Numerical study of quantum Hall effects in two-dimensional multi-band system: single- and multi-layer graphene

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Introduction

Quantum Hall Effects

- Hall conductance is topologically quantized.
- $\sigma_{xy} = -\frac{e^2}{h} c_F$, c_F: Chern number
- Most of previous calculations for c_F were limited to simplified models.
  - simple tight-binding model
  - "free electrons"
  - massless Dirac Fermion

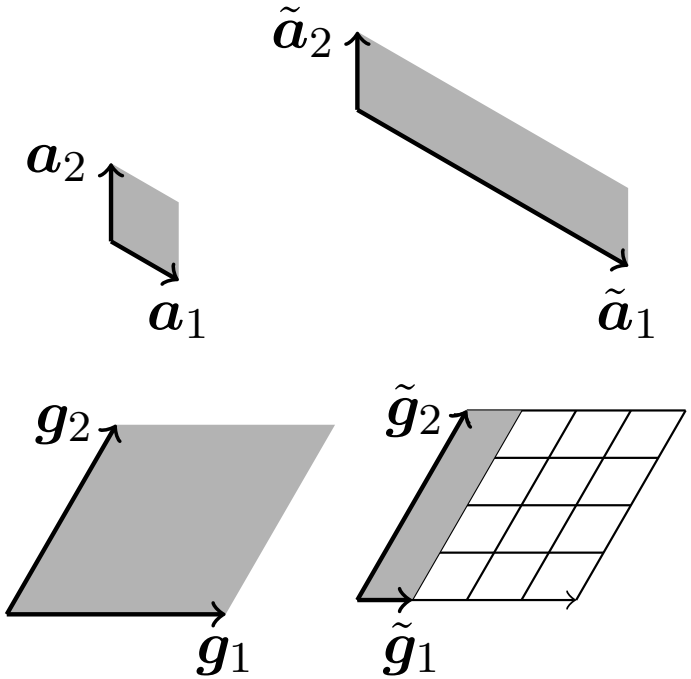
This work:

- QHE for "realistic band structure"
- Compute Chern numbers for realistic multi-band model.
  - Numerical demonstration
  - Application to graphene, multi-layer graphene, organic conductors.

Periodic system under uniform magnetic field

Magnetic flux in a unit cell $\phi = \frac{p}{q}$

$\phi = 0$	$\phi = \dfrac{p}{q}$
$\boldsymbol{a}_1, \boldsymbol{a}_2$	$\to \tilde{\boldsymbol{a}}_1 = q\boldsymbol{a_1}, \tilde{\boldsymbol{a}}_2 = \boldsymbol{a}_2$
unit cell: Ω	$\to q\Omega$
$\boldsymbol{g}_1$	$\to \tilde{\boldsymbol{g}}_1 = \dfrac{\boldsymbol{g}_1}{q}, \tilde{\boldsymbol{g}}_2 = \boldsymbol{g}_2$
BZ: Ω_{BZ}	$\to \Omega_{\mathrm{BZ}}/q$



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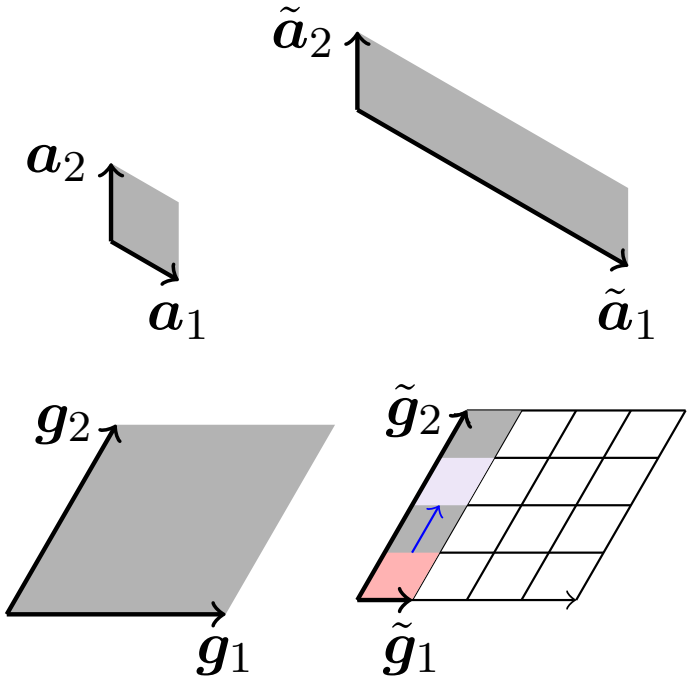


Utilize magnetic translational symmetry

$$\hat{T}_M(\boldsymbol{a}_1)\Psi_{\boldsymbol{k}} = \Psi_{\boldsymbol{k}+\frac{p}{q}\boldsymbol{g}_2}$$

Numerical calculations of Chern numbers

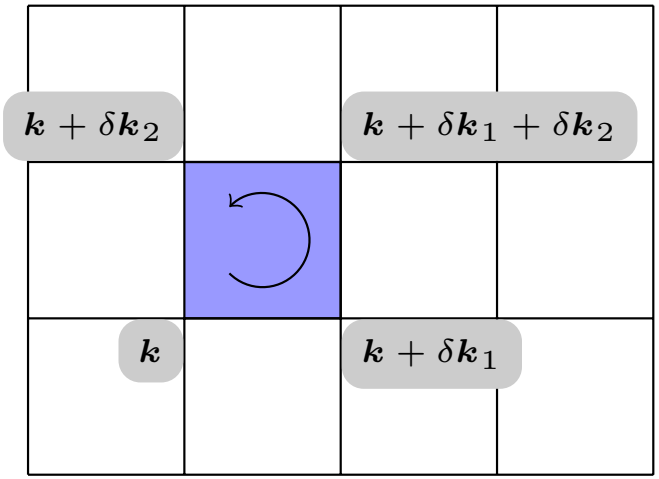
T. Fukui, Y. Hatsugai, and H. Suzuki, JPSJ, **74**, 1674 (2005)

- Divide (magnetic) BZ into uniform mesh points.
- Calculate eigenvectors:$\varepsilon_n(\boldsymbol{k}), |n;\boldsymbol{k}\rangle$
- Overlap integrals between adjacent mesh points:
  $U_{\boldsymbol{k_1},\boldsymbol{k_2}} \equiv \det(\langle n;\boldsymbol{k}_1|m;\boldsymbol{k_2}\rangle)$

Chern Number

$$\tilde{F}_{12}(\boldsymbol{k}) \equiv \mathrm{Arg}\{U_{\boldsymbol{k},\boldsymbol{k}+\delta\boldsymbol{k}_1} U_{\boldsymbol{k}+\delta\boldsymbol{k}_1,\boldsymbol{k}+\delta\boldsymbol{k}_1+\delta\boldsymbol{k}_2} U_{\boldsymbol{k}+\delta\boldsymbol{k}_1+\delta\boldsymbol{k}_2,\boldsymbol{k}+\delta\boldsymbol{k}_2} U_{\boldsymbol{k}+\delta\boldsymbol{k}_2,\boldsymbol{k}}\}$$

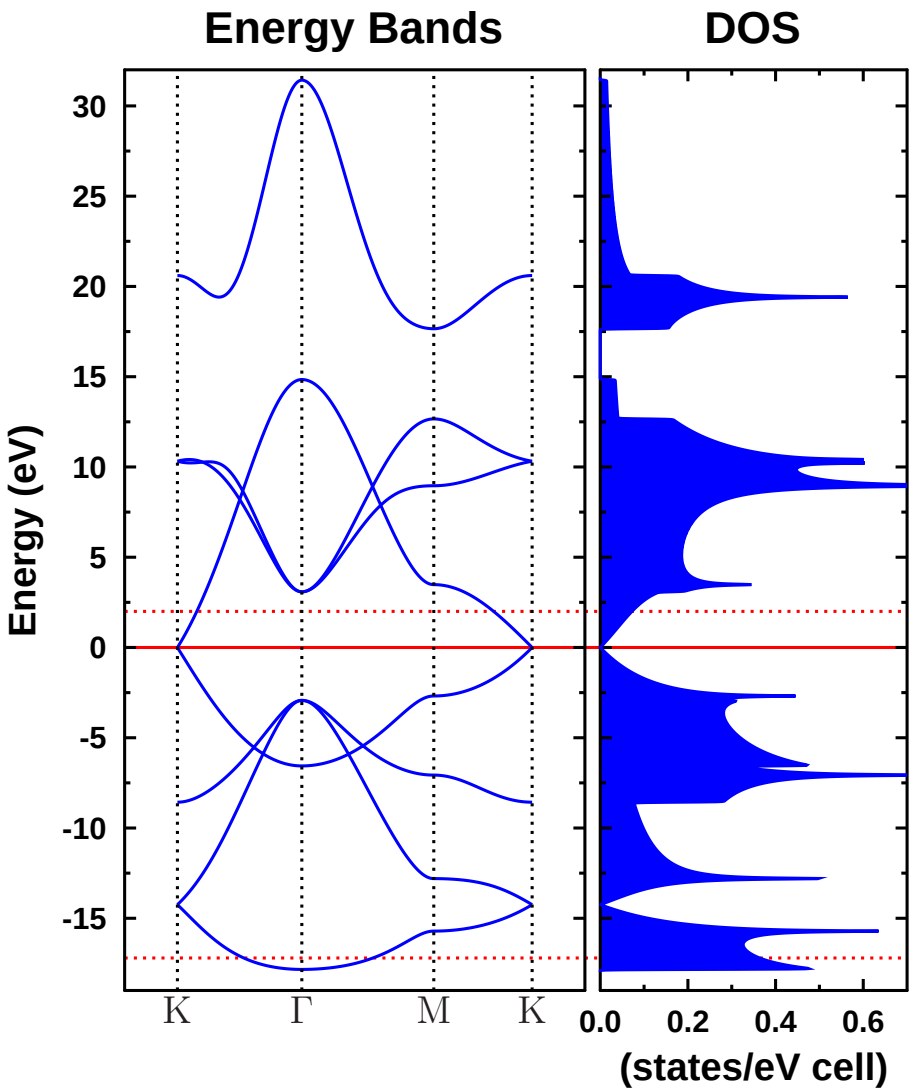
$$c_F = \frac{1}{2\pi}\sum_{\boldsymbol{k}} \tilde{F}_{12}(\boldsymbol{k})$$

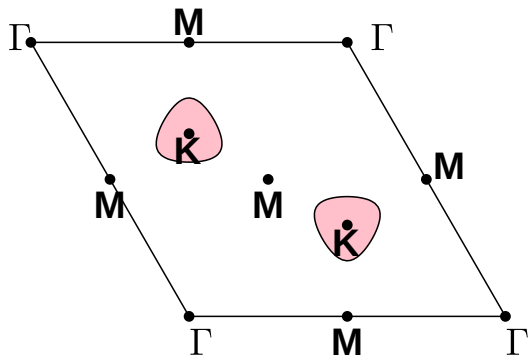


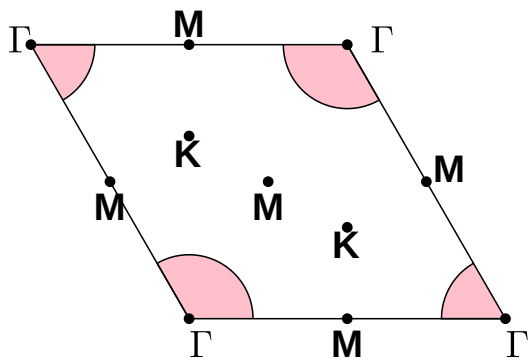
Graphene

Tight-binding model with s- and p- orbitals.
Nearest-Neighbor transfer and overlap integrals.
M.A and Y. Hatsugai, Phys. Rev. B79, 0705429 (2009)

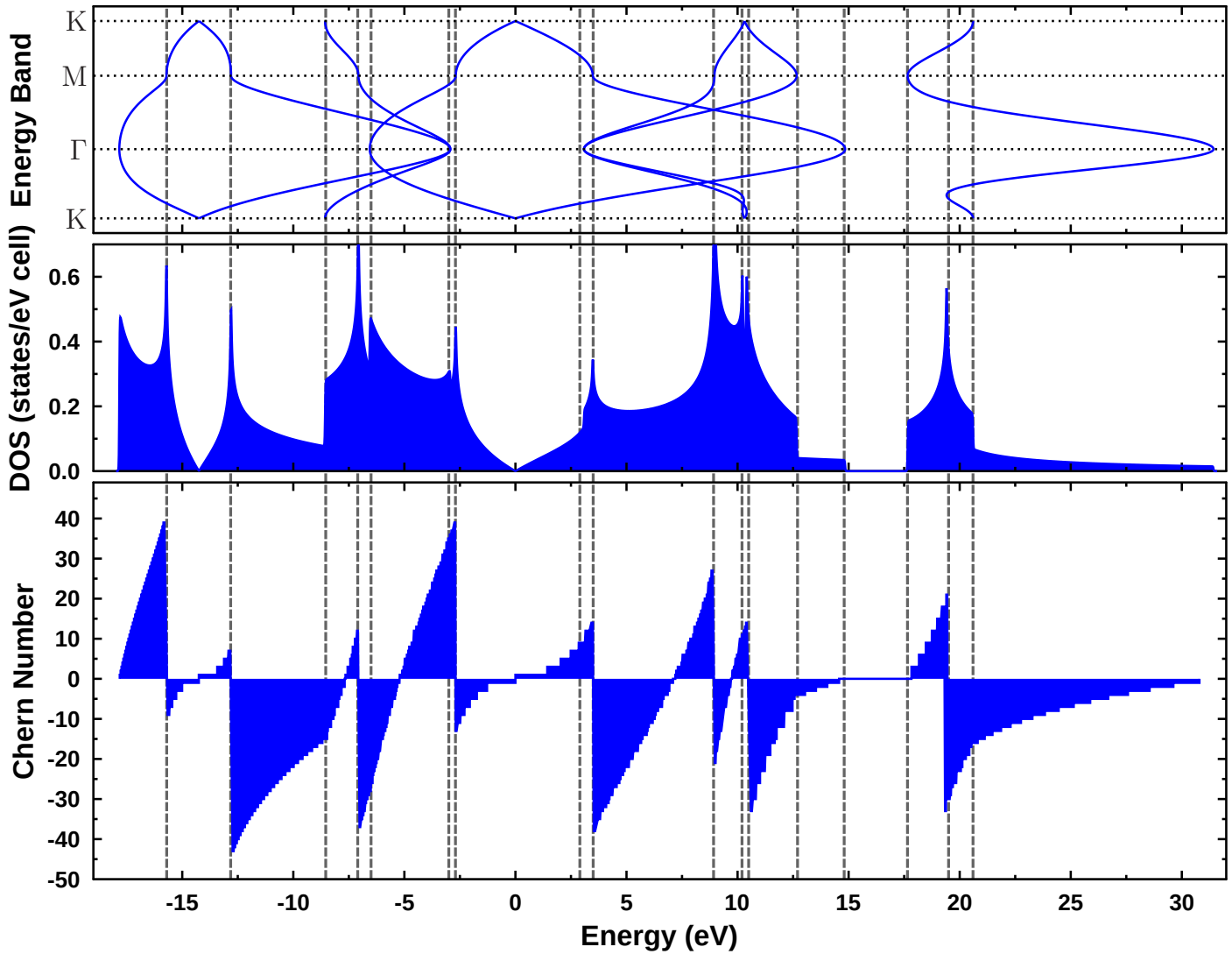
Graphene: Band Structure from Tight-Binding Model



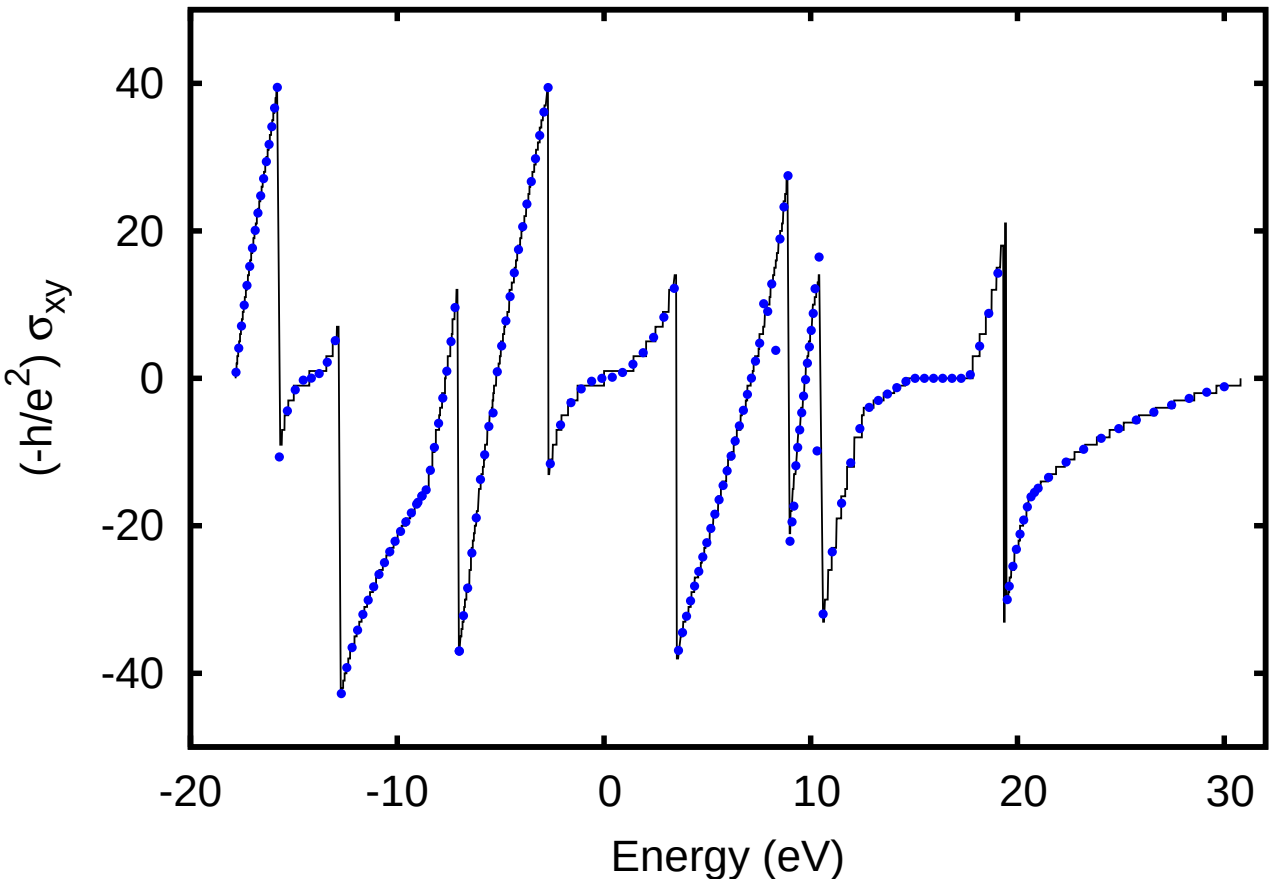




Chern number and van Hove singularities



Comparison with semi-classical theory



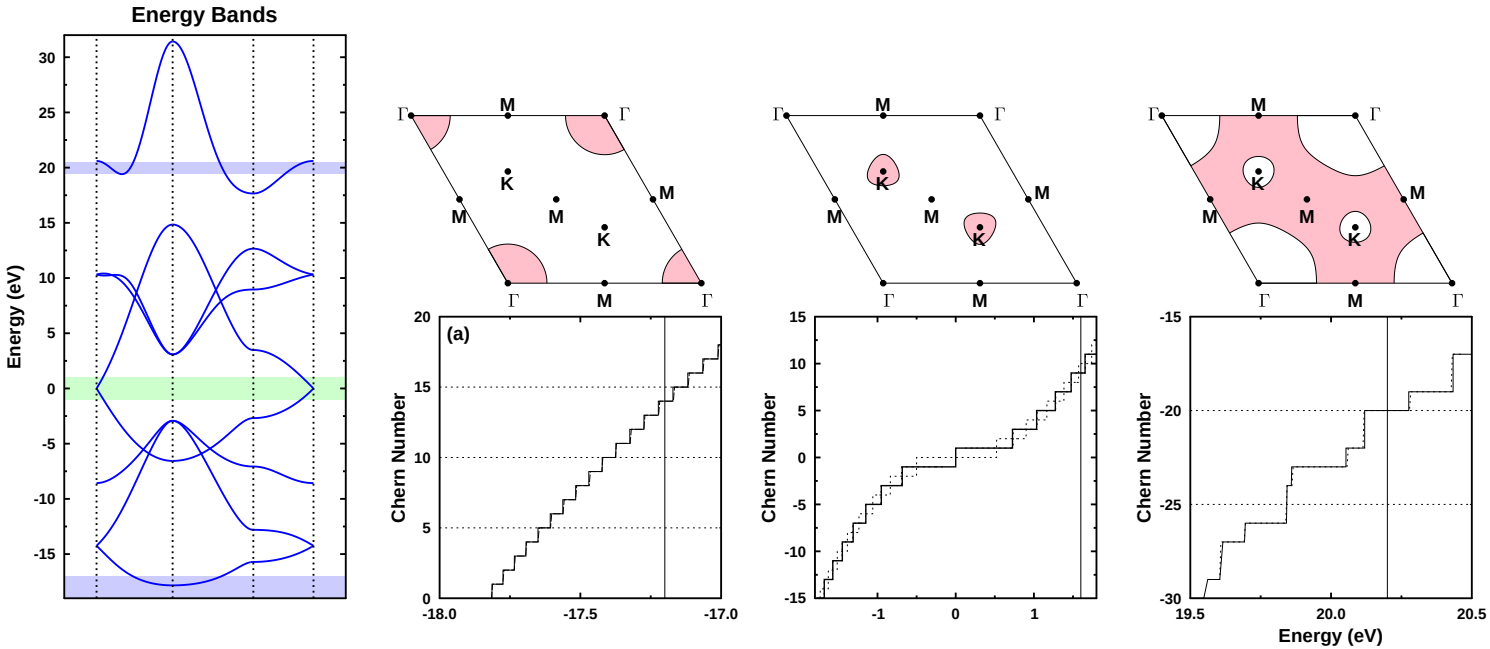
$$\sigma_{xy}^{c} = -\frac{ec}{(2\pi)^2 H} \sum_i S_i(\mu),$$

$S_i(\mu)$: directed area enclosed by Fermi surface.

$S_i(\mu) > 0$ (electron pocket)

$S_i(\mu) < 0$ (hole pocket)

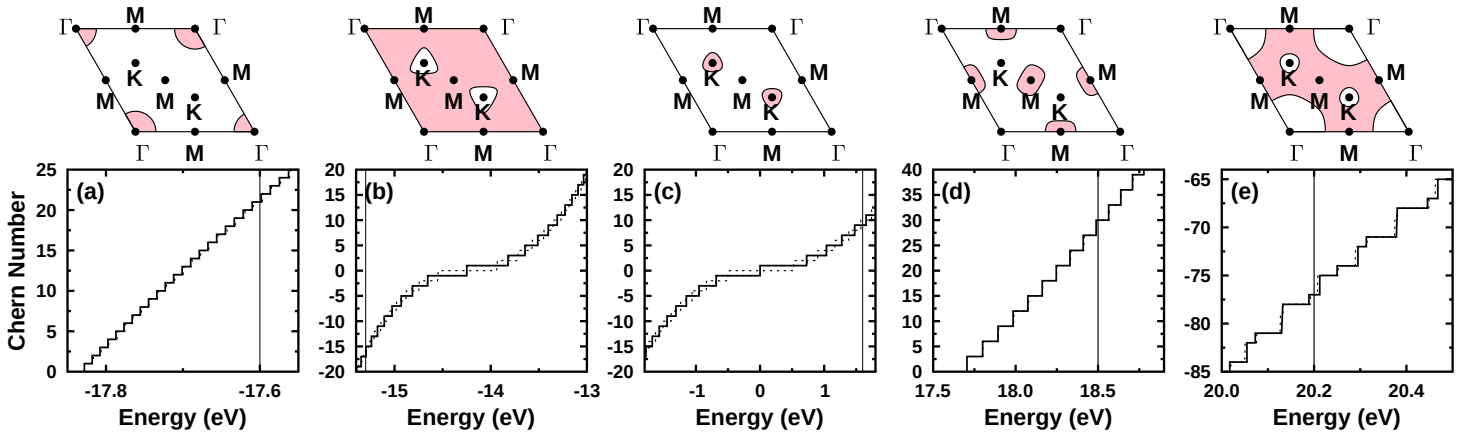
Quantum and semi-classical correspondence



semi-classical quantization: $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = (n+\gamma)\phi;\ \gamma = \frac{1}{2}$ or 0

(In some energy regions, simple quantization rule does not work.)

Limitation of semi-classical quantization?



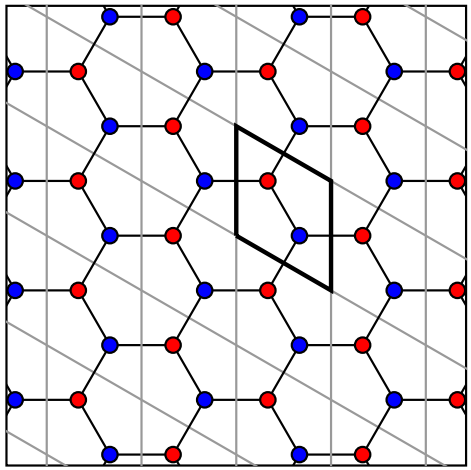
(1) Validity of semi-classical quantization

- Graphene with staggered on-site energy
- Bilayer graphene

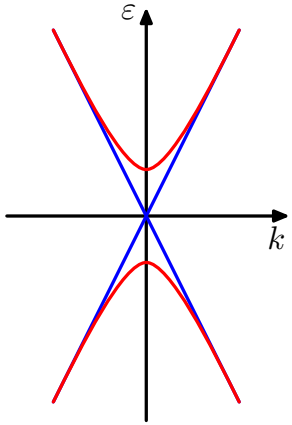
(2) Transition from Dirac fermion regime

Graphene(hexagonal lattice) with staggered on-site energy

π-band model



$\varepsilon_{\mathrm{A,B}} = \pm\Delta$



Near K(1/3,1/3), (2/3,2/3),

$$H = \begin{pmatrix} -\Delta & \delta k_x \pm i\delta k_y \\ \delta k_x \mp i\delta k_y & \Delta \end{pmatrix}$$

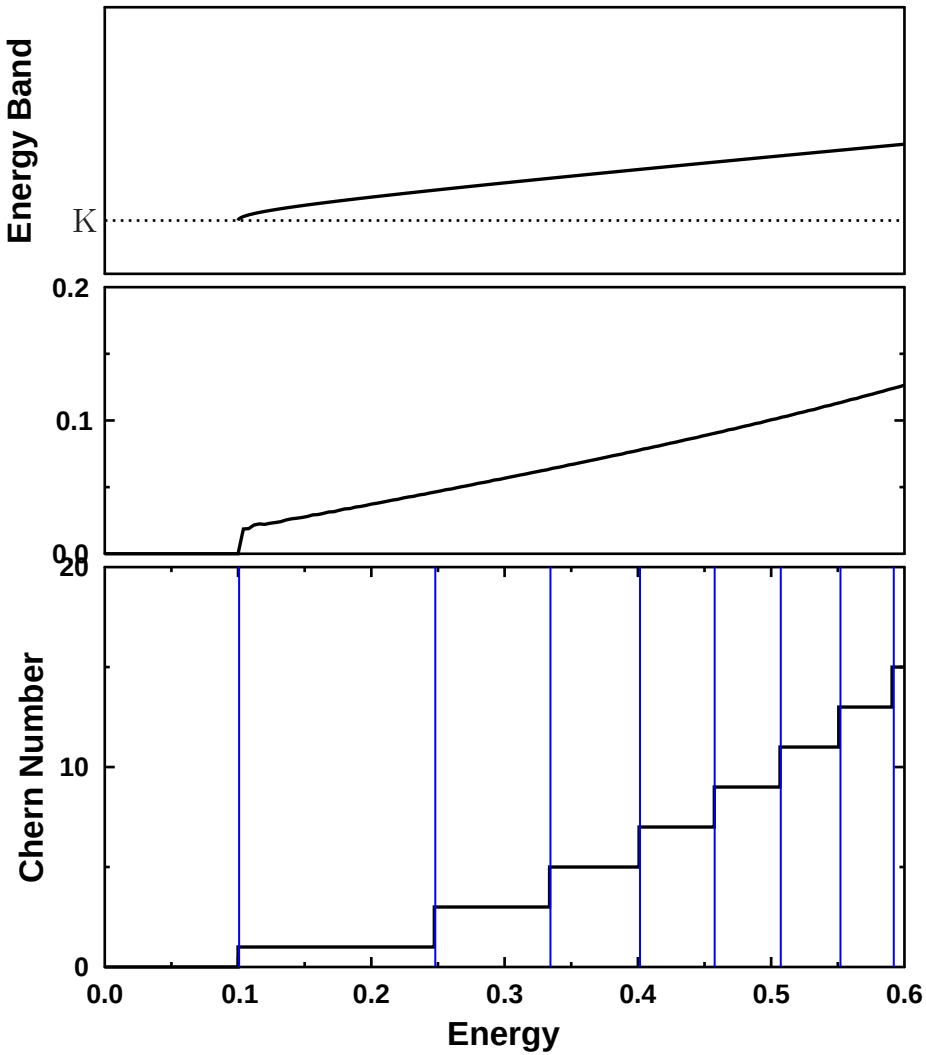
$$\Rightarrow \varepsilon(\boldsymbol{k}) = \pm\sqrt{\Delta^2 + \delta\boldsymbol{k}^2}$$

$$\approx \pm\left\{\Delta^2 + \frac{\delta\boldsymbol{k}^2}{2\Delta}\right\}$$

"Crosover" from $c_F = (2n+1)$ to $2n$?

NO

Quantized σ_{xy} for "massive" Dirac Fermion



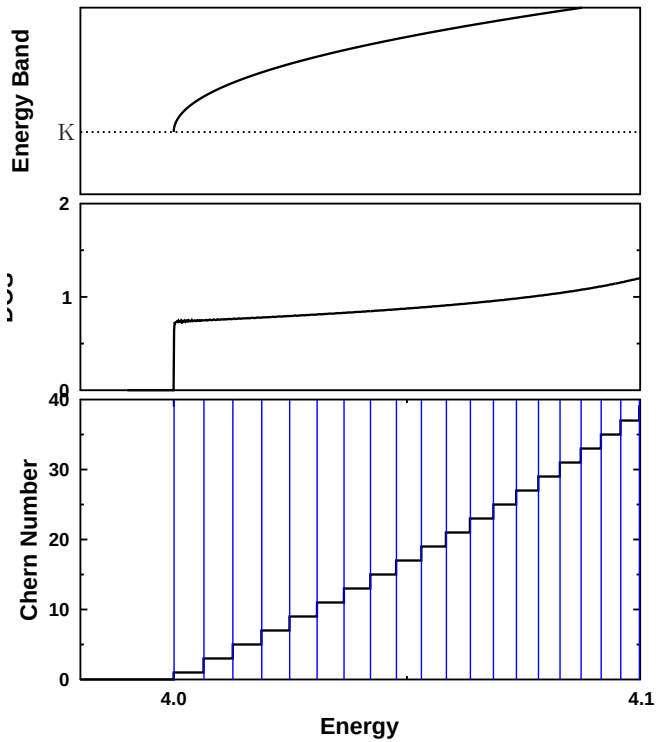
$\Delta = 0.1,\ \phi = \frac{1}{211}$

- $c_F = -3, -1, 0, 1, 3, \cdots$
- $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = n\phi$

H. Aoki, Y. Hatsugai, T. Fukui, International Journal of Modern Physics B21 1133, (2007)

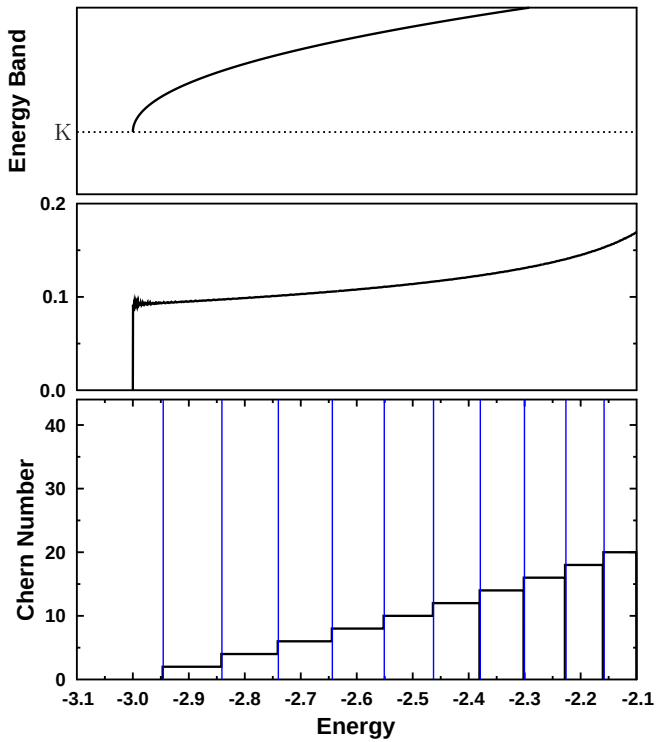
Quantized σ_{xy} for "massive" Dirac Fermion

$\Delta = 4,\ \phi = 1/100$



- $c_F = -3, -1, 0, 1, 3, \cdots$
- $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = n\phi$

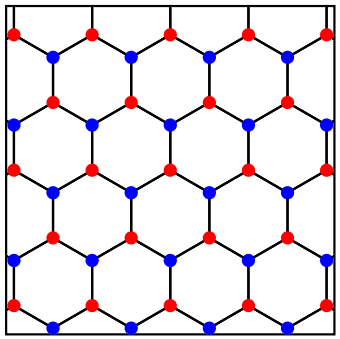
c.f.: Triangle-lattice



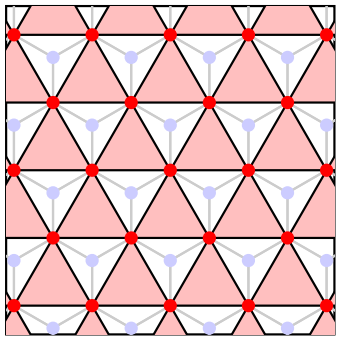
- $c_F = 0, 2, 4, 6, 8, 10 \cdots$
- $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = (n + \frac{1}{2})\phi$

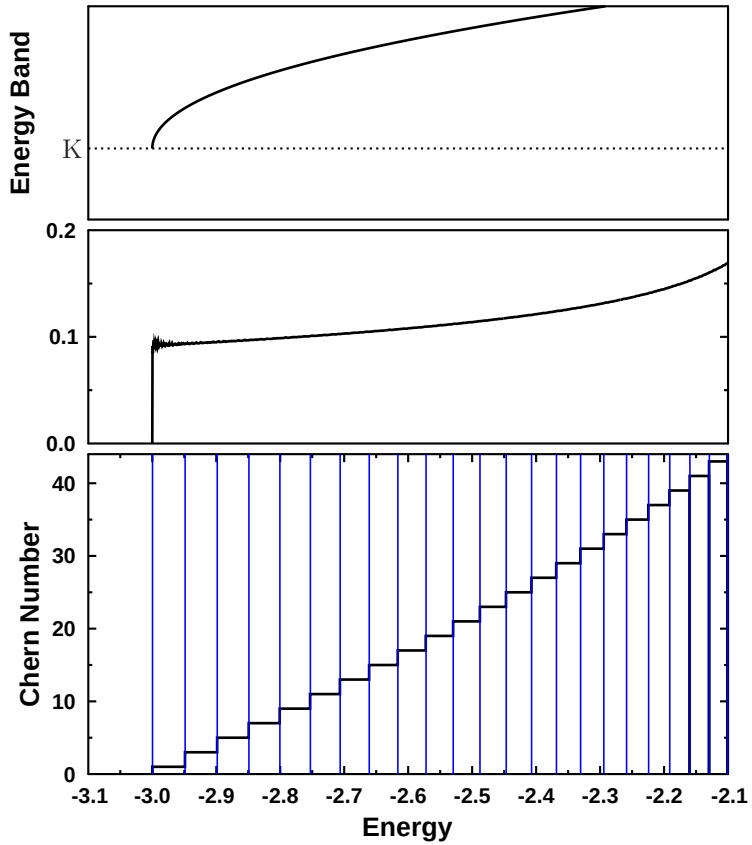
From Hexagonal to Triangle Lattice

Lattice Model



When $\Delta >> t$

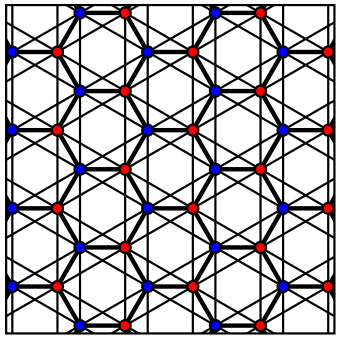




triangle lattice under non-uniform magnetic feild

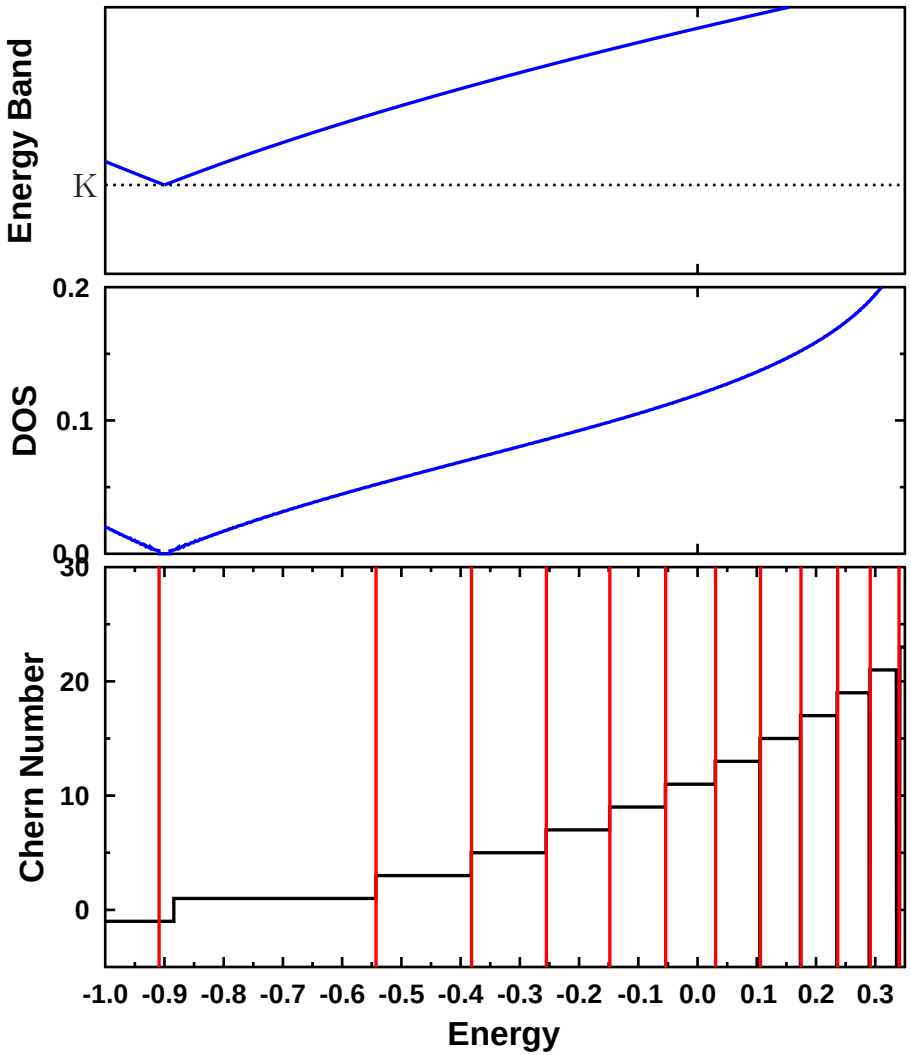
- $c_F = 0, 1, 3, \cdots$
- $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = n\phi$

Hexagonal with next-nearest transfer



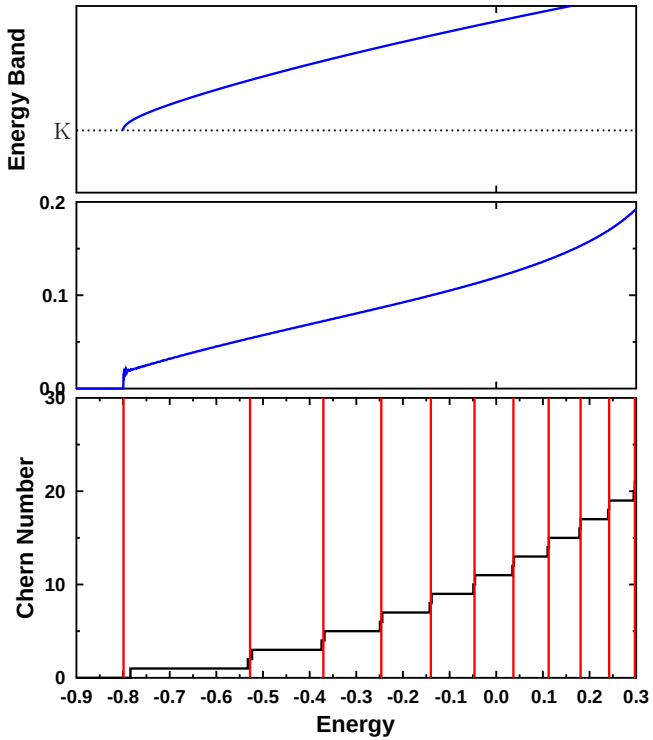
$t_2 = 0.3,\ \Delta = 0,\ \phi = 1/101$

- $c_F = \cdots, -3, -1, 1, 3, \cdots$
- $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = n\phi$

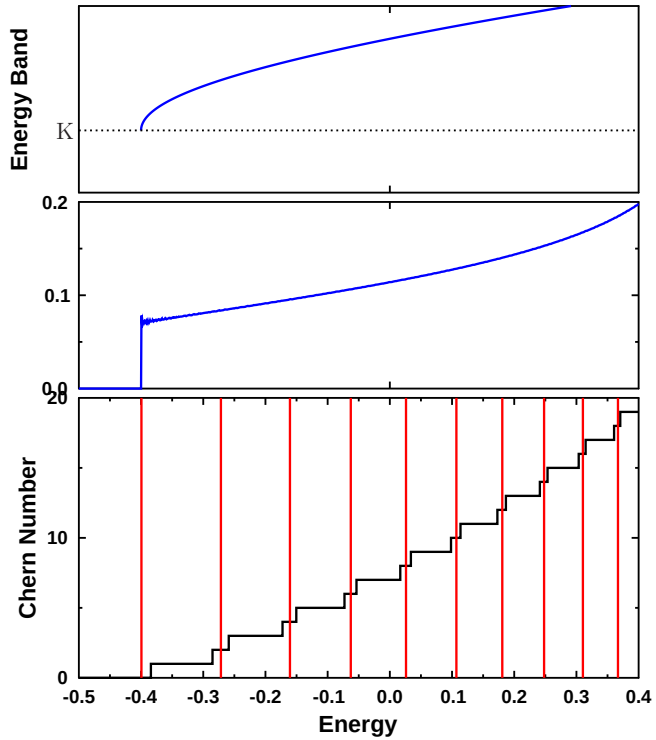


Hexagonal with next-nearest transfer $t_2 = 0.3$

$\Delta = 0.1$



$\Delta = 0.5$



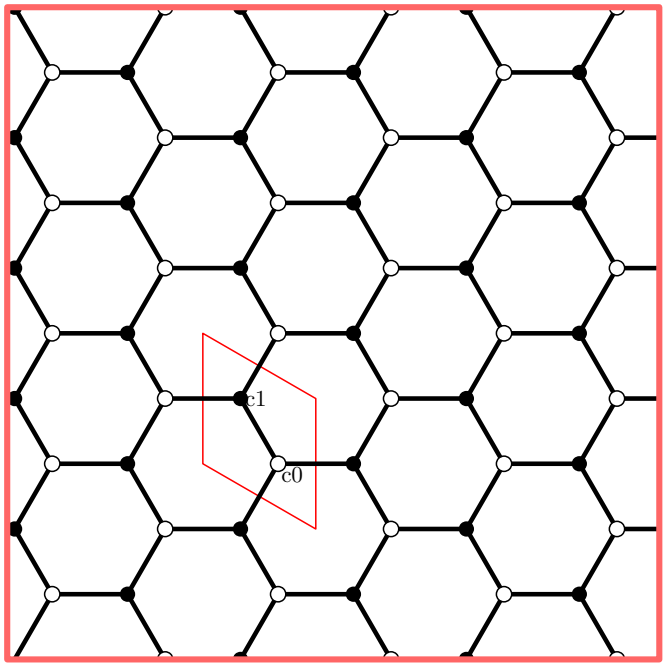
$\rightarrow c_F = \cdots, 0, 1, 2, 3, 4, \cdots$

When B = 0, Fermi surface consists of two "equivalent" electron pockets around K and K'. But, Landau quantization is different between K and K'.

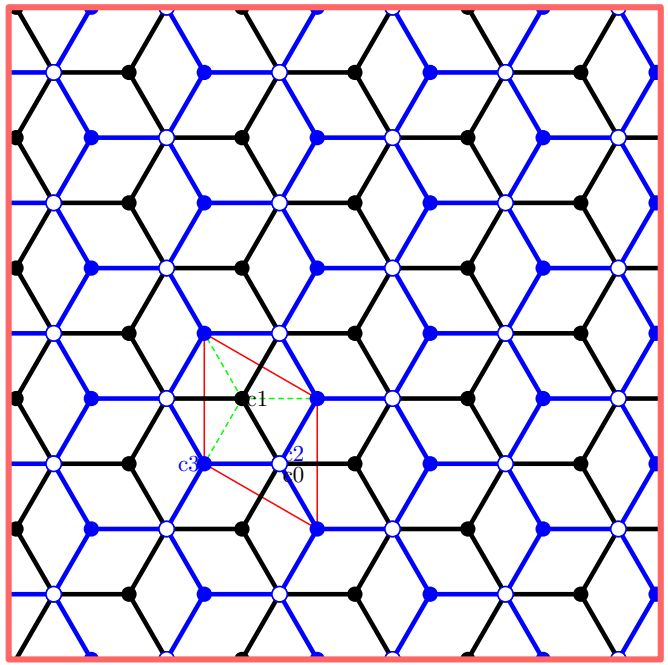
$\sigma_{xy} \neq$ (number of valley) $\times$ (integer)

Bilayer Graphene

Graphene



Bilayer graphene



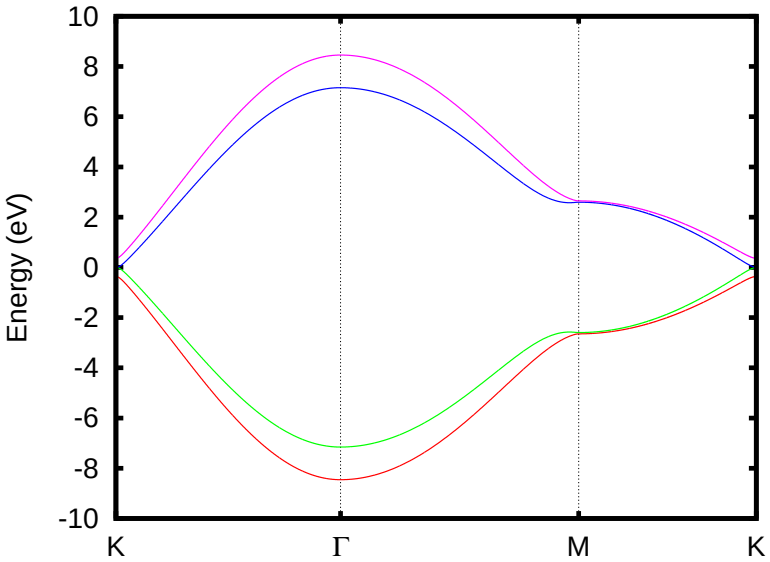
Transfer

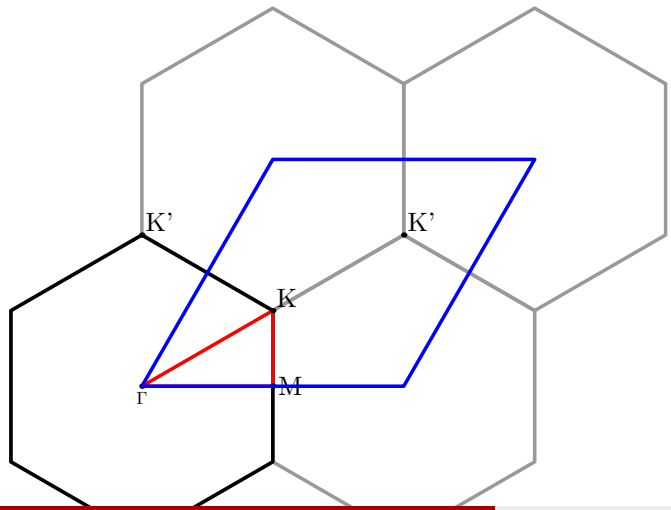
- c0 – c1:

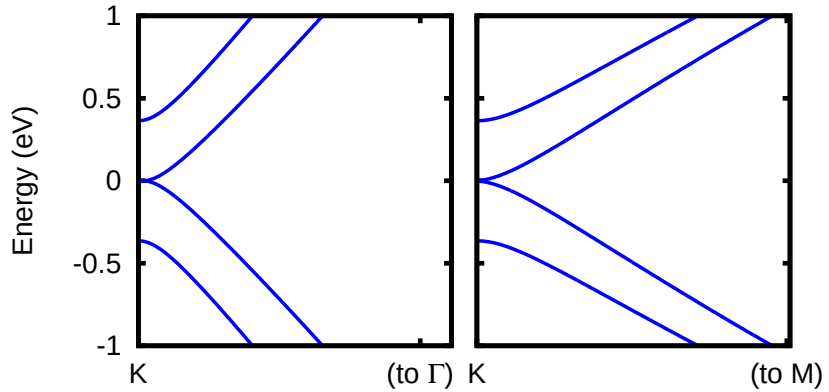
Transfer

- c0 – c1, c2 – c3: $\gamma_0 \approx 2.6\text{eV}$
- c0 – c2: $\gamma_1 \approx 0.4\text{eV}$
- c1 – c3: $\gamma_3 \approx 0.3\text{eV}$

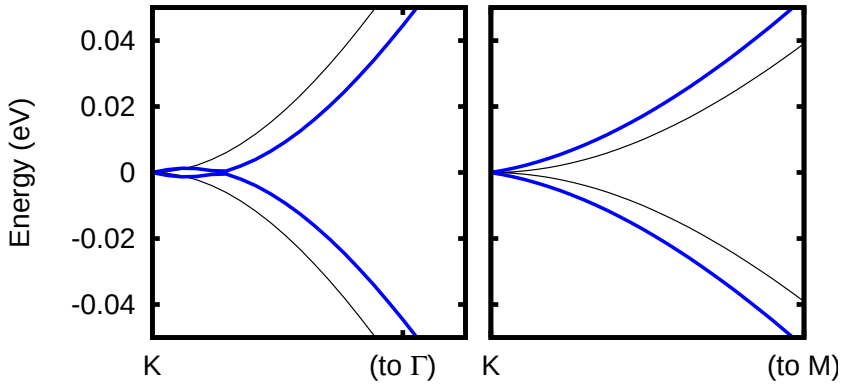
Bilayer Graphene: Energy Bands





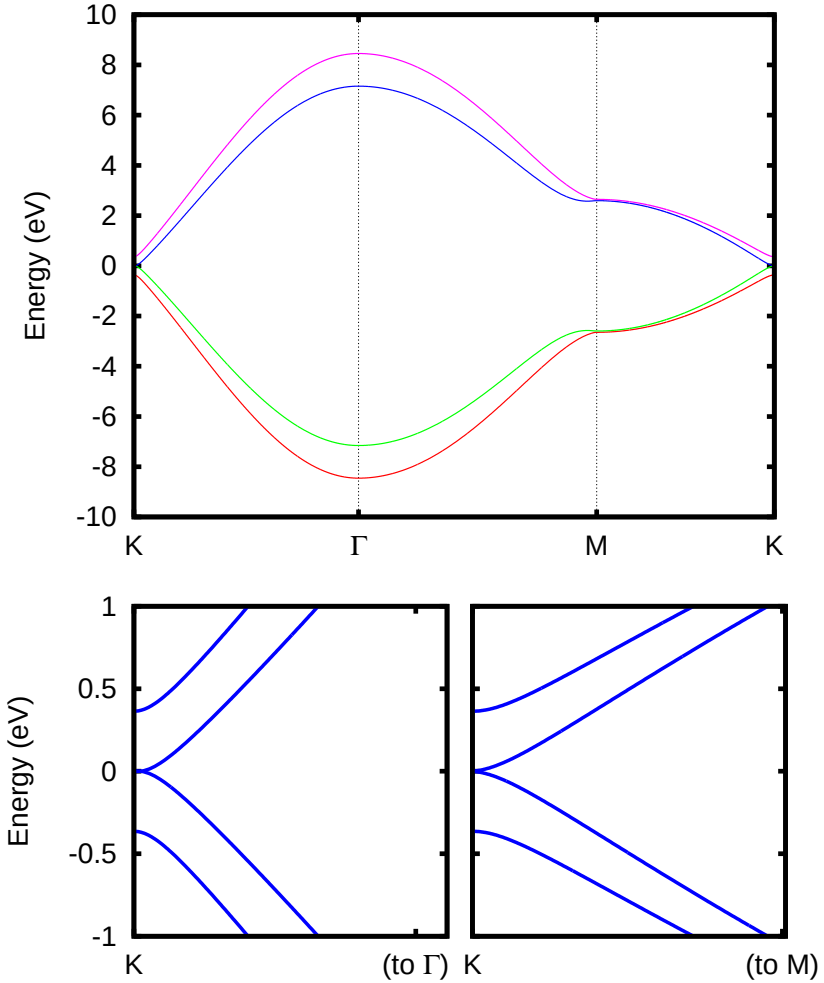


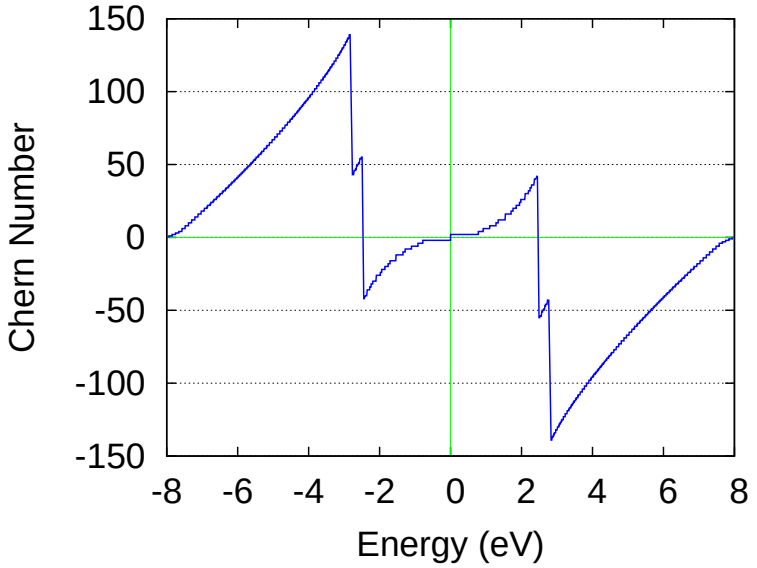
"Trigonal warping"

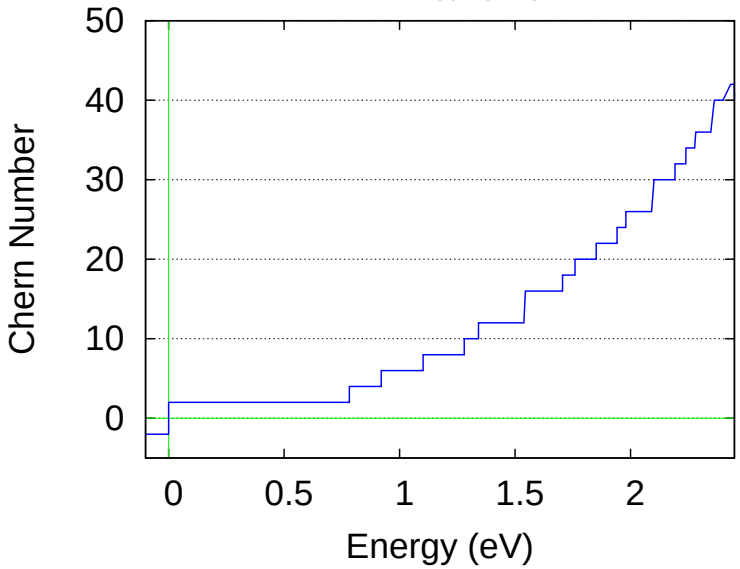


thin line: $\gamma_3 = 0$

Bilayer Graphene: Chern Number

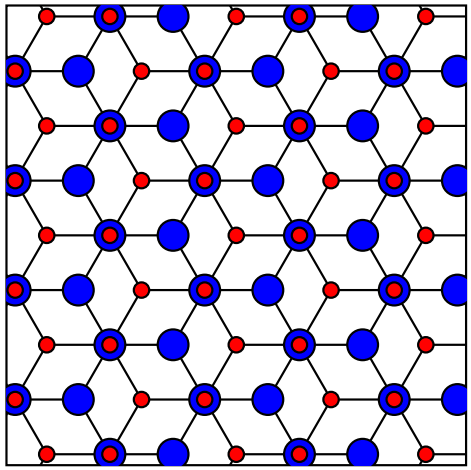






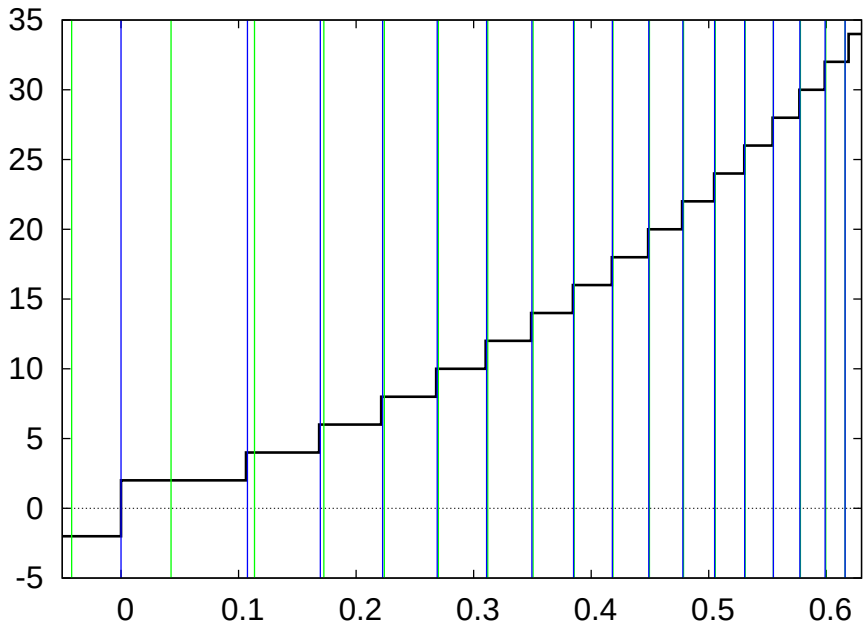
$$c_F = \cdots, -4, -2, 2, 4, 6, \cdots$$

Bilayer Graphene



$\gamma_0 = -1.0, \gamma_1 = -0.6$
$\phi = 1/100$

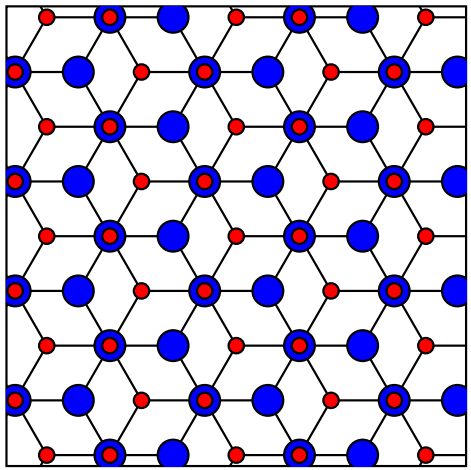
(exp. and theory) Nosvoselov et al, Nat. Phys. 2, 117 (2006)

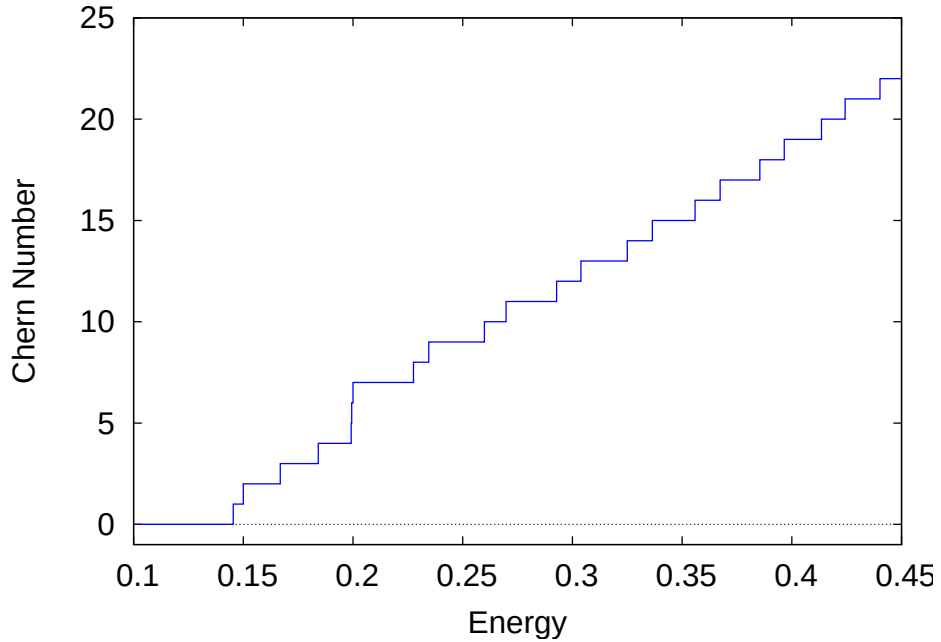


- $c_F = \cdots, -4, -2, 2, 4, 6, \cdots$
- $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = \pm\sqrt{n(n-1)}\phi$

Green line : $\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = (n + \frac{1}{2})\phi$

Bilayer Graphene with bias voltage





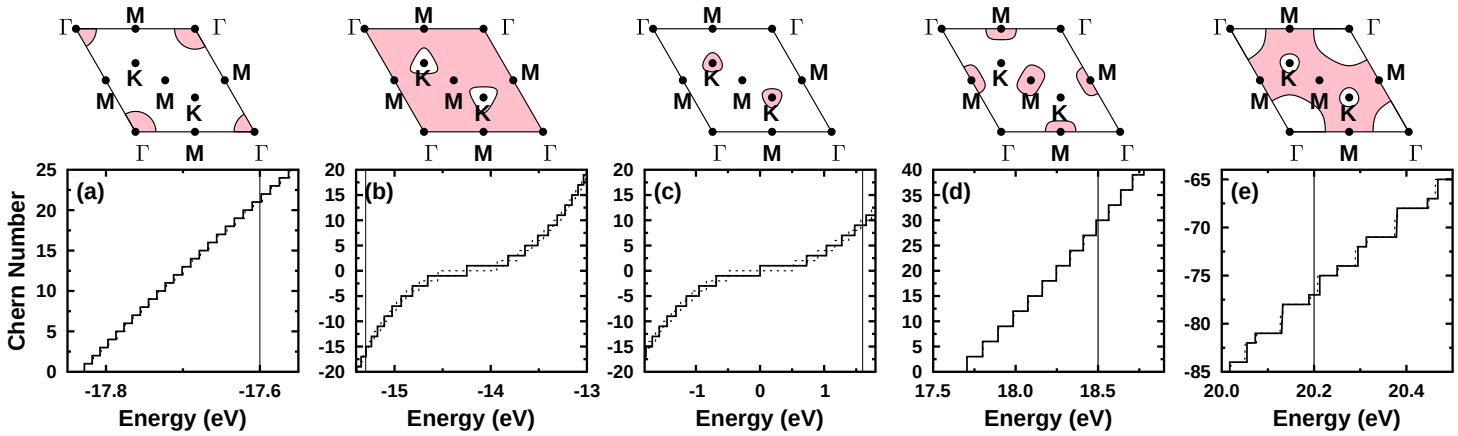
Different on-site energy for lower and upper layer.

$t_0 = -1, t_1 = -0.6,\ \Delta = 0.2$

(exp.) Castro et al, PRL, 99, 216802 (2007)

$c_F = \cdots, -1, 0, 1, 2, 3, 4, \cdots$

Additional plateaux appear.



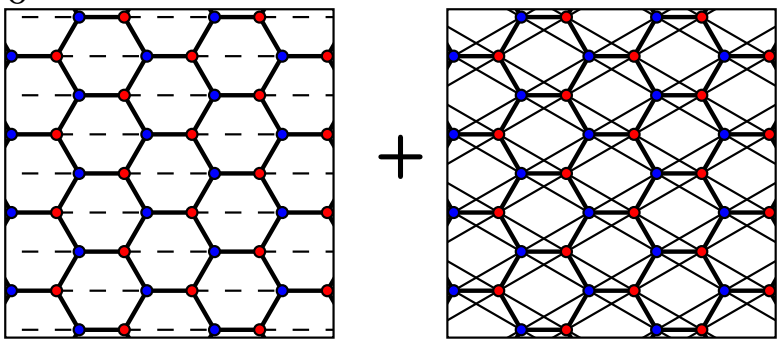
(1) Validity of semi-classical quantization

- Graphene with staggered on-site energy
- Bilayer graphene

(2) Transition from Dirac fermion regime

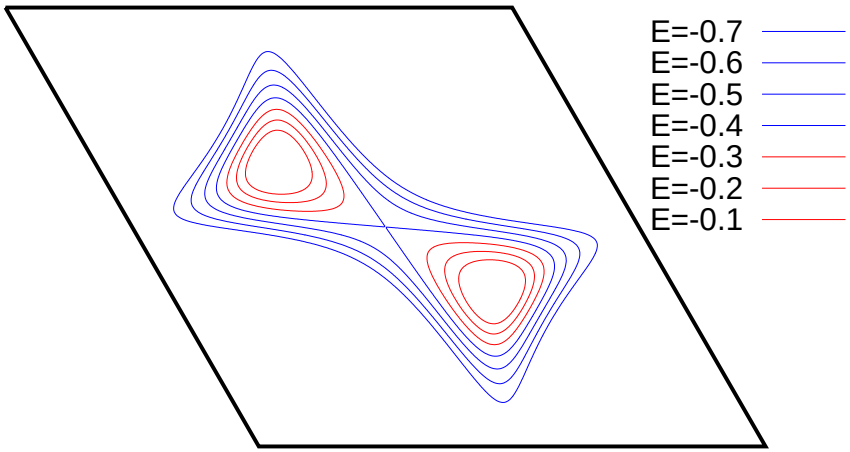
Fusion of two Dirac point: π-band model graphene+α

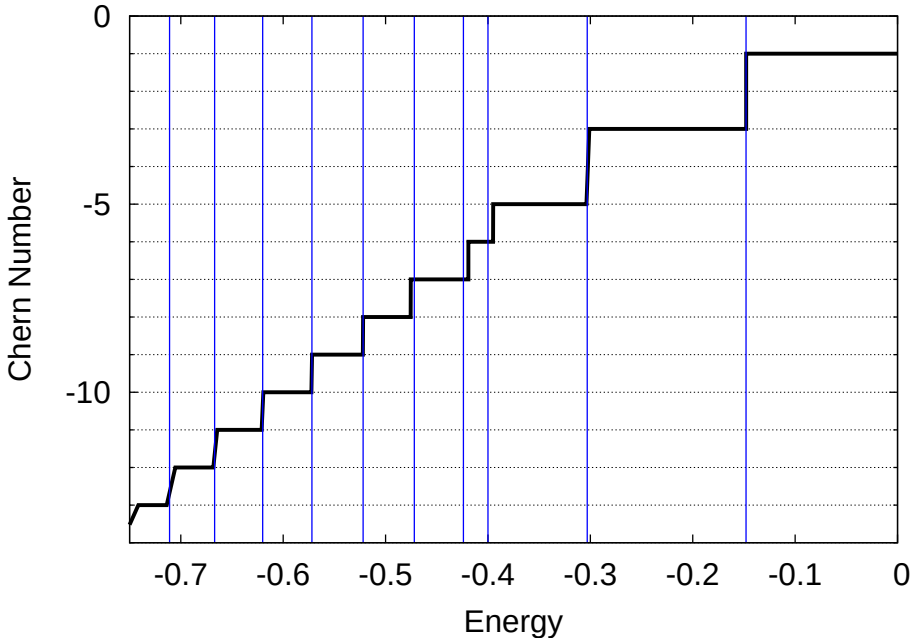
$t_0 = -1$



$t_1 = -0.2$ $t_2 = -0.1$

Two Dirac cones combine together.





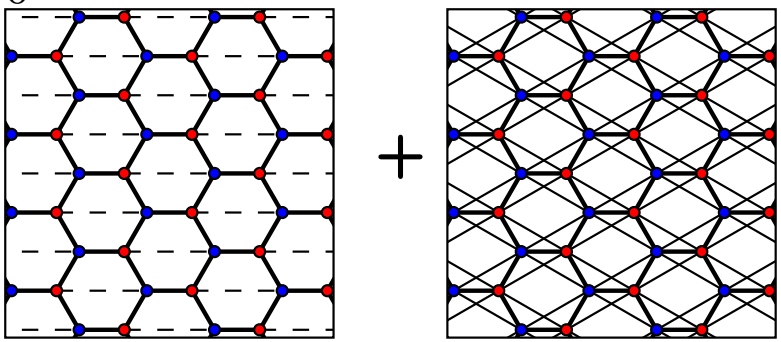
$c_F =$

$\cdots, -1, -3, -5, , -6, -7, -8, \cdots$

$$\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = n\phi, (n + \frac{1}{2})\phi$$

Fusion of two Dirac point: π-band model graphene+α

$t_0 = -1$



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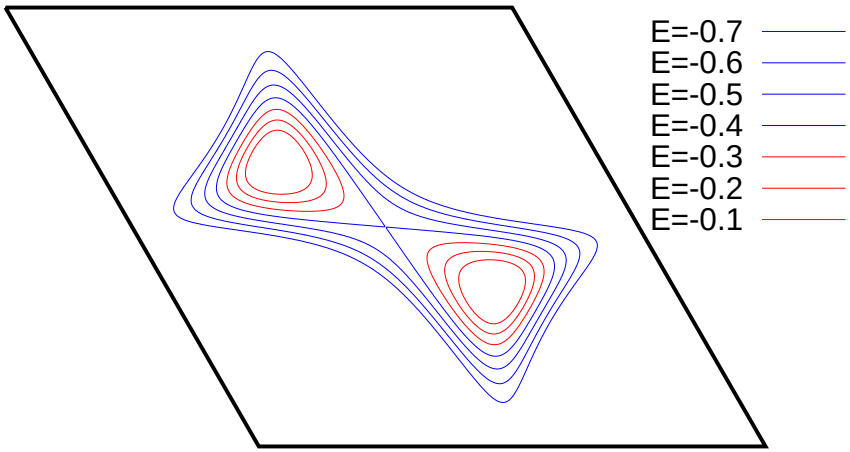
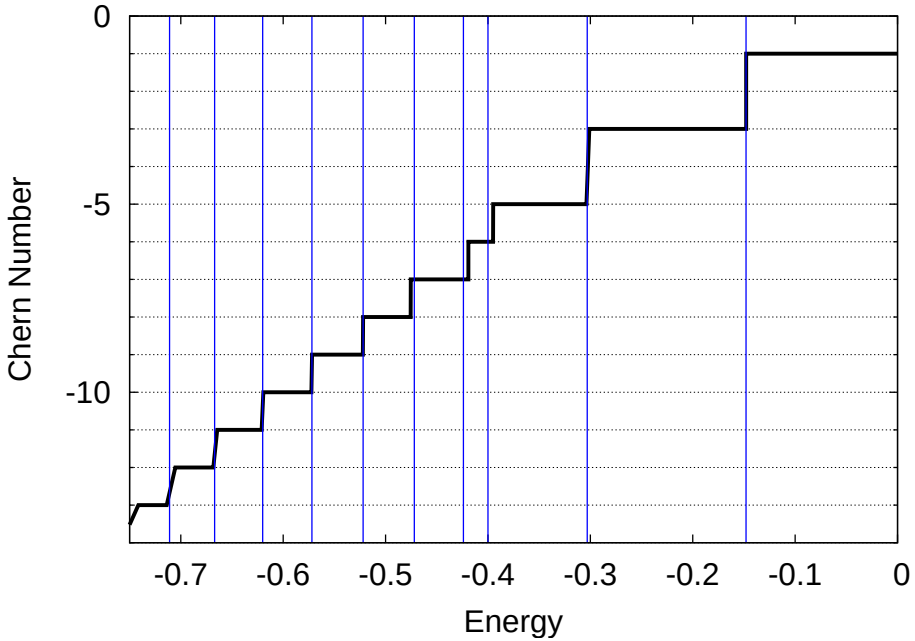


realized in organic conductors?



$c_F =$

$\cdots, -1, -3, -5, , -6, -7, -8, \cdots$

$$\frac{S(\varepsilon)}{\Omega_{\mathrm{BZ}}} = n\phi, (n + \frac{1}{2})\phi$$

Summary

- "Massive" Dirac Fermion on hexagonal lattice
  - Importance of next-nearest transfer
- Bilayer graphene
  - With bias voltage, new plateaux may appear.
- Two Dirac cone combines
  - semi-classical qunatization rule changes: $\gamma = 0, \rightarrow \frac{1}{2}$