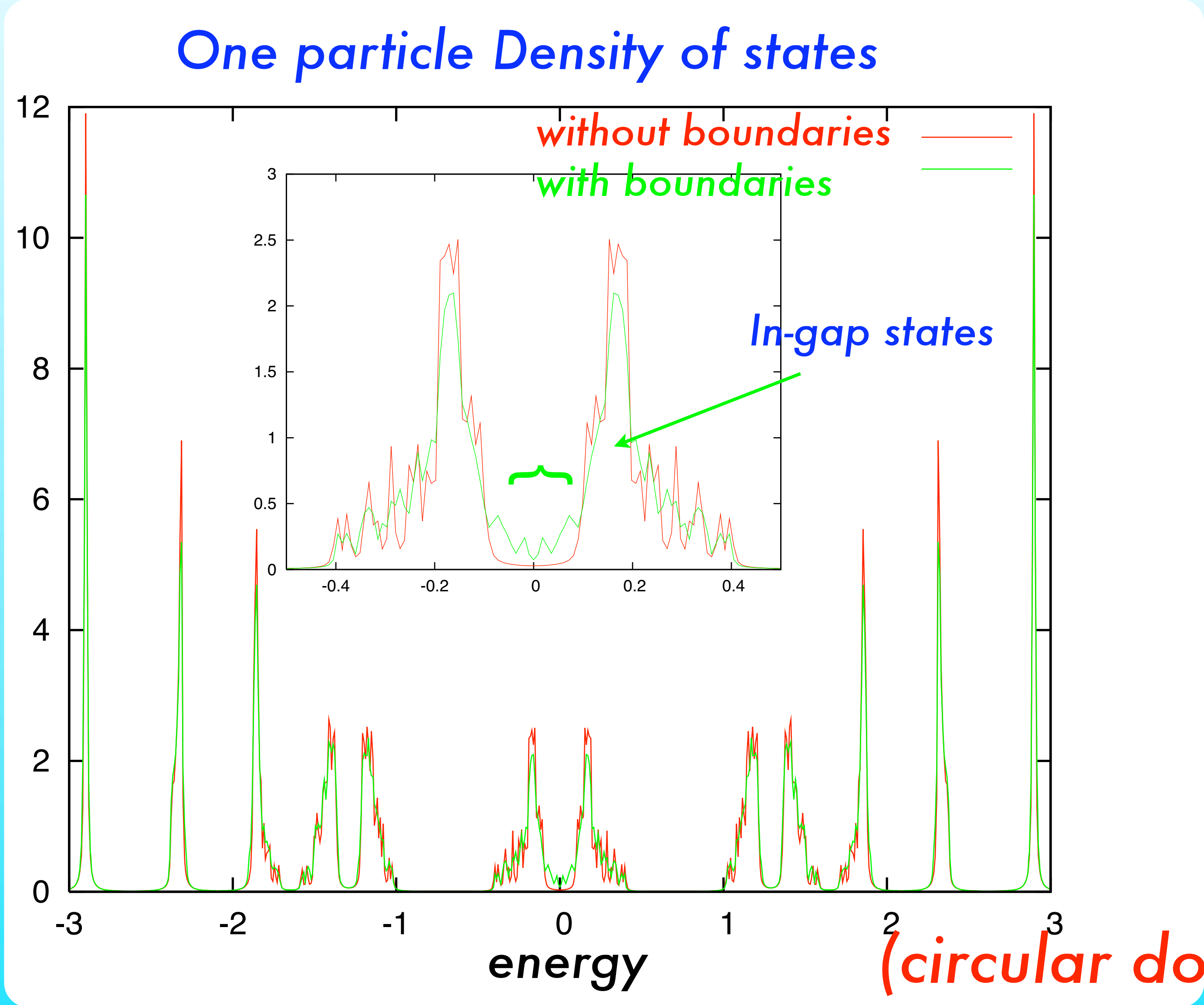


Snapshots ?



Y. Hatsugai, T. Fukui, H. Aoki, arXiv:0804.4762, Physica E 40, 1530 (2008).

In-gap states between the split E=0 Landau Level



(circular domain)

Summary

- Topological Aspects of Graphene
  - QHE by the Bulk
  - QHE by the edge
  - Bulk – Edge Correspondence
- Another Edge states of Graphene
  - without magnetic field
  - with magnetic field :
    Coexistence of the Bulk and edge states at E=0
    (STM observable)
- Possible quantum liquids with bond order
  - As a condensate of the loops by the edge states