Yukawa International Seminar 2007 (YKIS2007)

Interaction and Nanostructural Effects in Low-Dimensional Systems

Nov.5-30, 2007, Yukawa Institute for Theoretical Physics

Physics of graphene

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Purpose

Graphene

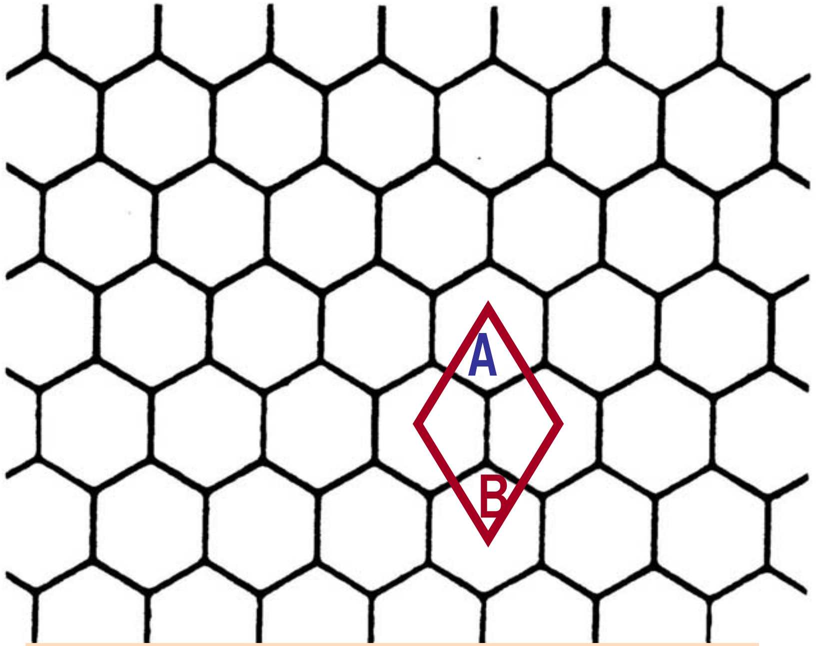
- atomically clean monolayer system
  with unusual (“massless Dirac”) dispersion
  Band structure, group theory

- anomalous integer QHE (one-body problem)
  topological quantum #
  bulk vs edge states

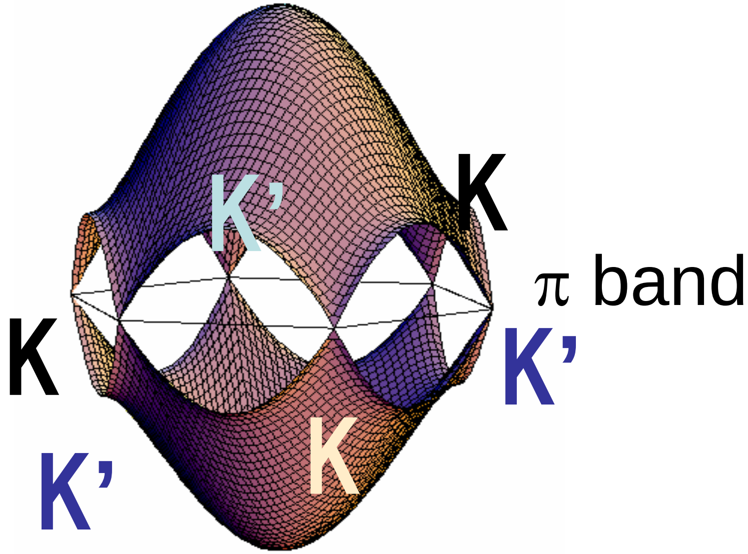
- Many-body states

Graphene – monolayer graphite

＊ Band structure: Wallece 1947
＊ Group theory: Lomer 1955

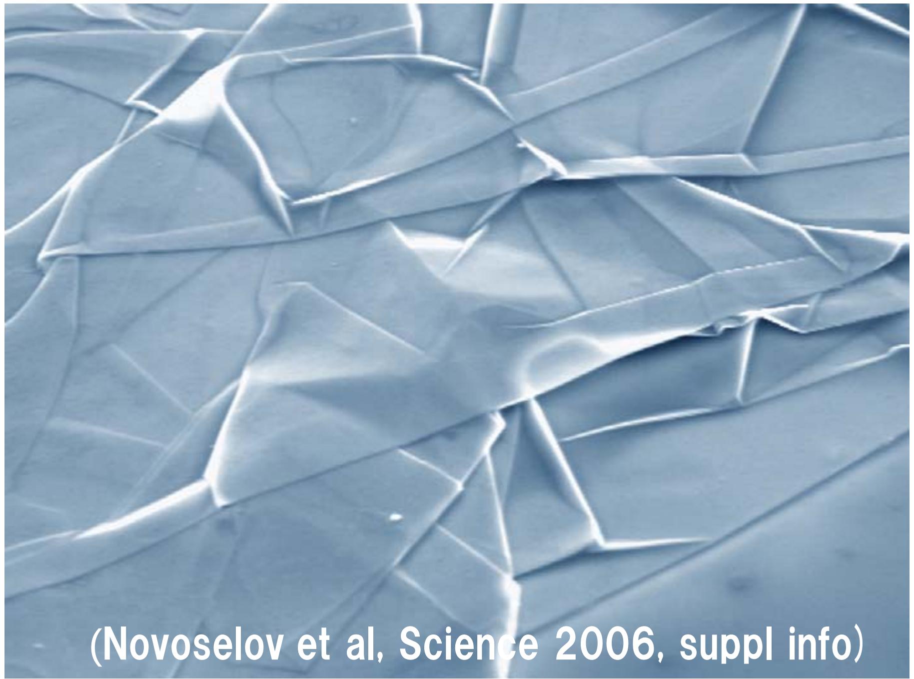


Honeycomb = Non-Bravais



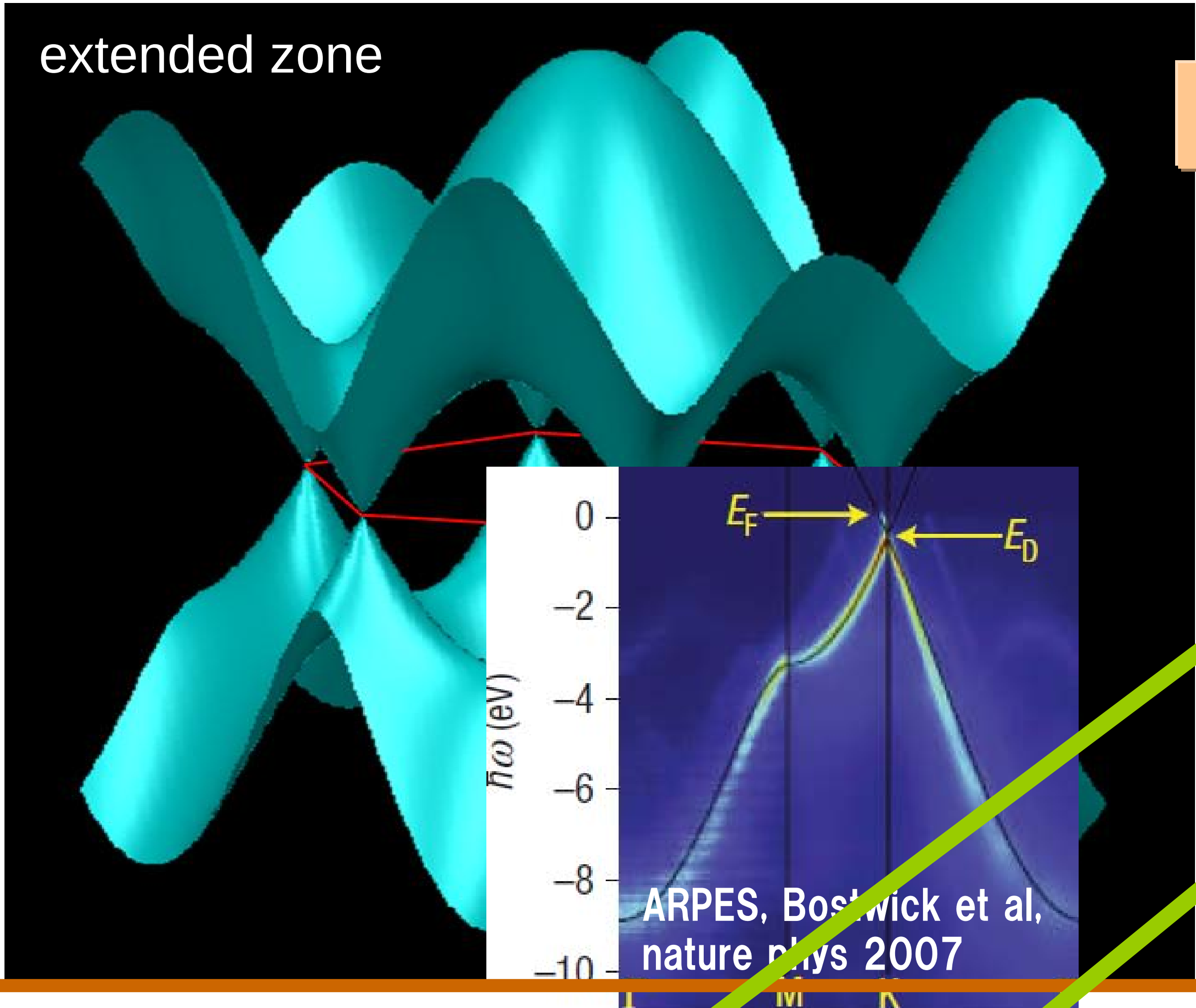
Mechanical exfoliation (Geim)
SiC decomposition (de Heer)
Benzene (Saiki)

(courtesy of Geim)

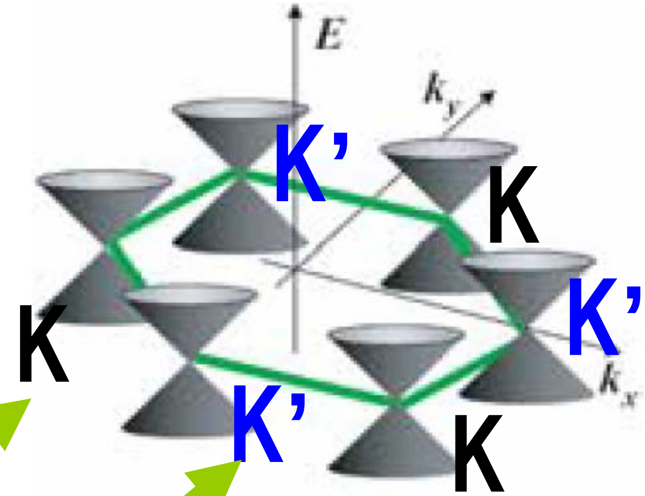


(Novoselov et al, Science 2006, suppl info)

Graphene's band dispersion



two massless Dirac points



T-reversal: K ⇔ K'

Effective-mass formalism

$$H_K = v_F(\sigma_x p_x + \sigma_y p_y) = v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

$$H_{K'} = v_F(-\sigma_x p_x + \sigma_y p_y) = v_F \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix}$$

Massless Dirac eqn for graphene

(Lomer, Proc Roy Soc 1955)

$$\begin{array}{cc}
 & \begin{array}{cc} \qquad\qquad \text{K} \qquad\qquad & \qquad\qquad \text{K}' \qquad\qquad \end{array} \\
\begin{array}{c} \text{K} \\ \\ \text{K}' \end{array} & \mathcal{H} = \dfrac{\gamma}{\hbar}\left(\begin{array}{cc|cc}
0 & \pi_x - i\pi_y & 0 & 0 \\
\pi_x + i\pi_y & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & \pi_x + i\pi_y \\
0 & 0 & \pi_x - i\pi_y & 0
\end{array}\right)
\end{array}$$

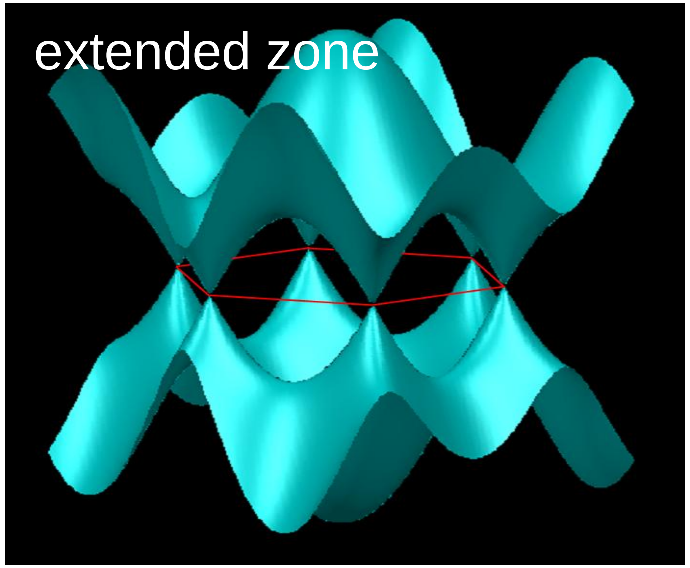
$$\hat{\boldsymbol{\pi}} = \hat{\mathbf{p}} + e\mathbf{A}/c$$

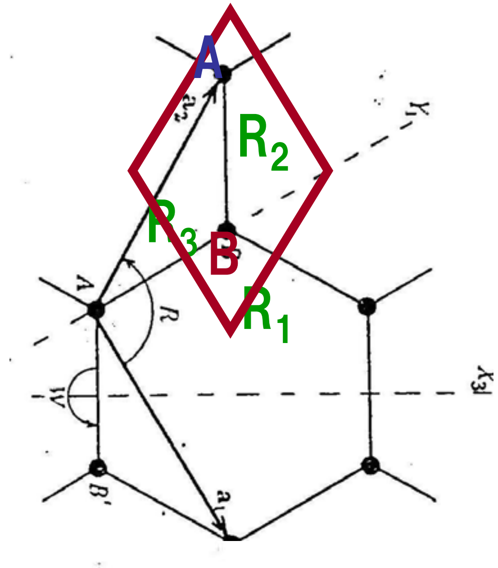
$$\mathbf{F}^{K}_{s\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{2L}}\exp(i\mathbf{k}\cdot\mathbf{r})\begin{pmatrix} s \\ e^{i\varphi(\mathbf{k})} \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{F}^{K'}_{s\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{2L}}\exp(i\mathbf{k}\cdot\mathbf{r})\begin{pmatrix} 0 \\ 0 \\ e^{i\varphi(\mathbf{k})} \\ s \end{pmatrix}$$

+ *B* [McClure, PR 104, 666 (1956)]

$$\mathbf{F}^{K}_{nk}(\mathbf{r}) = \frac{C_n}{\sqrt{L}}\exp(-iky)\begin{pmatrix} \mathrm{sgn}(n)\, i^{|n|-1}\phi_{|n|-1} \\ i^{|n|}\phi_{|n|} \\ 0 \\ 0 \end{pmatrix} \qquad \mathbf{F}^{K'}_{nk}(\mathbf{r}) = \frac{C_n}{\sqrt{L}}\exp(-iky)\begin{pmatrix} 0 \\ 0 \\ i^{|n|}\phi_{|n|} \\ \mathrm{sgn}(n)\, i^{|n|-1}\phi_{|n|-1} \end{pmatrix}$$

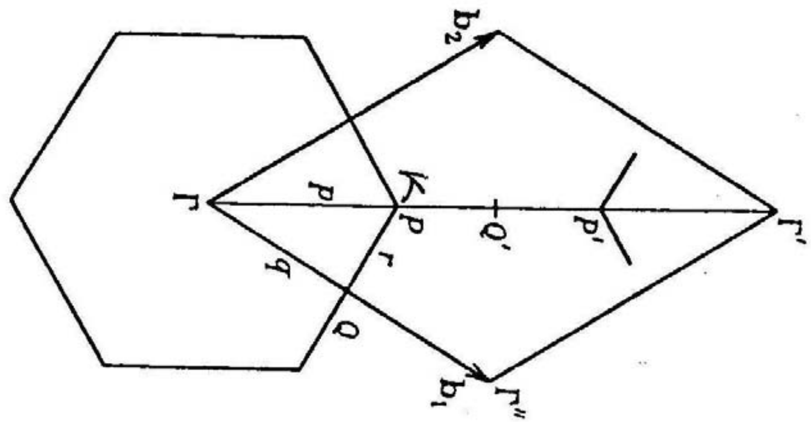
How does the massless Dirac appear on honeycomb (1)





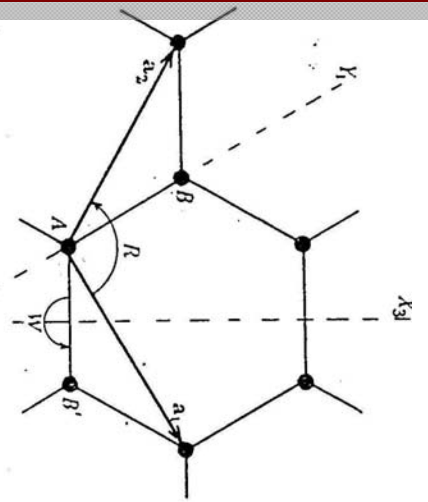
$$\mathcal{H}_{AB} = t(e^{i\vec{k}\cdot\vec{R}_1} + e^{i\vec{k}\cdot\vec{R}_2} + e^{i\vec{k}\cdot\vec{R}_3})$$

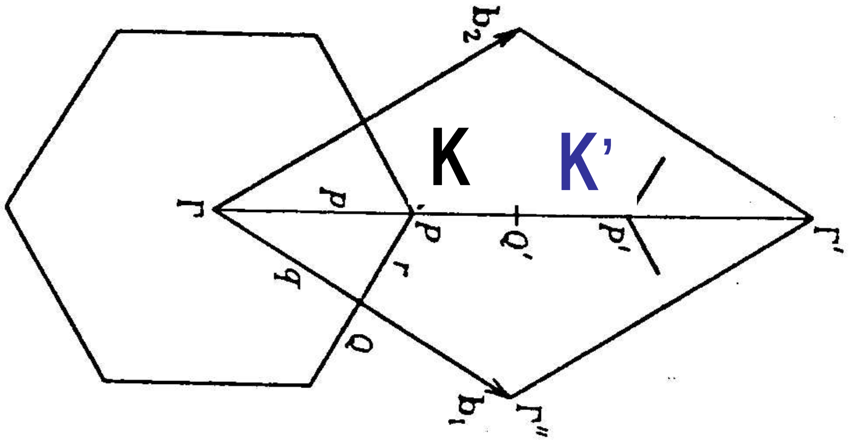
$$H = \begin{pmatrix} 0 & H_{AB} \\ H_{AB} & 0 \end{pmatrix}$$

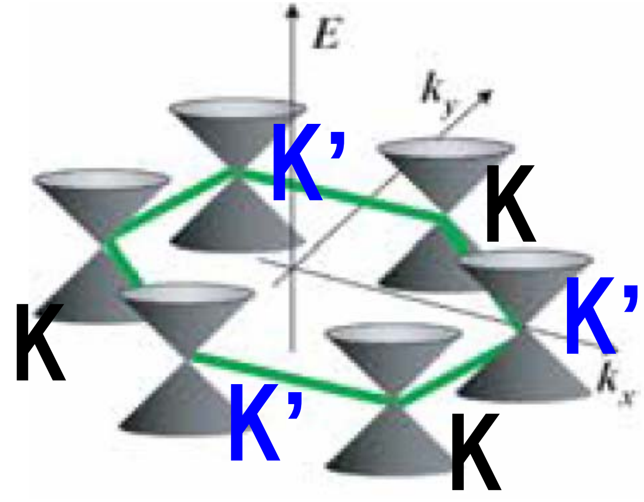


$$E_{g2D}(k_x, k_y) = \pm t \left\{ 1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right) \right\}^{1/2}$$

How does the massless Dirac appear on honeycomb (2)





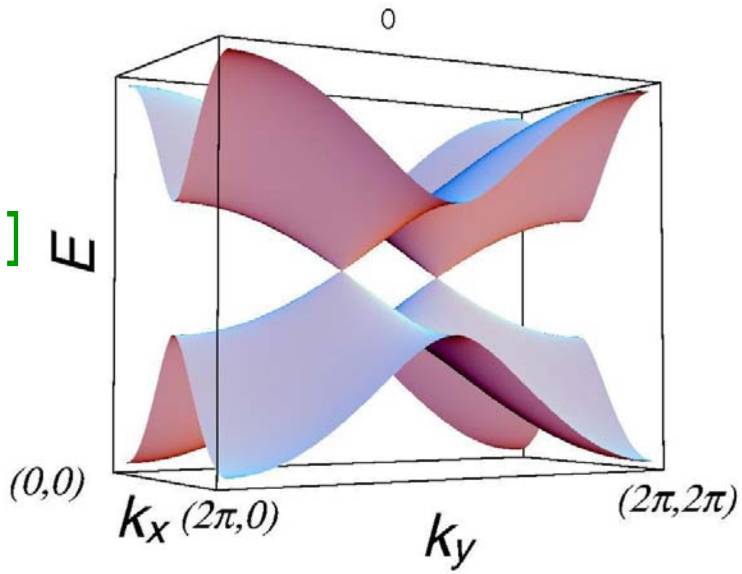


* Group theory (Lomer, Proc Roy Soc 1955)
2-dim representation at K and K'

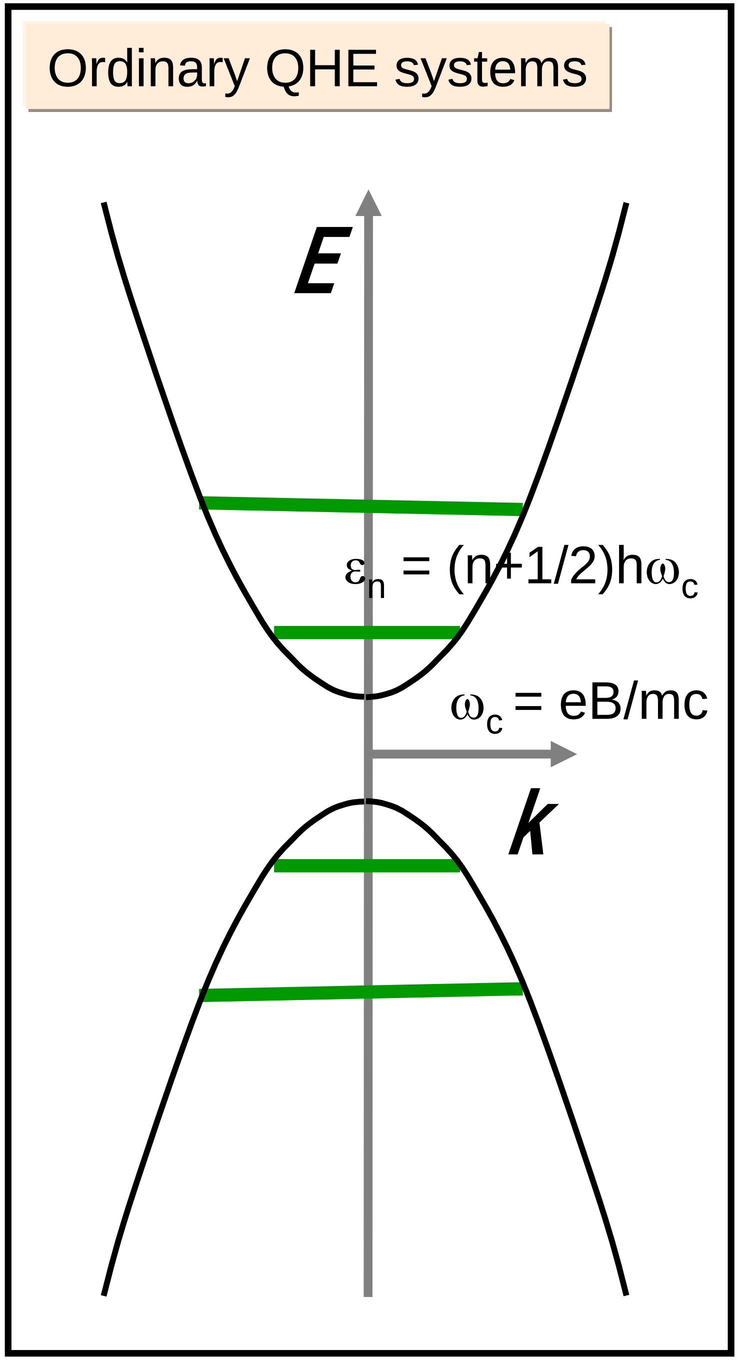
* k・p Hamiltonian [Wallece, PR 71, 622 (1947)]

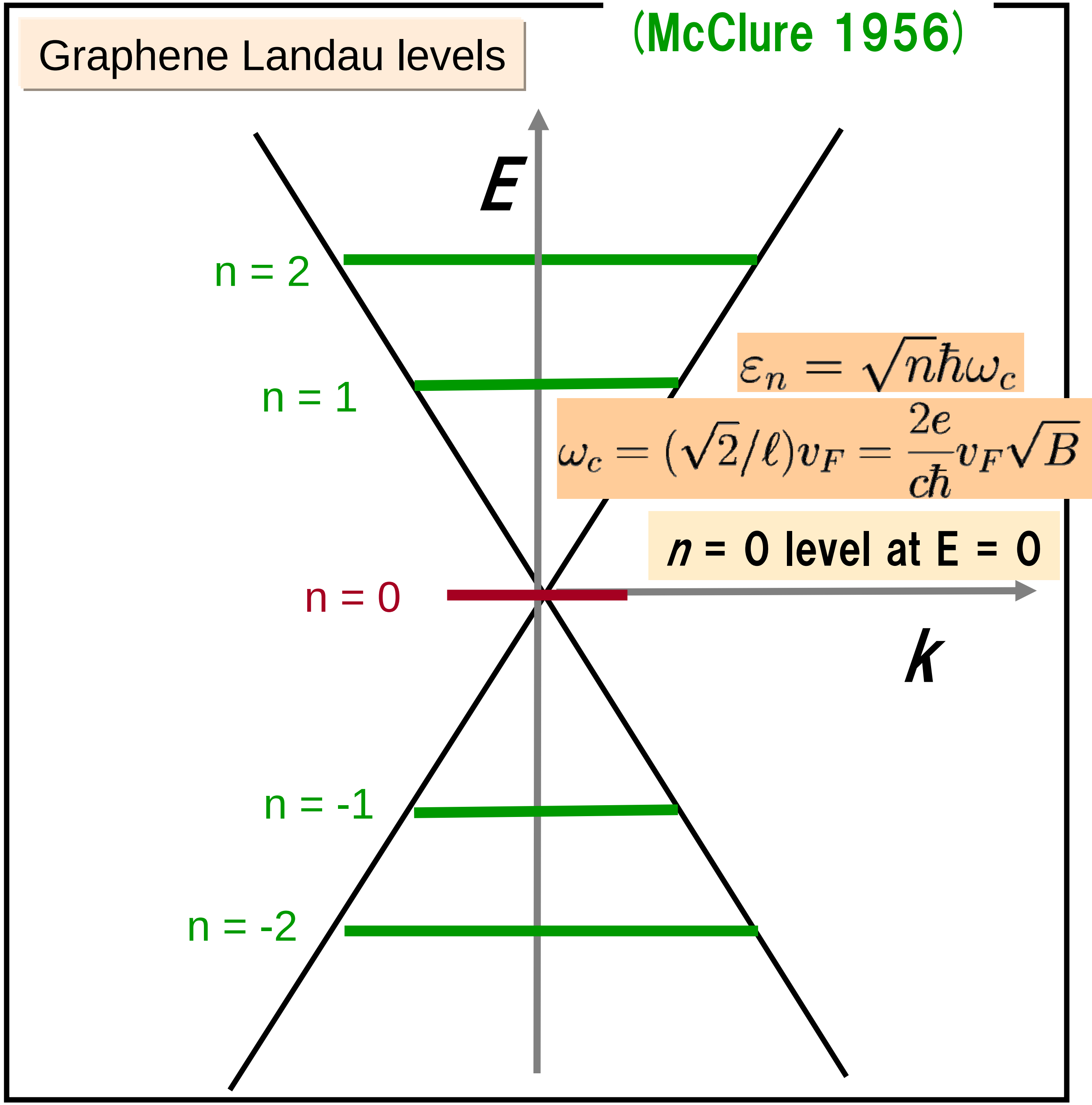
$$H = v_{\mathrm{F}}(\pm\sigma_x p_x + \sigma_y p_y)$$

+: K, -: K'



Graphene Landau levels





Massless Dirac →
a variety of anomalous phenomena observed / predicted

* QHE (Novoselov et al, Nature 2005;
  Zhang et al, Nature 2005)

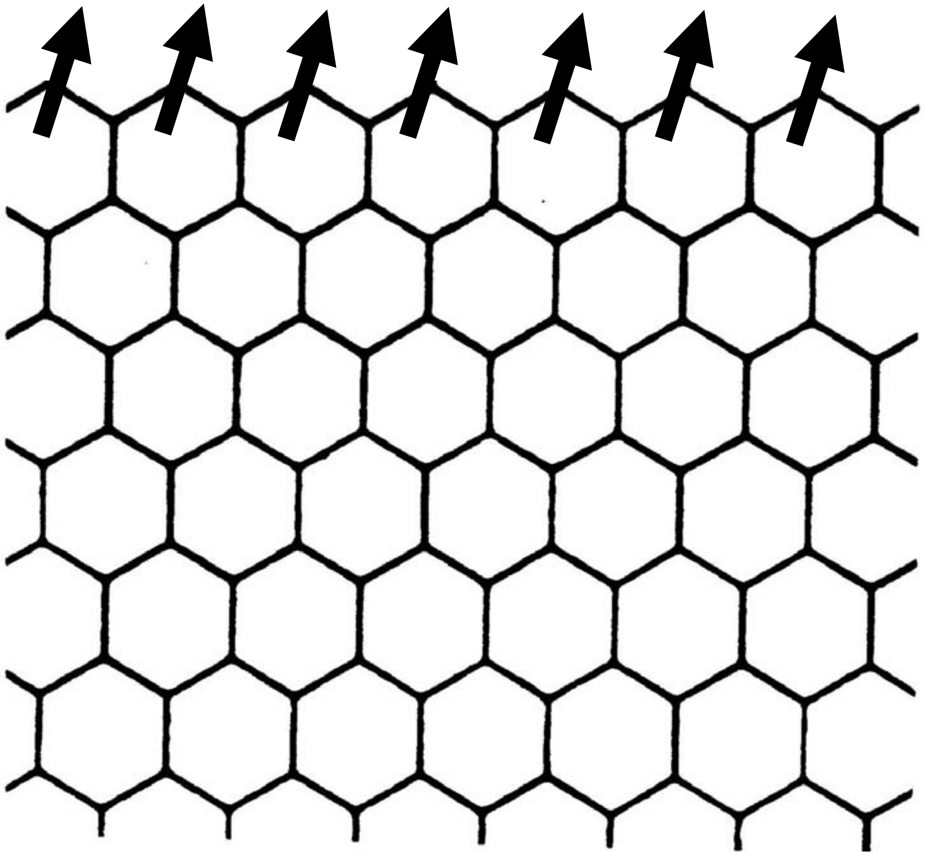
* Spin Hall effect (spin-orbit; Kane & Mele PRL 2005)
* Ferromagnetism (B =0; Peres et al, PRB 2005)
* FQHE (Apalkov & Chakraborty, PRL 2006)
* Superconductivity (Uchoa & Castro Neto, PRL 2007)
* Negative refractive index (Cheianov et al, Science 07)
* Klein paradox (Katsnelson et al, nature phys 2006)
* Gapped state (Nomura & MacDonald PRL 2006)
* Bond-ordered state (Hatsugai et al, 2007)
* Landau-level laser (Morimoto et al, 2007)

・・・

> 400 preprints on graphene in cond-mat in 2006-2007
(A review, incl. a brief history of graphene:
Andre Geim & Kostya Novoselov, nature materials 2007)

$B = 0$

Edge states in graphene



Band F in nonmagnetic materials ?

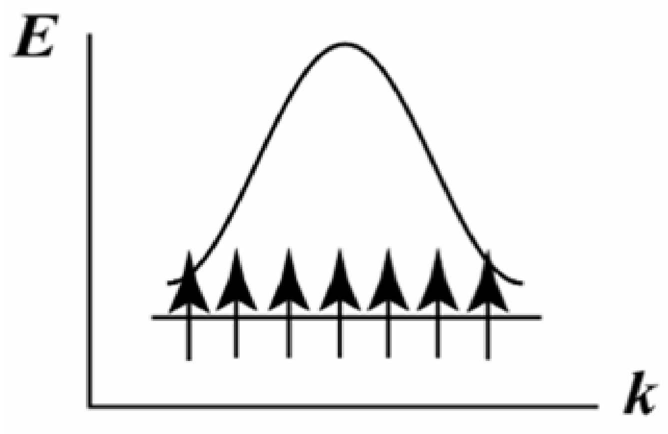
Criterion (Stoner's) for band F:

$UD(E_F) > 1$ --- too crude a criterion

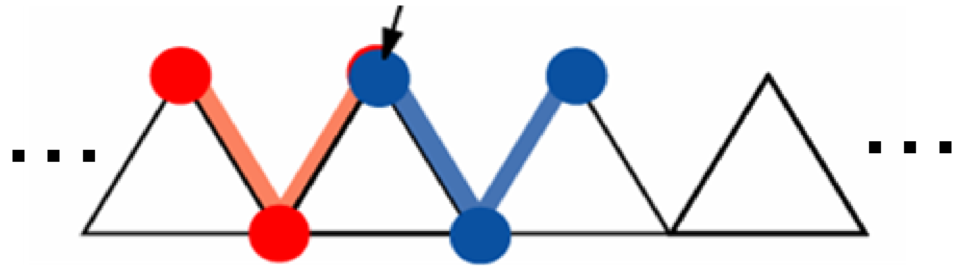
Flat-band ferromagnetism

(Lieb 1989; Mielke 1991; Tasaki 1992)

(a) Flat one-electron band

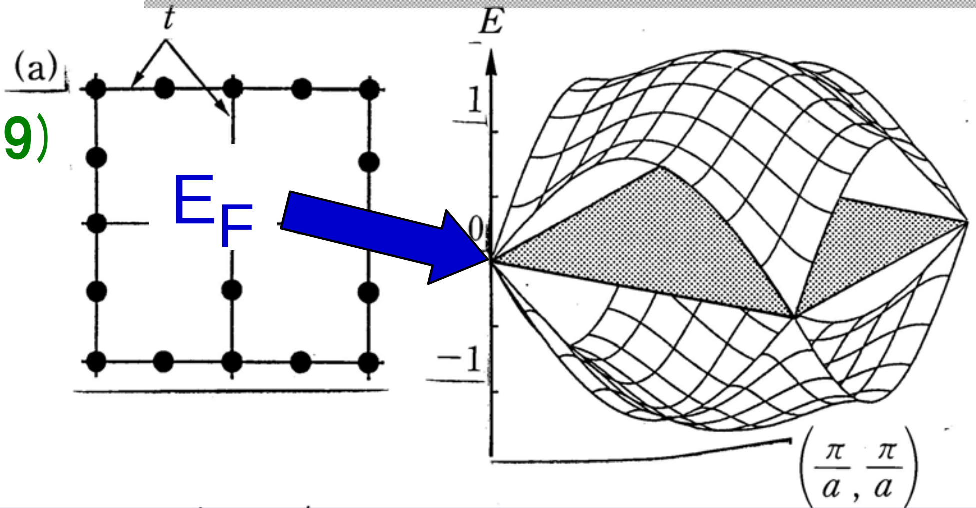


(b) Connectivity condition
(``Wannier" orbits overlap)
i.e., band ferromagnetism

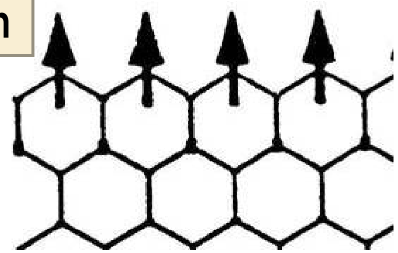


Hubbard model on flat-band systems

(Lieb, 1989)

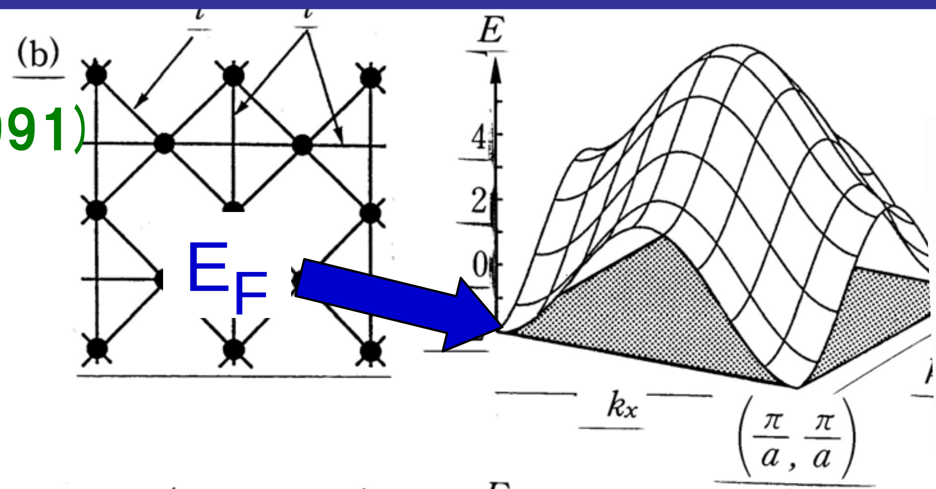


1D version

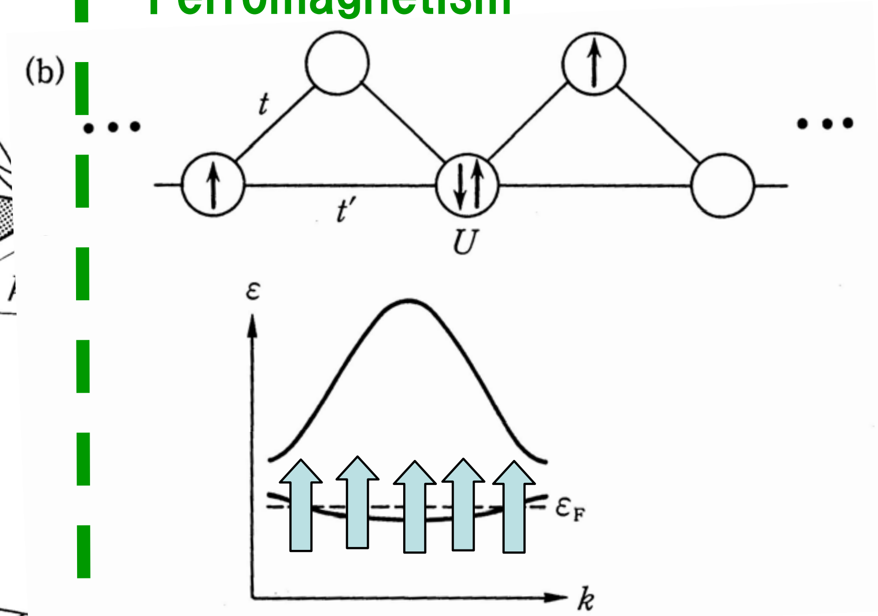


(Ovchinnikov rule
guaranteed for $0 < U < \infty$)

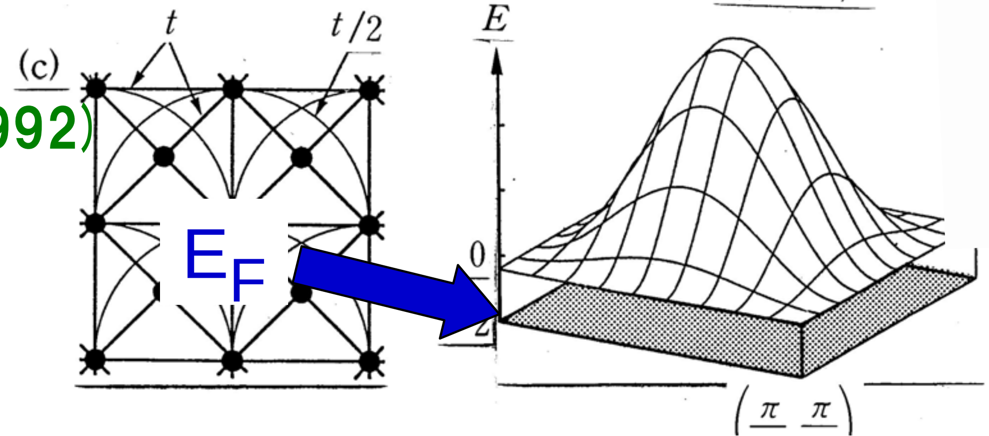
(Mielke, 1991)



Ferromagnetism



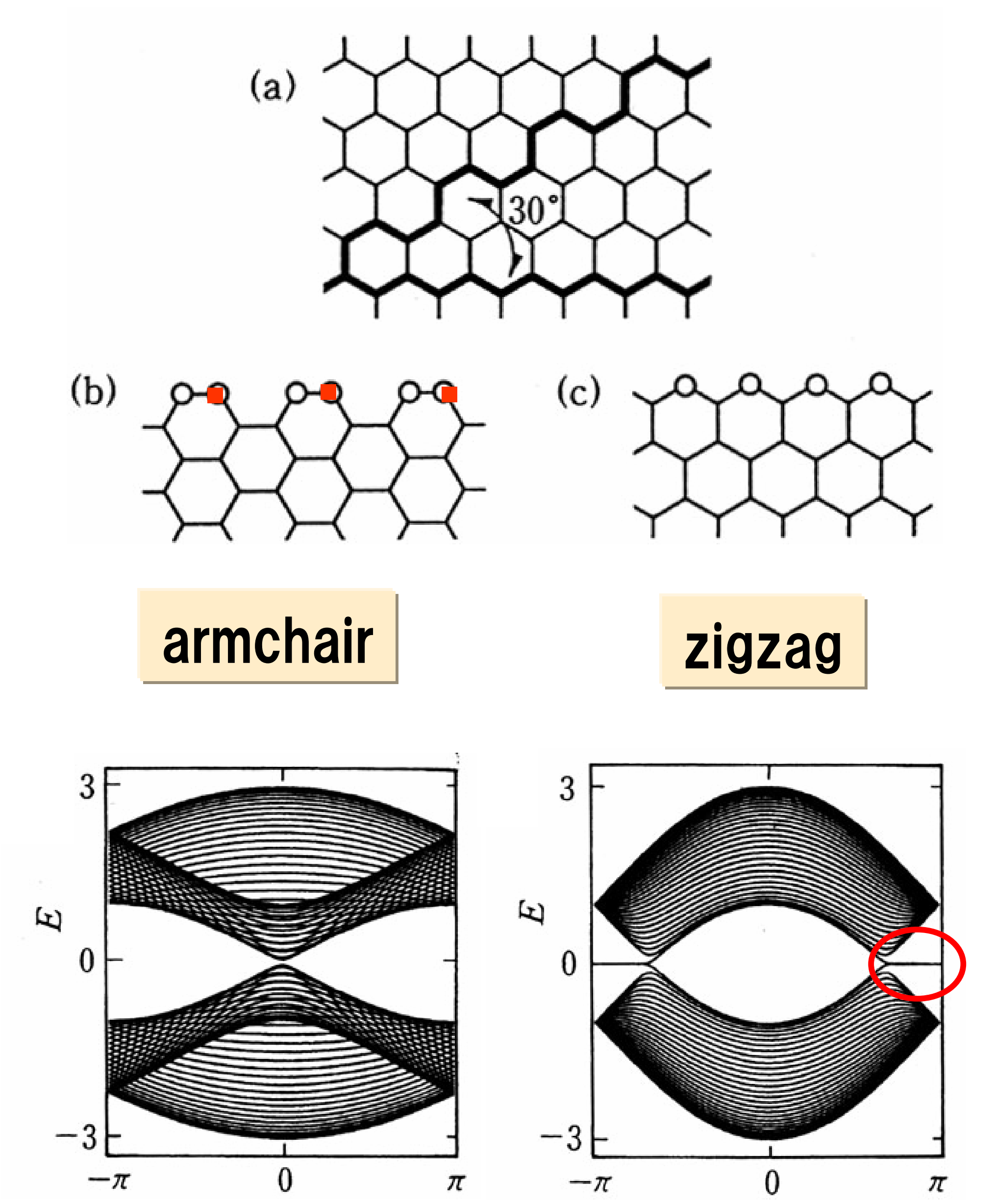
(Tasaki, 1992)

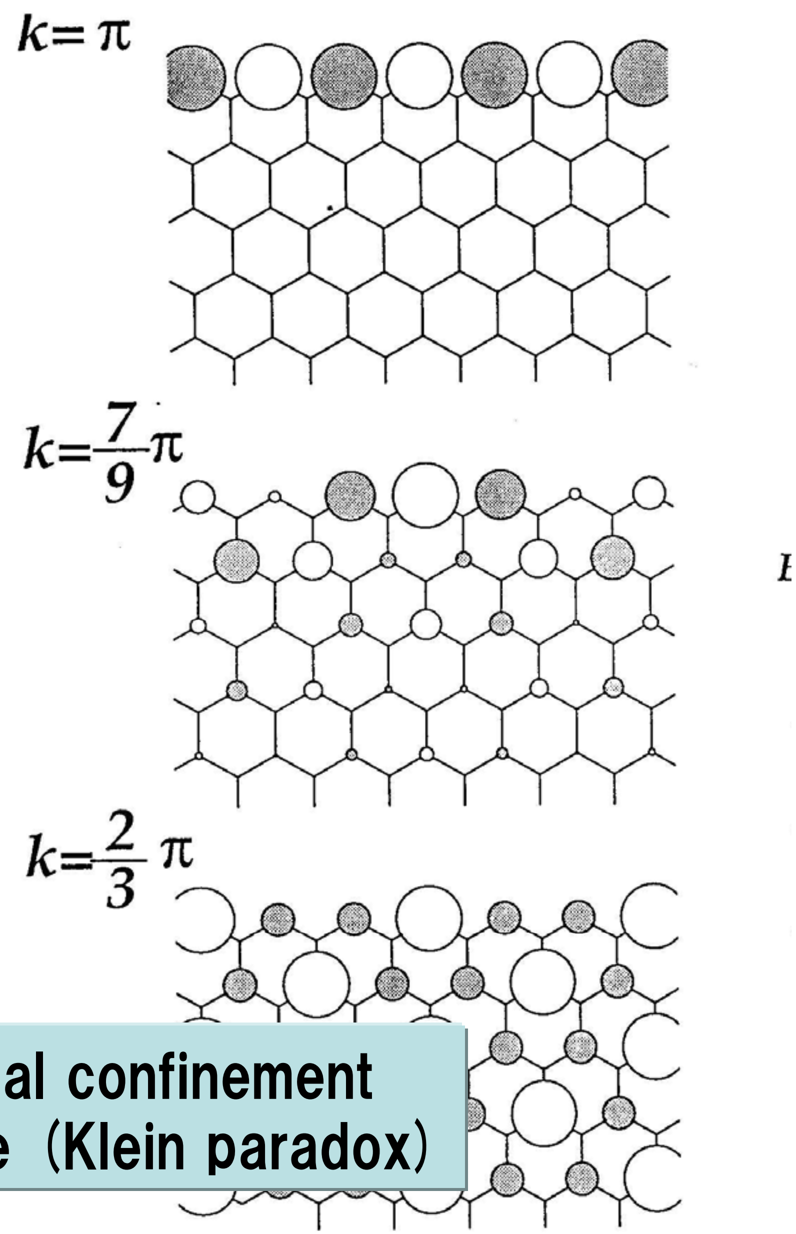


generalised Hund's coupling
(Kusakabe & Aoki, 1992)

Edge states in graphene

Nakata et al, PRB **54**, 17954 (1996)

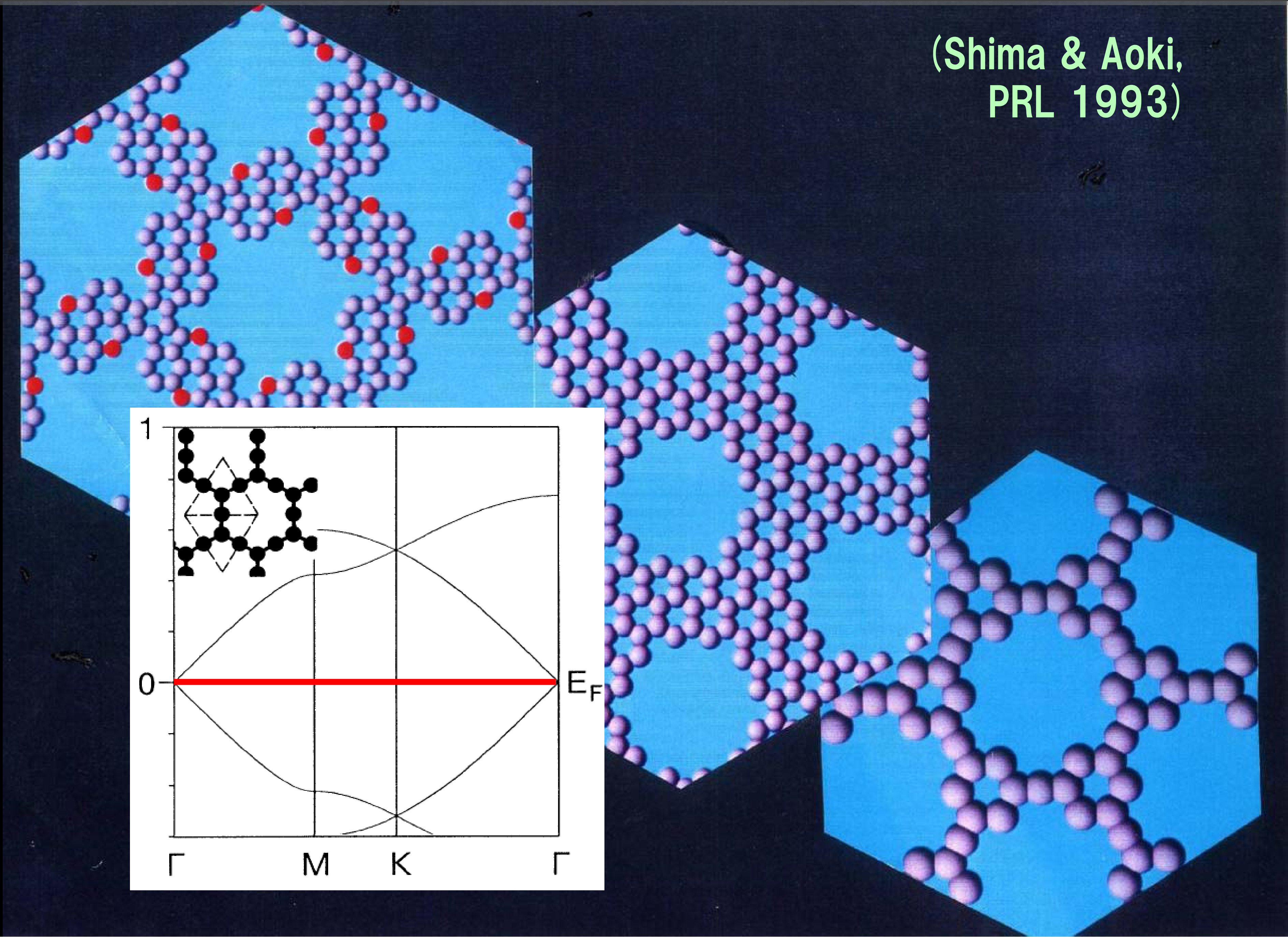




cf. Potential confinement impossible (Klein paradox)

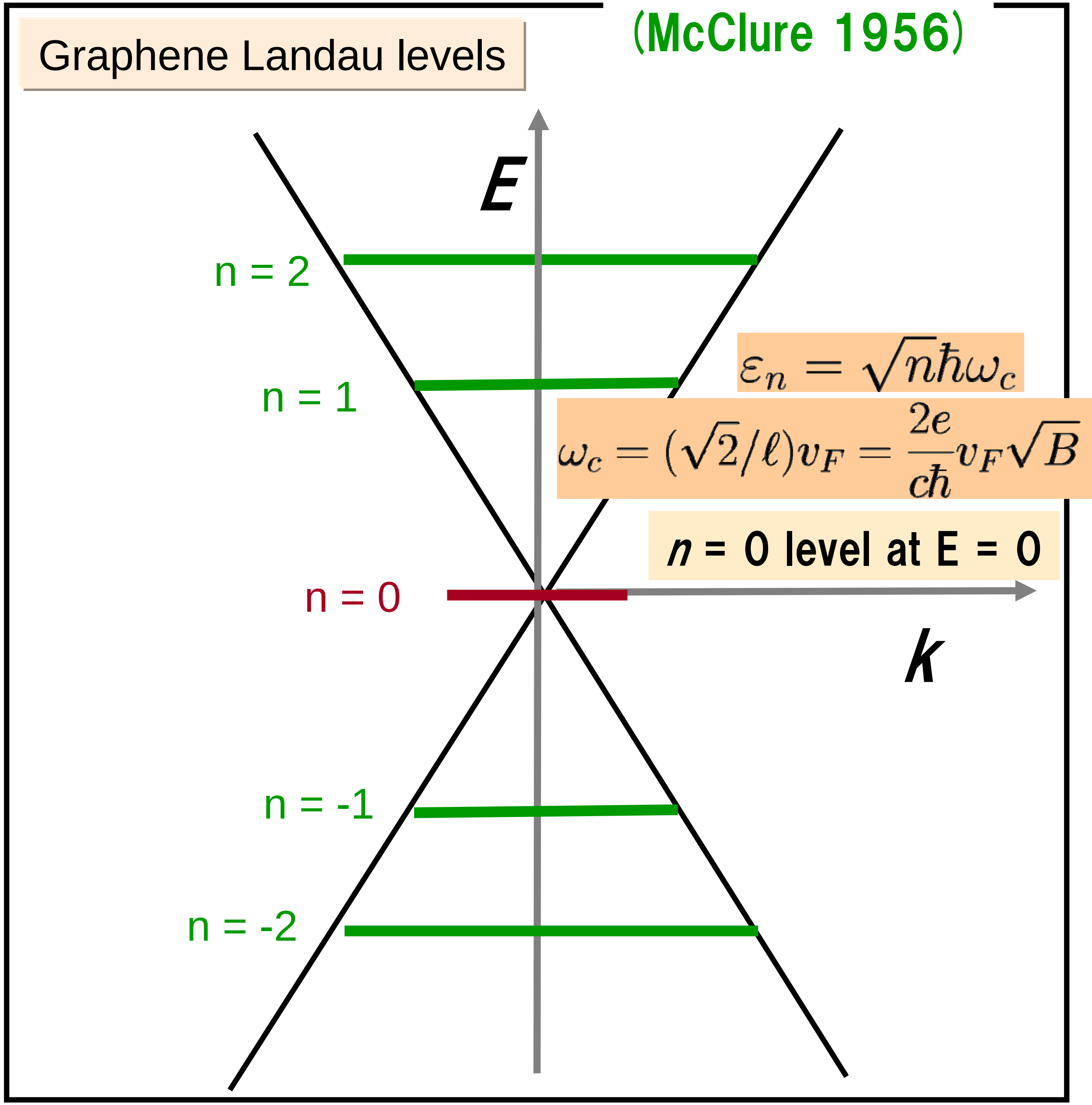
Long-period graphene

(Shima & Aoki, PRL 1993)



$B > 0$

Graphene Landau levels



Landau levels for massive Dirac particles

(MacDonald, PRB 1983)

Dirac eqn

$$[(\mathscr{E}-eEx)^2-(c\vec{p}-e\vec{A})^2 - m^2c^4 + e\hbar cH\,\sigma_z + ie\hbar cE\,\sigma_x]\phi = 0$$

Energy

$$\mathscr{E}(\vec{k}_\perp, n, \pm) = \frac{H}{\sqrt{H^2-E^2}} \times \{m^2c^4 + mc^2[\hbar\omega_c(2n+1\pm 1)]\}^{1/2}$$

non-relativistic

massless Dirac

$$\mathscr{E} = mc^2$$

↓ leading term in $h\omega_c/mc^2$ expansion

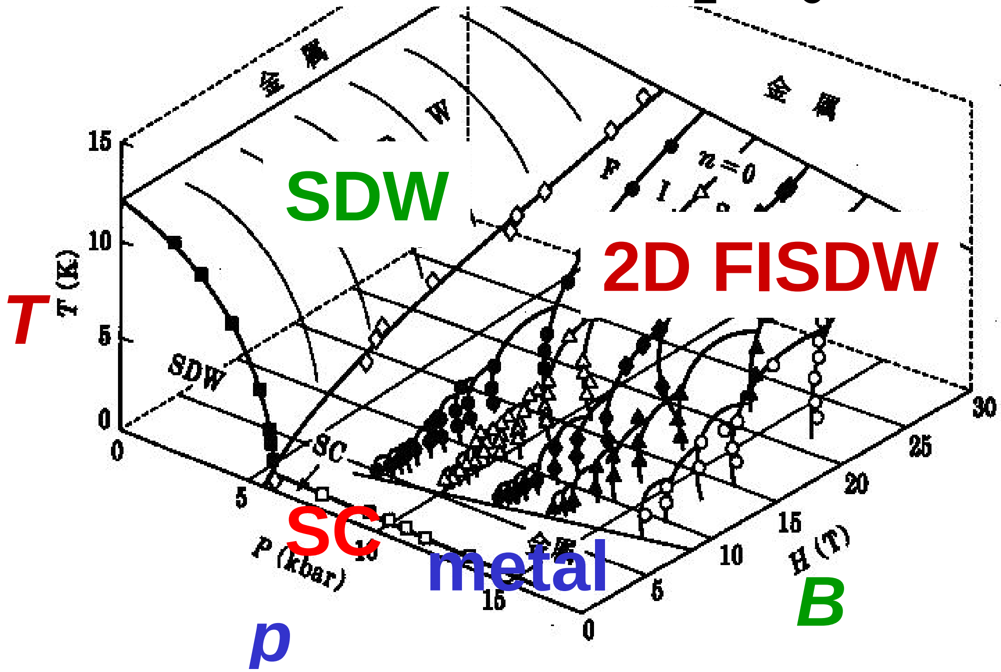
$$+\hbar\omega_c(n+1\pm\tfrac{1}{2}) + \frac{m}{2}\left(\frac{cE}{H}\right)^2 + \cdots$$

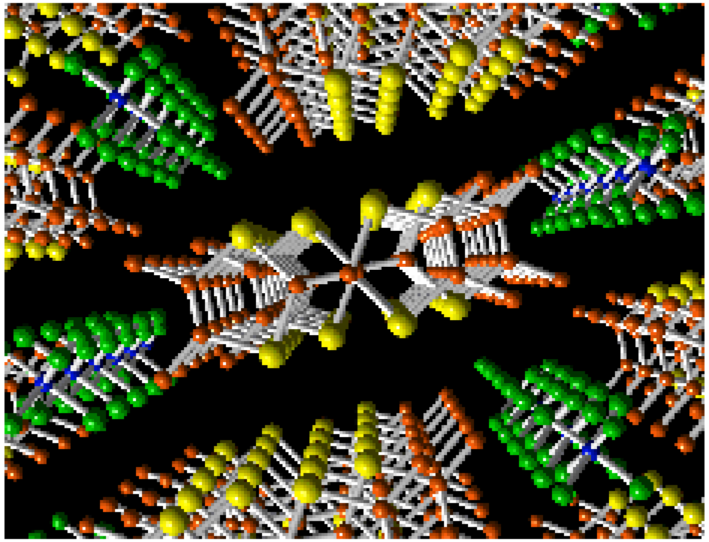
?

$\omega_c = eH/mc$

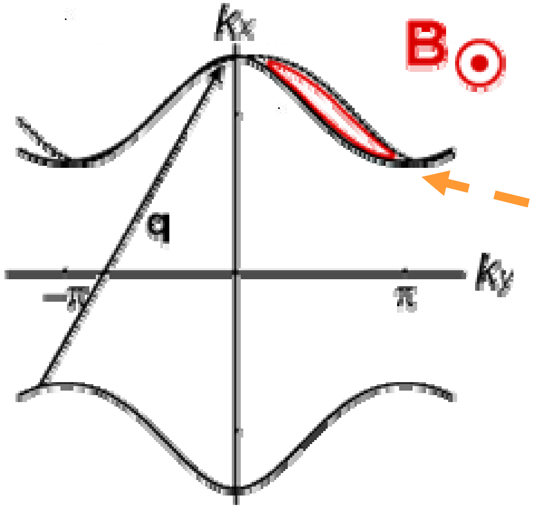
QHE can reflect band structures

q2D organic metal $(TMTSF)_2PF_6$ (Chaikin et al)





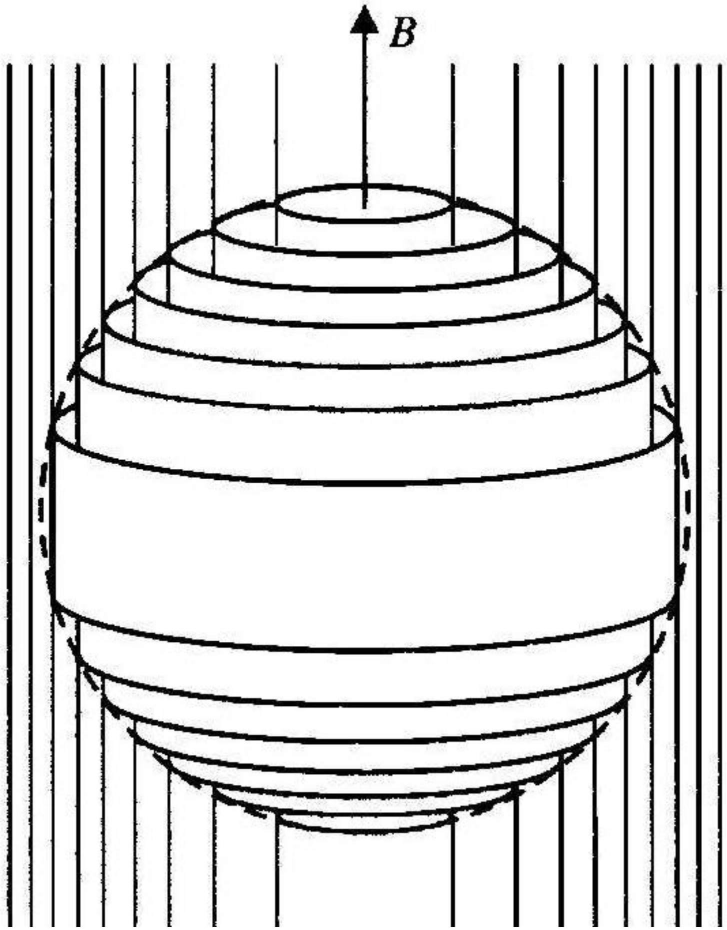
Lab. de Physique des Solides



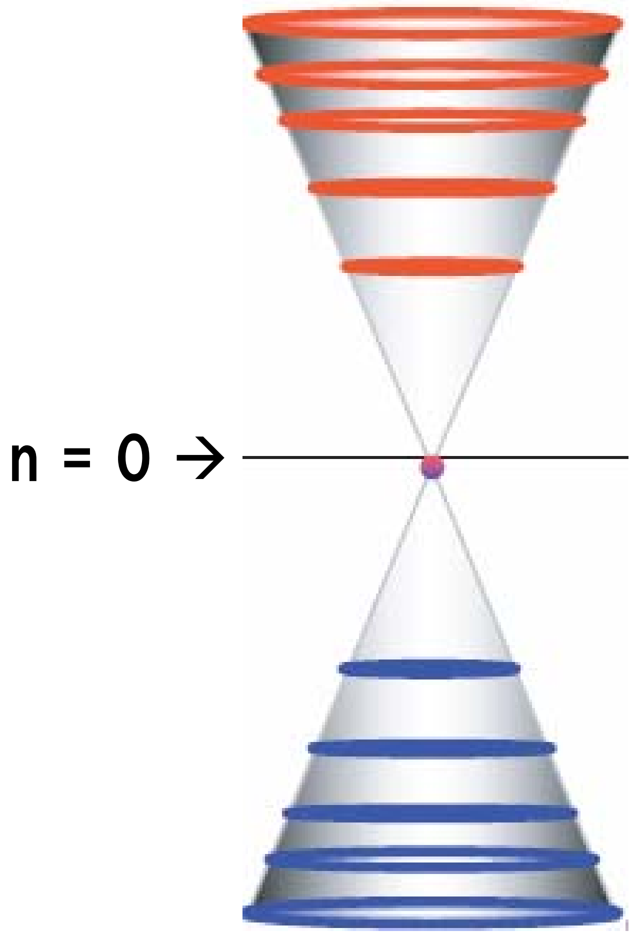
Incomplete nesting
→ Landau levels in Fermi pockets
→ IQHE

What's so special about graphene Landau level

Quantisation in *B*
↓ Onsager's semicl
"Landau tube"

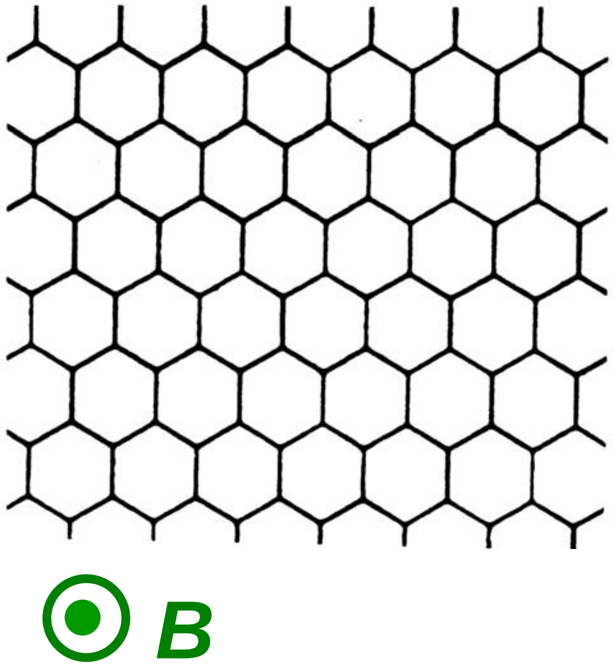


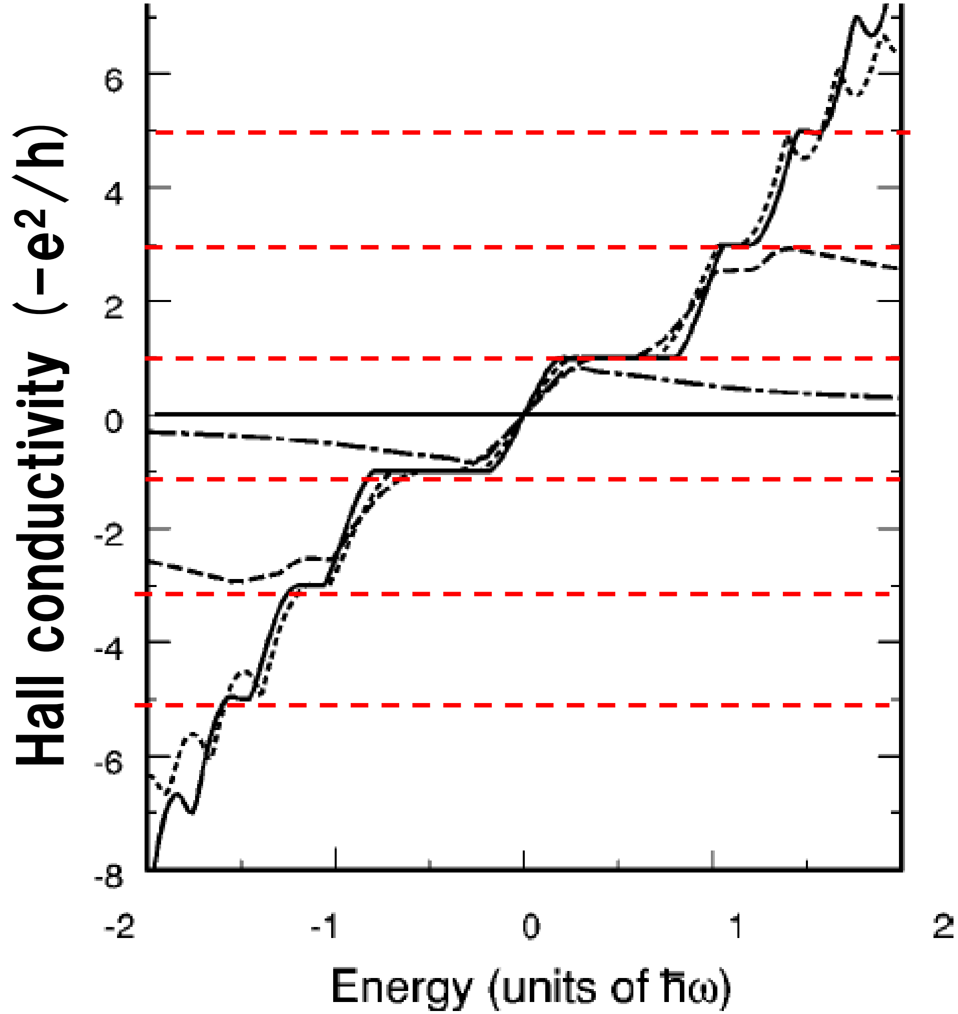
?



QHE in honeycomb lattice

(SCBA: Zheng & Ando, PRB 2002;
Gusynin & Sharapov, PRB, PRL 2005)





$\sigma_{xy} = (2n+1)(-e^2/h)$ steps

QHE in graphene

(Novoselov *et al*, Nature 2005; Nature Phys 2006; Zhang *et al*, Nature 2005)

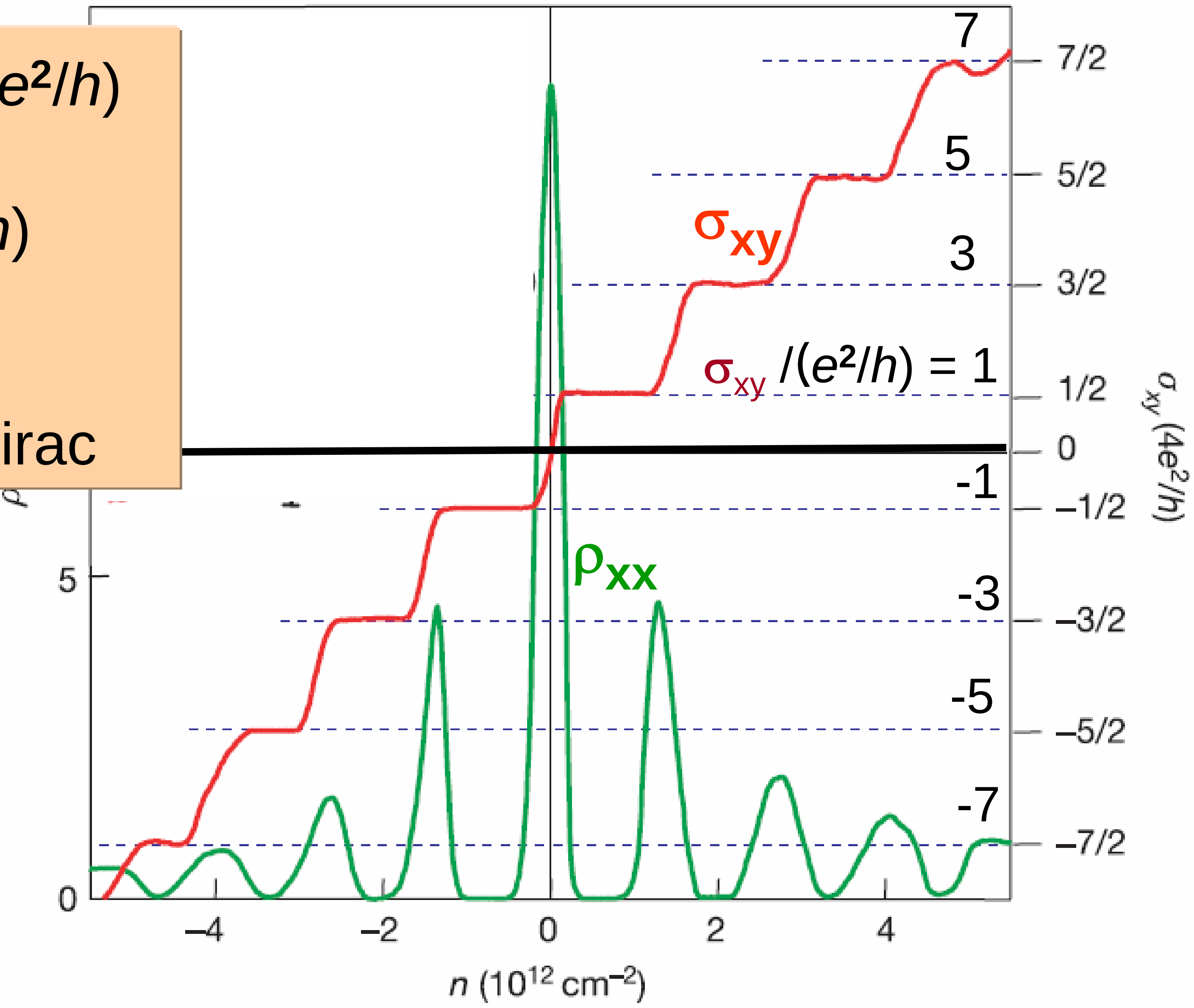
$B = 14\,\mathrm{T}$ and $T = 4\,\mathrm{K}$

$\sigma_{xy} = (2n+1)(-e^2/h)$

$2\,(n+1/2)(-e^2/h)$
(half-integer)

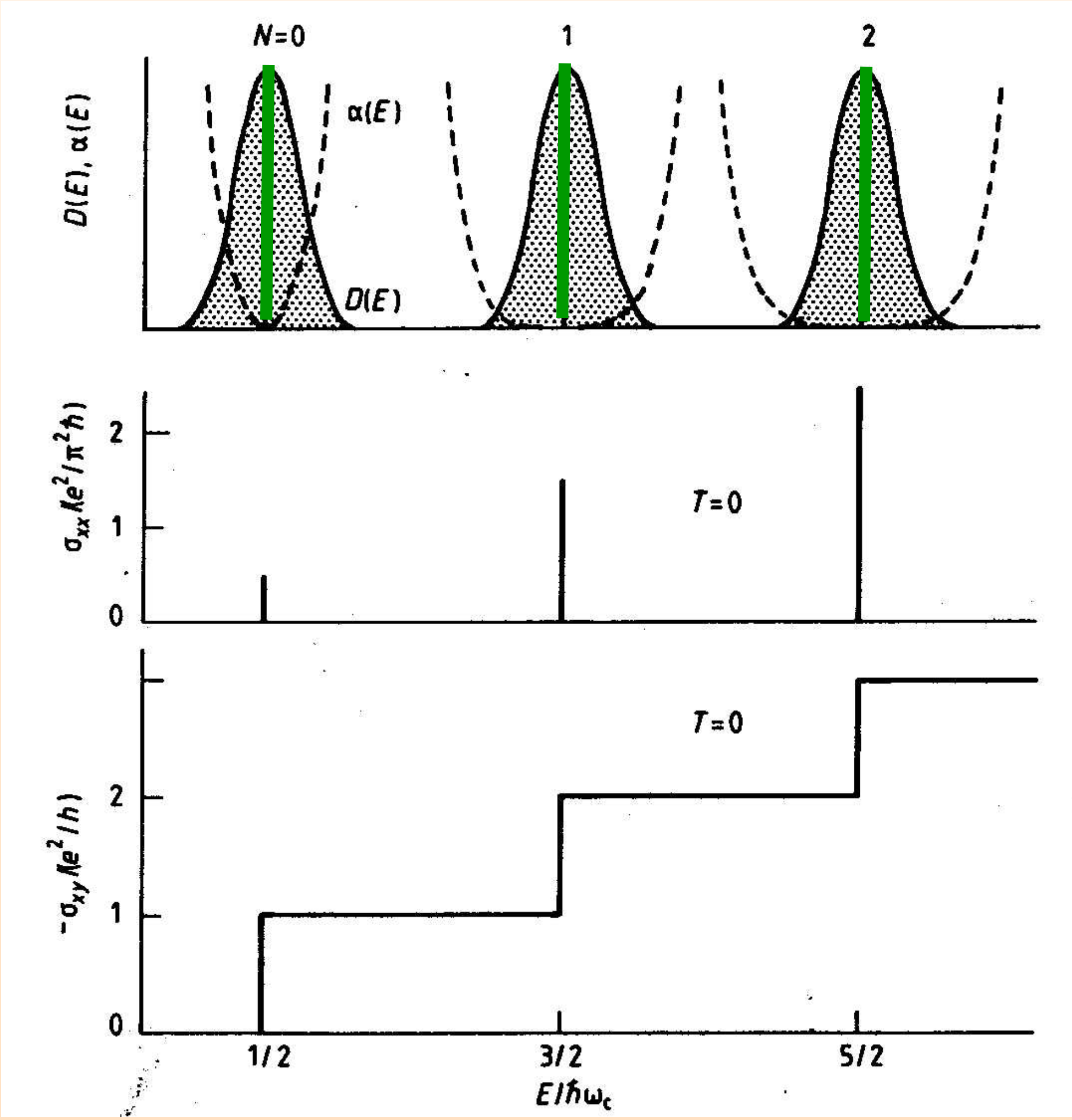
for massless Dirac

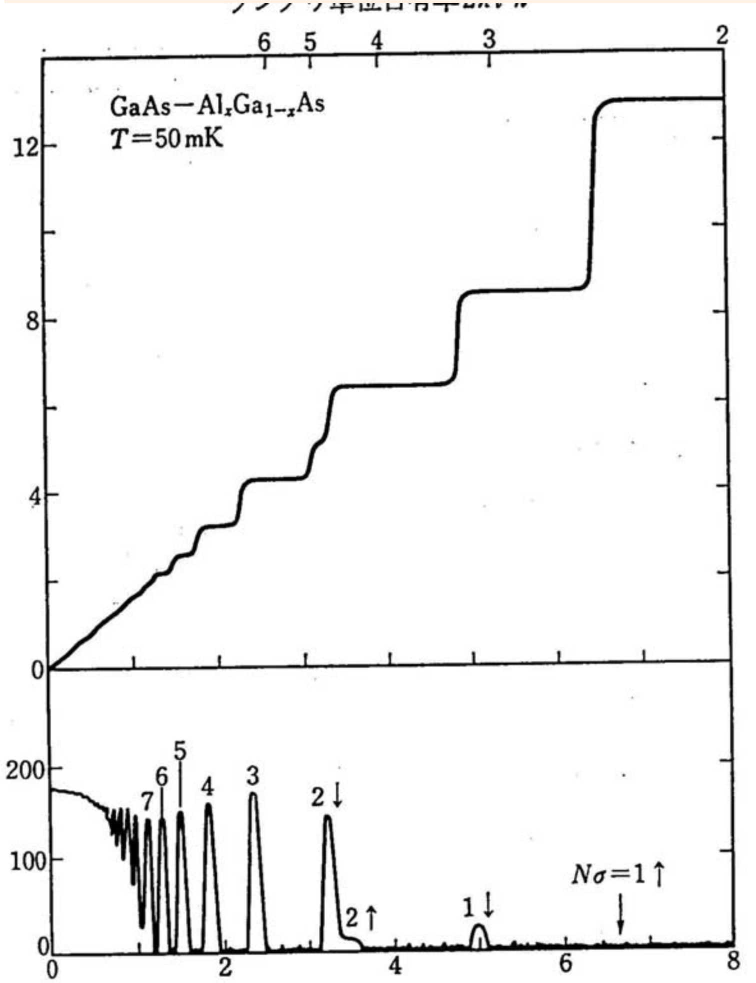
Valley degeneracy



Integer quantum Hall effect

(Aoki & Ando 1980)

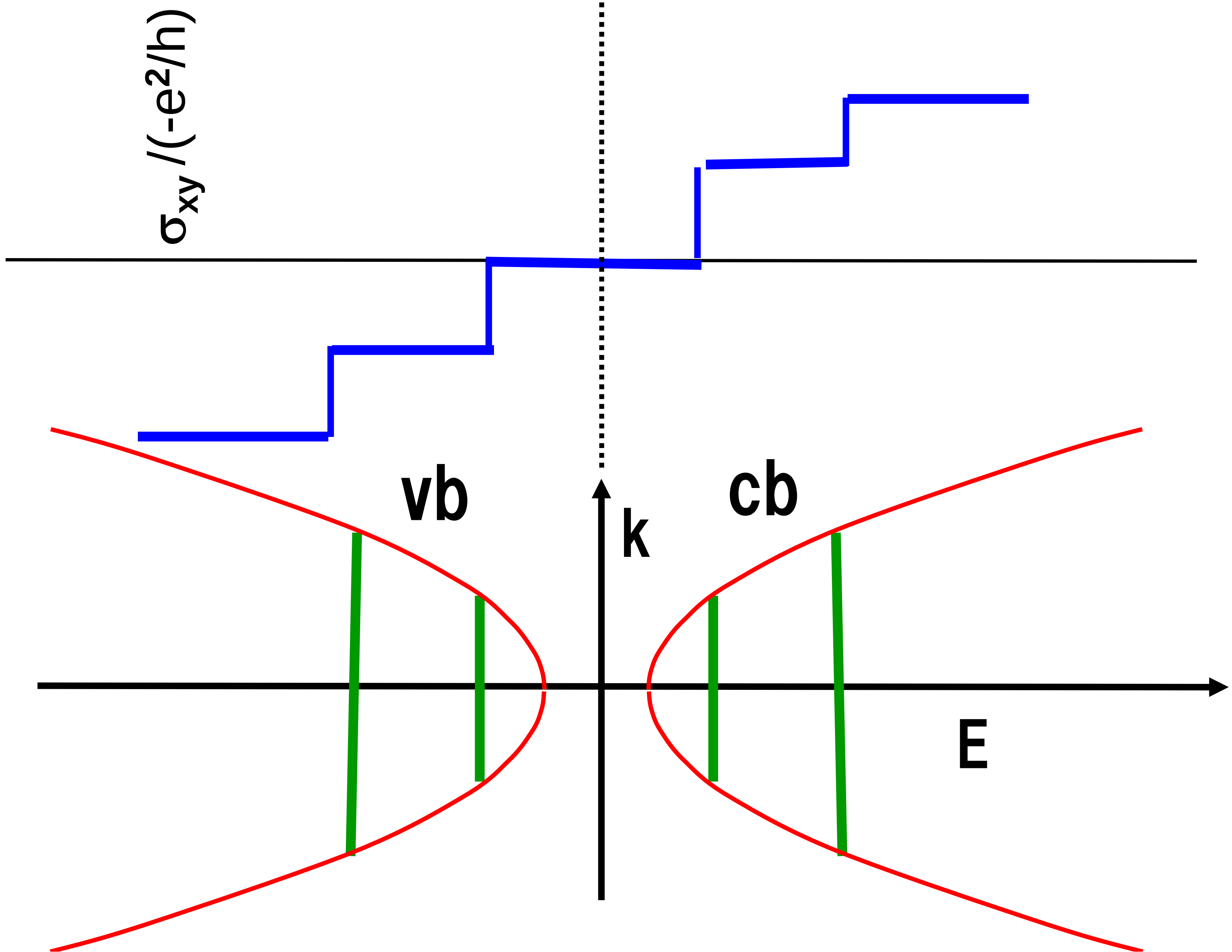




(Paalanen et al, 1982)

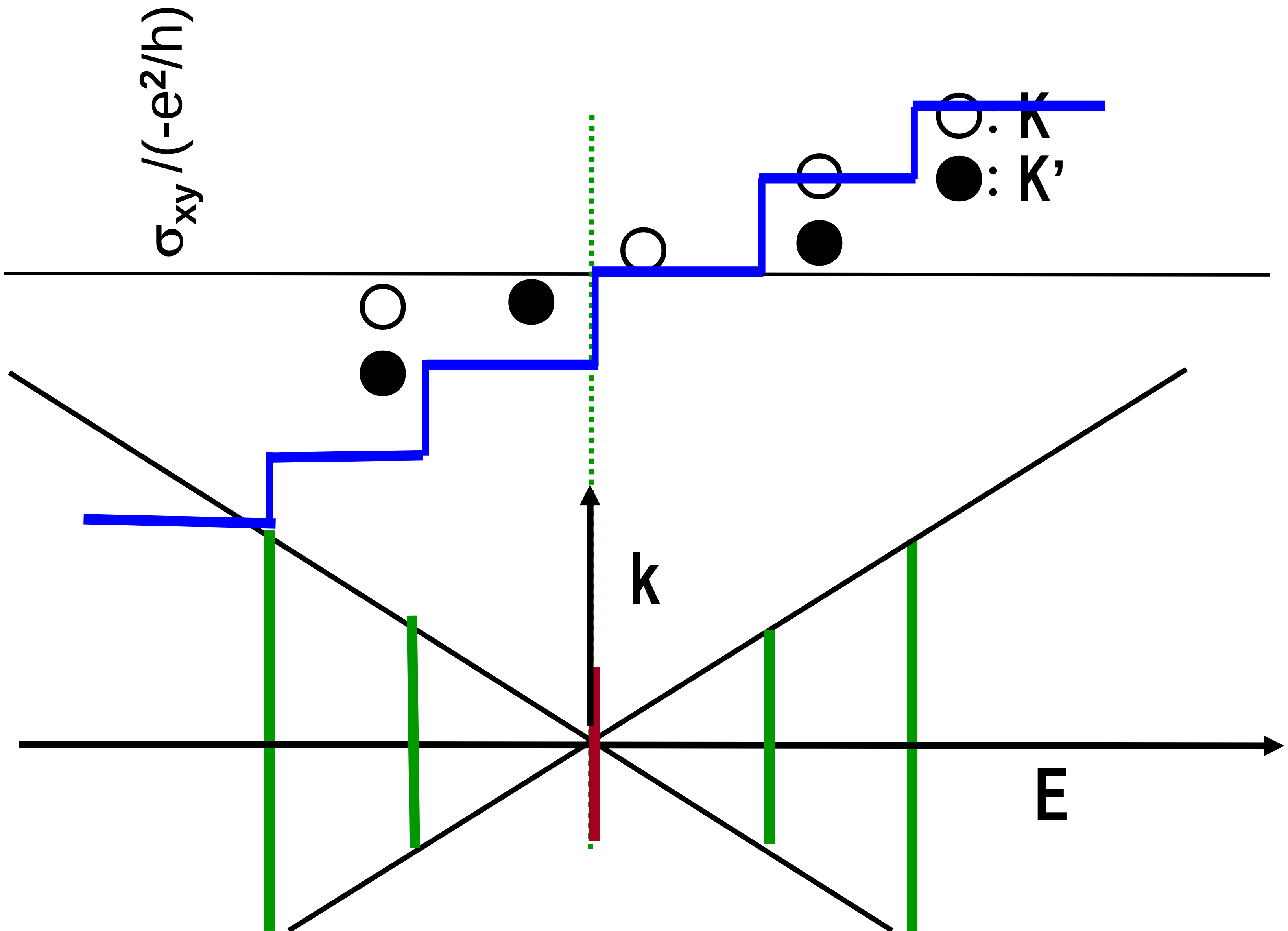
(Aoki, Rep Prog Phys 1987)

QHE in ordinary valence / conduction bands



QHE for massless Dirac

Can we interpret this in terms of topoogical quantum # ?



Hall conductivity = a topological number

(Thouless, Kohmoto, Nightingale & den Nijs, 1982)

Linear response

$$\sigma_{xy} = -i\frac{1}{L^2}\sum_{\alpha,\beta} f(\varepsilon_\alpha)\frac{\langle\alpha|J_x|\beta\rangle\langle\beta|J_y|\alpha\rangle - \langle\alpha|J_y|\beta\rangle\langle\beta|J_x|\alpha\rangle}{(\varepsilon_\alpha - \varepsilon_\beta)^2}$$

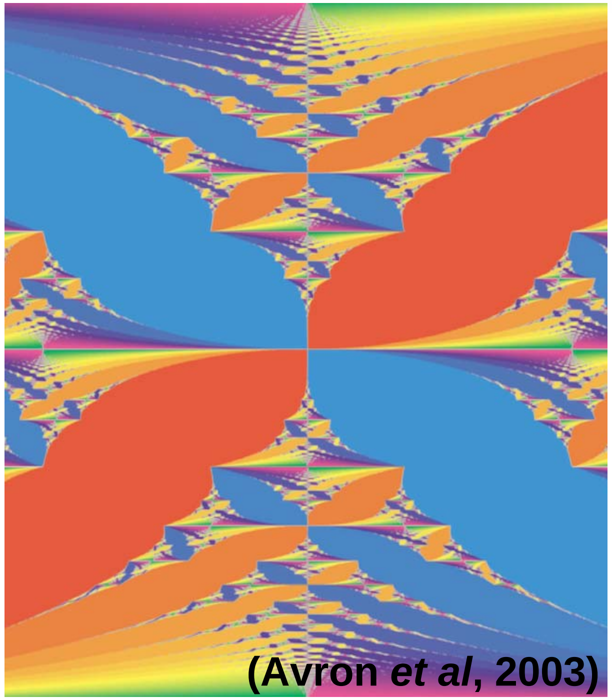
clean, periodic systems

Berry's "curvature"

$$= -i\frac{e^2}{L^2}\sum_{n,\vec{k}} f(\varepsilon_{n\vec{k}})\left[\vec{\nabla}_{\vec{k}} \times \langle n\vec{k}|\vec{\nabla}_{\vec{k}}|n\vec{k}\rangle\right]_z$$

"Gauss-Bonnet"

$= \Sigma_n^{\text{band}}$ (Chern #)$_n$



(Avron *et al*, 2003)

disordered systems

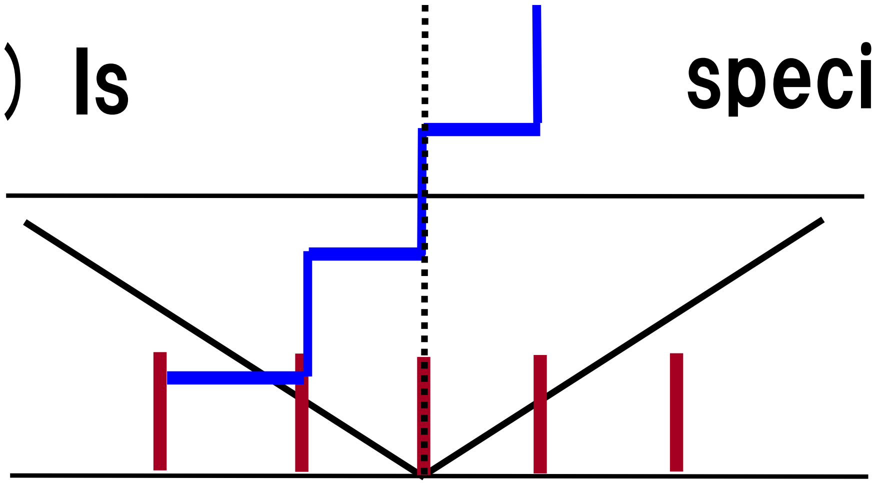
(Aoki & Ando, 1986)

distribution of topological #
in disordered systems
(Aoki & Ando, 1986;
Huo & Bhatt, 1992;
Yang & Bhatt, 1999)

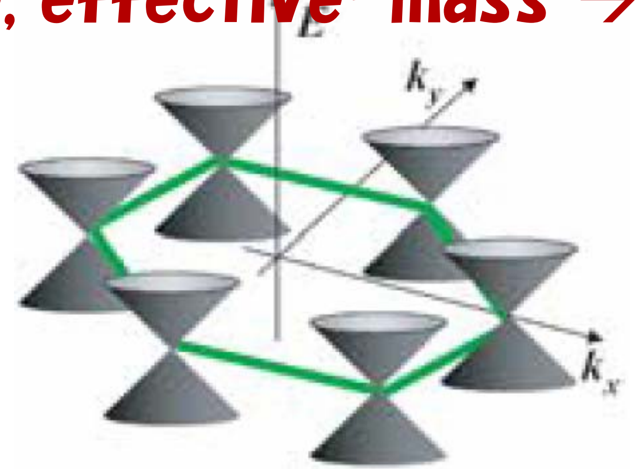
Questions about graphene IQHE

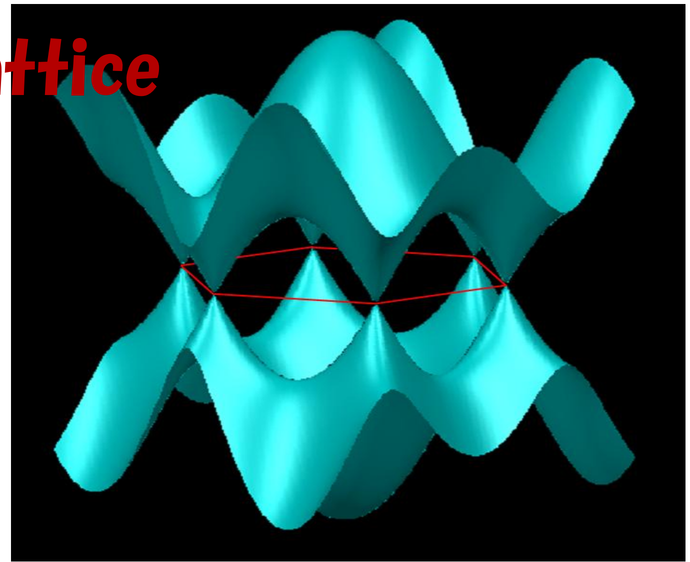
(A) How does the topological nature appear ?

(B) How do the edge states look like ?

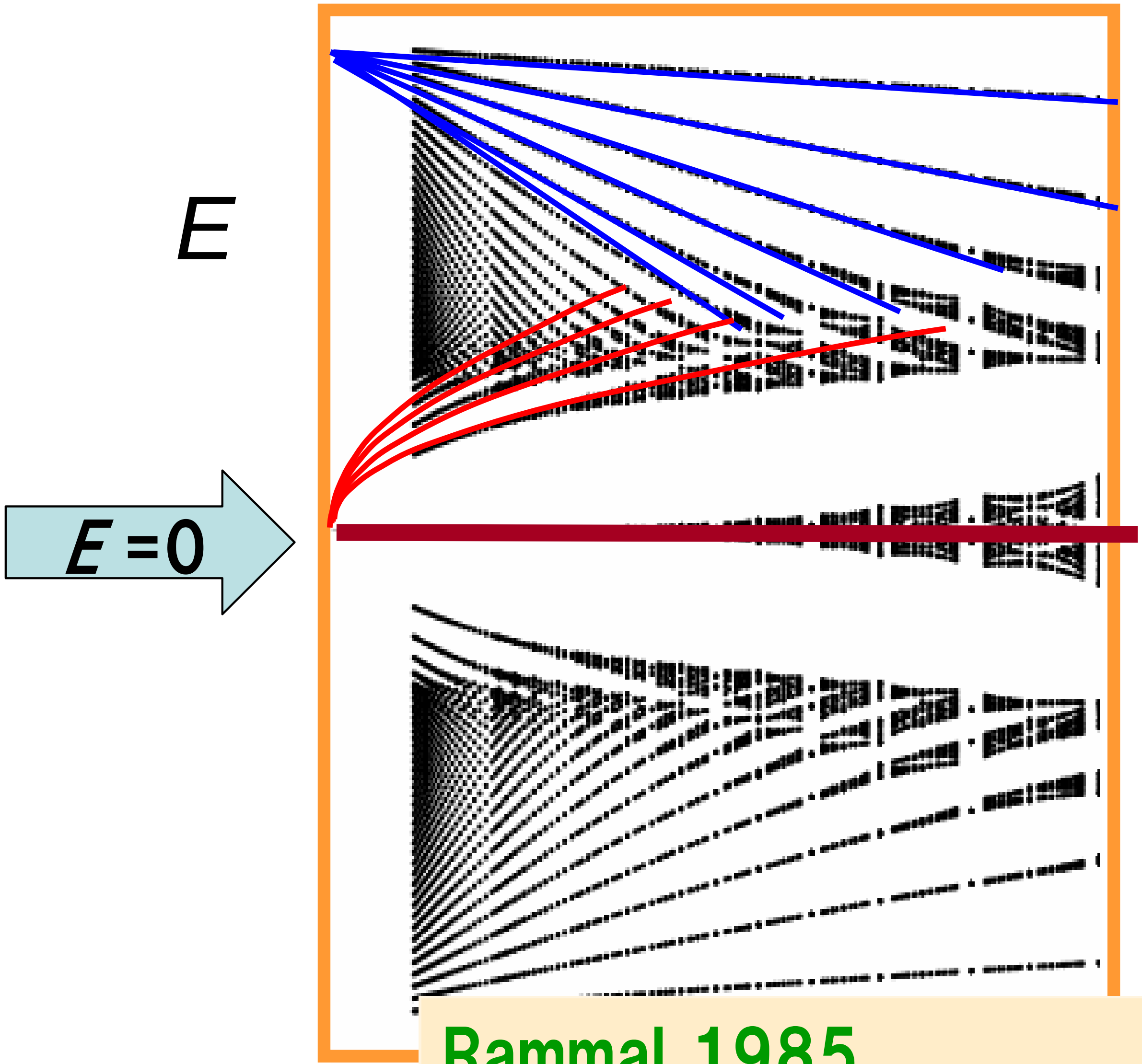
(C) Is  specific to honeycomb?

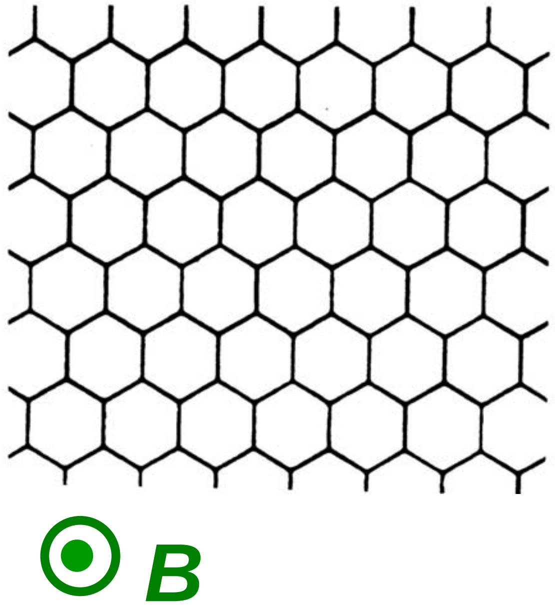
For these, effective-mass → original lattice





Whole spectrum for honeycomb lattice



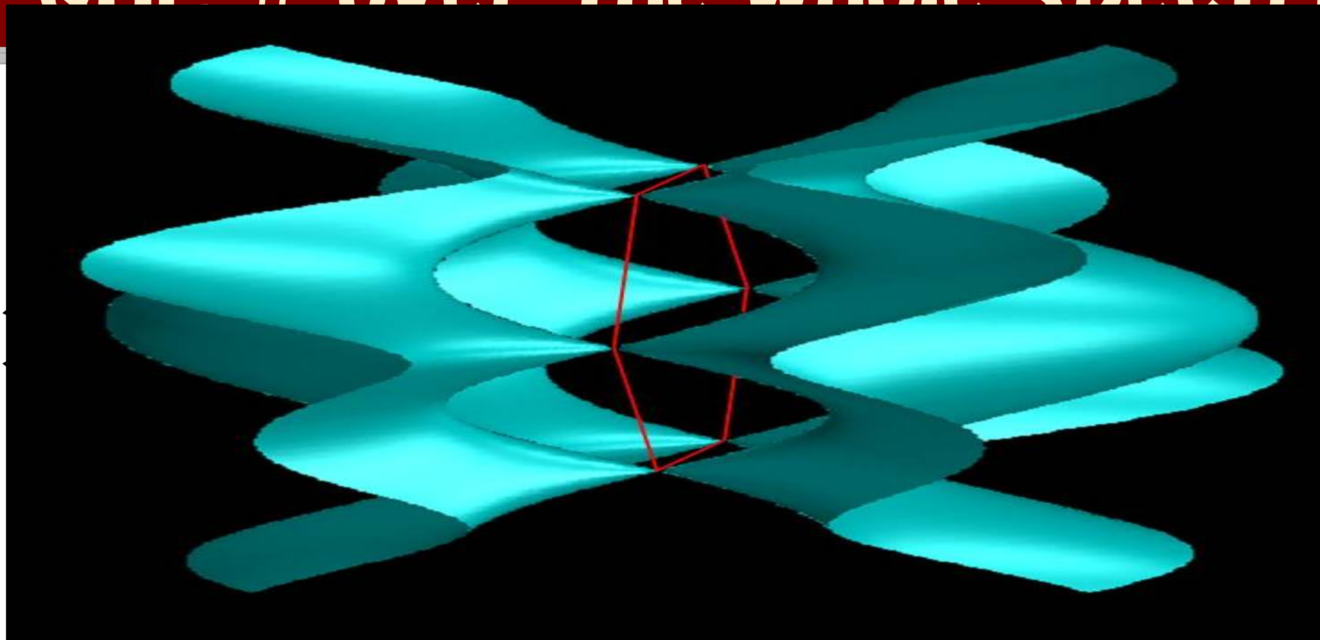


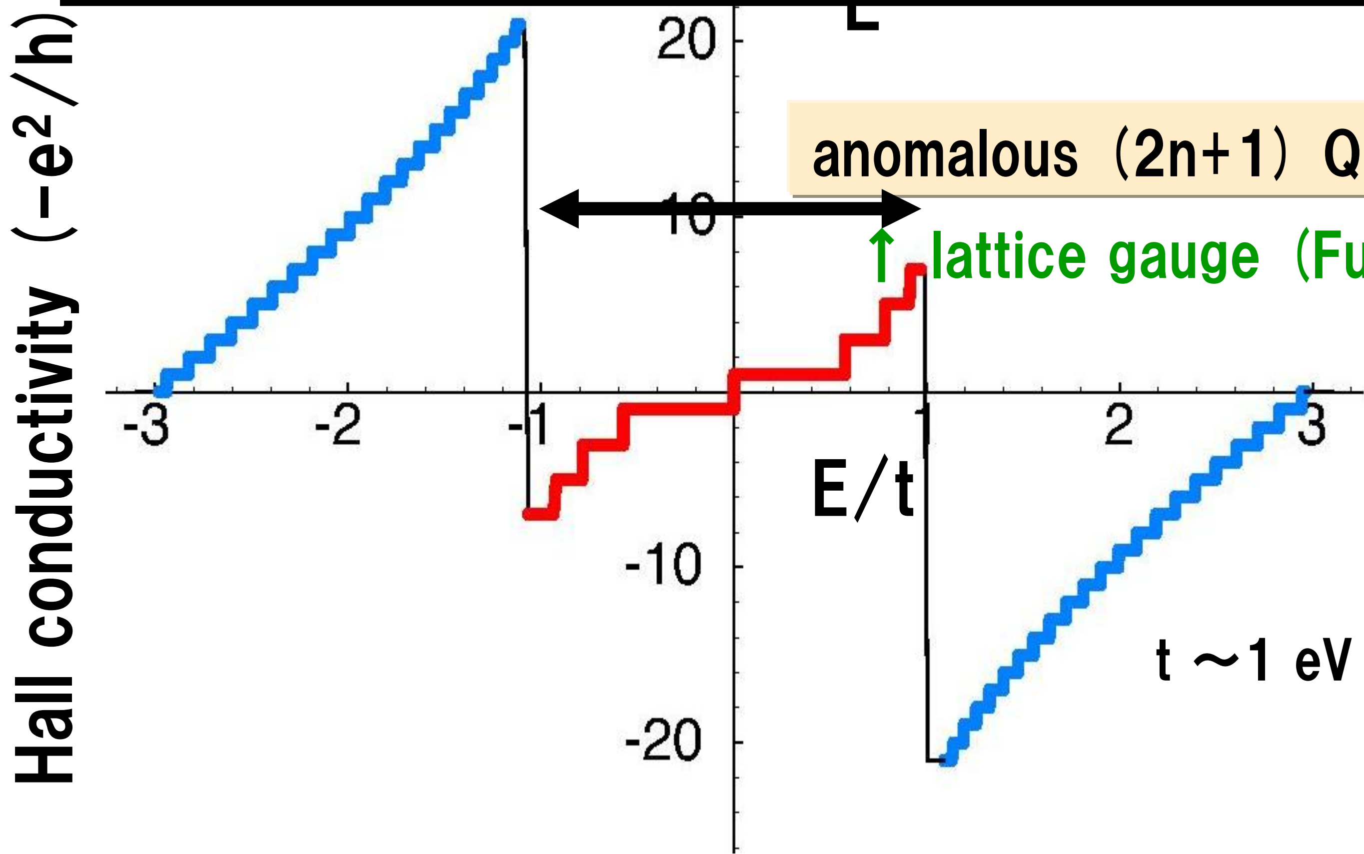
Rammal 1985

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

QHE # over the whole spectrum

oki, PRB 2006)



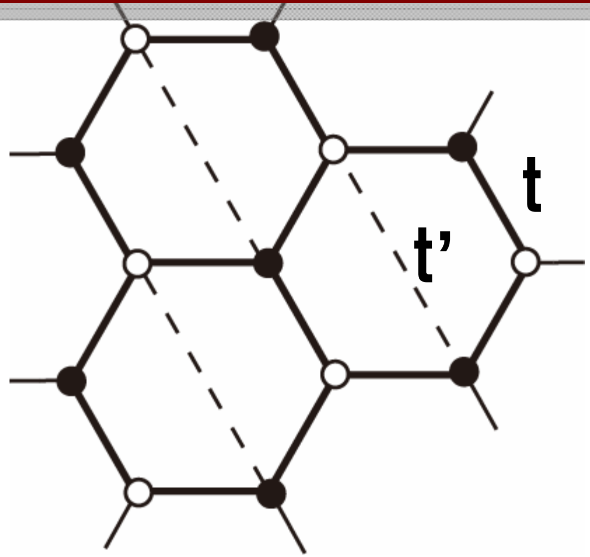


anomalous (2n+1) QHE:

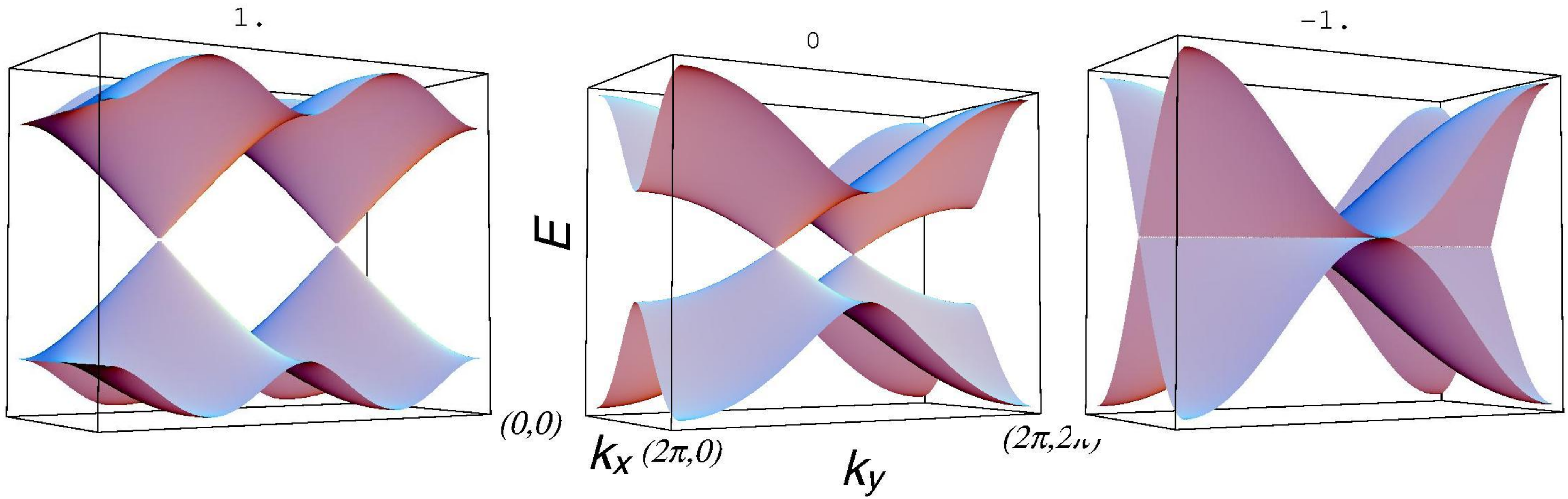
↑ lattice gauge (Fukui & Hatsugai)

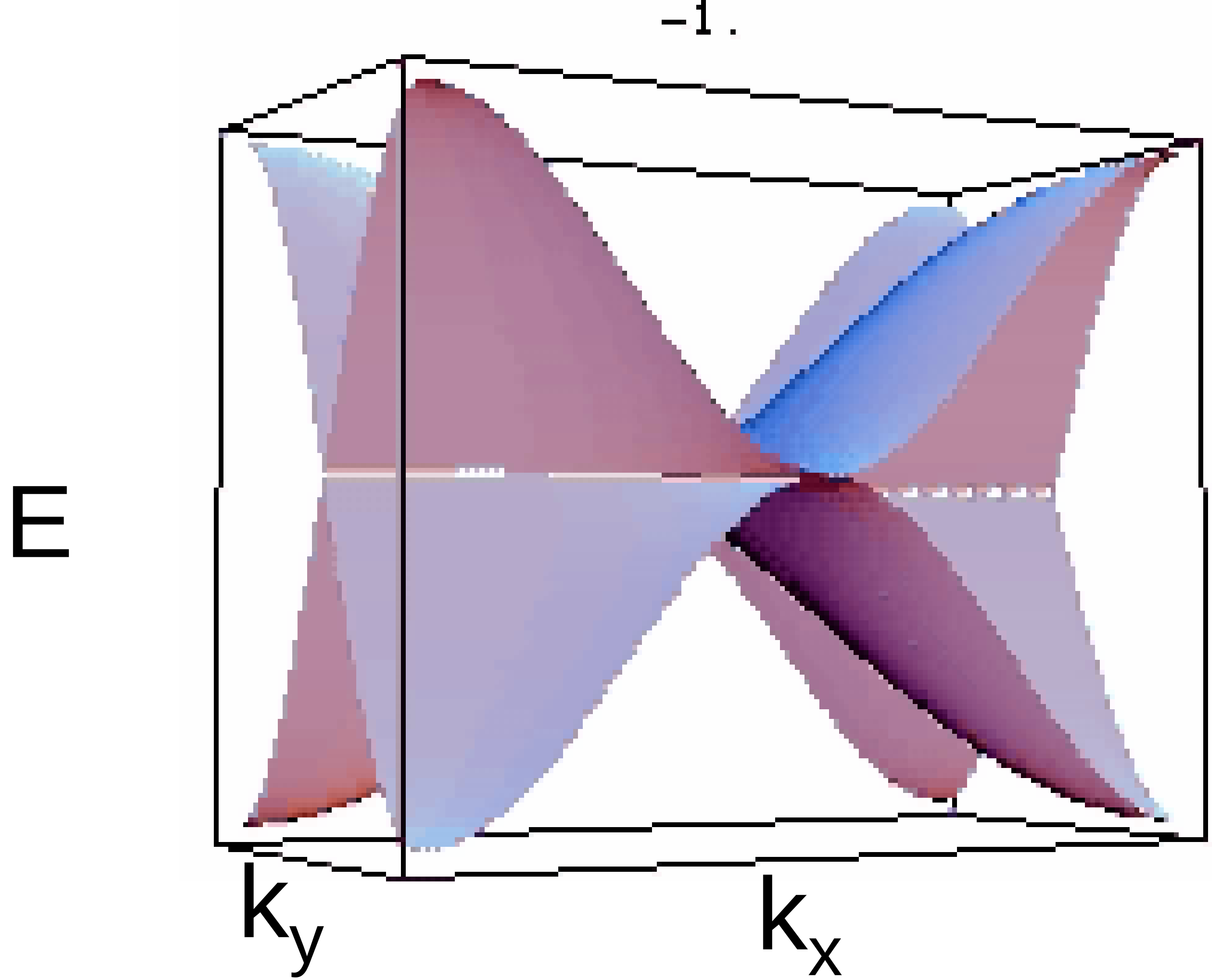
t ∼1 eV for graphene

"Massless Dirac" for a sequence of



t'=−1: π−flux lattice   t'=0: honeycomb   t'=+1: square





•Not specific to graphene

but shared by a class of non-Bravais lattices ?

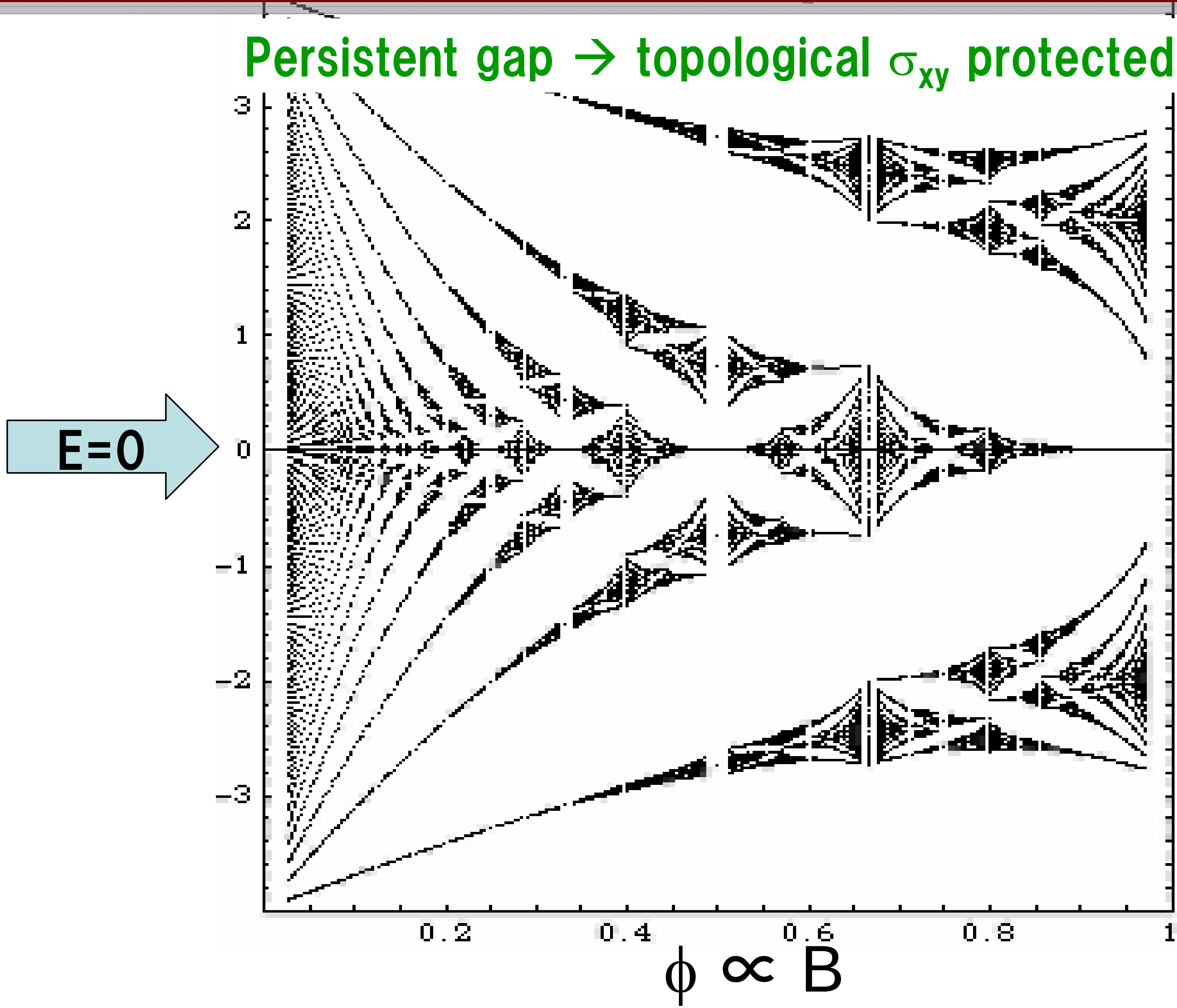
cf. recent organic system

* Dirac cones seem to always appear in pairs

--- Nielsen-Ninomiya

Adiabatic continuity for QHE

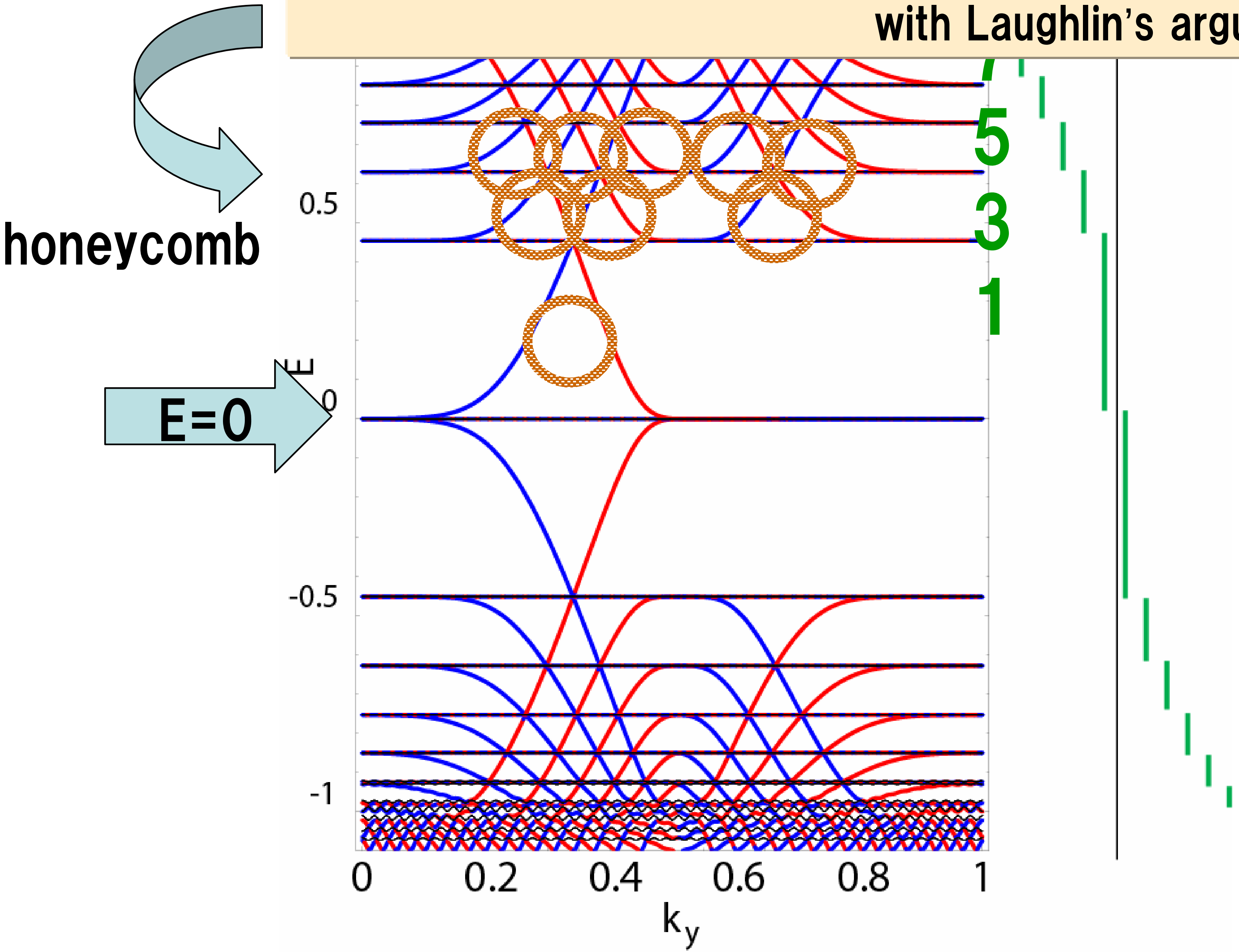
Persistent gap → topological σ_{xy} protected



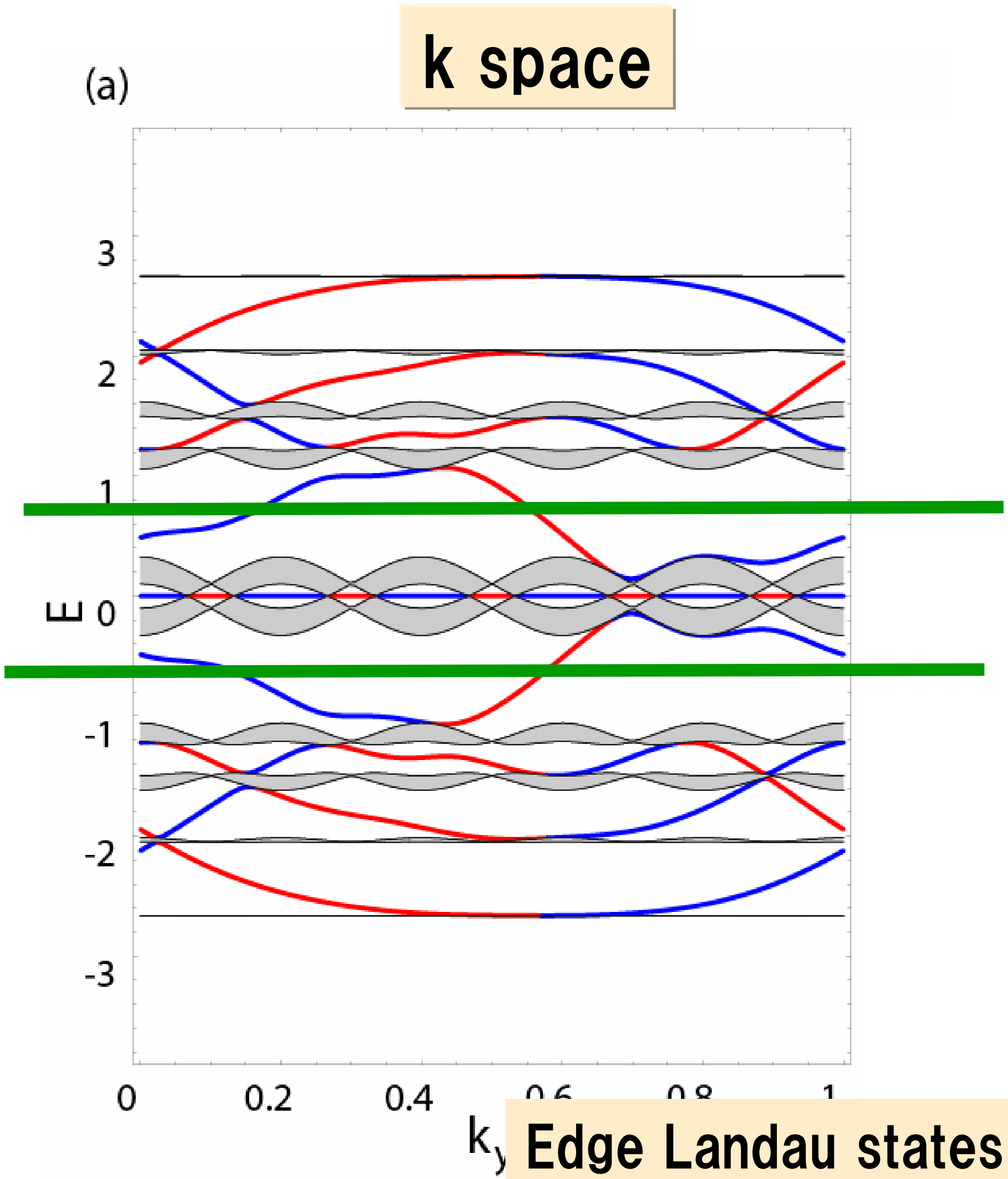
$\sigma_{xy}^{bulk} = \sigma_{xy}^{edge}$ *in honeycomb*

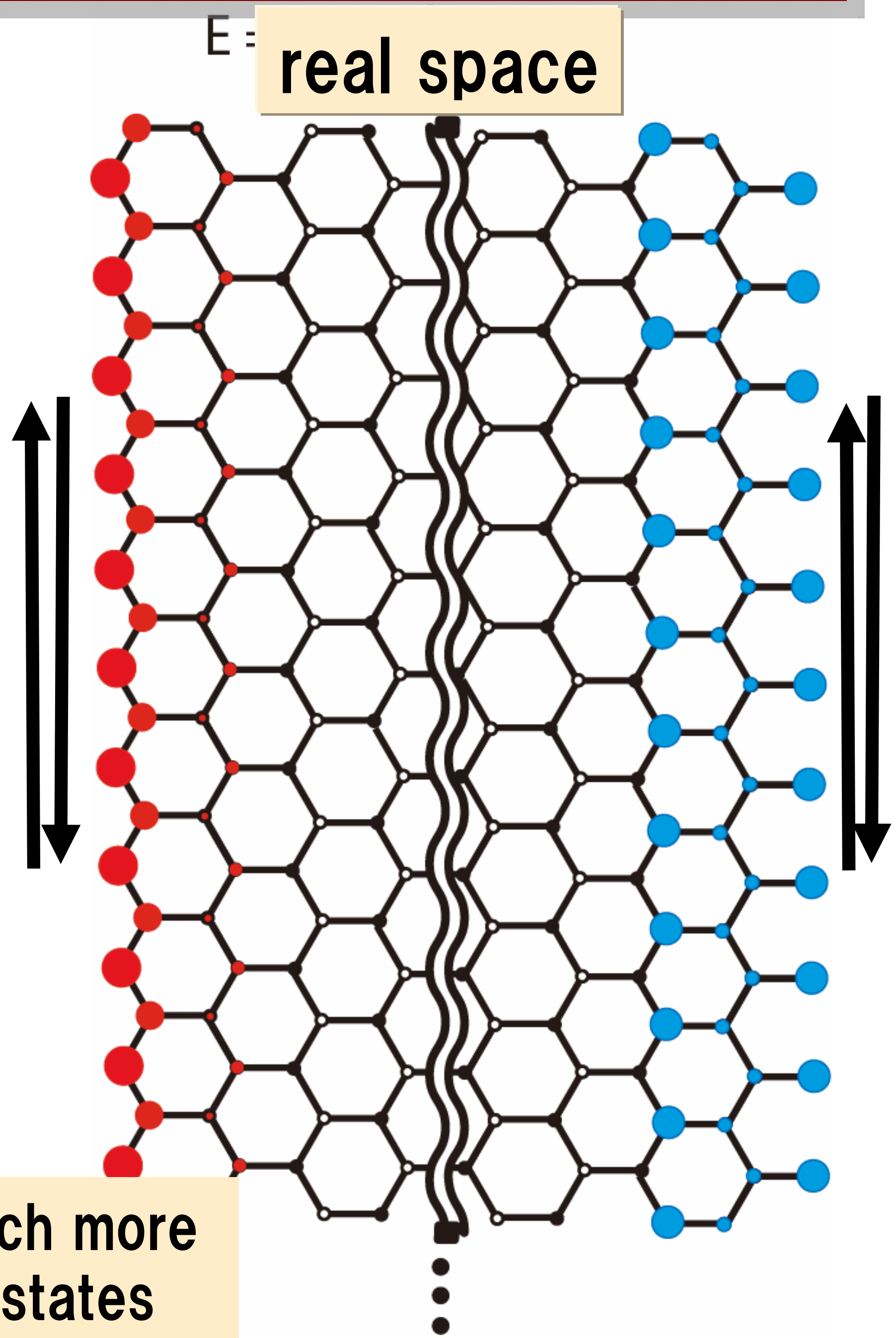
Ordinary QHE: $\sigma_{xy}^{bulk} = \sigma_{xy}^{edge}$ ←Hatsugai, 1993

with Laughlin's argument



Edge Landau states



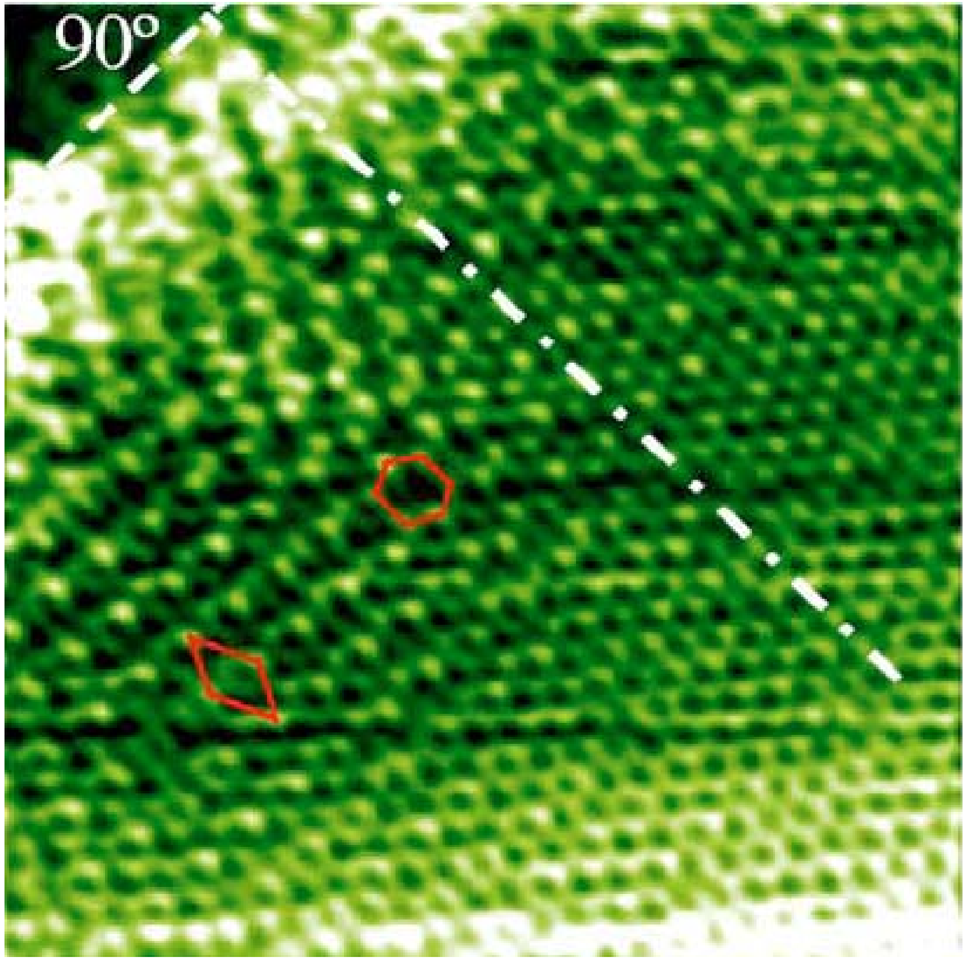


Edge Landau states much more robust than B=0 edge states

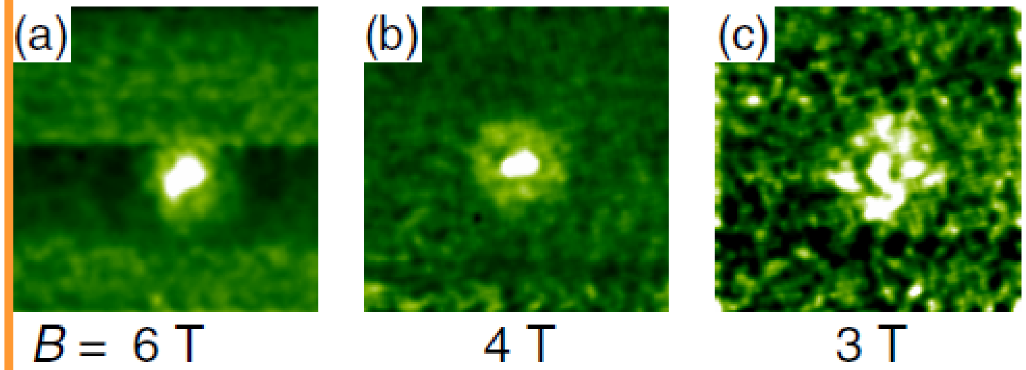
Boundary states with STM

* STM for graphite:

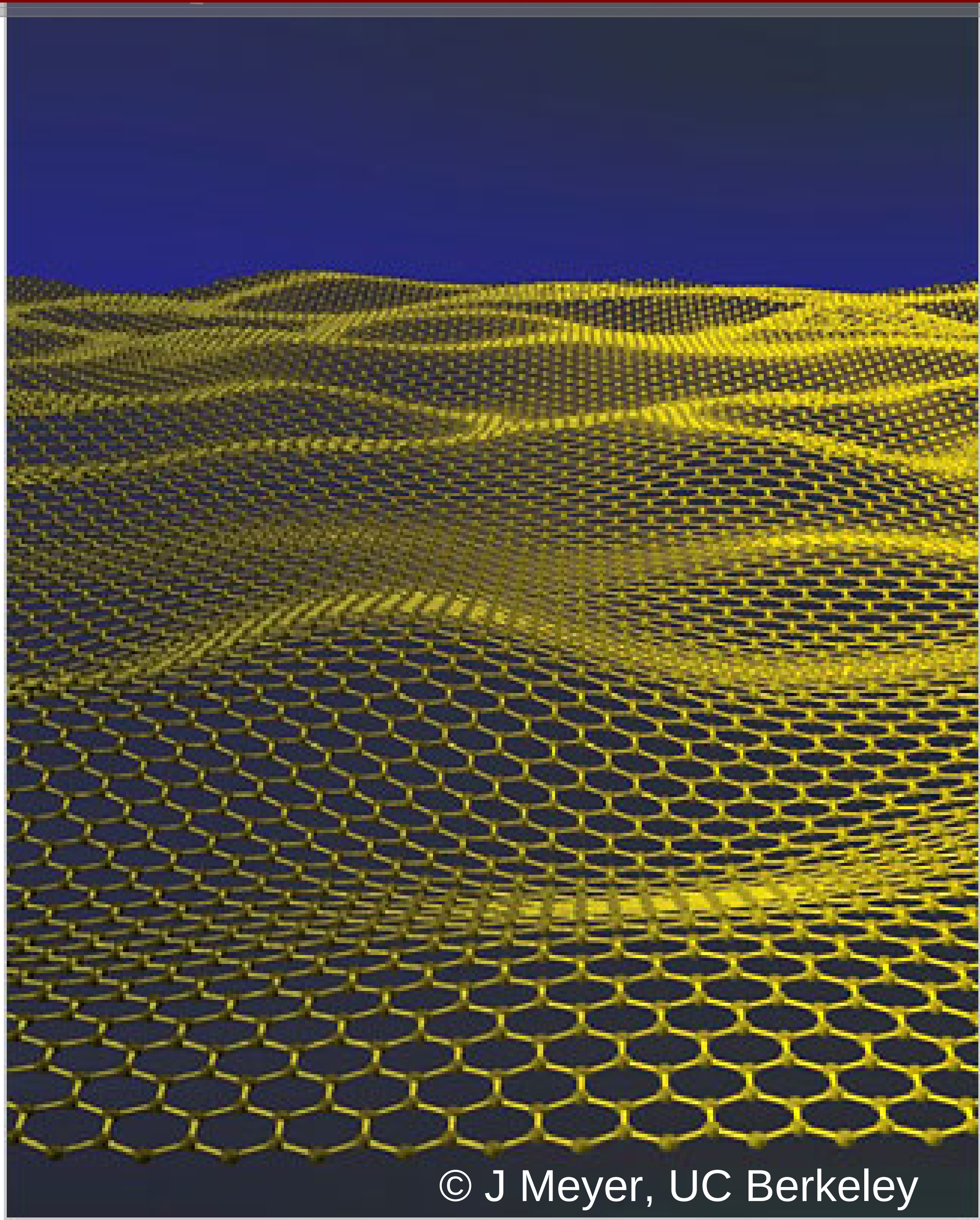
Edge (Niimi et al, PRB 2006)



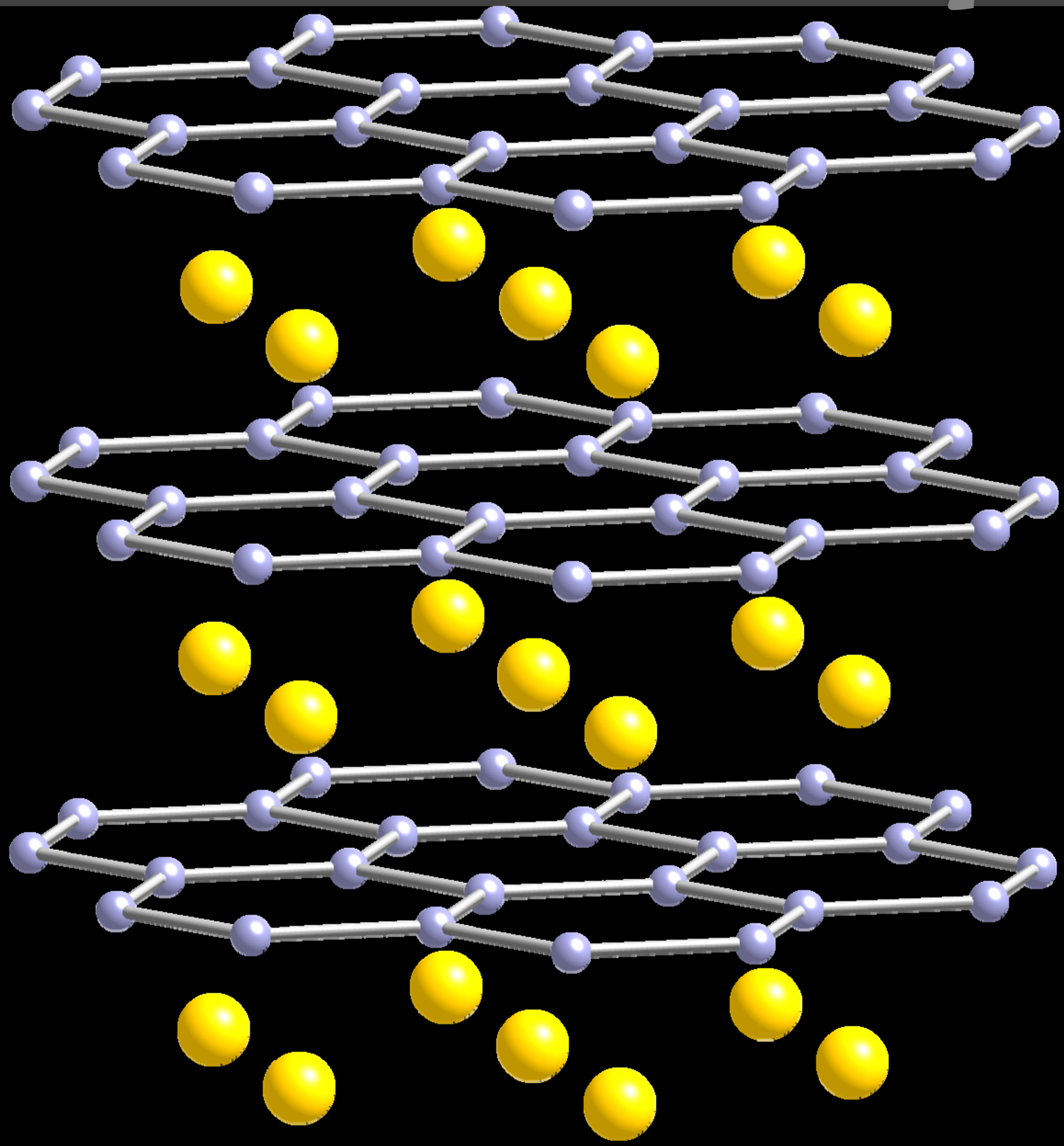
Point defect in B
(Niimi et al, PRL 2006)



2D crystals should not exist



Related structures: GIC, MgB_2



MgB_2 bandstructure

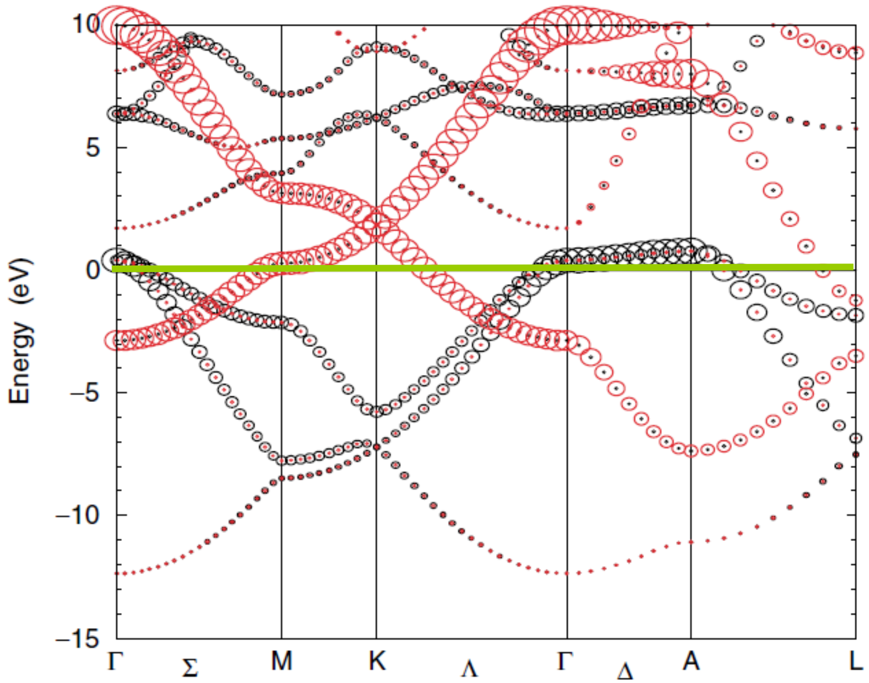
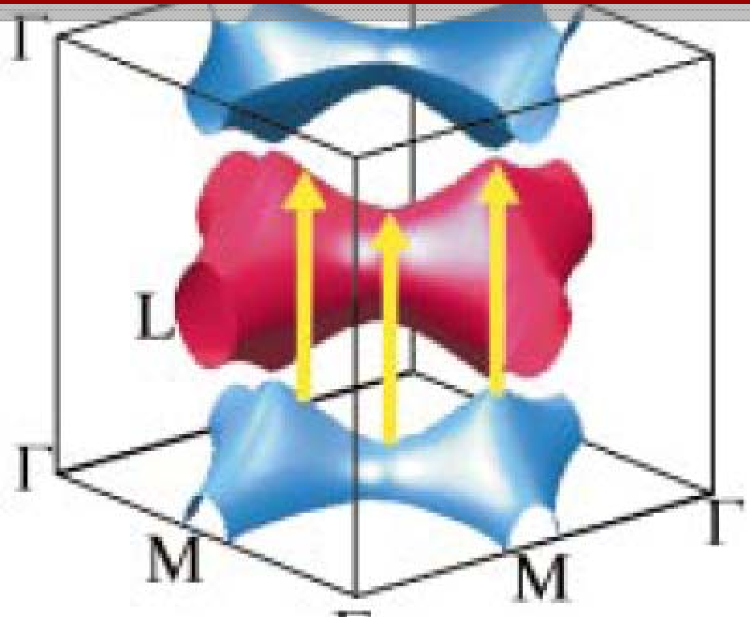
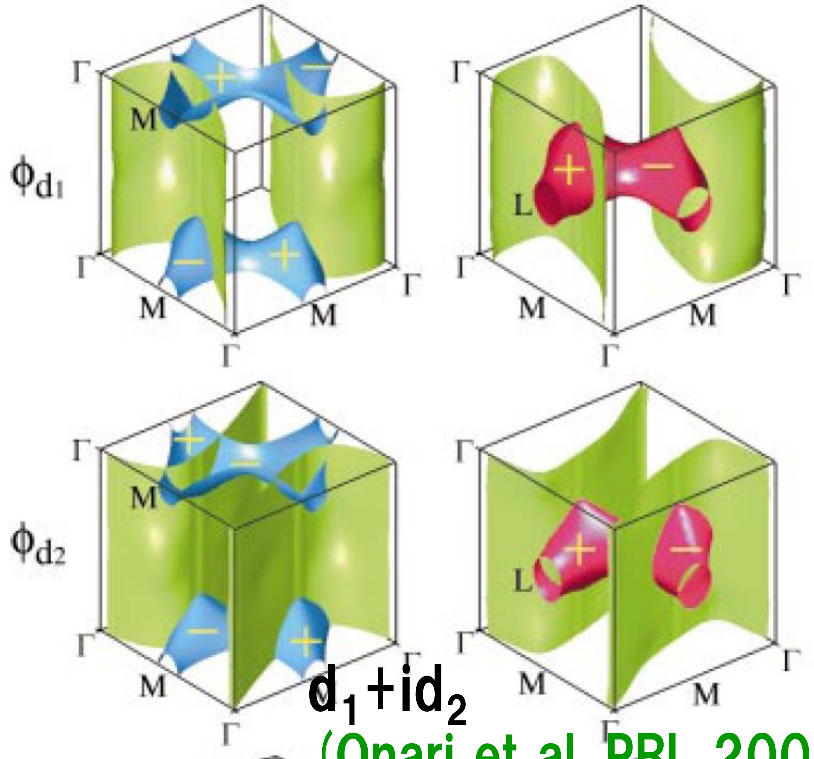


FIG. 1 (color). Band structure of MgB_2 with the B p character. The radii of the red (black) circles are proportional to the B p_z (B $p_{x,y}$) character.

(Kortus et al, PRL 2001)





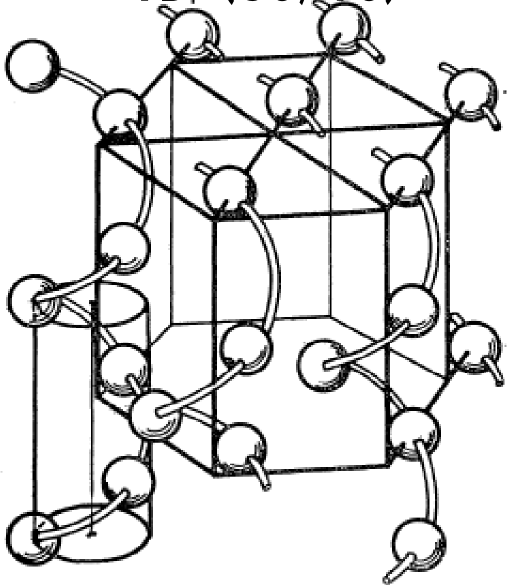
d_1+id_2

(Onari et al, PRL 2002)

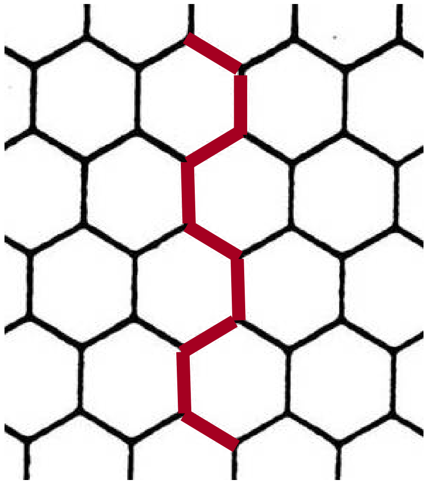
cf. p wave SC becomes
p + ip at K point in honeycomb
(Uchoa & Castro Neto, PRL 2007)

Why the bands stick together at Bz edges

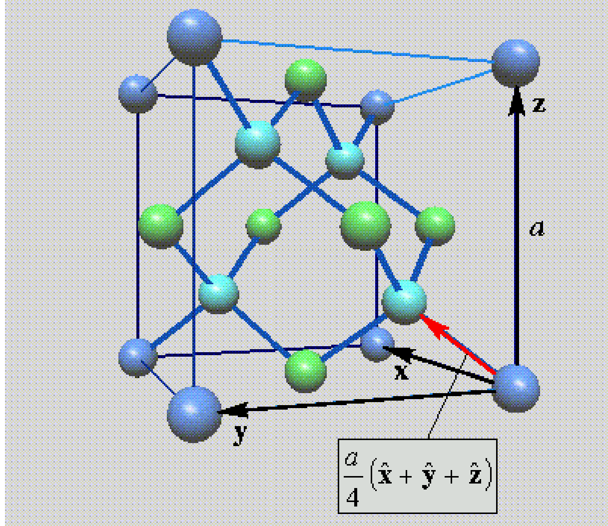
1D (Se, Te)



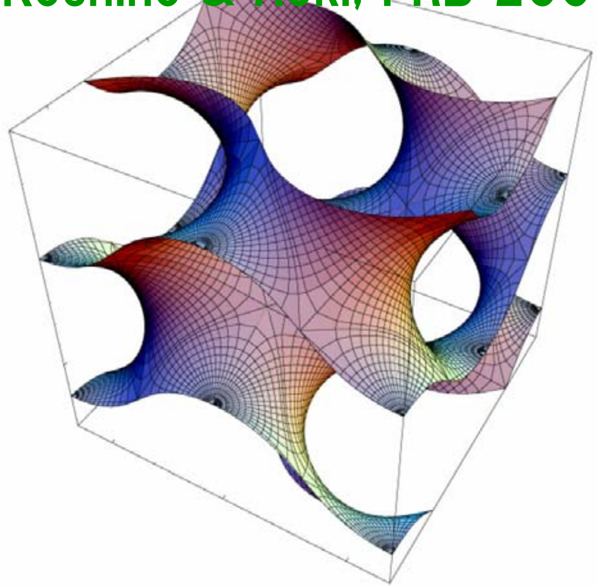
2D (graphite)



3D (diamond)

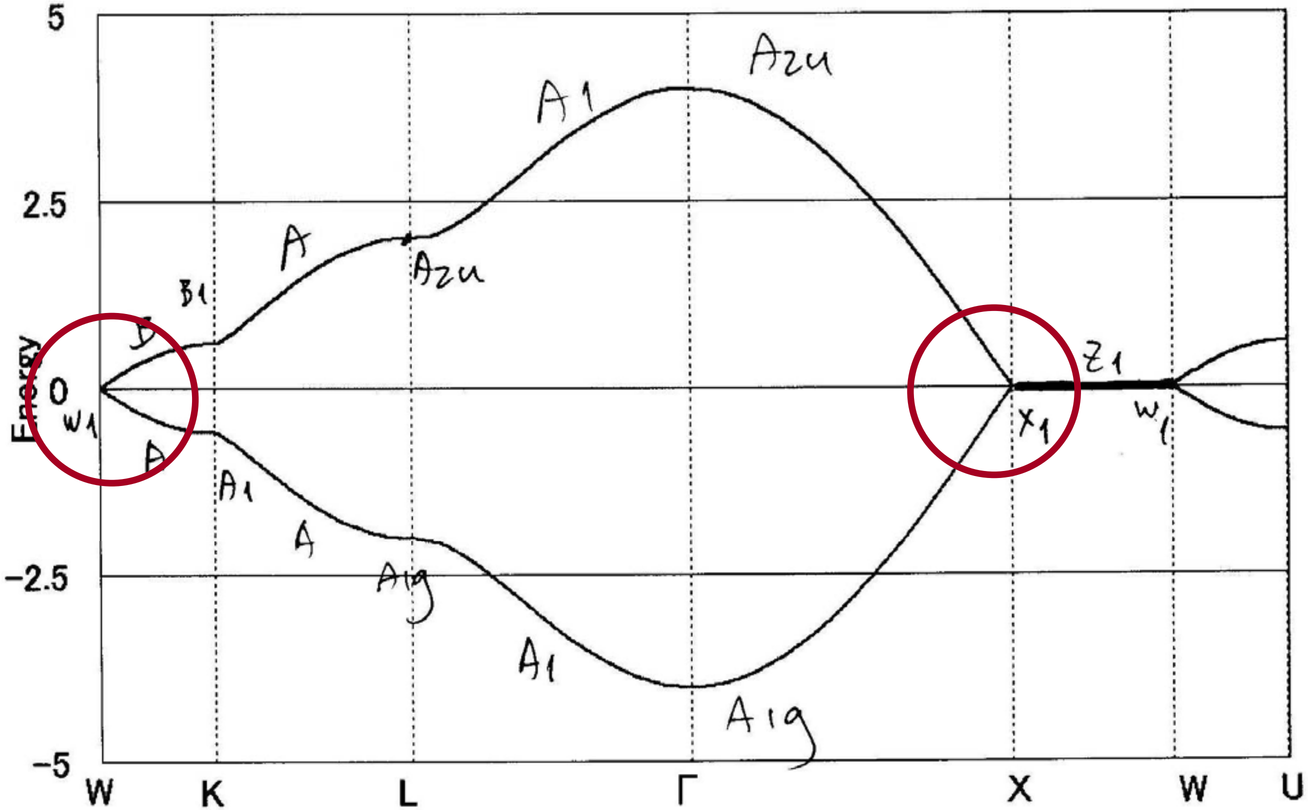


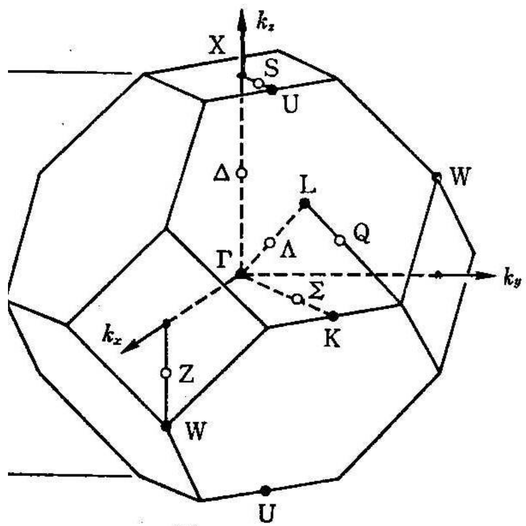
(gyroid system:
[Koshino & Aoki, PRB 2005])



helical symmetry → band sticking
(see, eg, Heine 1960)

Band for diamond (s orbits)

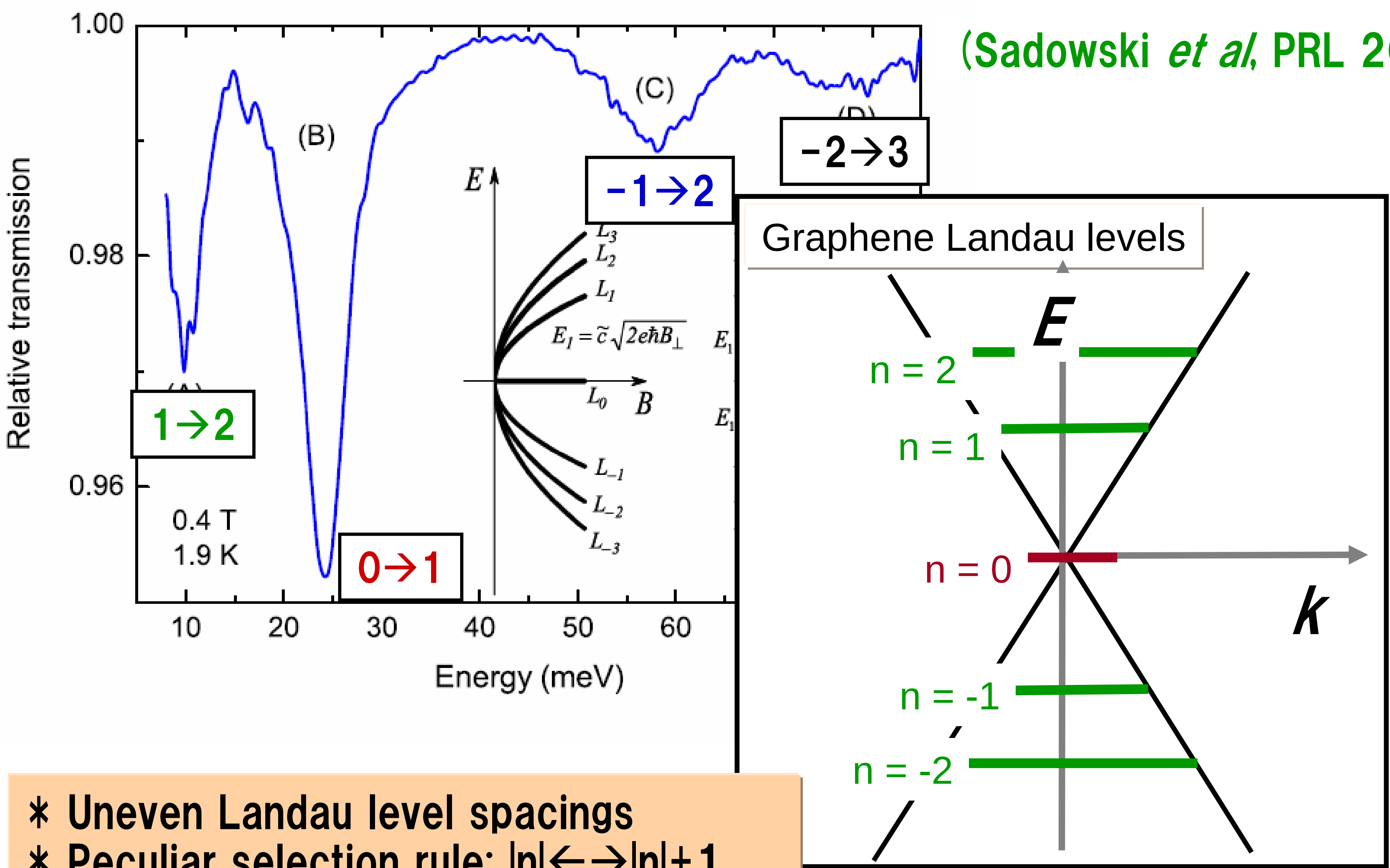




(b)

Optical spectroscopy for graphene Landau levels

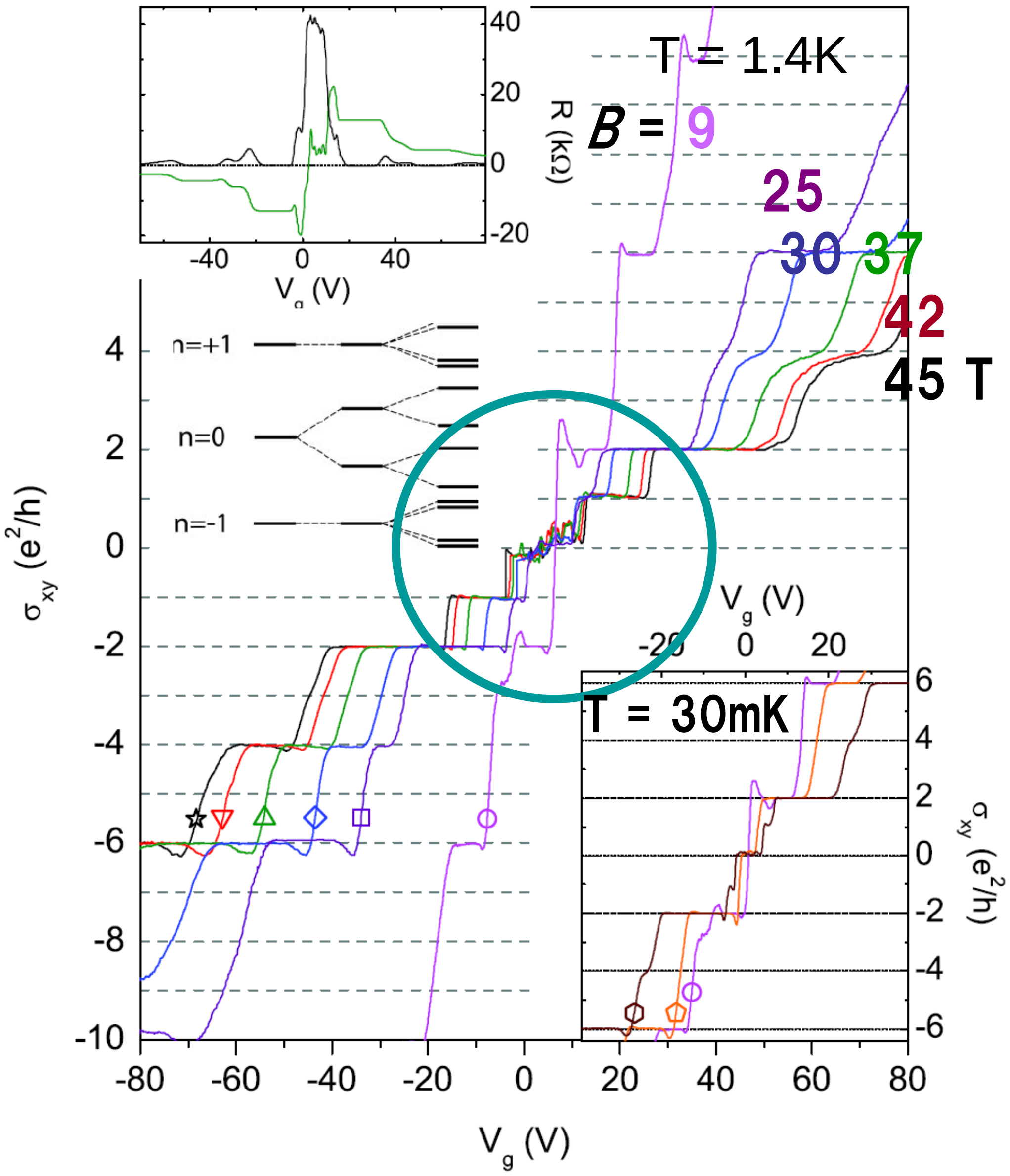
(Sadowski *et al*, PRL 2006)



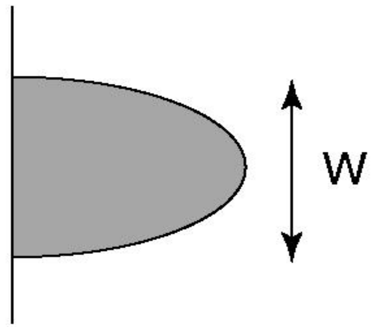
* Uneven Landau level spacings
* Peculiar selection rule: |n|←→|n|+1 (usually, n←→n+1)

Observed splitting of Landau levels

(Zhang et al, PRL 2006)



Correlated electron systems



$$\frac{U}{W} = \text{large}$$

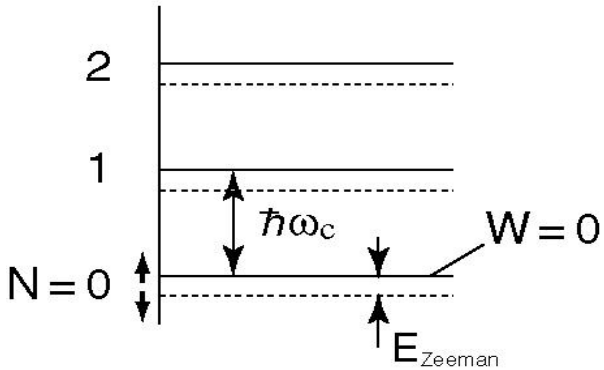
$\rightarrow$ strong correlation

band filling

n=1 Mott transition

n≠1 Superconductivity
Stripe
⋮

FQHE systems



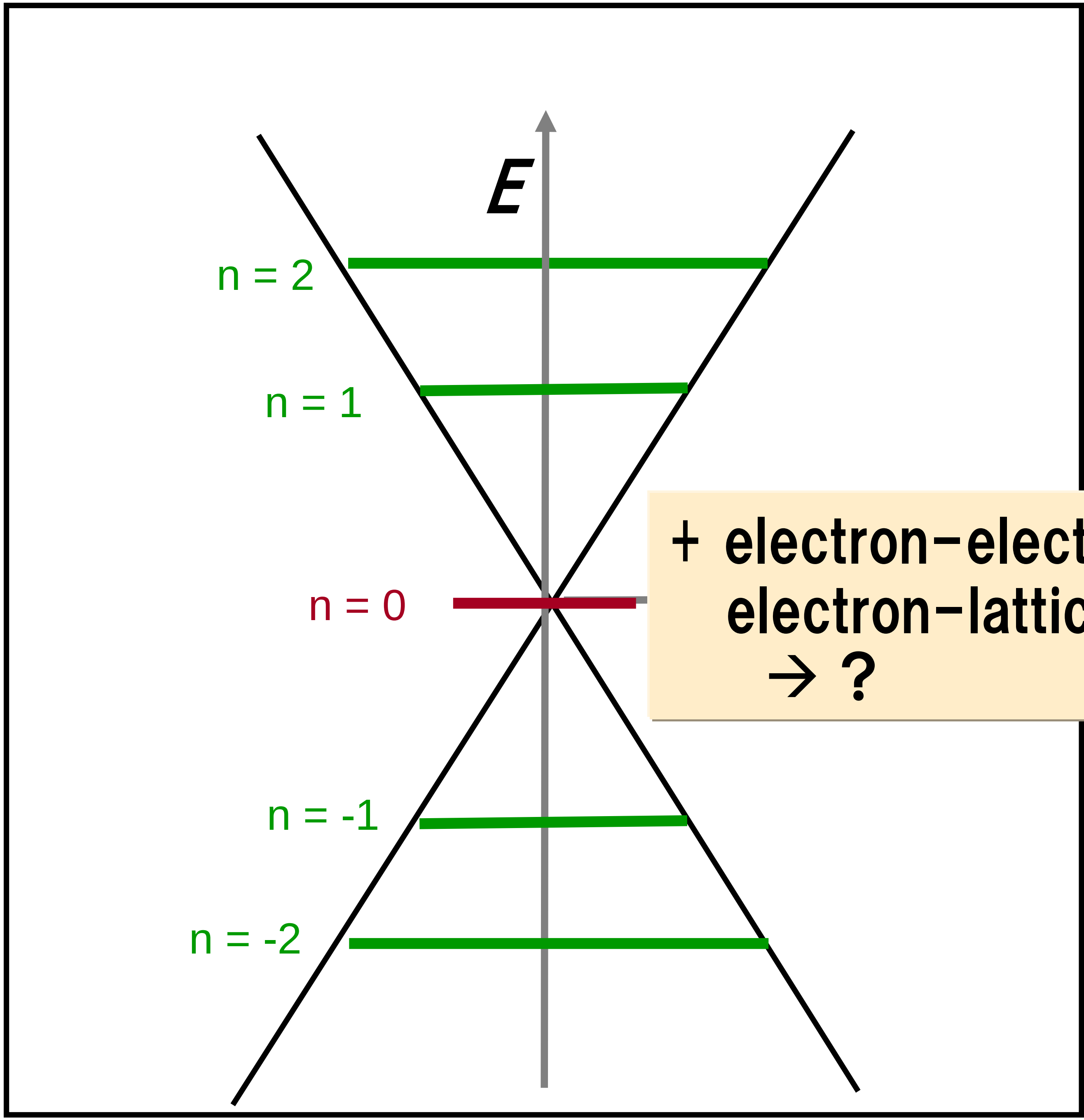
$$\frac{U}{W} = \infty$$

$\frac{U}{\hbar\omega_c}$, $\frac{U}{E_{Zeeman}}$: controllable

$\nu = \frac{1}{\text{odd}}$ Laughlin's QL

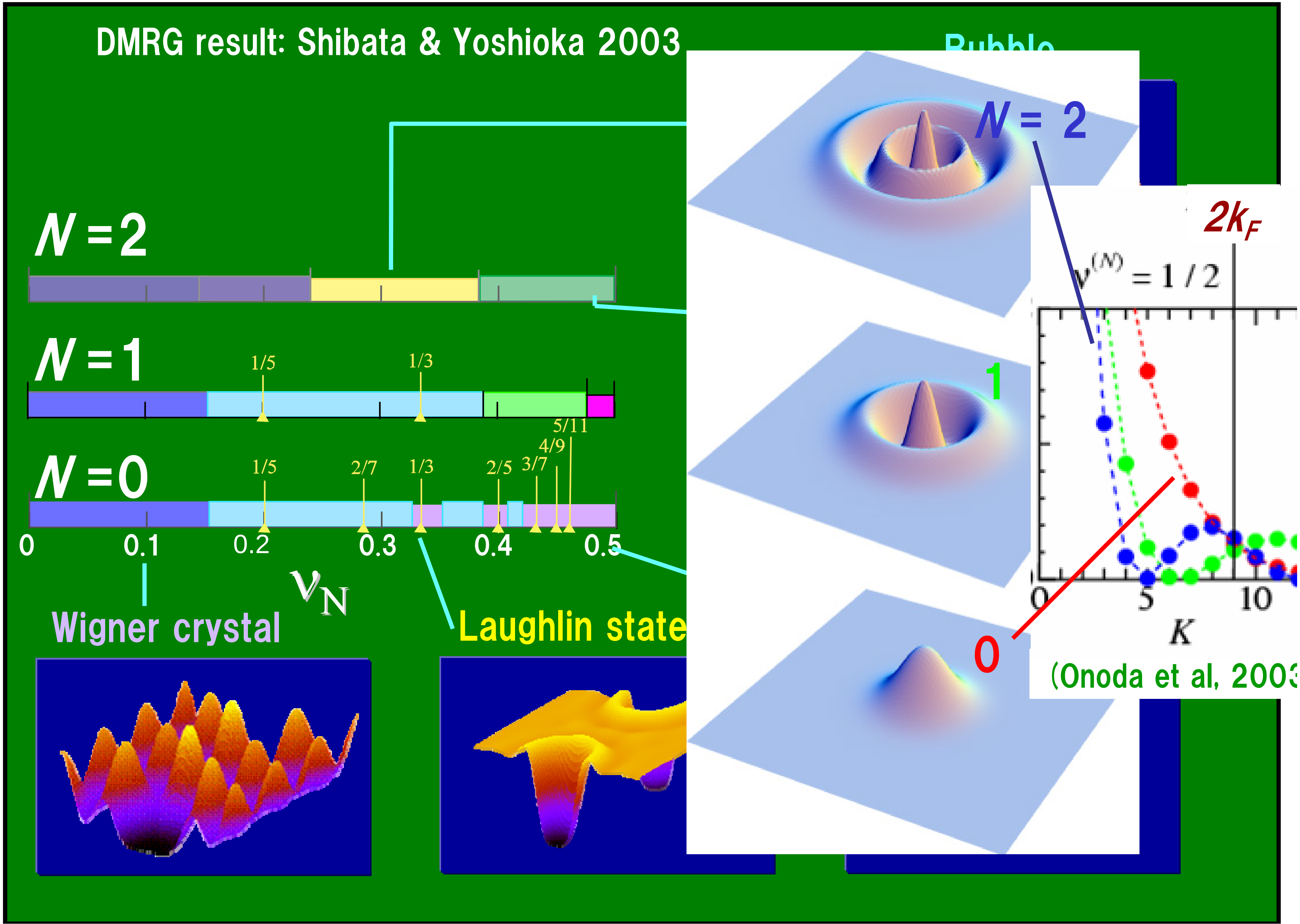
$\nu = \frac{*}{\text{even}}$ (marginal?) FL
BCS state?
stripe
⋮

Many-body effects in graphene Landau levels



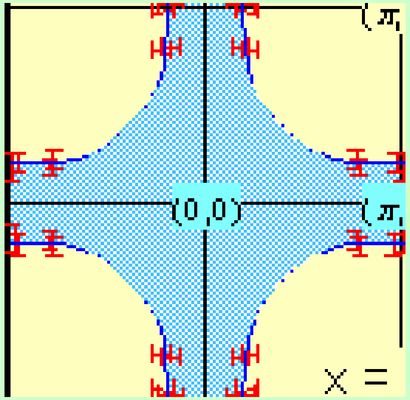
+ electron-electron interaction,
electron-lattice interaction
→ ?

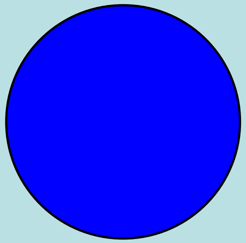
Various phases in the quantum Hall system

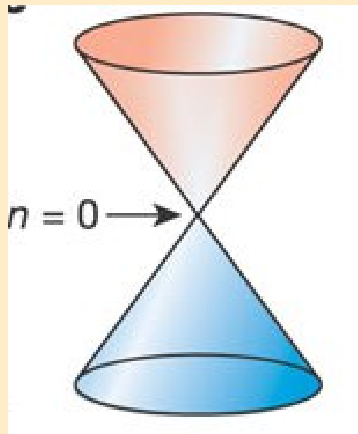


As strongly-correlated systems:

HTC	FQHE	graphene
Coulomb	gauge field	
anisotropic	isotropic	





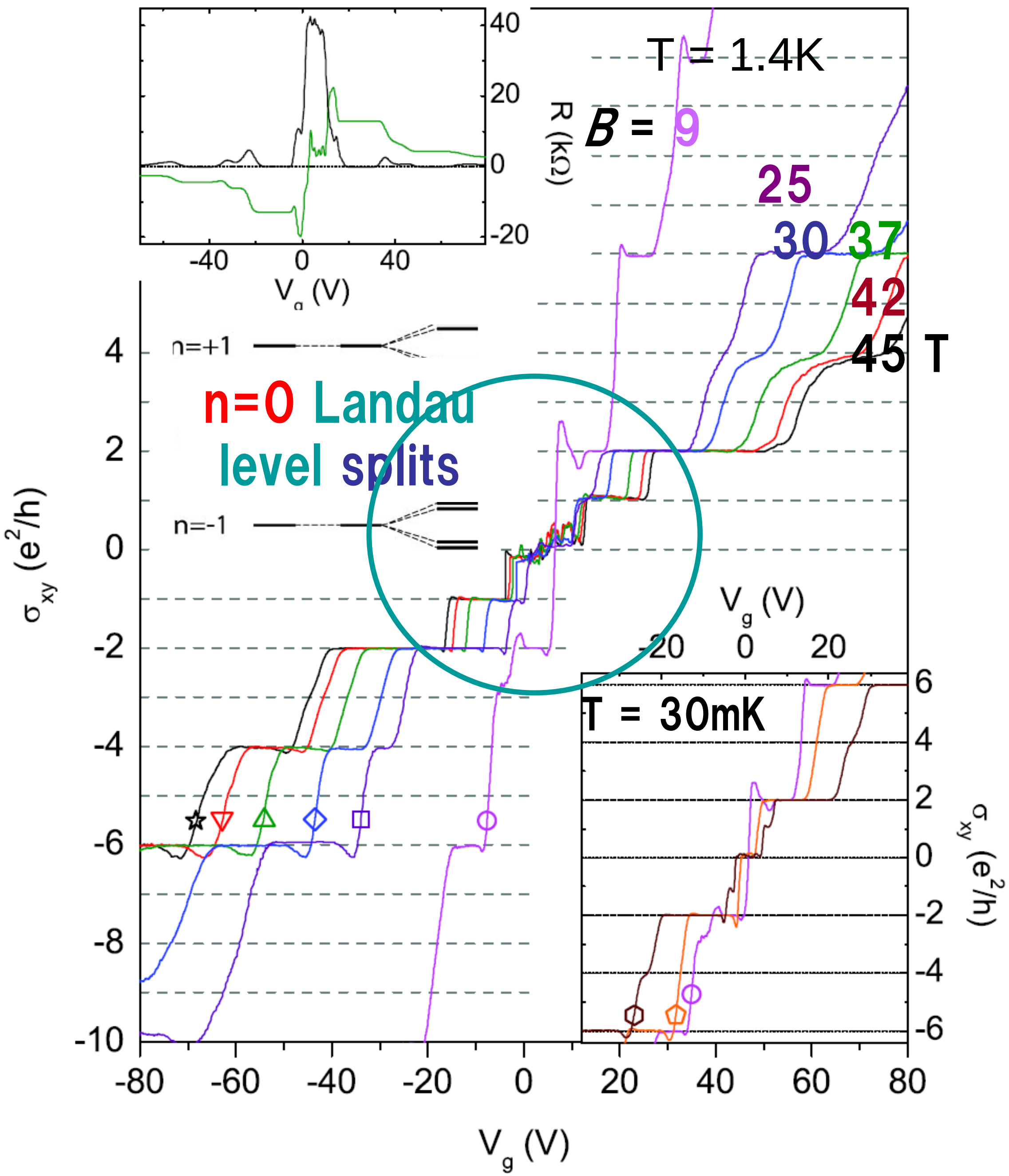


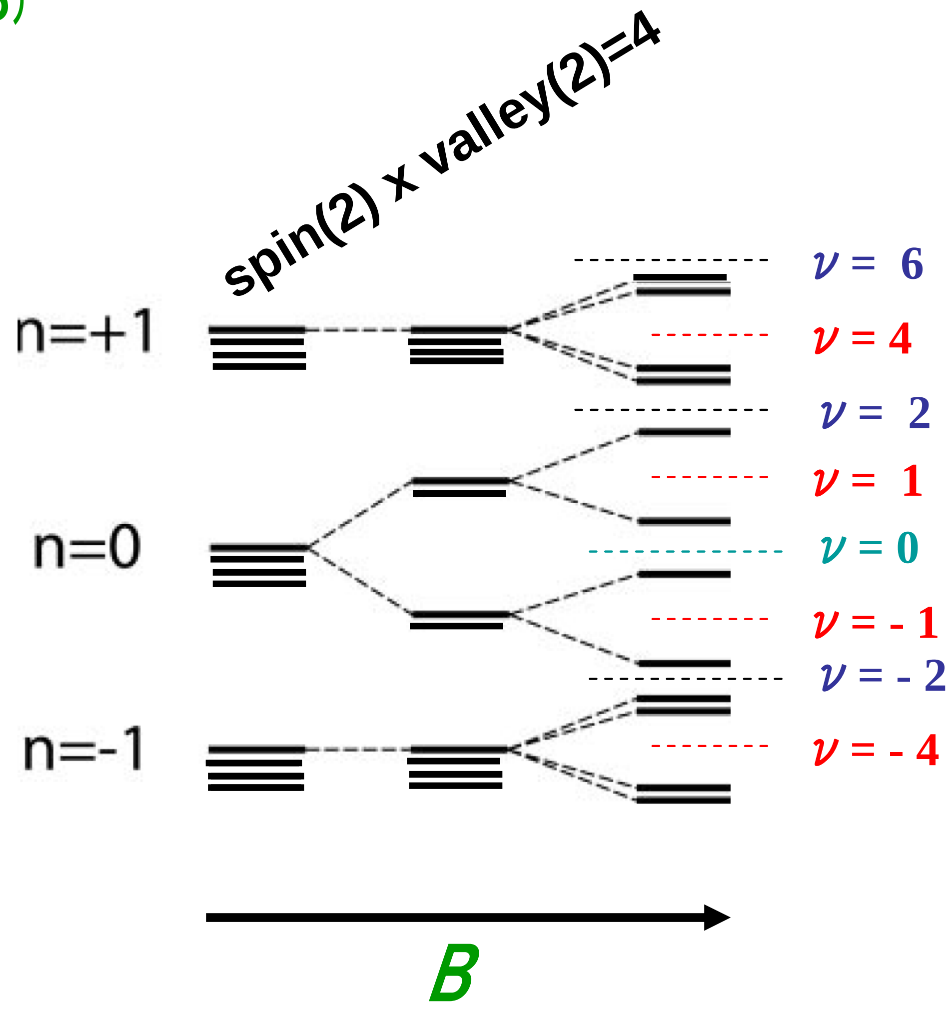
Reminds us of Kohn-Luttinger 1965

every metal $\xrightarrow[T \to 0]{}$ normal states become instable

Observed splitting of Landau levels

(Zhang et al, PRL 2006)





Proposed mechanisms for split Landau levels

* Excitonic gap (Gusynin et al, PRB 2006)

* SU(4)-breaking (Nomura & MacDonald, PRL 2007)

* FQHE (Apalkov & Chakraborty, PRL 2006)

* Peierls distortion (Fuchs & Lederer, PRL 2007)

☑ Bond order (Hatsugai et al, 2007)

・・・

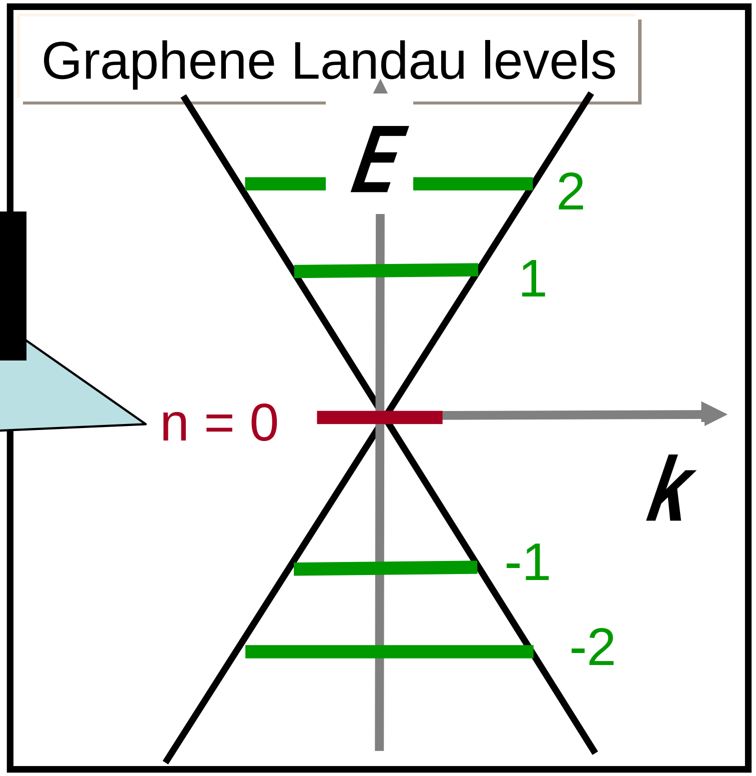
Bond ordering

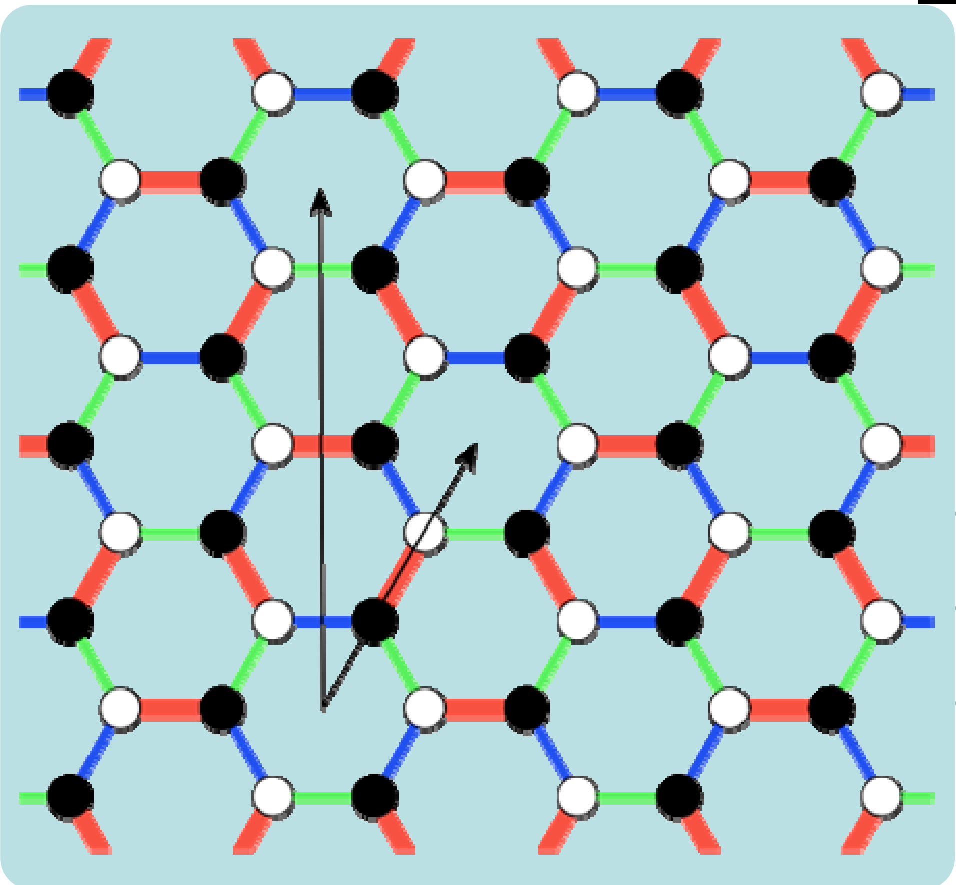
(Hatsugai, Fukui & Aoki, 2007)

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

(Affleck-Marston 1988)

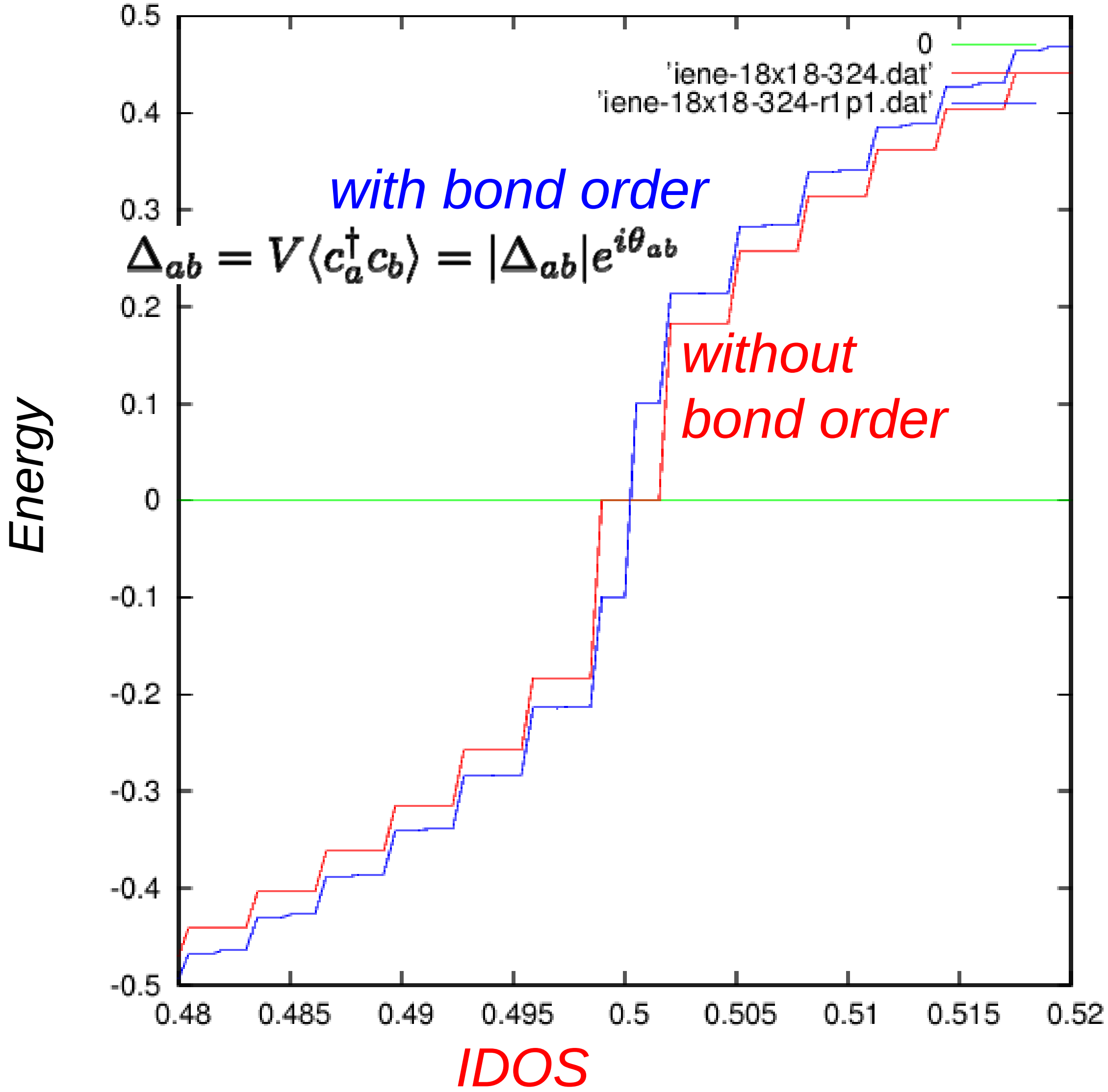
stabilised due to D (E) = ∞

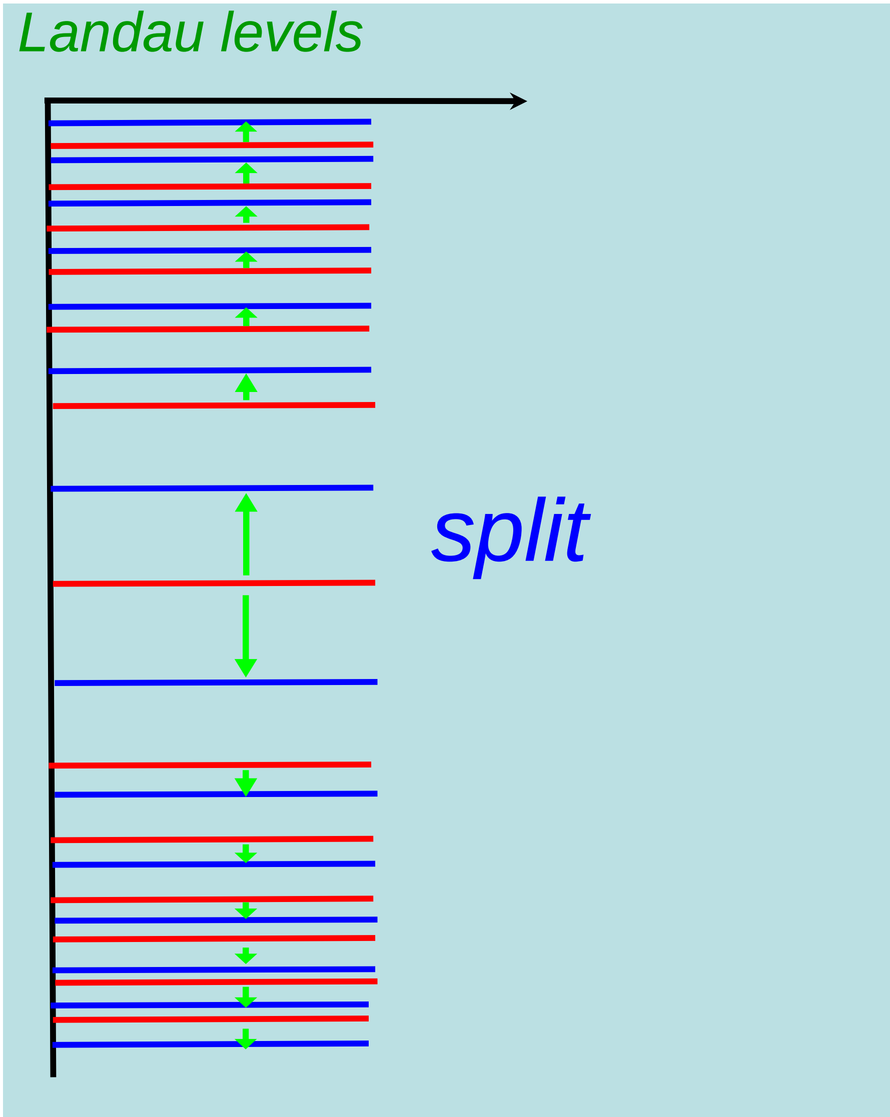




- "Kekulean" pattern
- but the chiral symm preserved
- 3-fold degenerate

Gap opening with the bond ordering

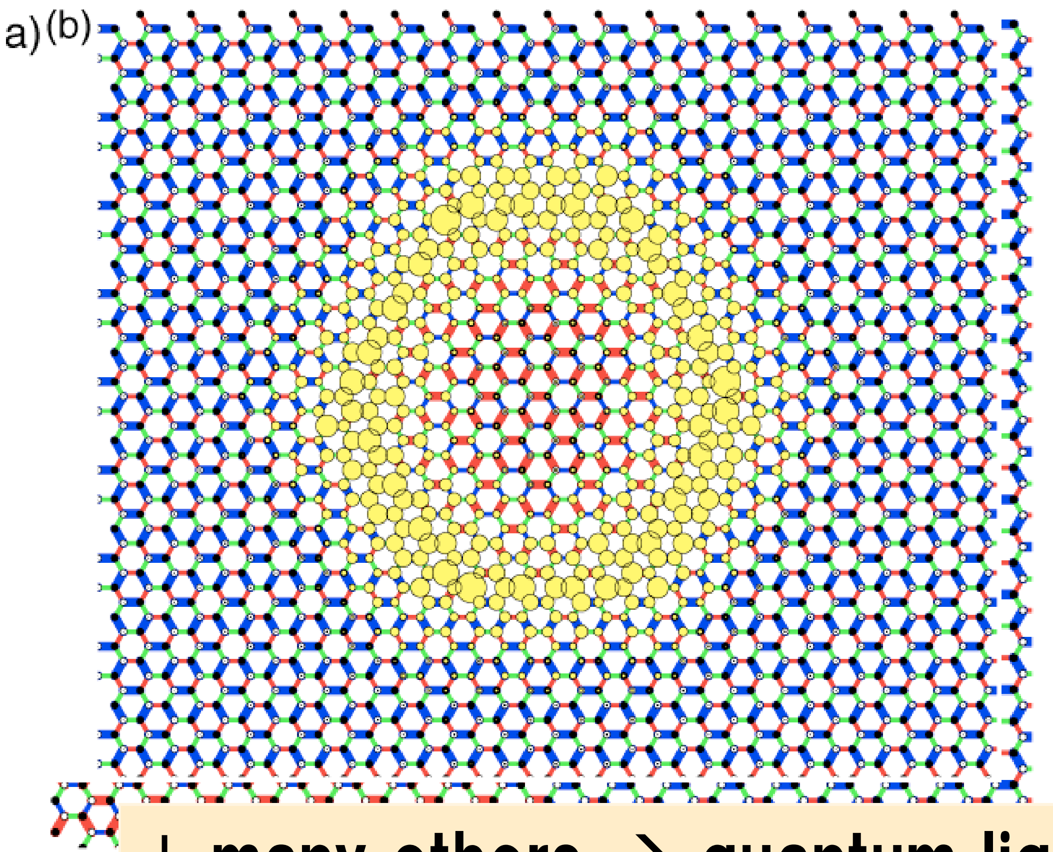


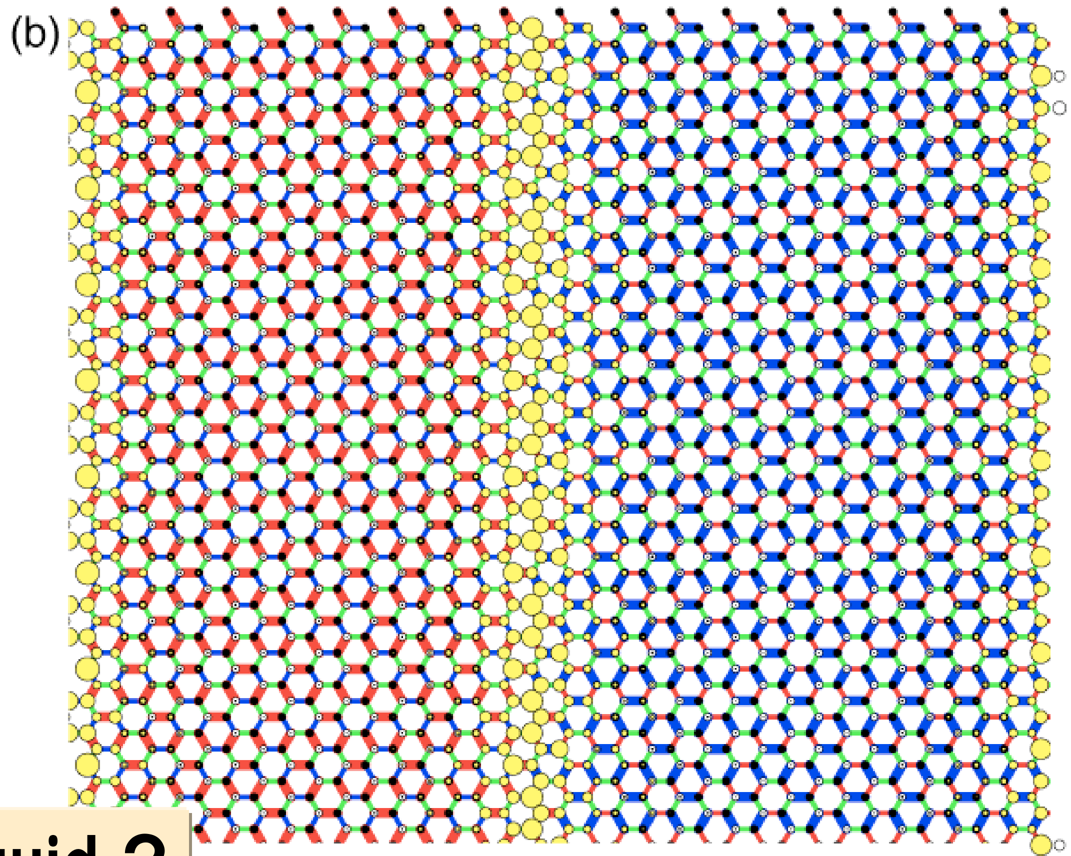


18 x 18, ϕ =1/324

Domain structures in bond ordering

Charge Density of the in-gap states





+ many others → quantum liquid ?

Summary

Graphene: one-body

- massless Dirac + B → peculiar QHE
- QHE: topological
  → bulk-edge correspondence

Graphene: many-body

- Landau level + interaction
  → various instabilities expected

Future problems

- re-doing the condensed-matt phys picking up anomalies on the way