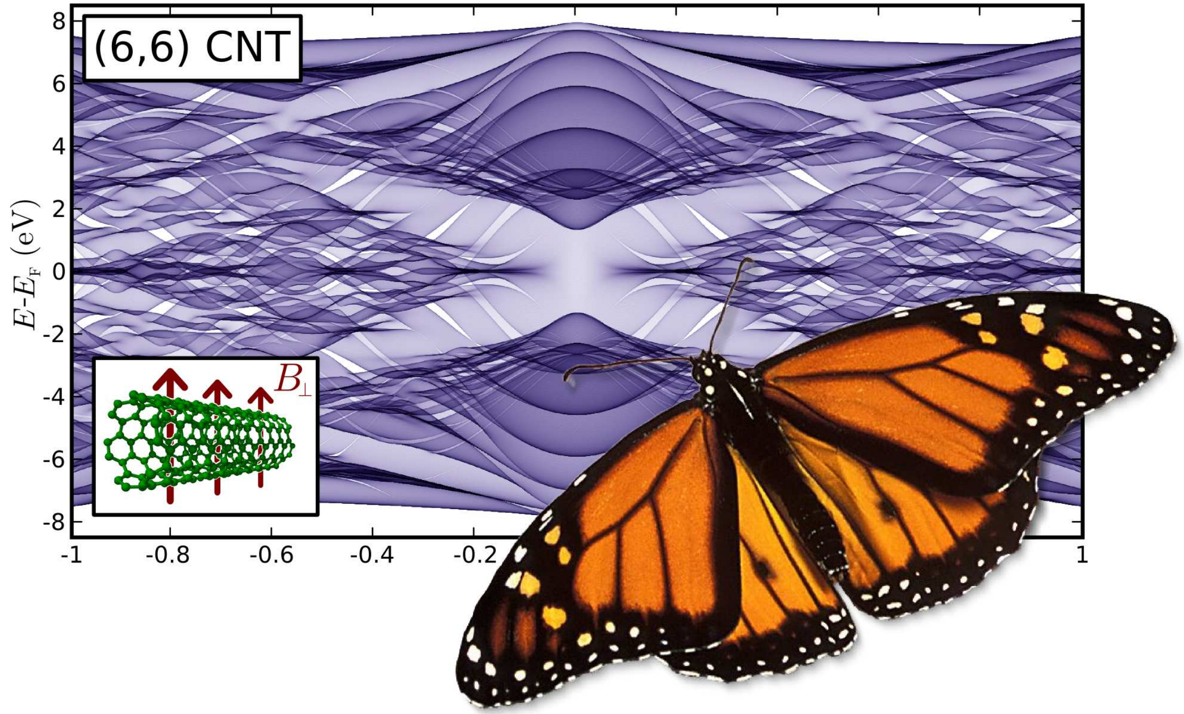
Hofstadter butterflies of graphene layers and carbon nanotubes

Norbert Nemec

Molecular Computing Group

Institut für theoretische Physik

Universität Regensburg



- N. Nemec and G. Cuniberti, Phys. Rev. B (Rapid Comm.) to appear [cond-mat/0612369]
- N. Nemec and G. Cuniberti, Phys. Rev. B **74**, 165411 (2006)

Outline

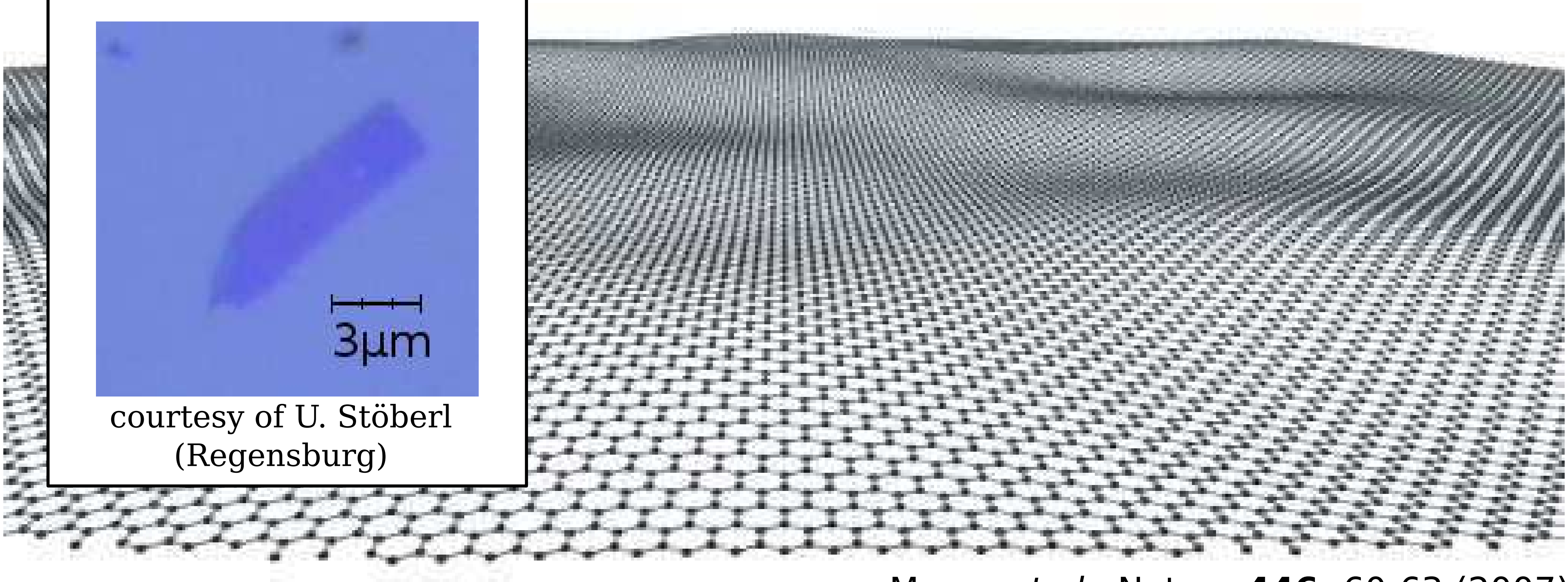
- Motivation:
  anomalous QHE in graphene layers

- Theory:
  graphene band structure and magnetoelectronic spectrum

- Bilayer graphene:
  effects of interlayer interaction beyond Bernal stacking

- Double wall carbon nanotubes:
  varying stacking around the circumference

Motivation: Graphene



courtesy of U. Stöberl
(Regensburg)

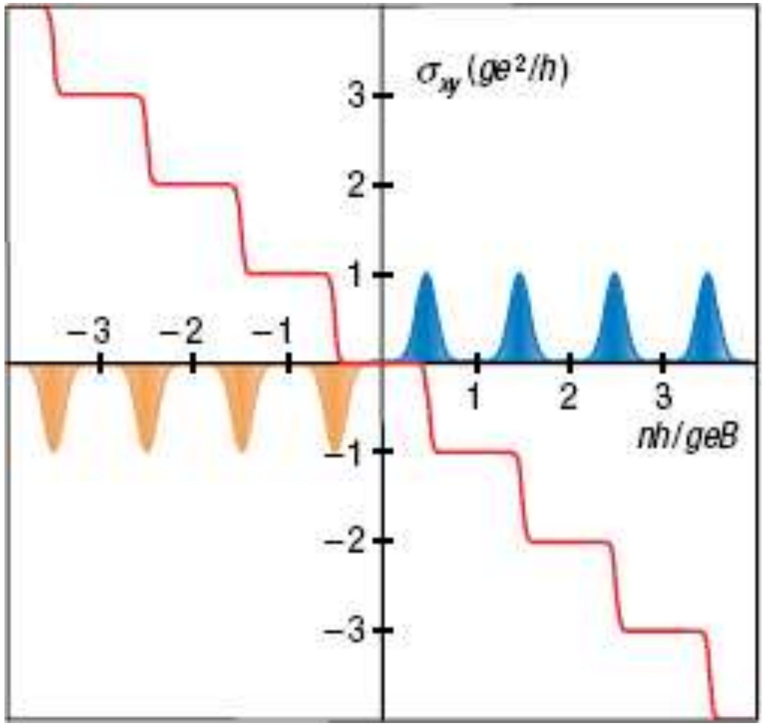
Meyer *et al.*, Nature **446,** 60-63 (2007)

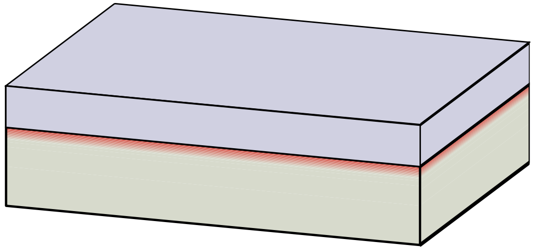
(remember: HL 37.5 this morning)

Motivation: Quantum Hall effect (QHE)

2D semiconductor

$$\sigma_{xy} = \frac{e^2}{h} g_s n$$

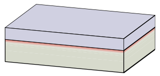




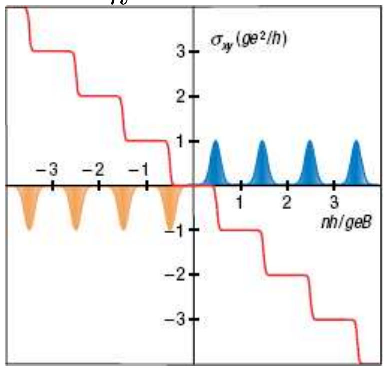
von Klitzing *et al*., Phys. Rev. Lett. **45**, 494 (1980)

Odd-integer QHE in graphene

2D semiconductor

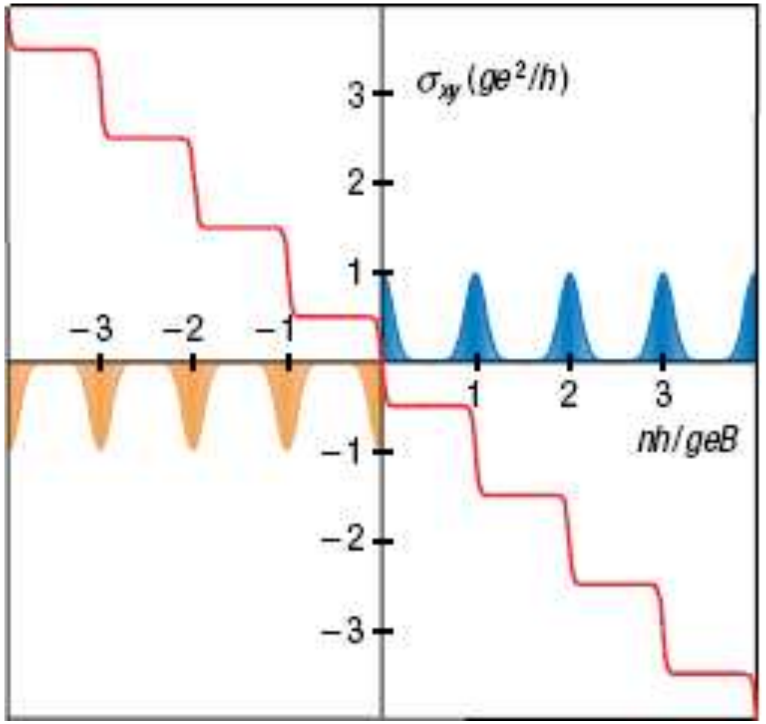


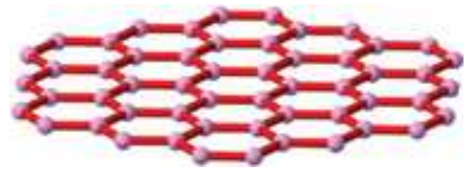
$$\sigma_{xy} = \frac{e^2}{h} g_s n$$



monolayer graphene

$$\sigma_{xy} = \frac{e^2}{h} g_s \left(n + \frac{1}{2} \right)$$



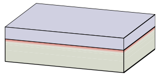


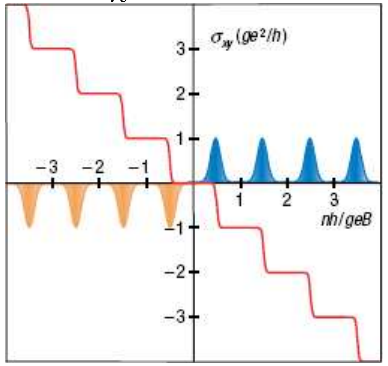
Zhang *et al.* / Novoselov *et al.*, Nature **438** (2006)

Nonzero QHE in bilayer graphene

2D semiconductor

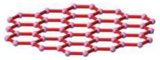
$\sigma_{xy} = \frac{e^2}{h} g_s n$

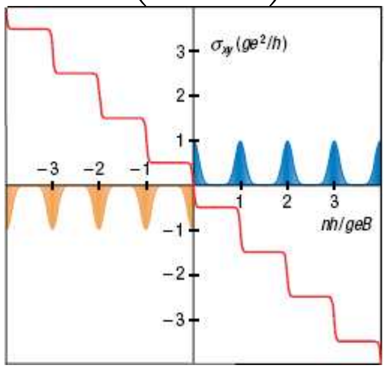


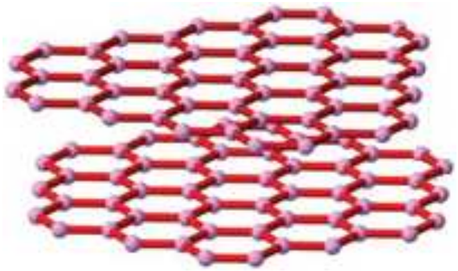


monolayer graphene

$\sigma_{xy} = \frac{e^2}{h} g_s \left(n + \frac{1}{2}\right)$

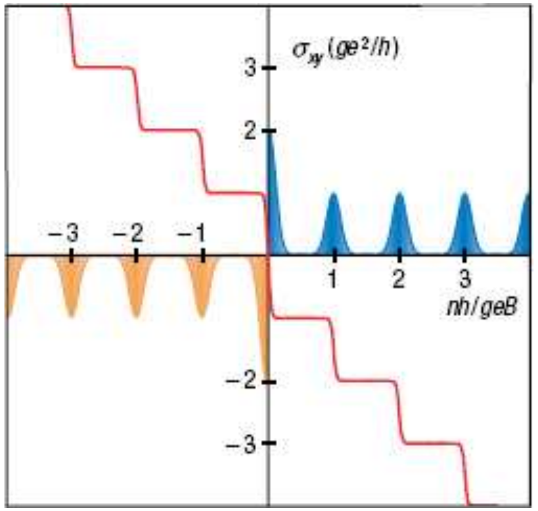


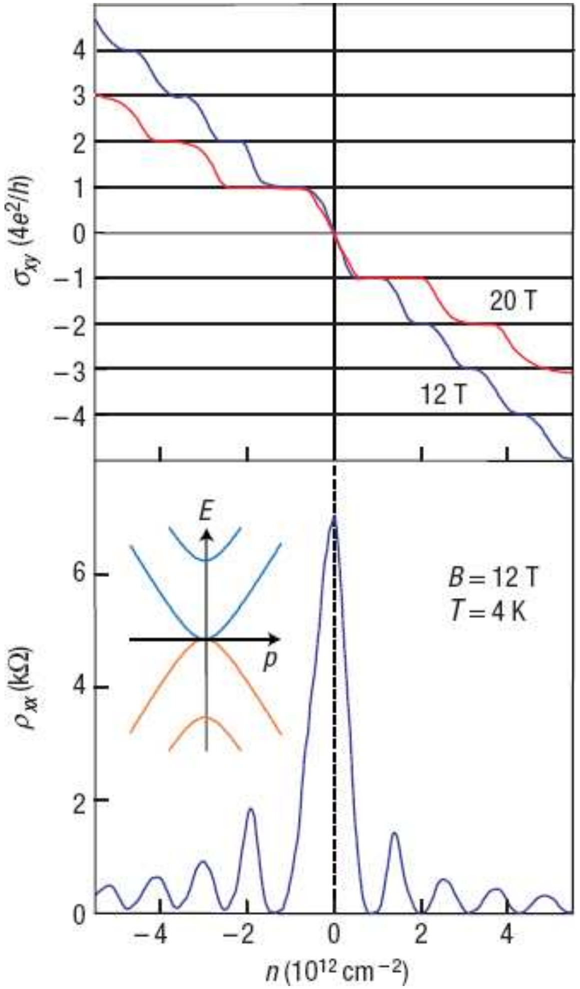




bilayer graphene

$$\sigma_{xy} = \frac{e^2}{h} g_s n,\ \boldsymbol{n \neq 0}$$





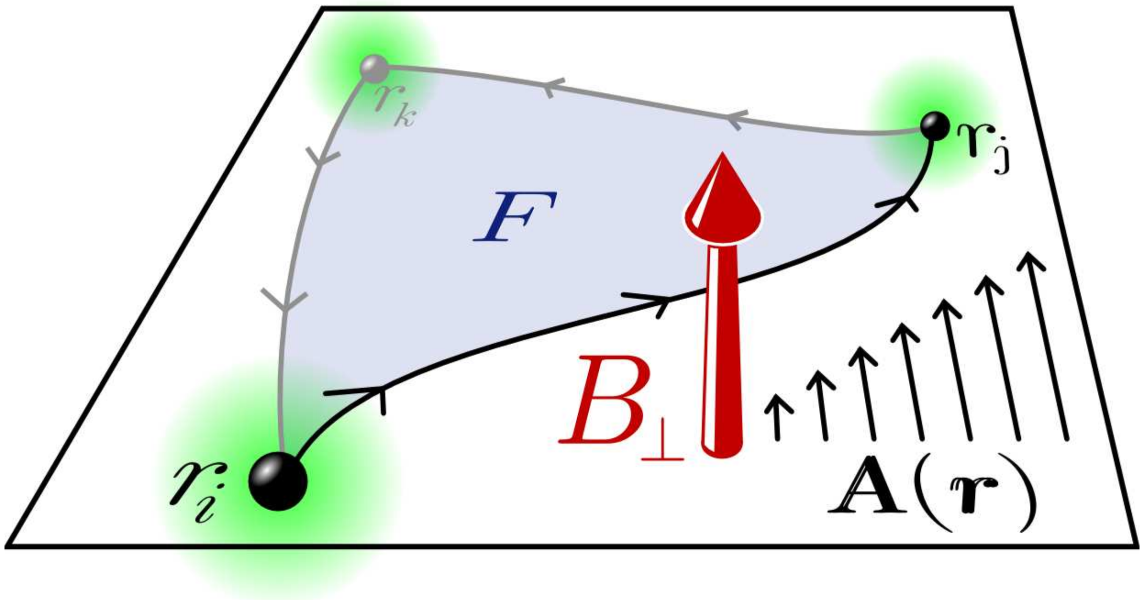
Novoselov *et al.*, Nat. Phys. **2**, 177-180 (2006)

Theory: Peierls substitution

$$\gamma_{ij}(\boldsymbol{B}) \;=\; \gamma_{ij}^{0}\exp\left(\frac{2\pi\mathrm{i}}{\Phi_0}\int_{\boldsymbol{r}_i}^{\boldsymbol{r}_j}\mathrm{d}\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})\right)$$

magnetic field: $\boldsymbol{B}(\boldsymbol{r}) \;=\; \nabla\times\boldsymbol{A}(\boldsymbol{r})$
gauge field: $\boldsymbol{A}(\boldsymbol{r})$ (*"vector potential"*)
flux quantum: $\Phi_0 = h/e$

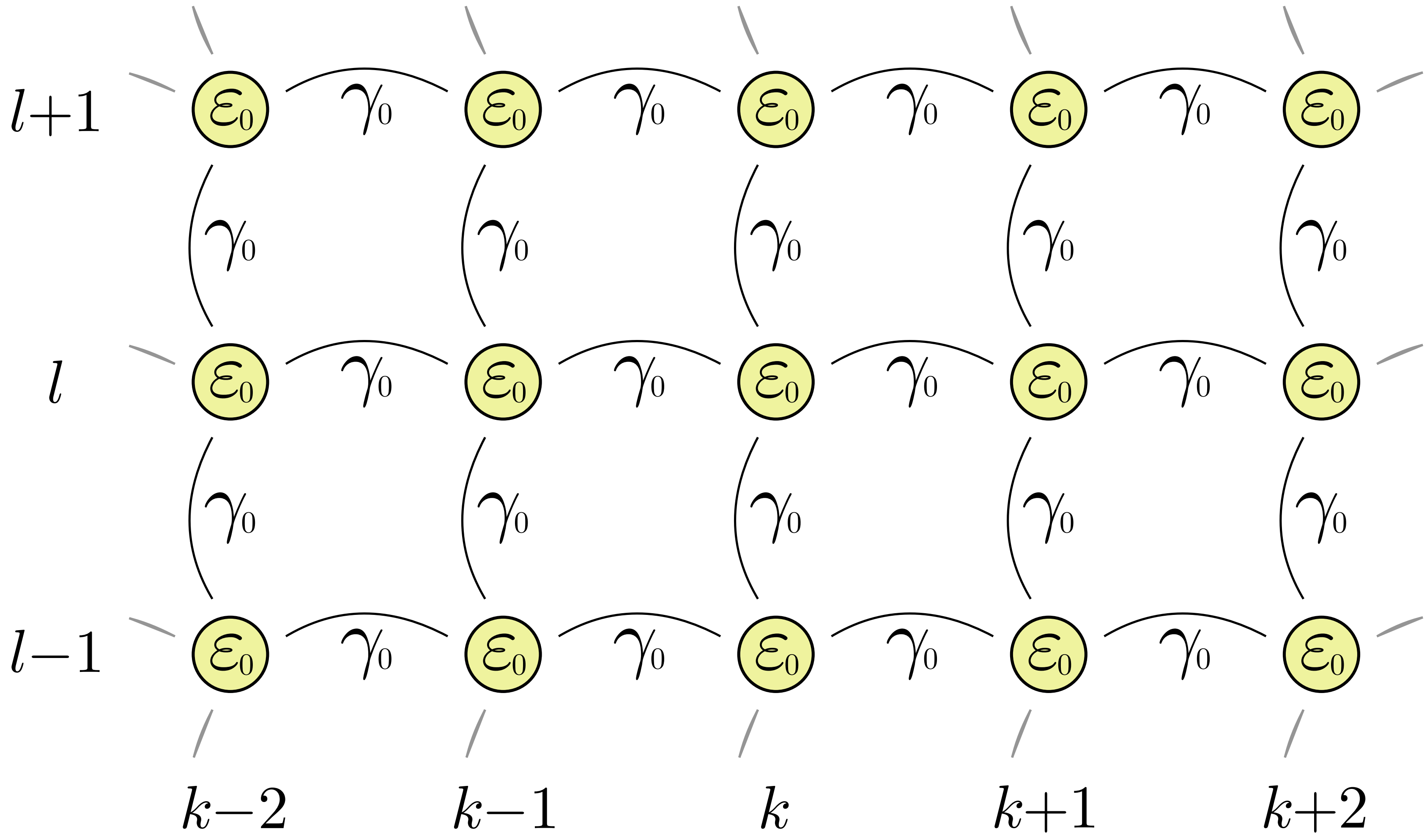
Peierls, Z. Phys. **80**, 763 (1933)



Phase of circular path given by enclosed area F:

$$\varphi_{i\to j\to k\to i} = \exp\left(2\pi\mathrm{i}\frac{F B_\perp}{\Phi_0}\right)$$

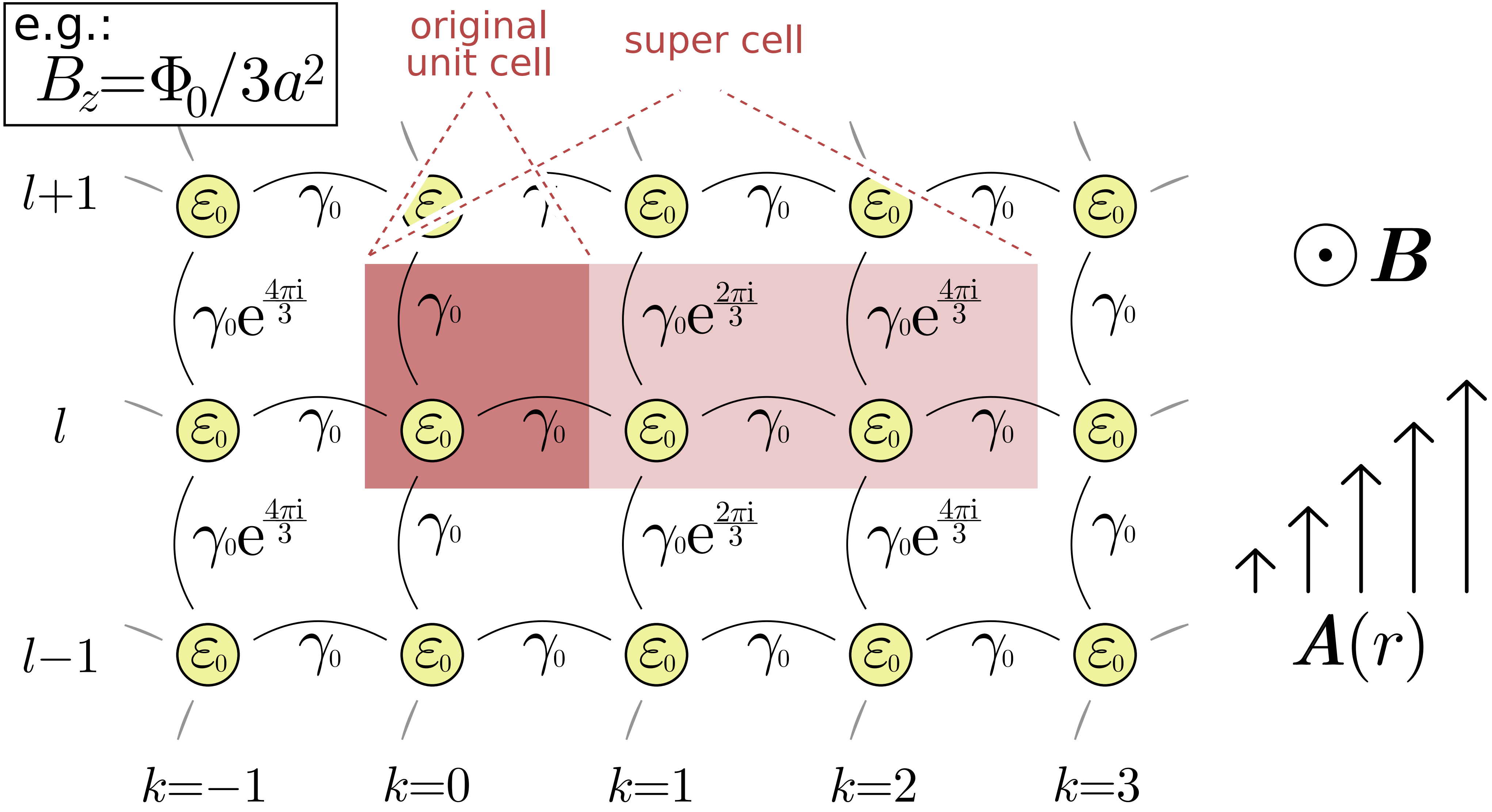
The original Hofstadter butterfly (I)



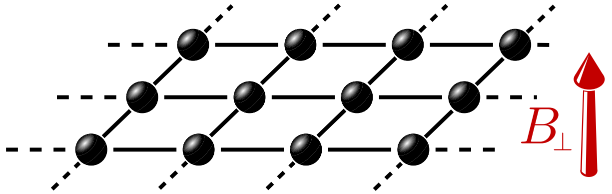
(lattice constant a)

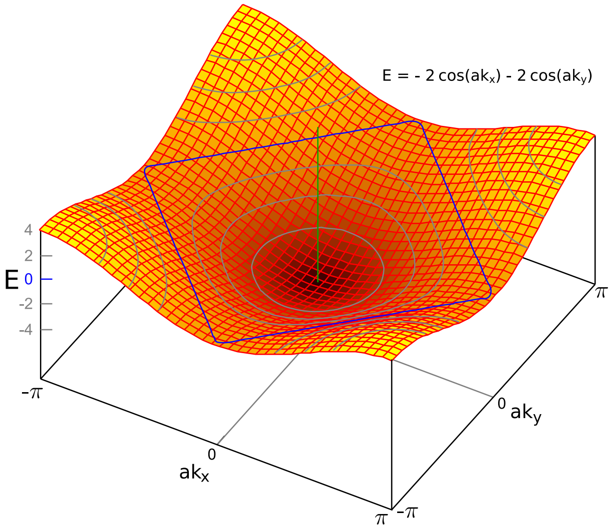
The original Hofstadter butterfly (II)

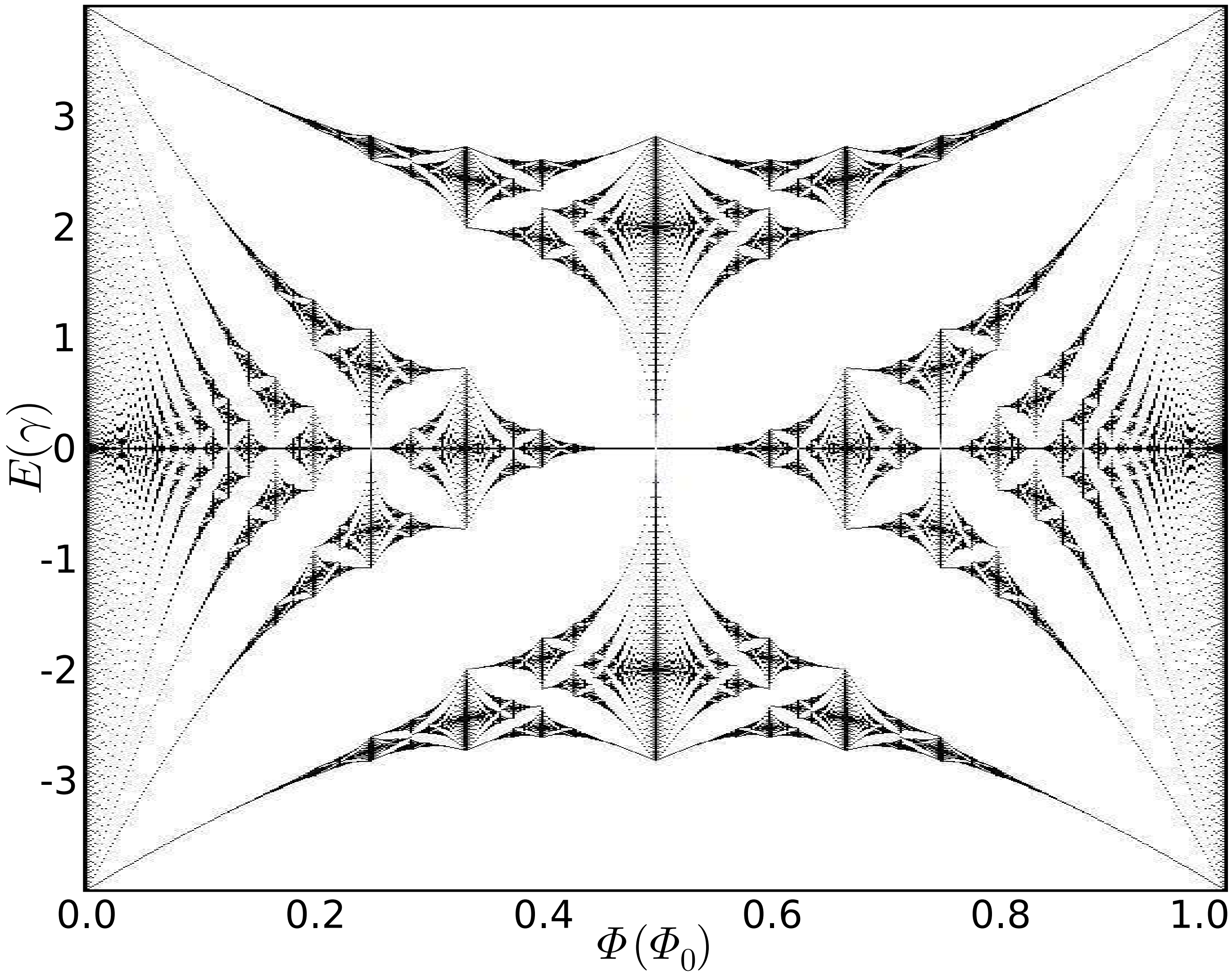
e.g.:
$B_z = \Phi_0 / 3a^2$



The original Hofstadter butterfly

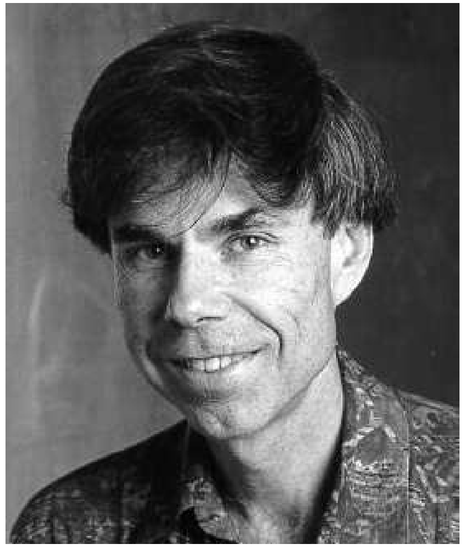






1975 in Regensburg...

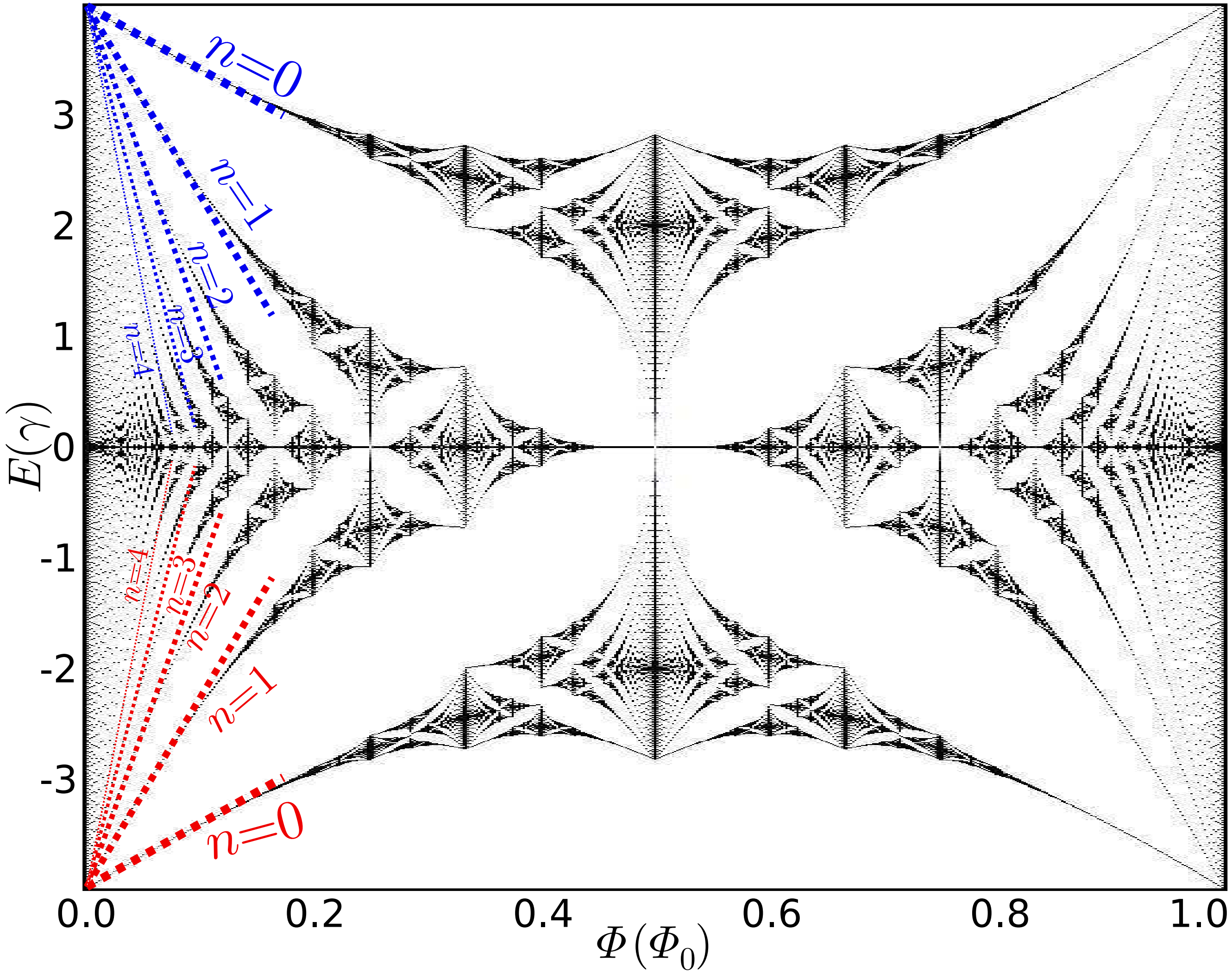
HP 9820A ("Rumpelstilzchen")
(8MHz/16bit CPU, 3432 byte RAM...)

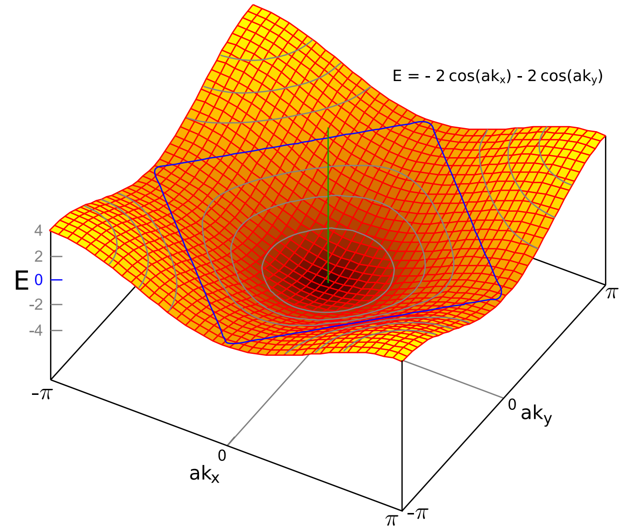


D. Hofstadter
G. Wannier
G. Obermair

Phys. Rev. B **14**, 2239 (1976)

Conventional Landau levels



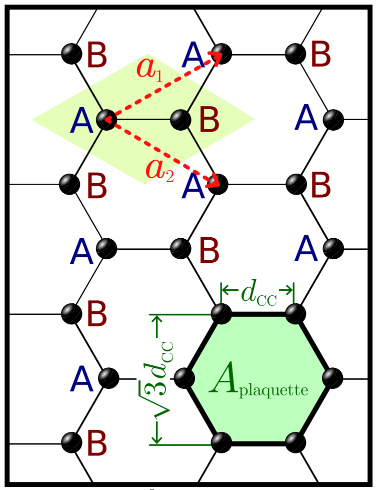


$\rightarrow$ Landau levels at band band edges with effective mass $m^* = \frac{\hbar^2}{2\gamma a^2}$:

$$E = +4\gamma - \frac{\hbar e}{m^*} B_\perp \left(n + \frac{1}{2}\right)$$

$$E = -4\gamma + \frac{\hbar e}{m^*} B_\perp \left(n + \frac{1}{2}\right)$$

Band structure of graphene



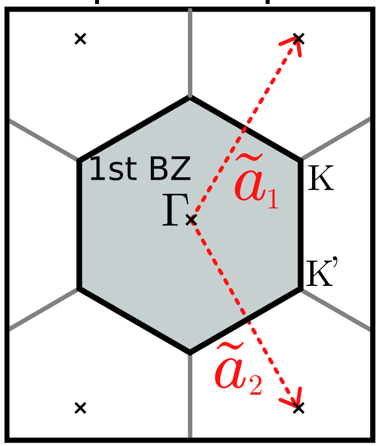
real space

hexagonal lattice, 2-atom basis:

$$\mathcal{H}(\boldsymbol{k}) = \varepsilon_0 - \gamma_0 \begin{pmatrix} 0 & 1 + e^{\mathrm{i}\boldsymbol{k}\boldsymbol{a}_1} + e^{\mathrm{i}\boldsymbol{k}\boldsymbol{a}_2} \\ 1 + e^{-\mathrm{i}\boldsymbol{k}\boldsymbol{a}_1} + e^{-\mathrm{i}\boldsymbol{k}\boldsymbol{a}_2} & 0 \end{pmatrix}$$

$$E(\boldsymbol{k}) = \varepsilon_0 \pm \gamma_0 \left| 1 + e^{\mathrm{i}\boldsymbol{k}\boldsymbol{a}_1} + e^{\mathrm{i}\boldsymbol{k}\boldsymbol{a}_2} \right|$$

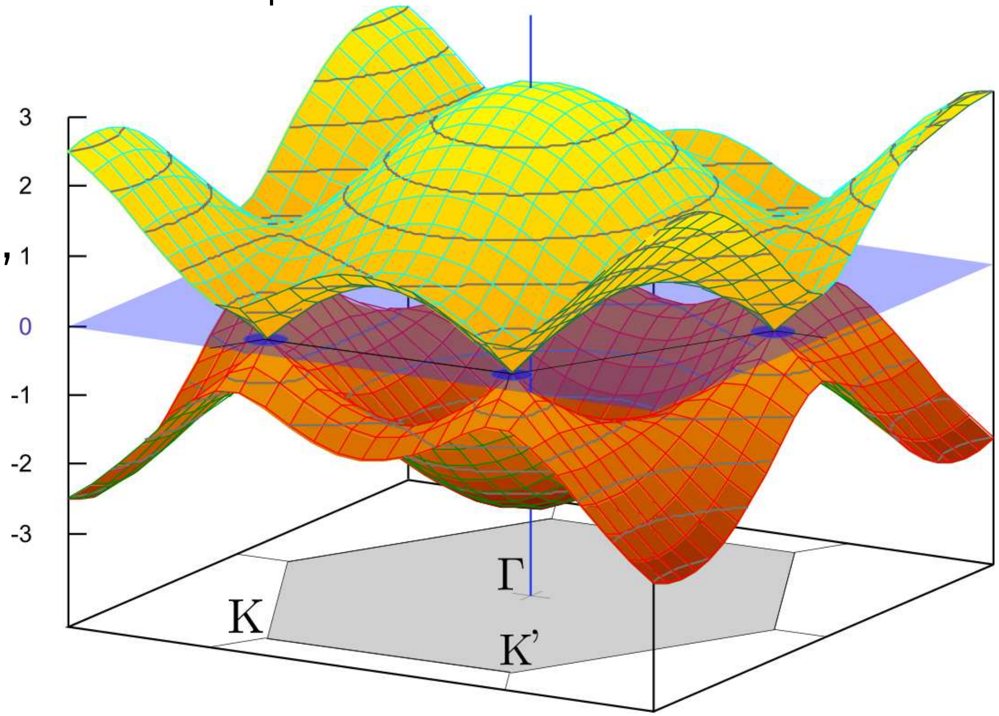
reciprocal space



$\Rightarrow$ pointlike Fermi-“surface” at K-points

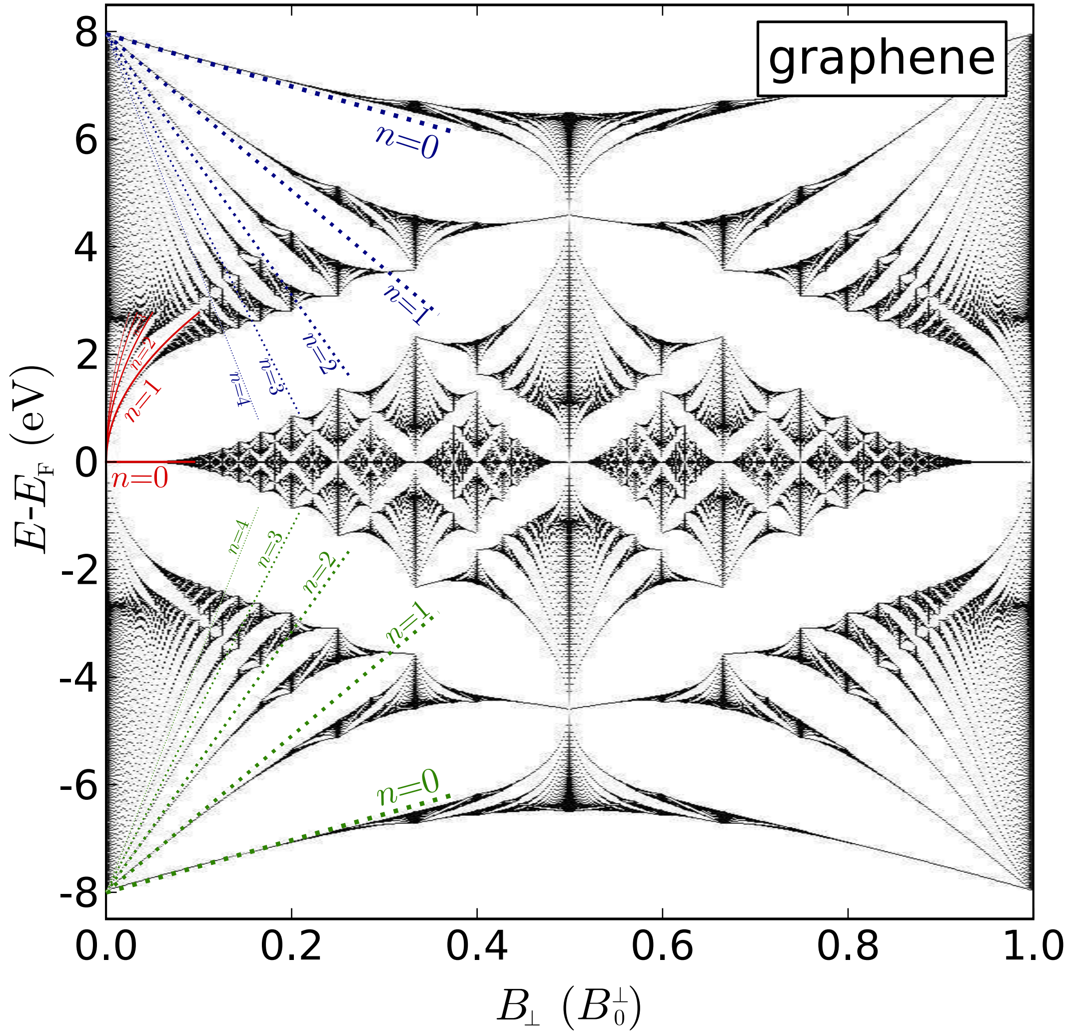
$\Rightarrow$ semi-metallic character

$\Rightarrow$ massless bands at E_{F} (Dirac-like theory)



Wallace, Phys. Rev. **71**, 622 (1947)

Hofstadter butterfly of graphene



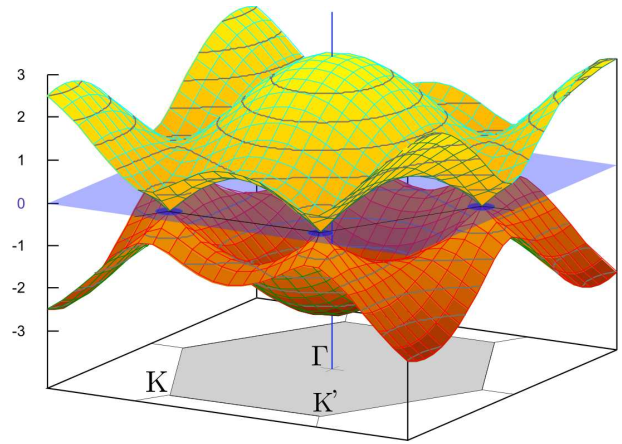
Rammal, J. Phys. (Paris) **46**, 1345 (1985)

(standard) Landau levels ("LL"):

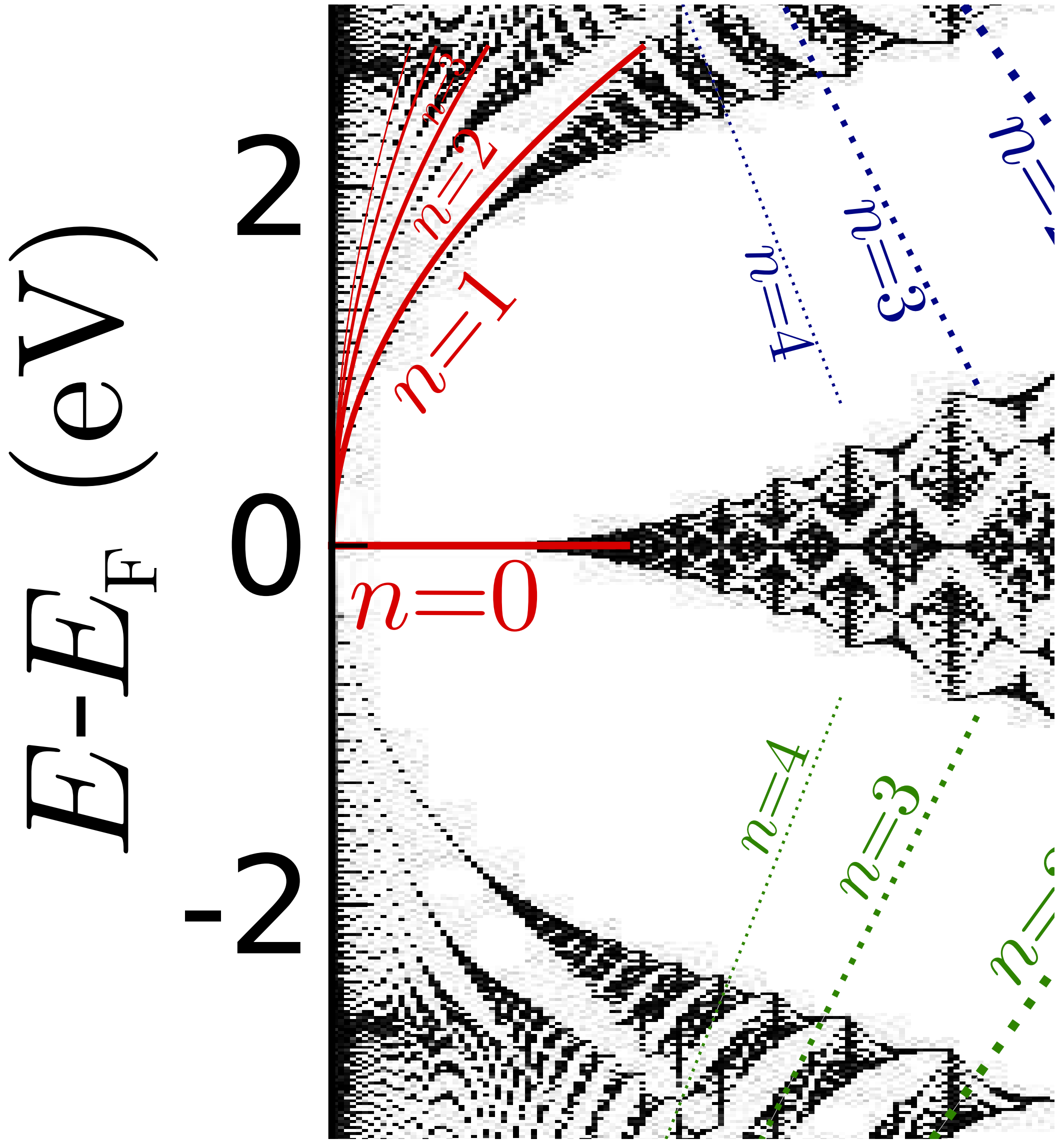
$$E - E_{\min} \propto \frac{\hbar e}{m^*} B \left(n + \frac{1}{2} \right)$$

$$E_{\max} - E \propto \frac{\hbar e}{m^*} B \left(n + \frac{1}{2} \right)$$

effective mass: $m^* = \frac{2\hbar^2}{\gamma a^2}$



Hofstadter butterfly of graphene



(standard) Landau levels ("LL"):

$$E - E_{\min} \propto \frac{\hbar e}{m^*} B \left(n + \frac{1}{2}\right)$$

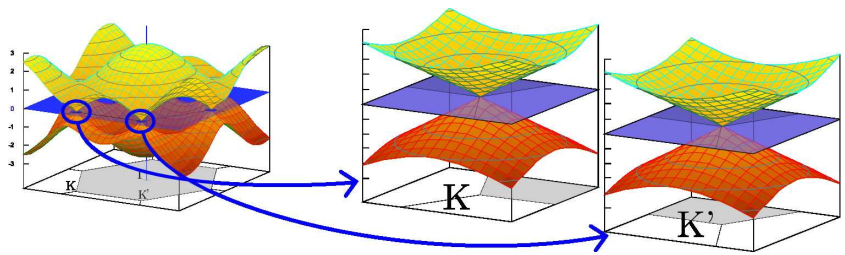
$$E_{\max} - E \propto \frac{\hbar e}{m^*} B \left(n + \frac{1}{2}\right)$$

relativistic LL: $(v_{\mathrm{F}} = \sqrt{3}\gamma a / 2\hbar)$

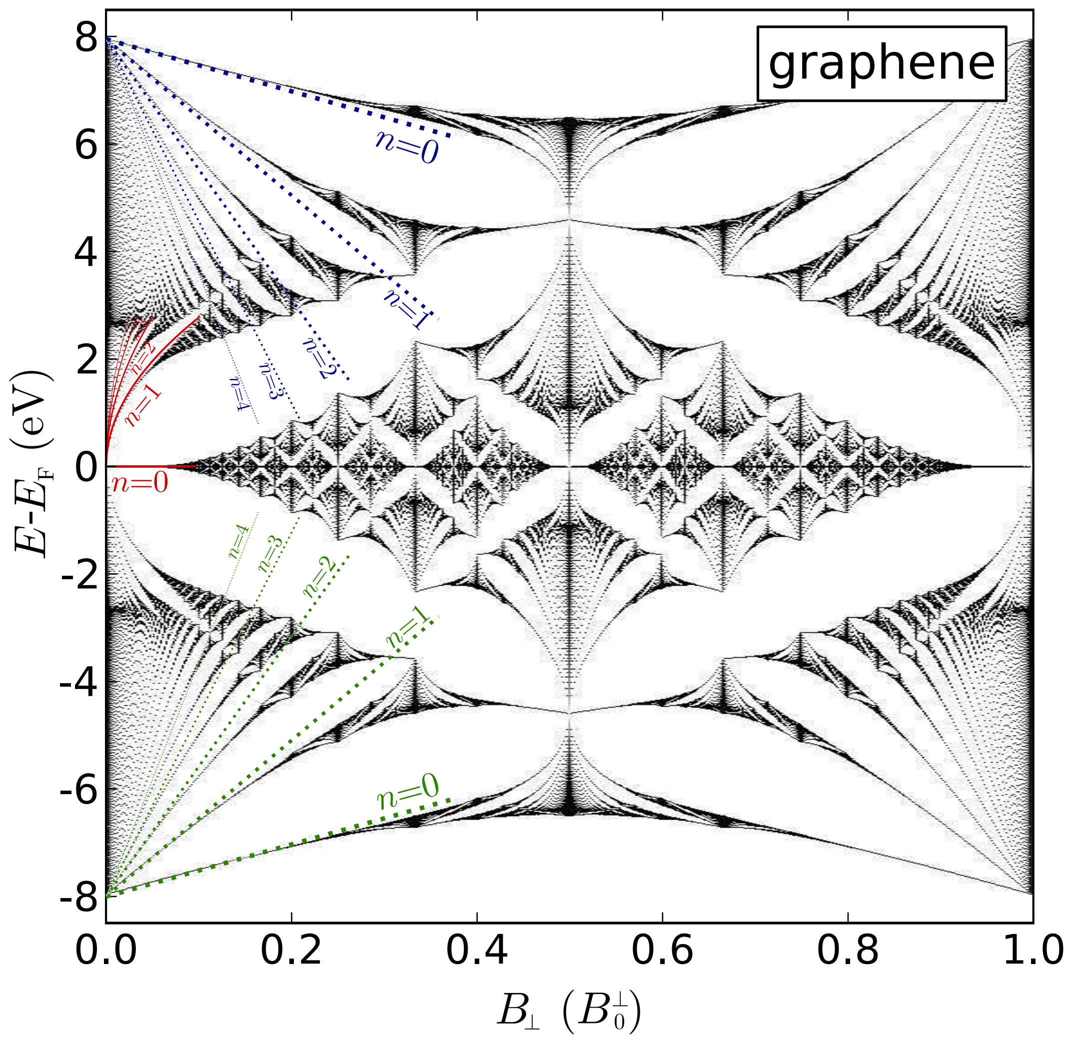
$$E - E_{\mathrm{F}} = \pm\, v_{\mathrm{F}} \sqrt{2e\hbar\, B\, n}$$

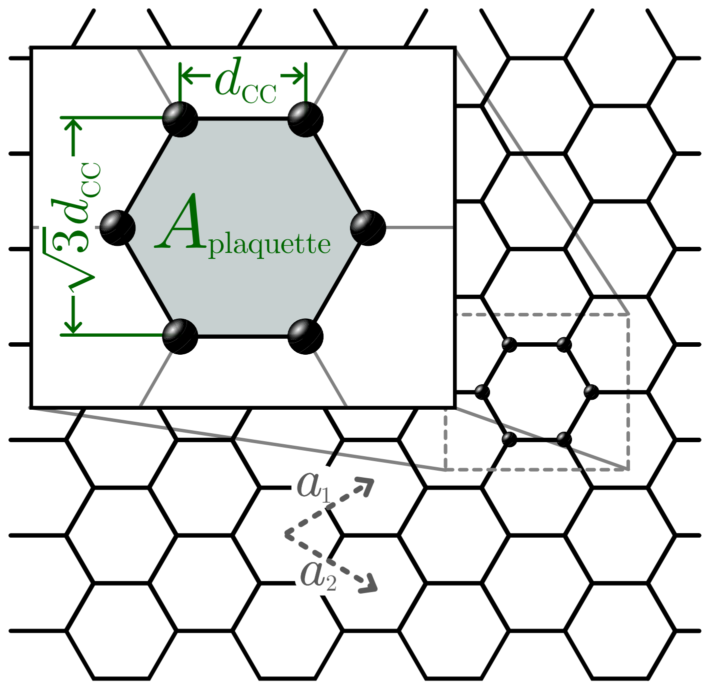
supersymmetric LL ("SuSyLL"):

$$E = E_{\mathrm{F}}$$



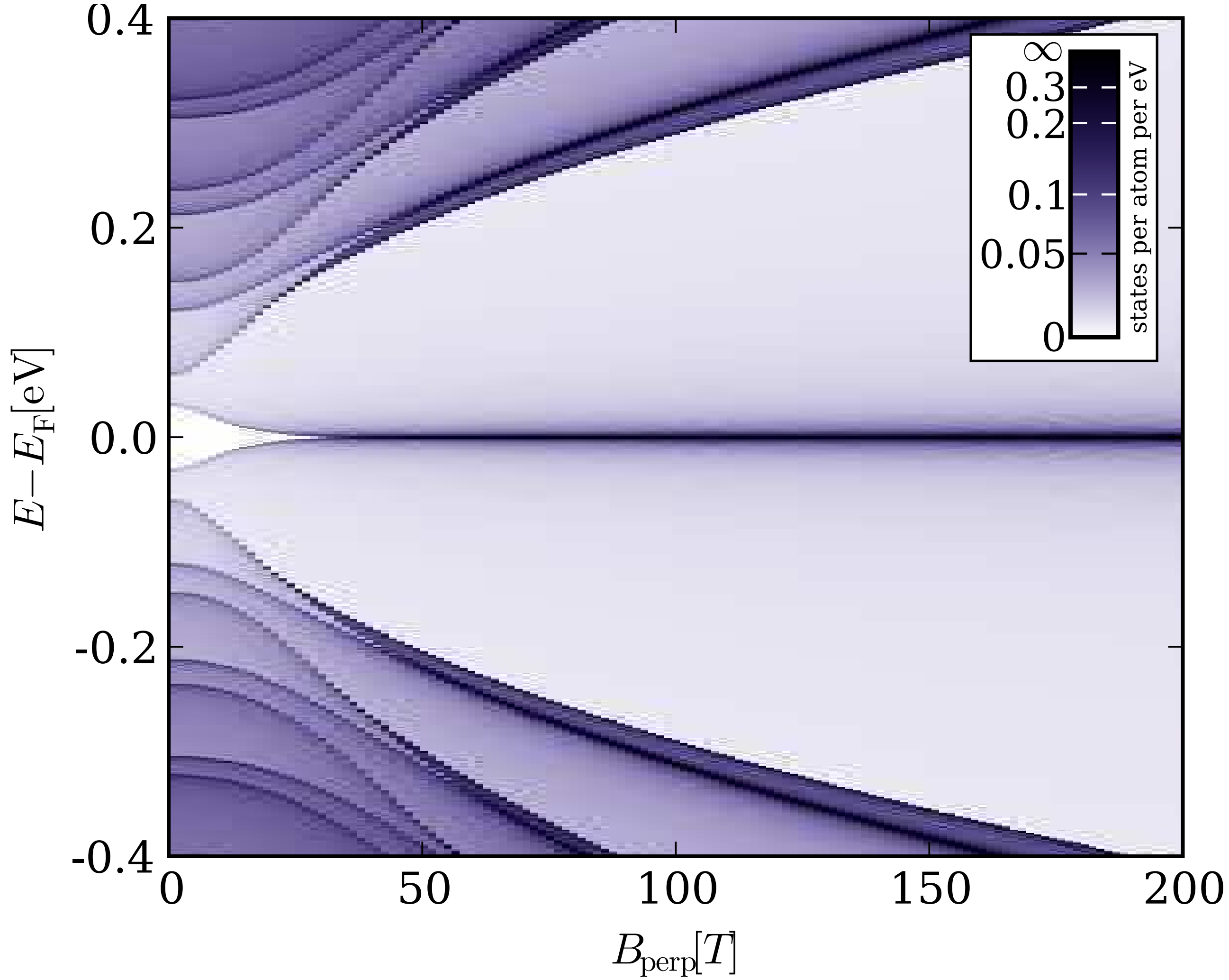
Hofstadter butterfly of graphene

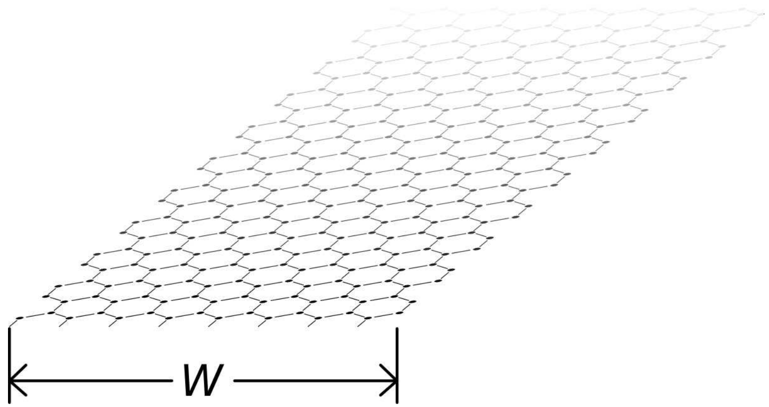




$$
\begin{aligned}
B_0^\perp &= \Phi_0 / A_{\text{plaquette}} \\
&\approx 79\,\mathrm{kT}\ (!!)
\end{aligned}
$$

Graphene nanoribbon

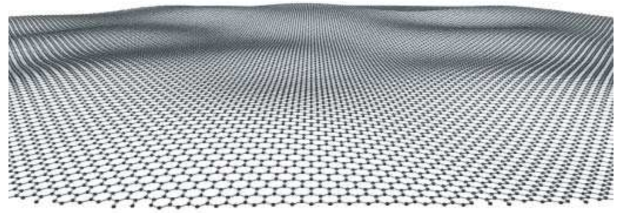


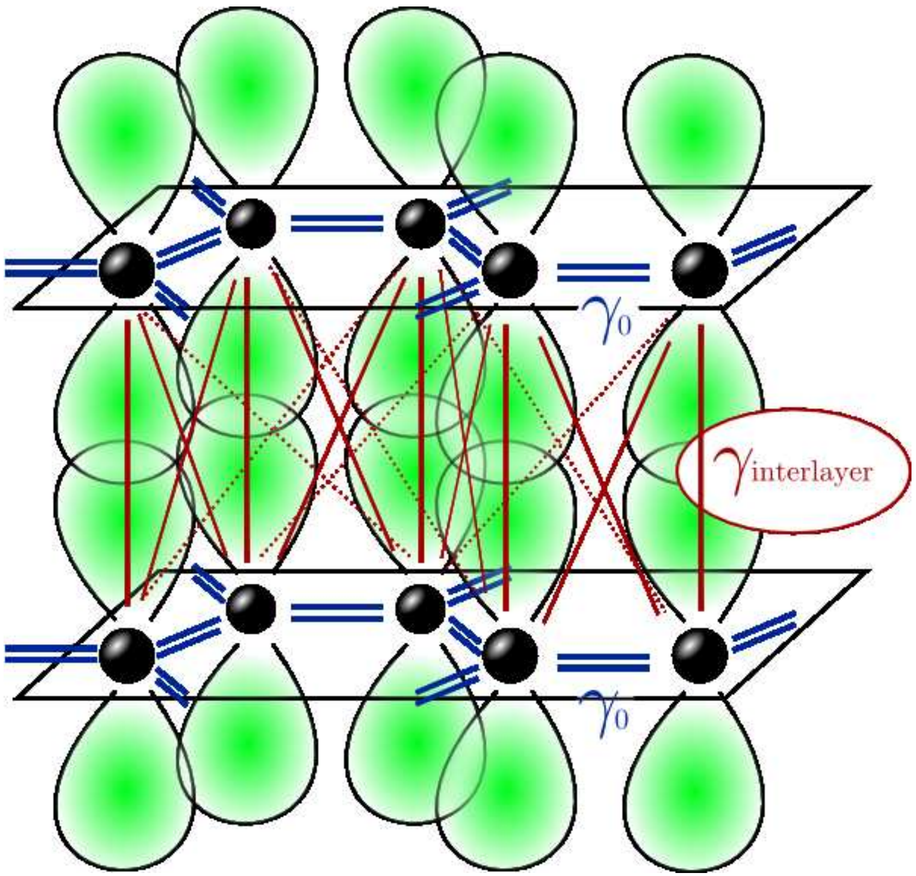


(80,0)-armchair ribbon
$W = 20\text{nm}$

see also:
Peres *et al.*
PRB **73**, 241403 (2006)

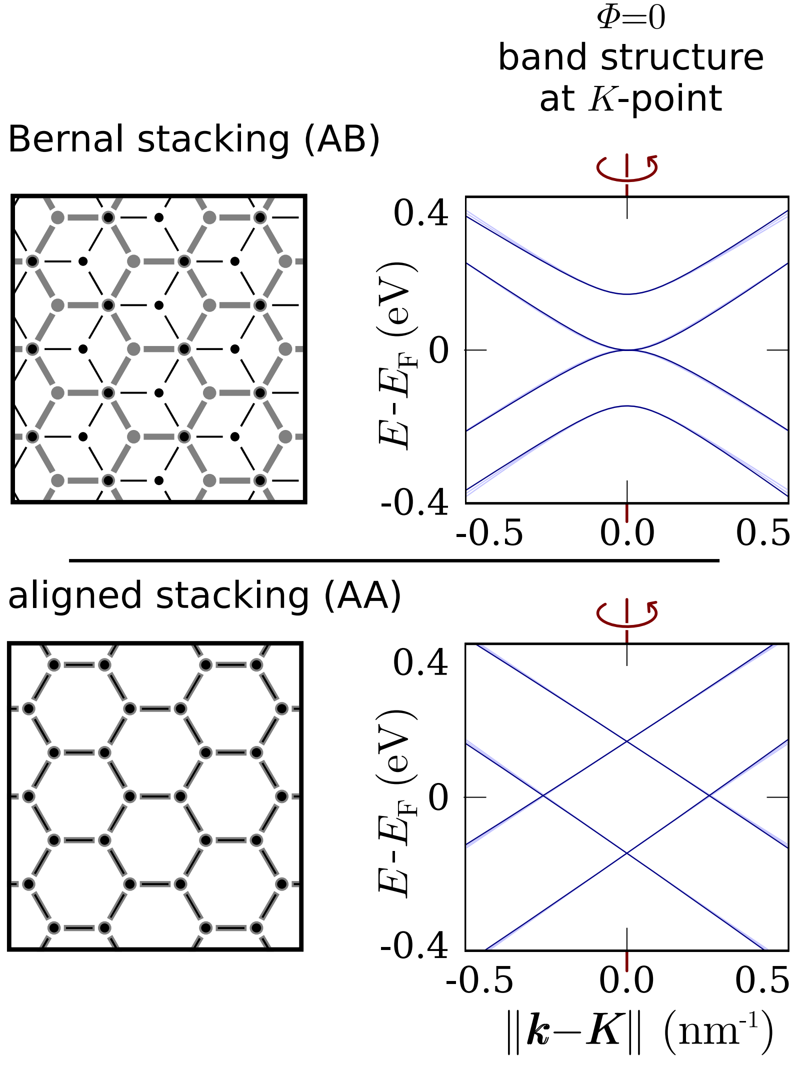
Bilayer graphene





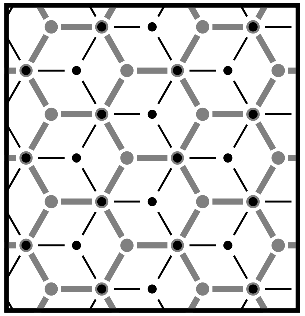
$$\gamma_{ij}^{\text{interlayer}} = \frac{\gamma_0}{8}\exp\left(\frac{d_{ij}-d_0}{\delta}\right)$$

$$\beta = \frac{\gamma_0}{8},\ d_0 = 3.34\,\text{Å},\ \delta = 0.45\,\text{Å}$$



N. Nemec and G. Cuniberti, Phys. Rev. B (Rapid Comm.) to appear. [cond-mat/0612369]

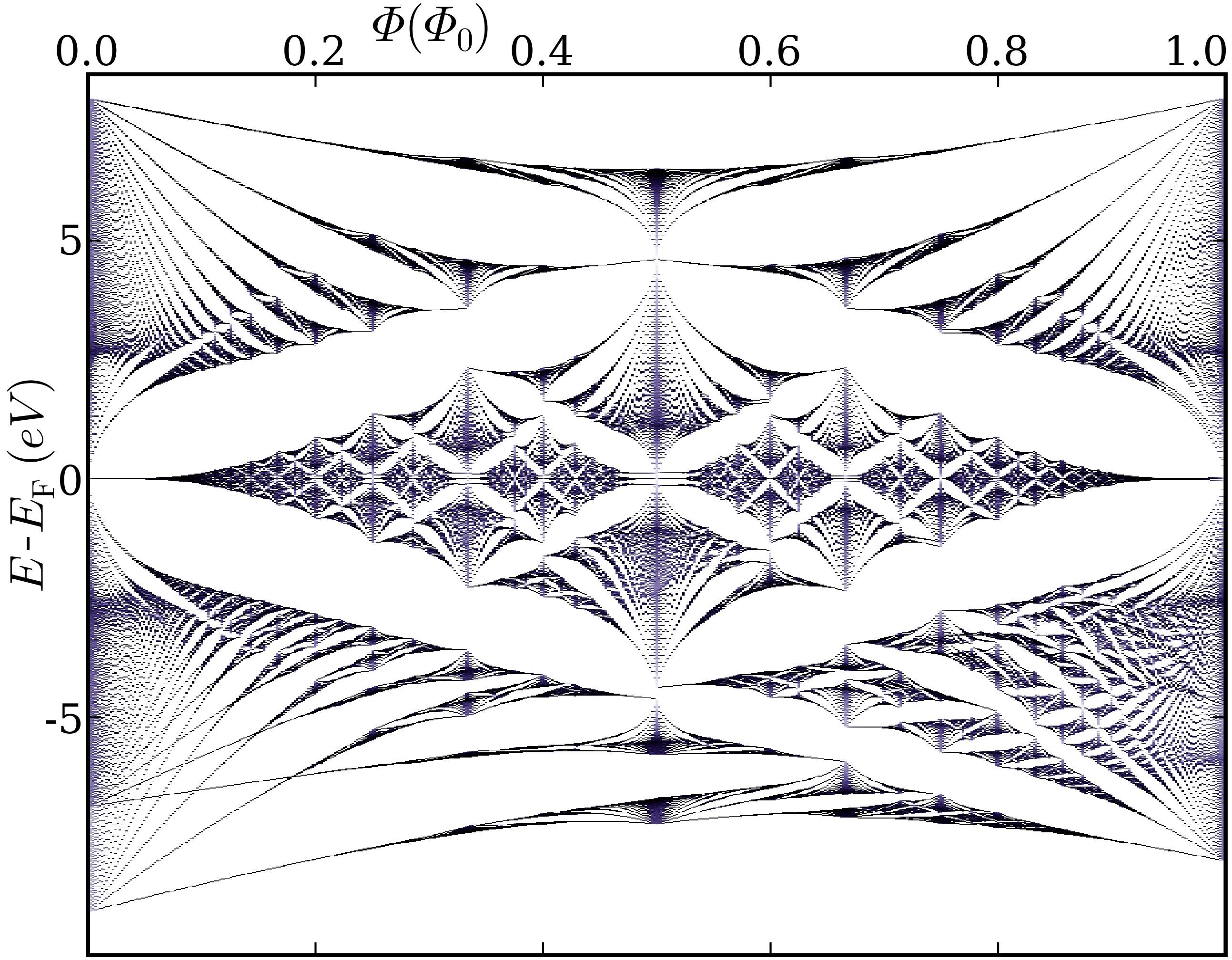
Hofstadter butterfly of bilayer graphene



Bernal-
stacking

broken symmetries:
$\rightarrow \Phi_0$-periodicity
$\rightarrow$ electron-hole

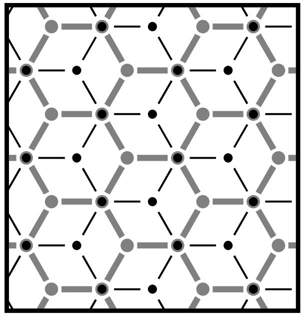
SuSyLL protected
by symmetry



see also: Novoselov *et al.*, Nature Physics **2**, 177 (2006)

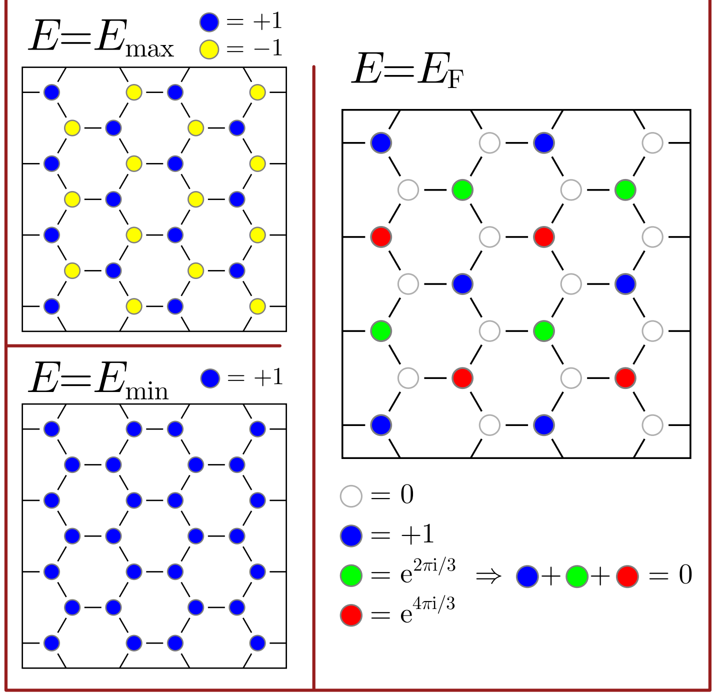
N. Nemec and G. Cuniberti, Phys. Rev. B (Rapid Comm.) to appear. [cond-mat/0612369]

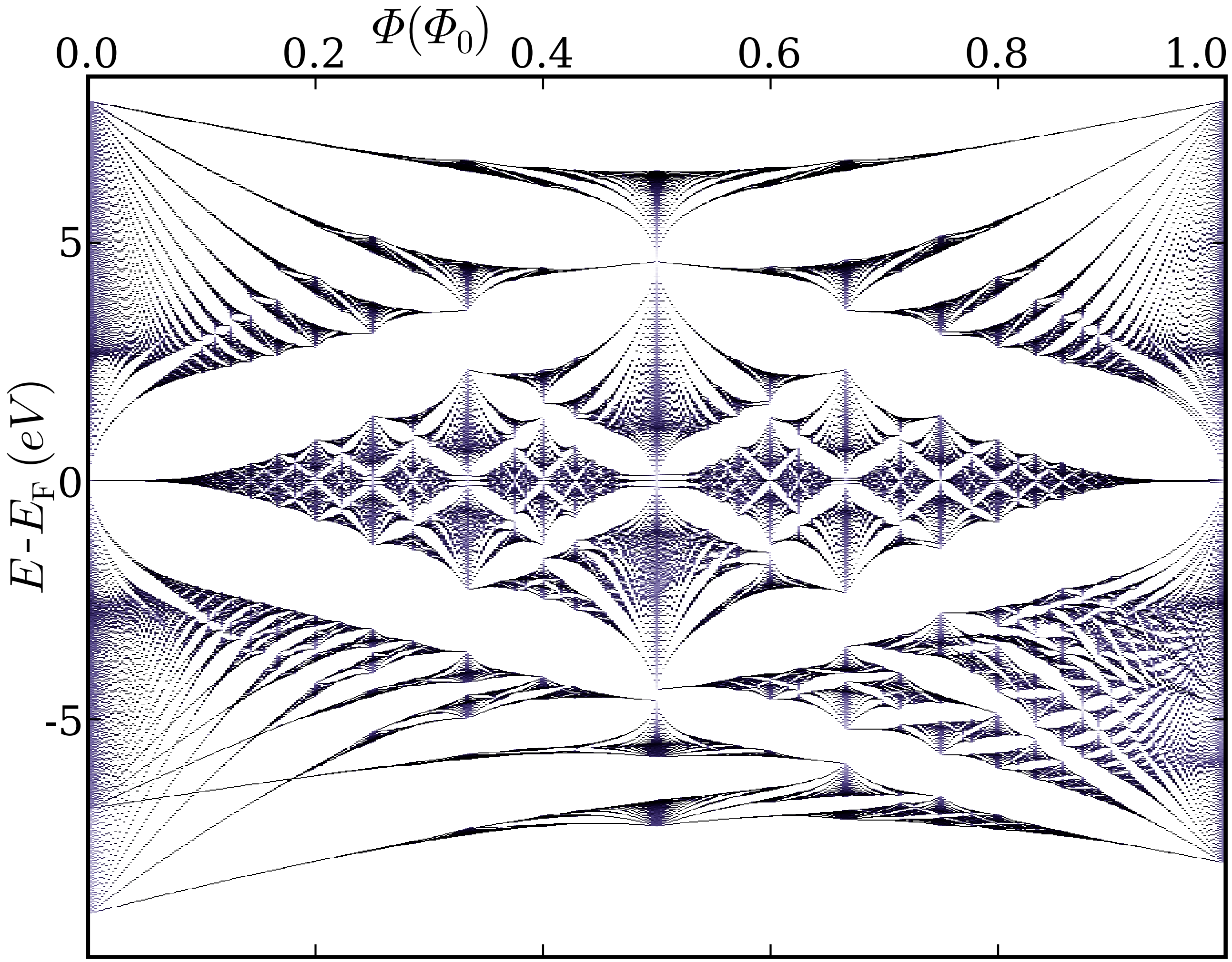
e-h asymmetry



Bernal-stacking

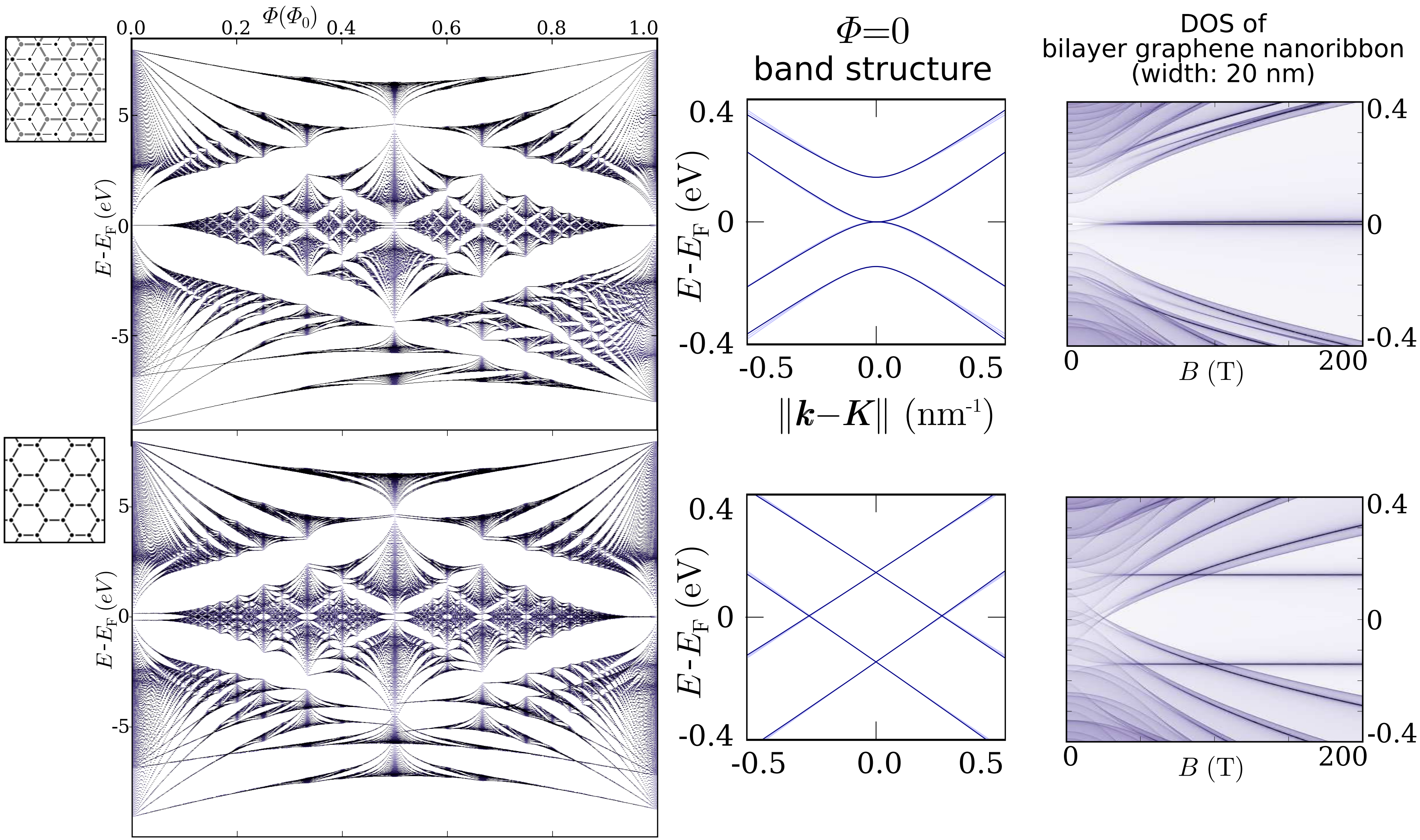
Wavefcns in graphene **monolayer**





N. Nemec and G. Cuniberti, Phys. Rev. B (Rapid Comm.) to appear. [cond-mat/0612369]

Shifted bilayer graphene

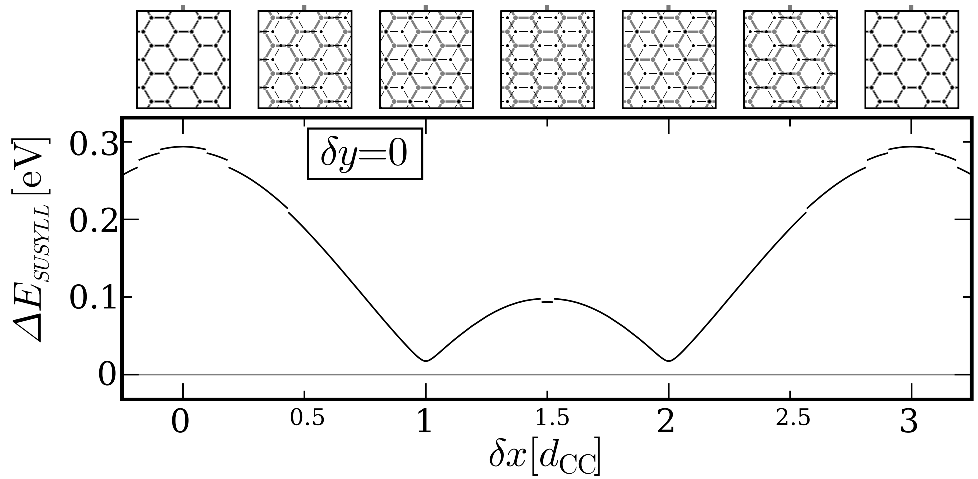


N. Nemec and G. Cuniberti, Phys. Rev. B (Rapid Comm.) to appear. [cond-mat/0612369]

Split of the SUSYLL

Bernal stacking:
SuSyLL protected against split

Shifted configurations:
SuSyLL split by varying amounts

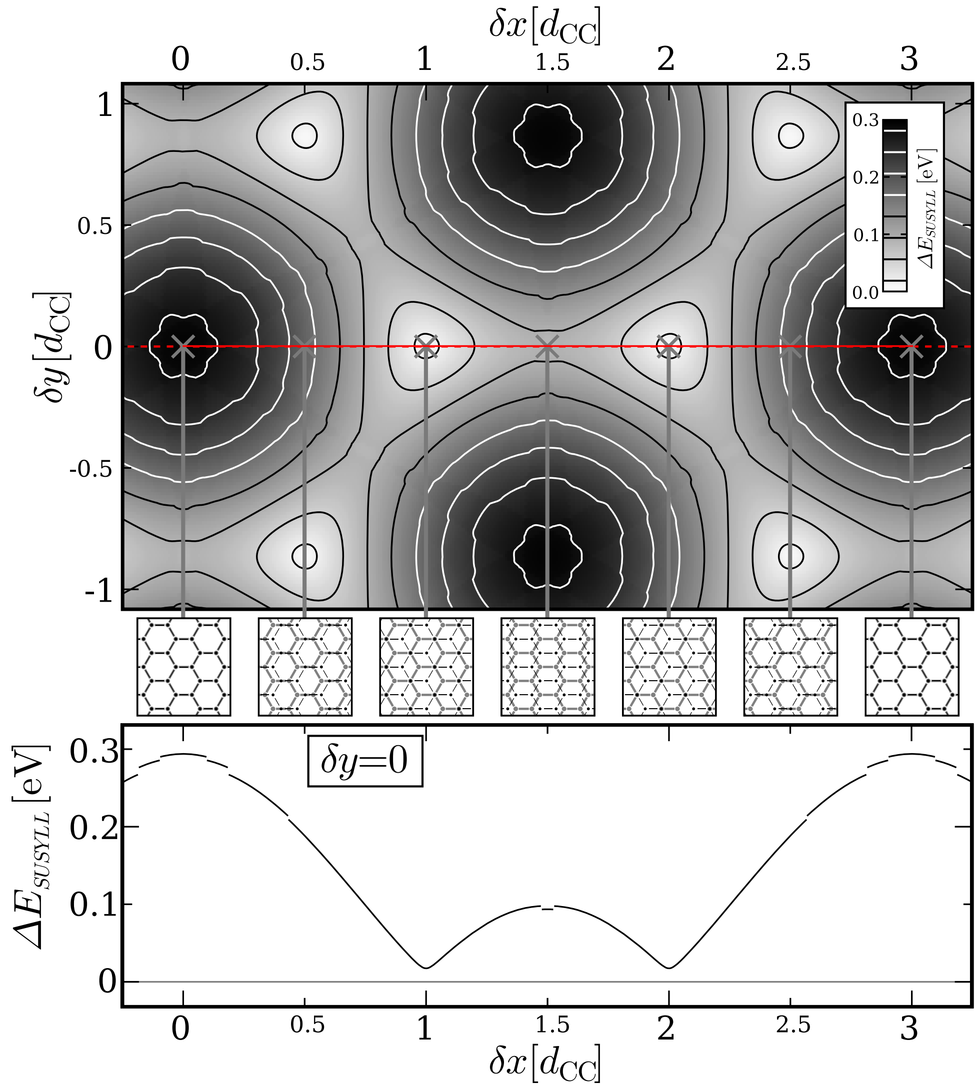


N. Nemec and G. Cuniberti, Phys. Rev. B (Rapid Comm.) to appear. [cond-mat/0612369]

Split of the SUSYLL

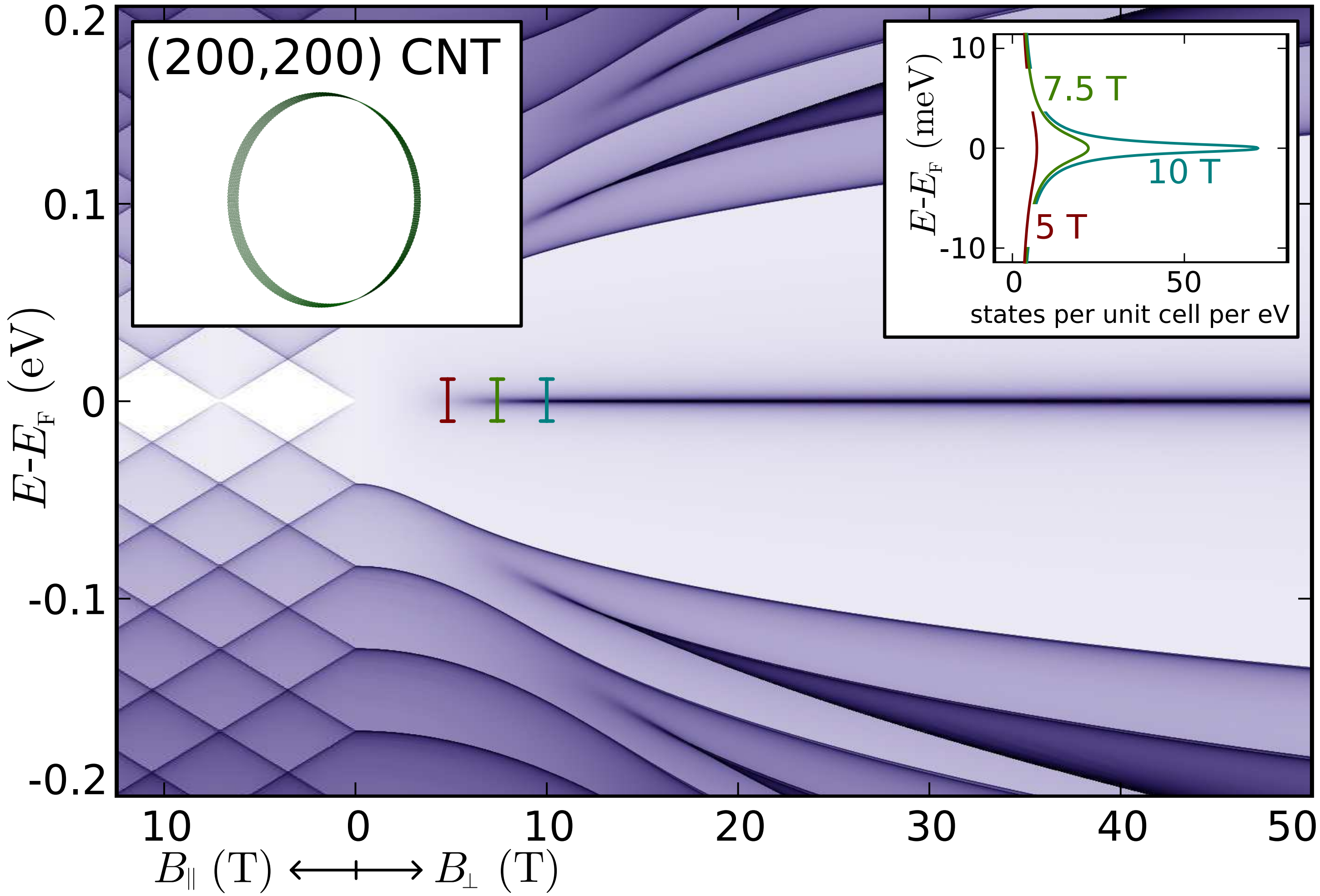
Bernal stacking:
SuSyLL protected against split

Shifted configurations:
SuSyLL split by varying amounts



N. Nemec and G. Cuniberti, Phys. Rev. B (Rapid Comm.) to appear. [cond-mat/0612369]

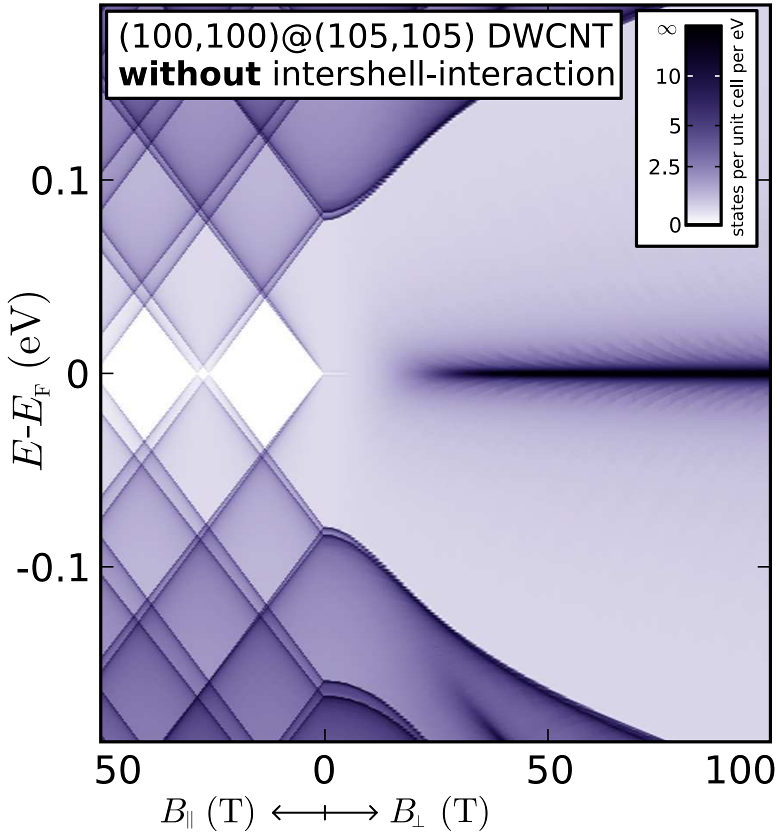
Carbon nanotubes at accessible fields



- scaling behavior: $\mathrm{DOS}_{(m,m)}(E,\boldsymbol{B}) = \mathrm{DOS}_{(m',m')}\left(\frac{m}{m'}E, \frac{m^2}{m'^2}\boldsymbol{B}\right)$

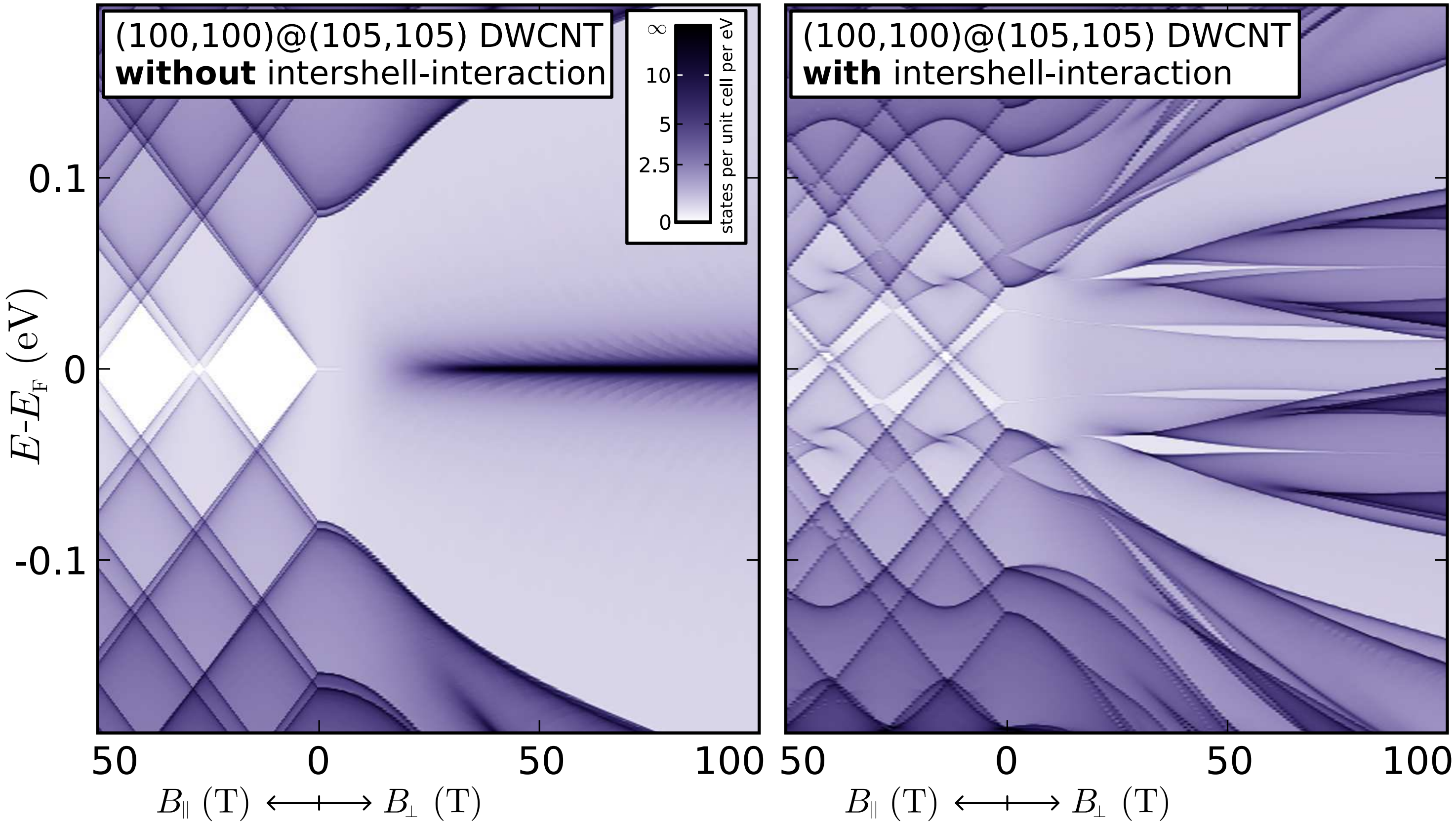
N. Nemec and G. Cuniberti, Phys. Rev. B **74**, 165411 (2006)

Inter-shell effects in MWCNT



- no interaction $\Rightarrow$ $\mathrm{DOS} = \mathrm{DOS}_{\mathrm{inner}} + \mathrm{DOS}_{\mathrm{outer}}$

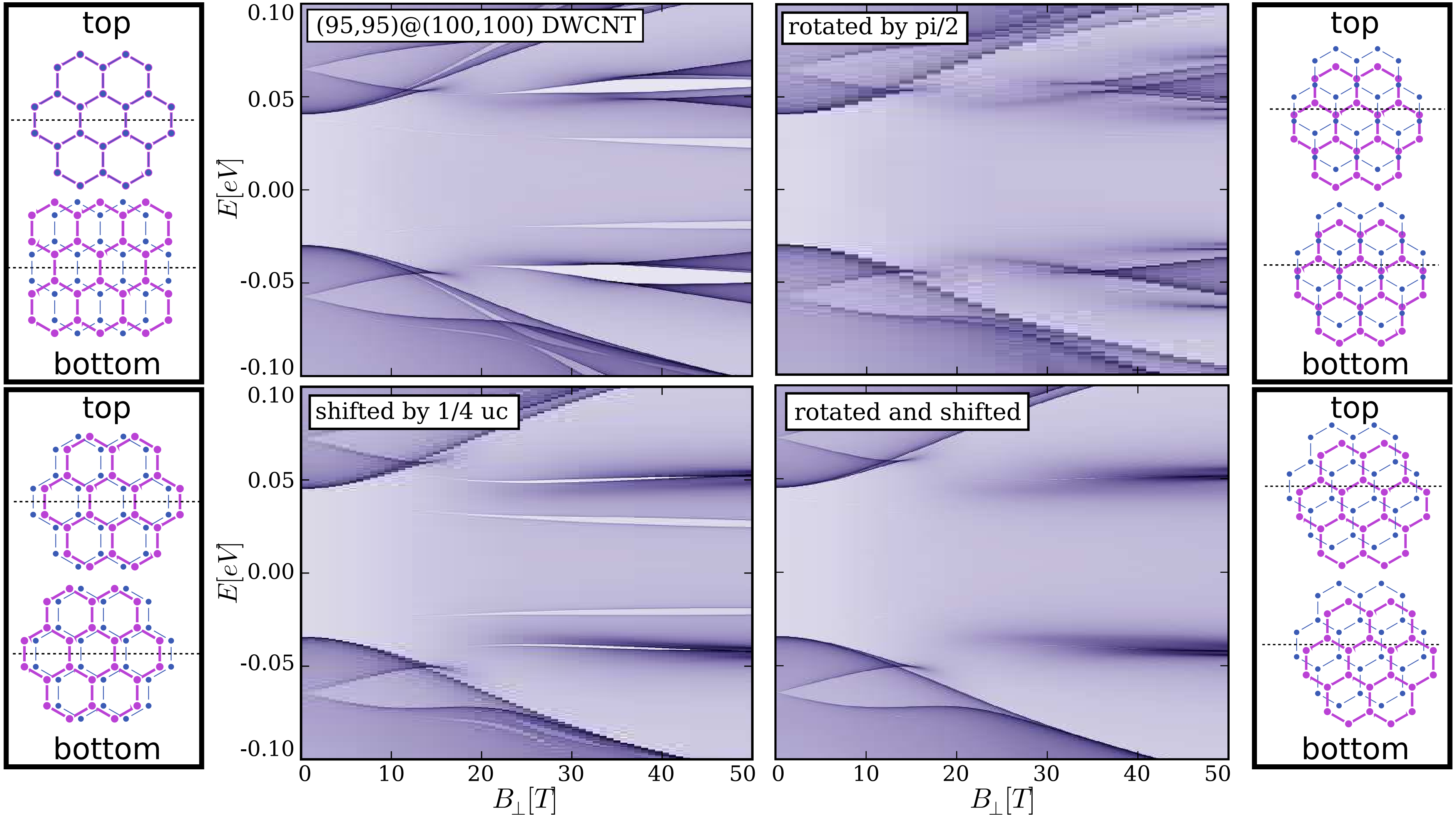
Inter-shell effects in MWCNT



- no interaction $\Rightarrow$ $\mathrm{DOS} = \mathrm{DOS}_{\mathrm{inner}} + \mathrm{DOS}_{\mathrm{outer}}$
- SuSyLL split up by intershell-interaction

work in progress

Inter-shell effects in MWCNT



$\Delta E \approx 0.1\mathrm{eV}$ *independent of relative positions !!*

work in progress

Summary

- Graphene: *Dirac electrons* at E_F $\rightarrow$ relativistic LL & SuSyLL
- SuSyLL in graphene: ΔE_SuSy *varies* with relative shift of layers
- DWCNT: $\Delta E_\mathrm{SuSy} \approx 0.1\,\mathrm{eV}$

Outlook

- more detailed modelling of interlayer interaction
- effects on magnetotransport
  e.g. Fabry-Perot, *see also: HL 49.1, 17^{30} (H17)*
- role of defects
  see also: HL 49.3, 18^{00} (H17)