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FINLAND

Flat bands in graphene-based systems

Tero T. Heikkilä

Nanoscience Center/Department of Physics,
University of Jyväskylä, Finland

ACADEMY OF FINLAND
RESEARCH FUNDING AND EXPERTISE

Codes available at
https://gitlab.jyu.fi/jyucmt/

Collaborators

Teemu Peltonen
Univ. Jyväskylä

Aleksi Julku
Aalto University

Risto Ojajärvi
Univ. Jyväskylä

Grigori Volovik
Low Temp Lab, Aalto University
Landau Institute, Moscow

Päivi Törmä
Aalto University

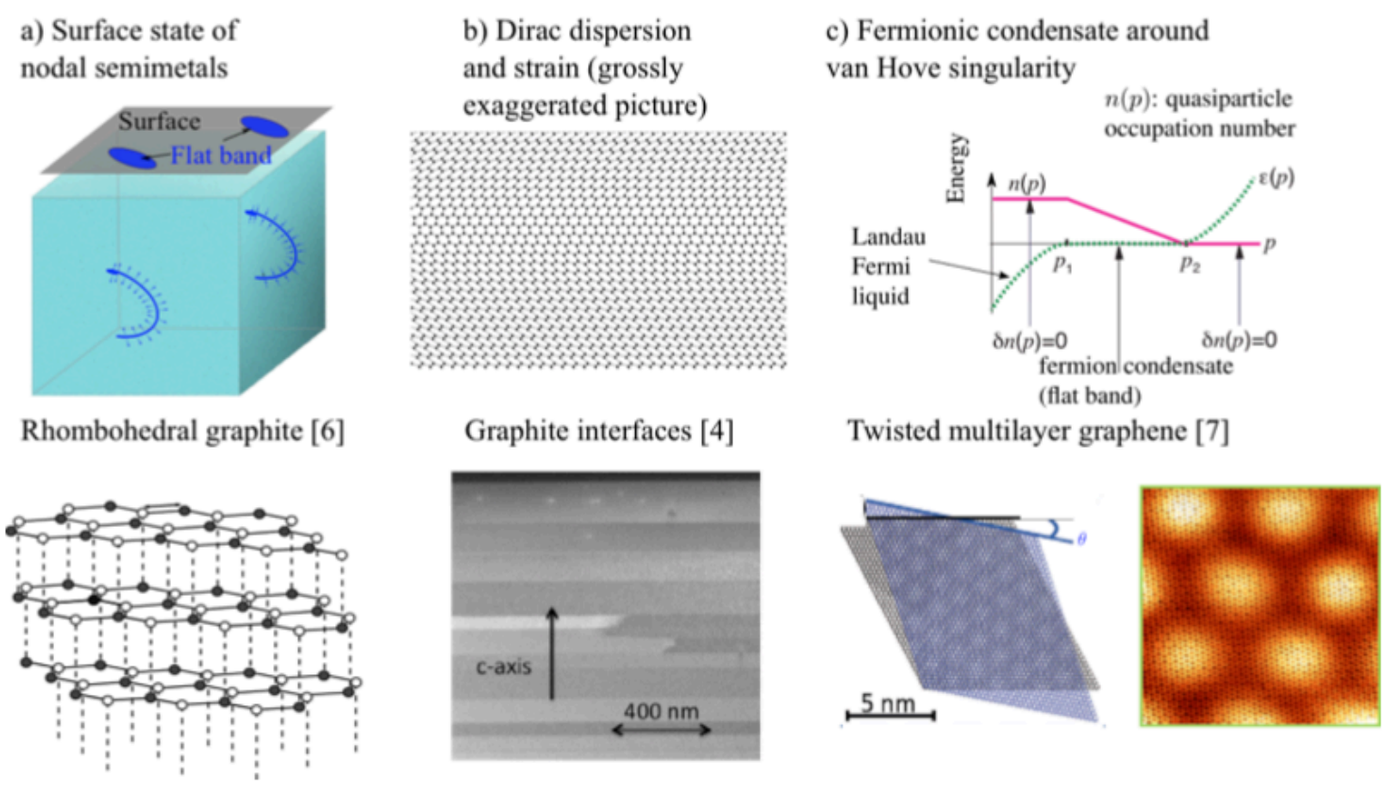
Timo Hyart
Univ. Jyväskylä
(now in Warsaw)

Nikolai Kopnin
Low Temp Lab, Aalto University
Landau Institute, Moscow
in memoriam

Ville Kauppila, Ari Harju, Mari Ijäs, Liang Long, Jaakko Nissinen, Aalto University
Faluke Aikebaier, Univ. Jyväskylä

Contents

- Flat bands and superconductivity
- Stacked graphene -based flat band
- Strained graphene -based flat band
- Flat bands from twisted graphene bilayers

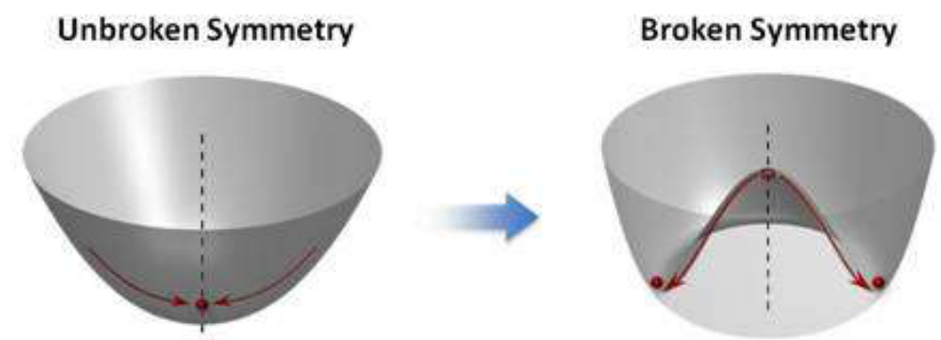


Funding proposal SUPERFLAT 2015
Unfortunately unsuccessful…

Superconductivity: mean field

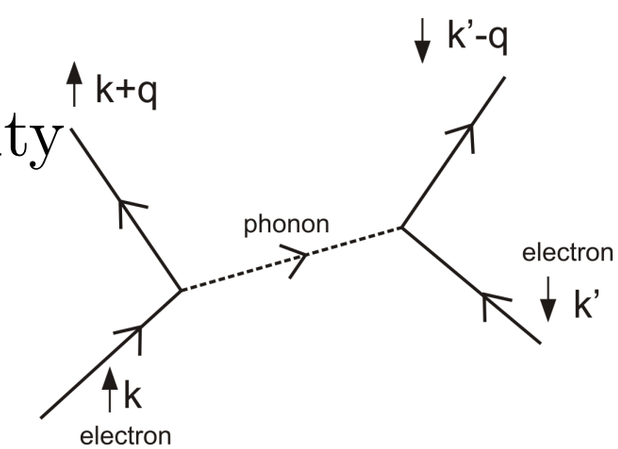
Order parameter: $\Delta = \lambda \langle \psi_\sigma \psi'_\sigma \rangle$

Supercurrent: $\Delta = |\Delta| e^{i\phi(\mathbf{r})} \Rightarrow \mathbf{j} = D_s \nabla \phi$



BCS mean field theory: $k_B T_C \sim \Delta$ depends on the competition between

- Attractive interaction mediated by a coupling to a spectrum of bosonic modes, strength λ
- Conduction electron dispersion, bandwidth δE and density of states ν_F at $E = E_F$
- Boson characteristic frequency ω_c

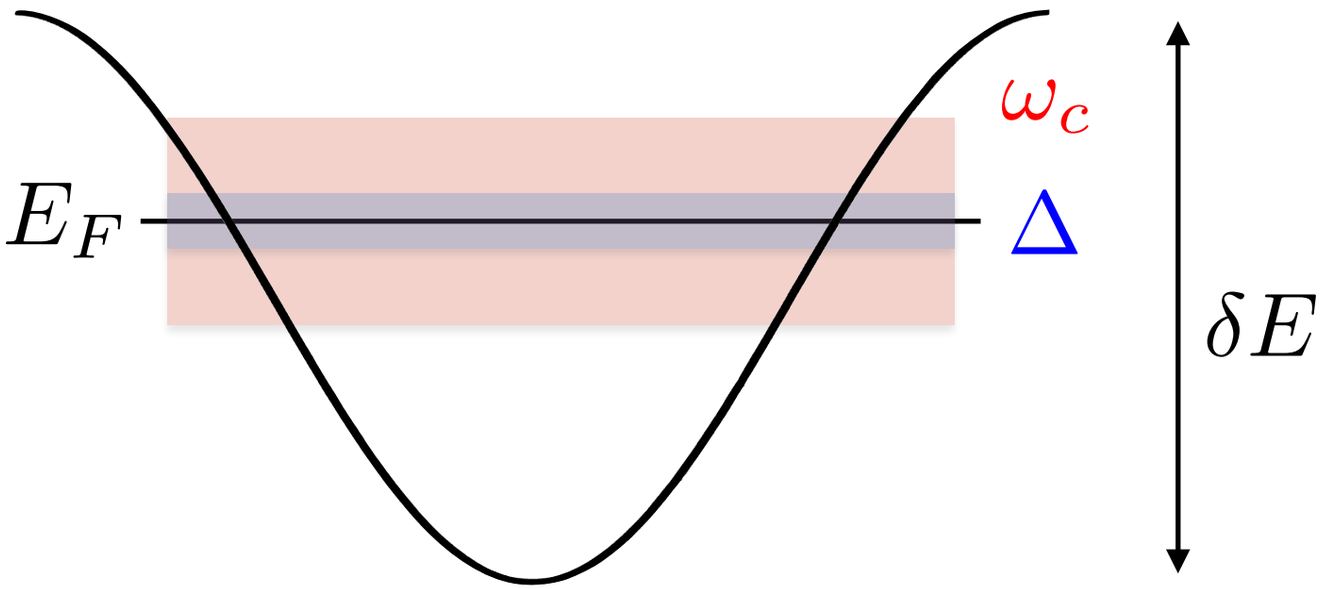


Picture sources: Phys. org, Wikimedia Commons

BCS theory

$[\lambda] = \mathrm{Jm}^d$

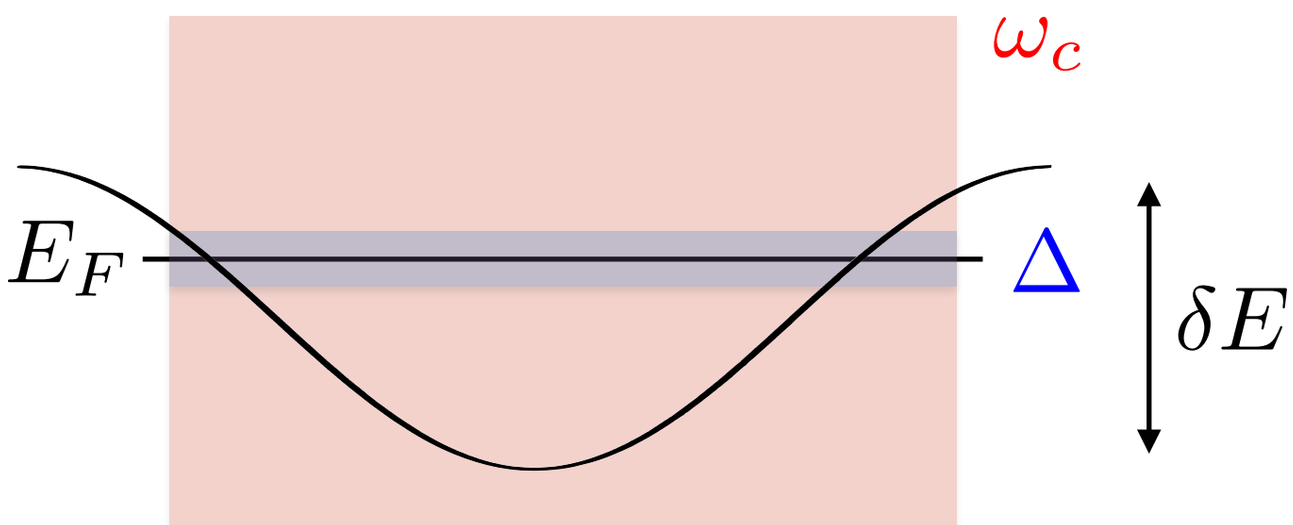
Conventional metals



$$T_c, \Delta \sim \omega_c e^{-1/(\lambda \nu_F)}$$

Bardeen, Cooper & Schrieffer, 1957

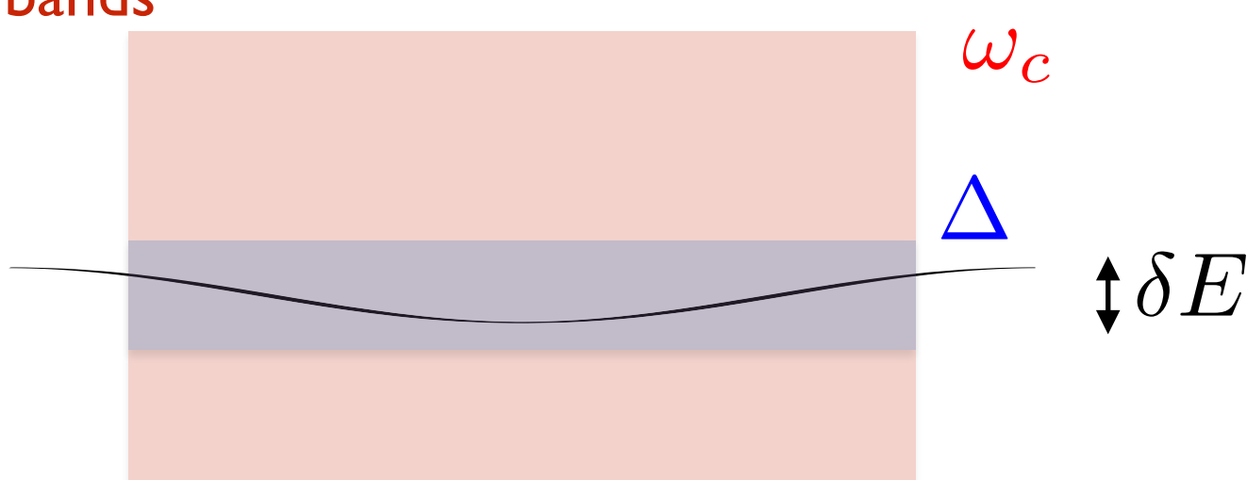
Narrow bands



$$T_c, \Delta \sim \delta E e^{-1/(\lambda \nu_F)}$$

$$(\text{also: larger } \nu_F)$$

Flat bands



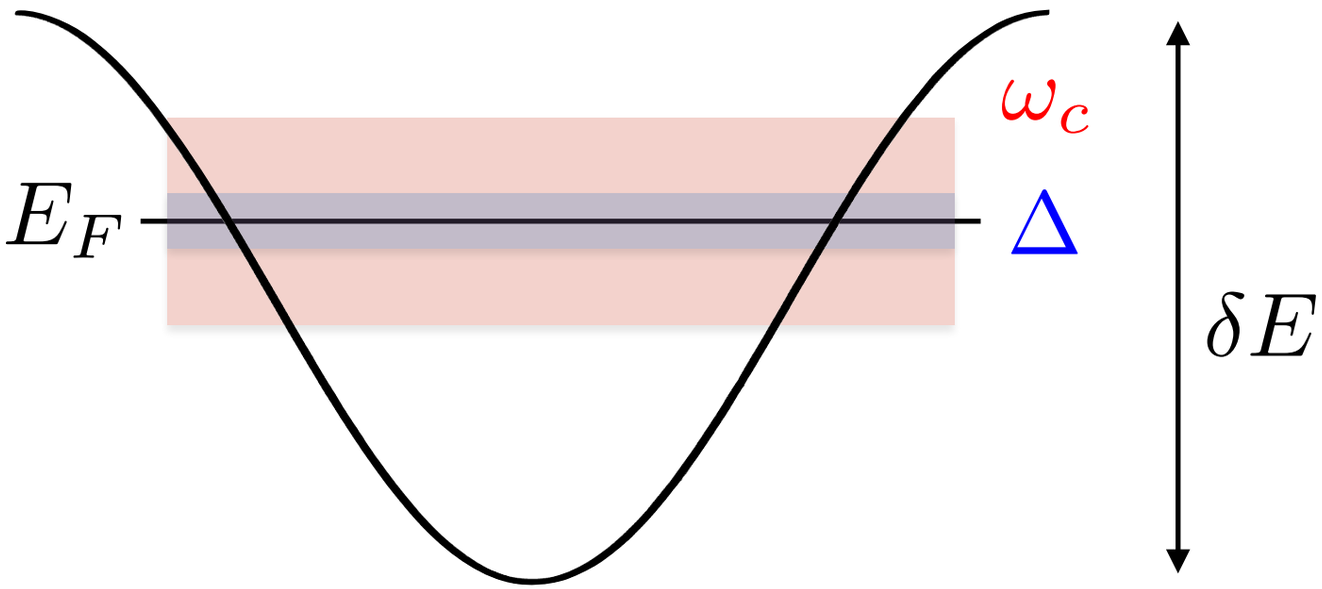
Flat band size!

$$T_c \sim \Delta = \frac{\lambda \Omega_{\mathrm{FB}}}{2\pi}$$

Belyaev, JETP (1960)
Khodel & Shaginyan, JETP Lett. (1990)
Kopnin, TTH, G.E. Volovik, PRB **83**, 220503 (R) (2011)
Tasaki, PRL (1992); Mielke & Tasaki Commun. Math. Phys. (1993)
(flat-band magnetism)

BCS theory

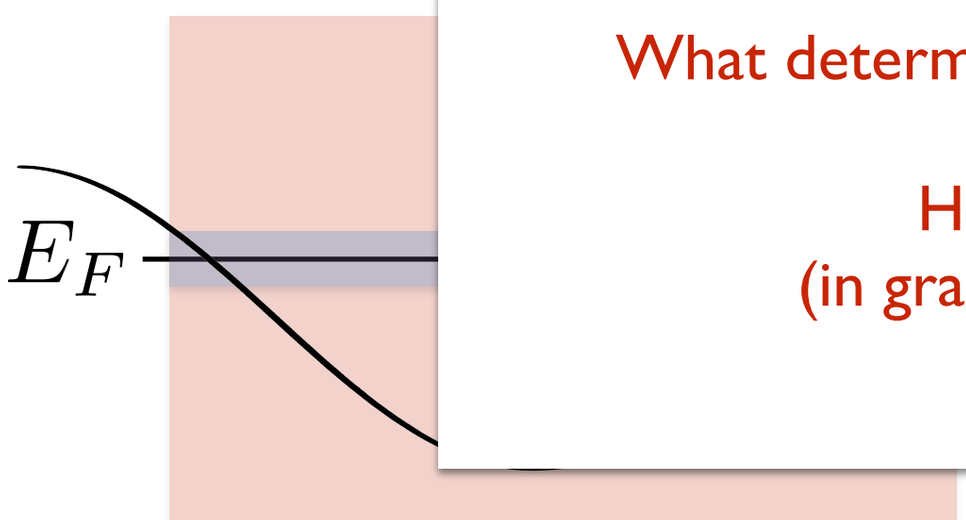
Conventional metals



$$T_c, \Delta \sim \omega_c e^{-1/(\lambda \nu_F)}$$

Bardeen, Cooper & Schrieffer, 1957

Narrow bands



$$Ee^{-1/(\lambda \nu_F)}$$

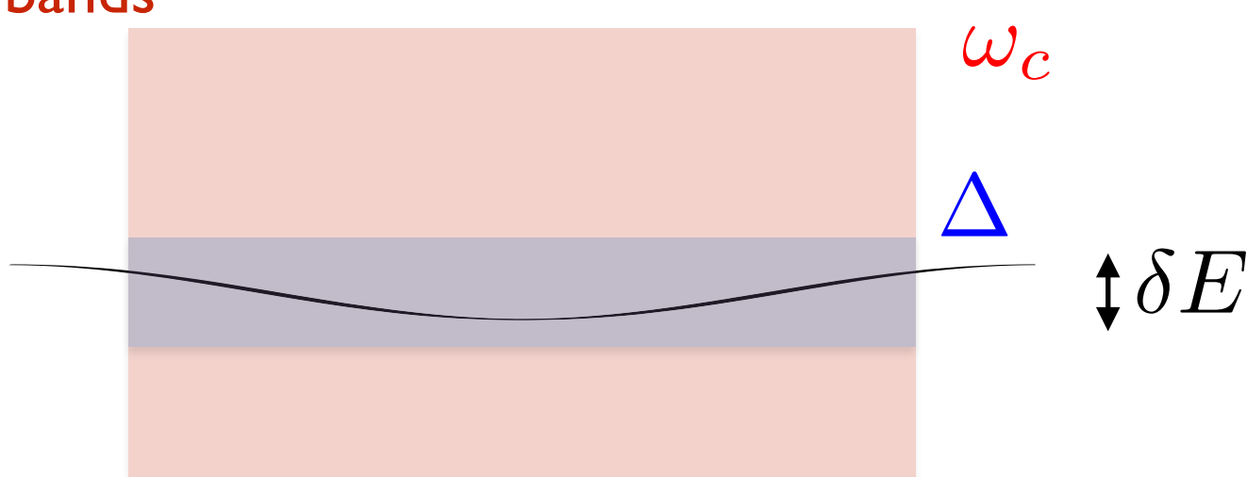
also: larger ν_F)

What determines the size of the flat band?

How to maximise it
(in graphene based systems)?

Flat band size!

Flat bands



$$T_c \sim \Delta = \frac{\lambda \Omega_{\mathrm{FB}}}{2\pi}$$

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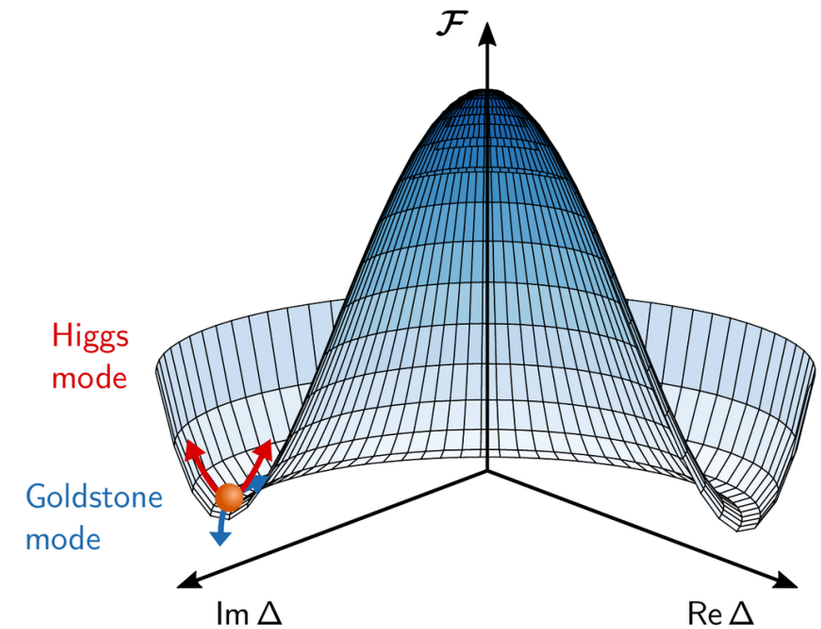
Tasaki, PRL (1992); Mielke & Tasaki Commun. Math. Phys. (1993)
(flat-band magnetism)

Possible caveats



Picture stolen from Dirk Manske

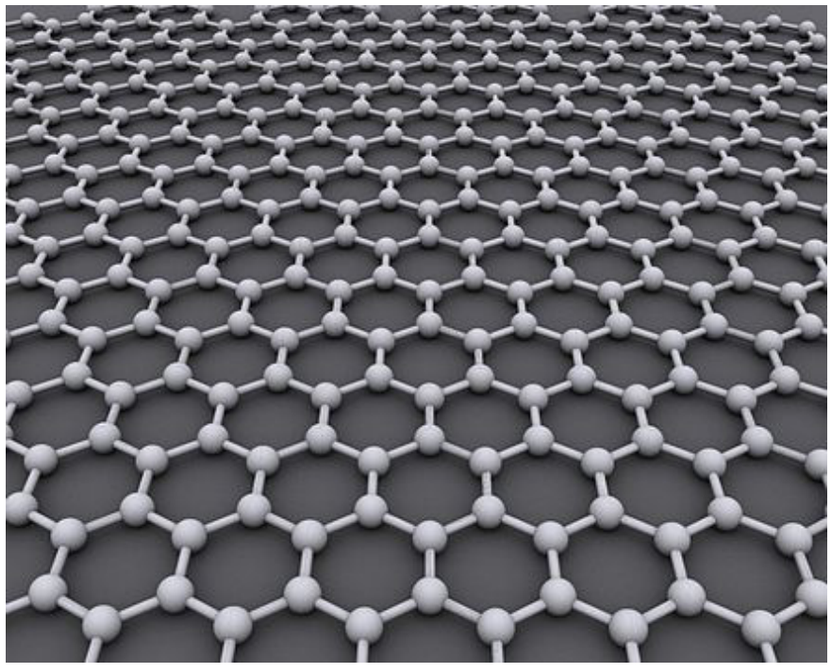
- Validity of the mean-field theory
  - Ok for *T=0* (e.g., Josephson effect)
  - Phase fluctuations (Goldstone): BKT transition, consider geometric contribution to superfluid weight!

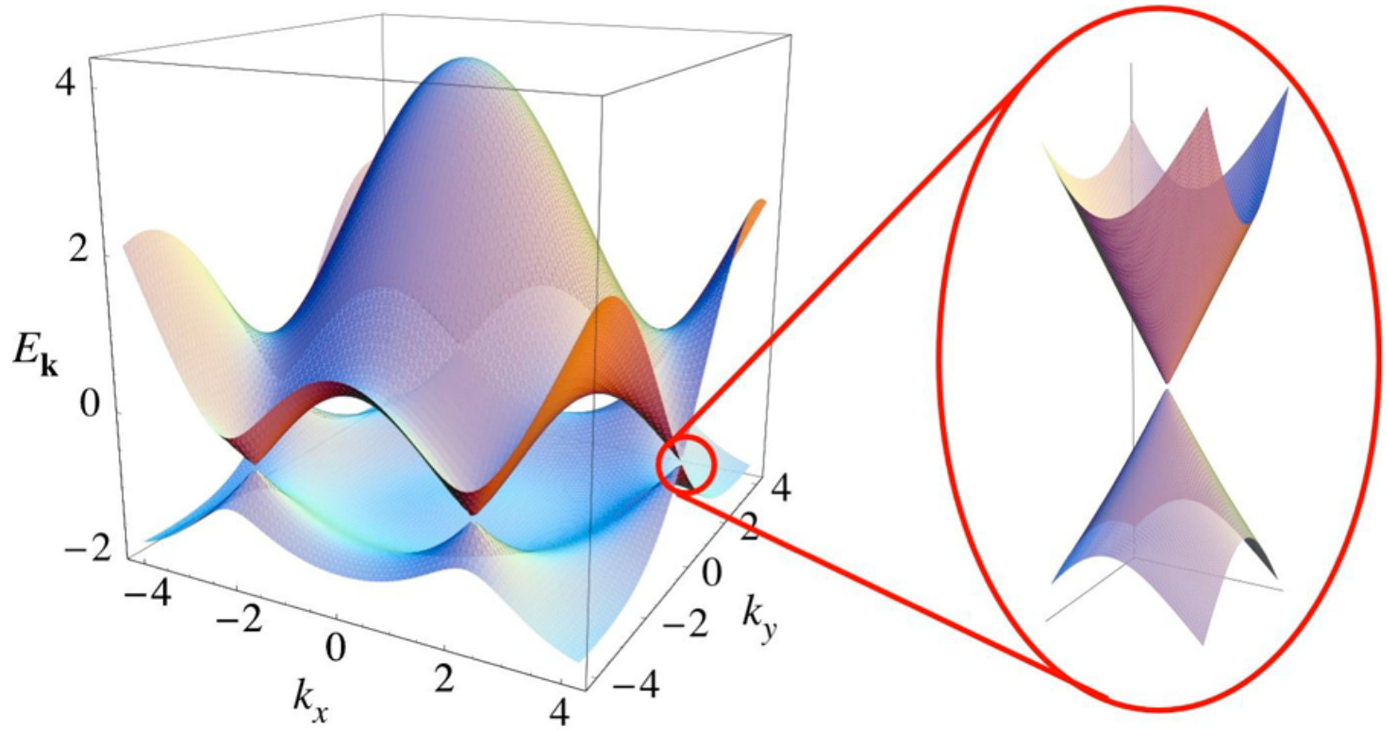
    But: $T_{\mathrm{BKT}} \lesssim T_c^{\mathrm{mf}} \sim \Delta$
  - Amplitude fluctuations (Higgs): another way to kill the mean field! $\mathrm{Gi} \sim T_C/E_F \sim 1$
- Electron-phonon model: Migdal theorem not valid: only lowest-order result
- Of course there can be also other correlated states

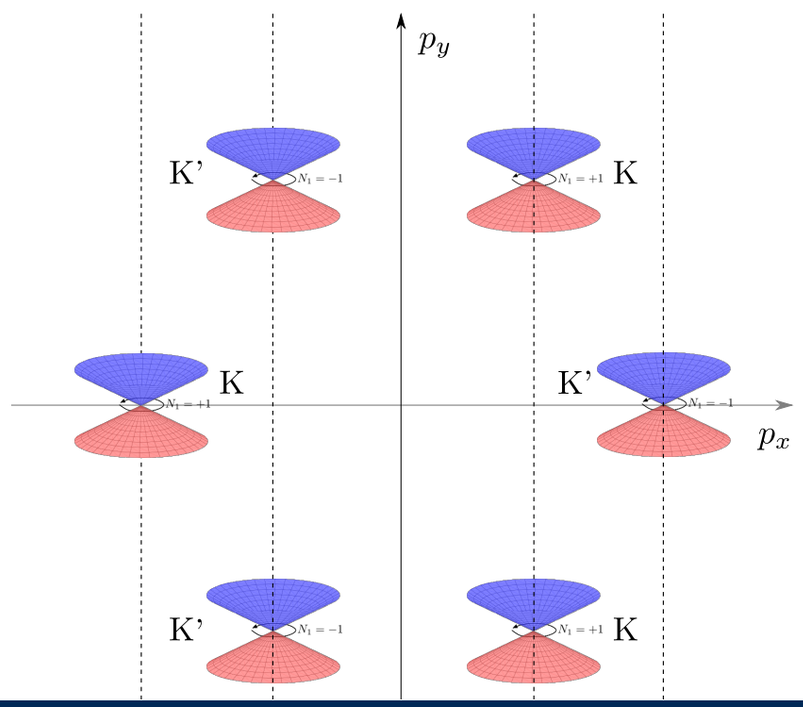
Recent beyond mean field works (Flat-band superconductivity):
- Tovmasyan, et al. PRB 2016
- Wang, et al., PRB 2020
- Hofmann, et al., PRB 2020

Migdal:
$\omega_D \ll E_F$
$\Rightarrow$ self-consistent
Born ok

Now: flat bands from graphene



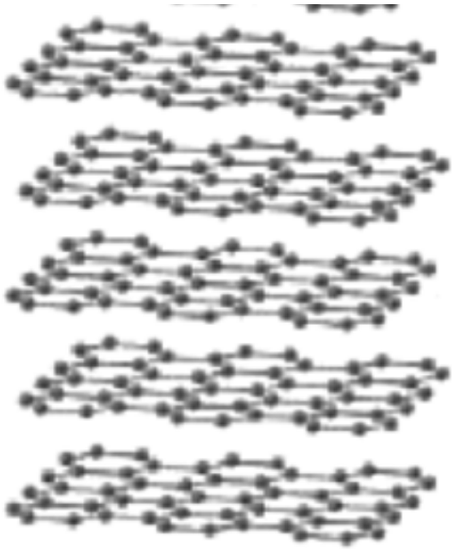




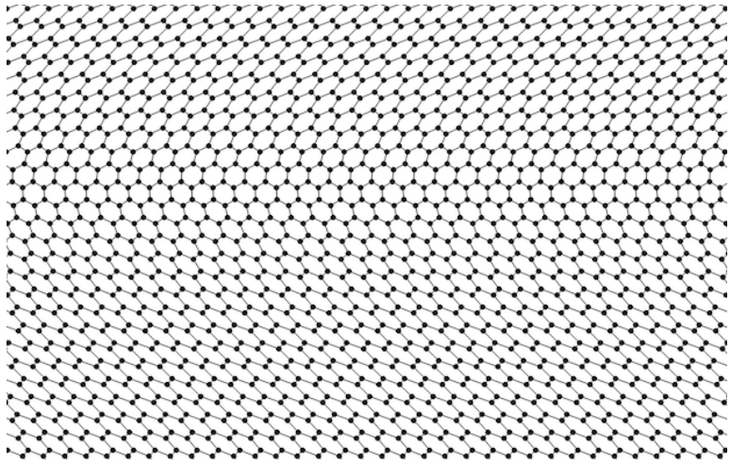
$$H = v_F \sigma \cdot p = v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

$$\mathbf{p} = \mathbf{k} - \mathbf{K}$$

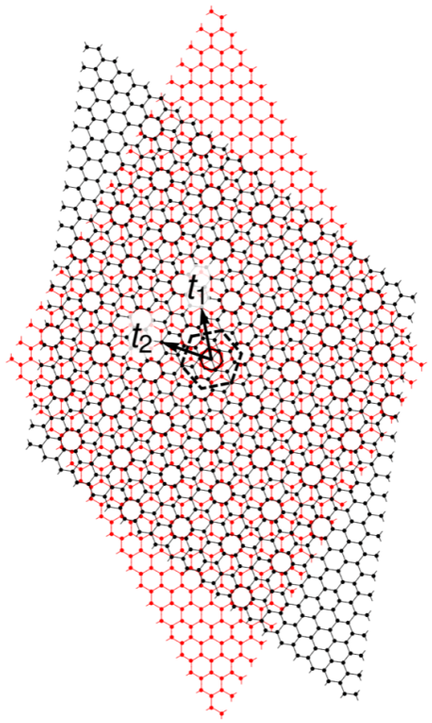
- Stacked graphene



- Periodically strained graphene

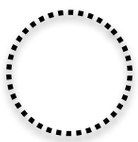


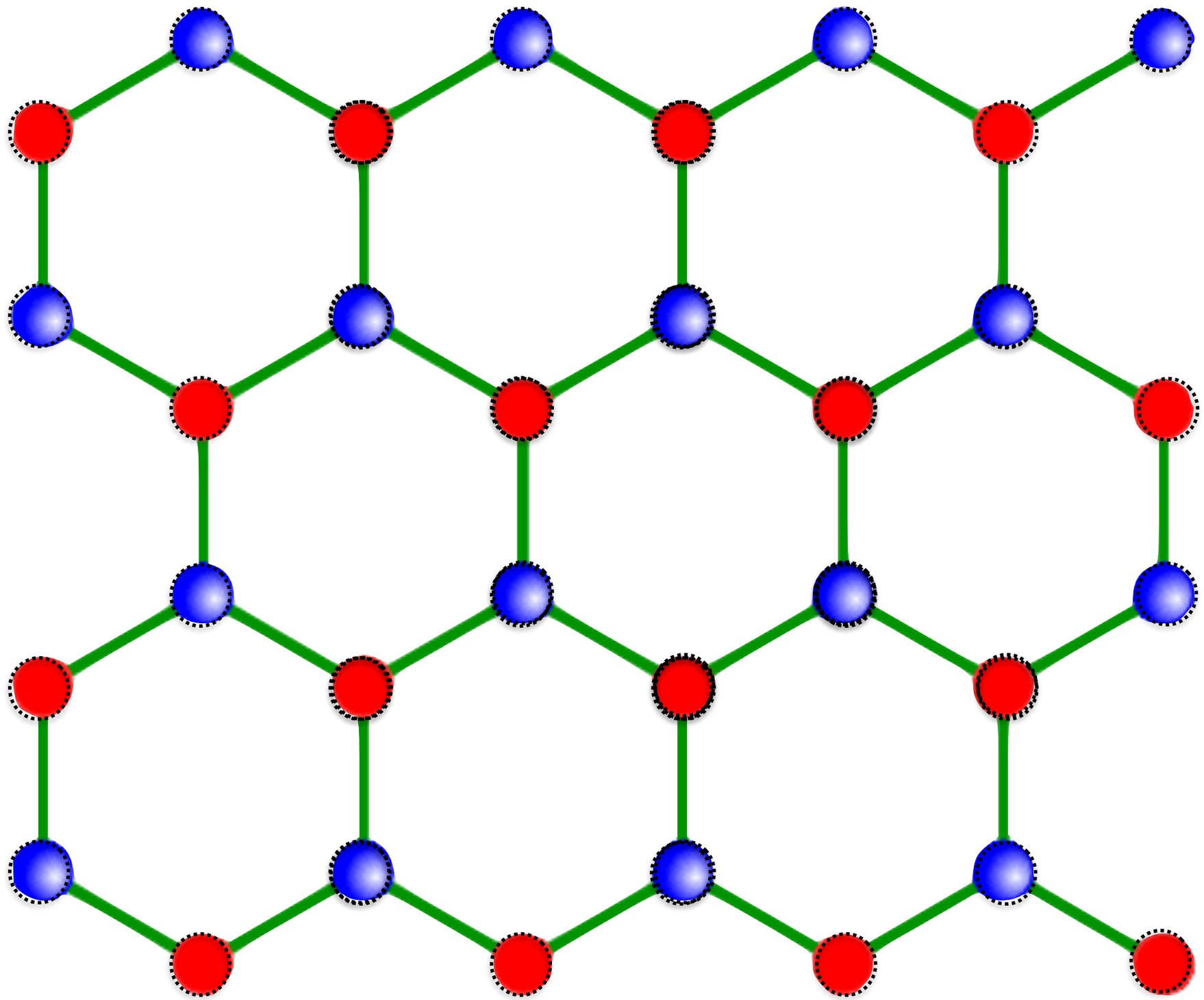
- Twisted bilayer graphene



Bernal stacking of pairs of layers

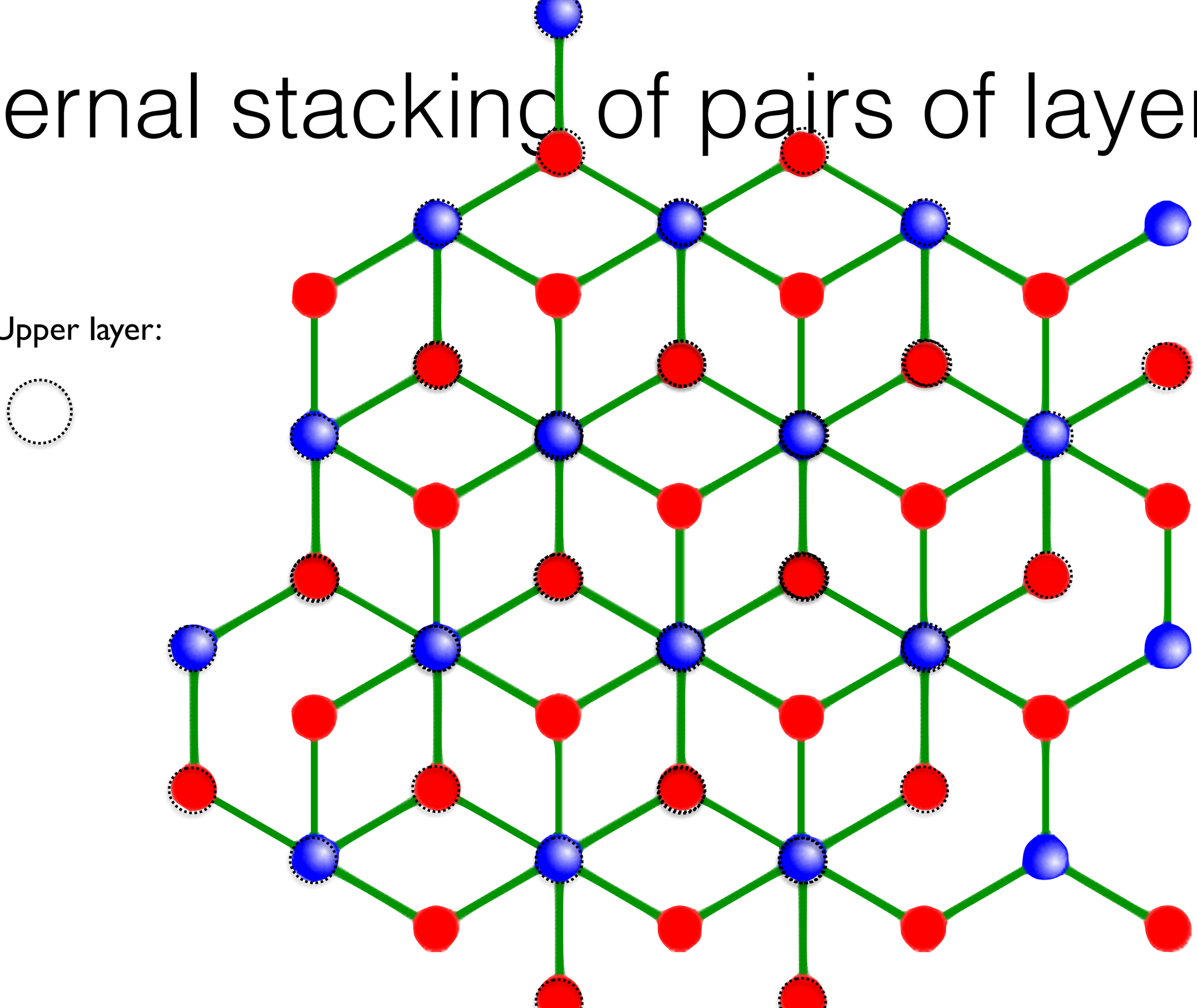
Upper layer:





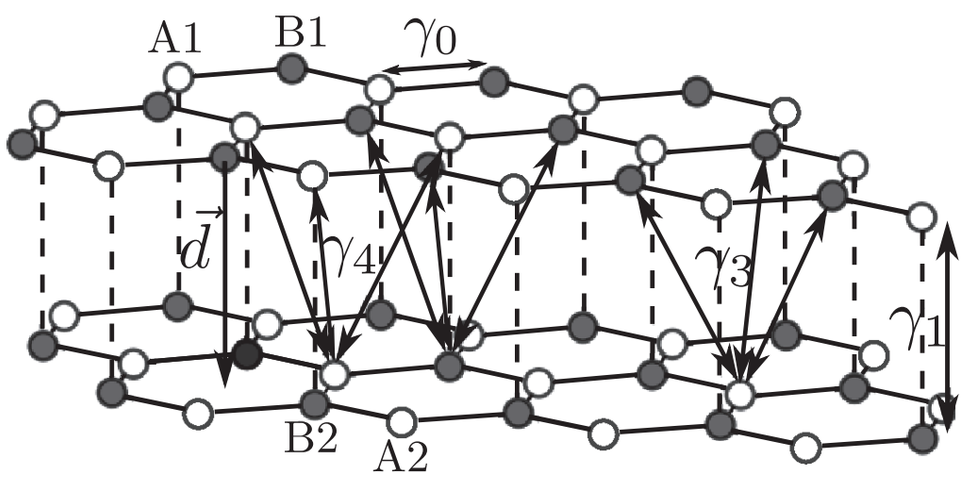
Bernal stacking of pairs of layers

Upper layer:

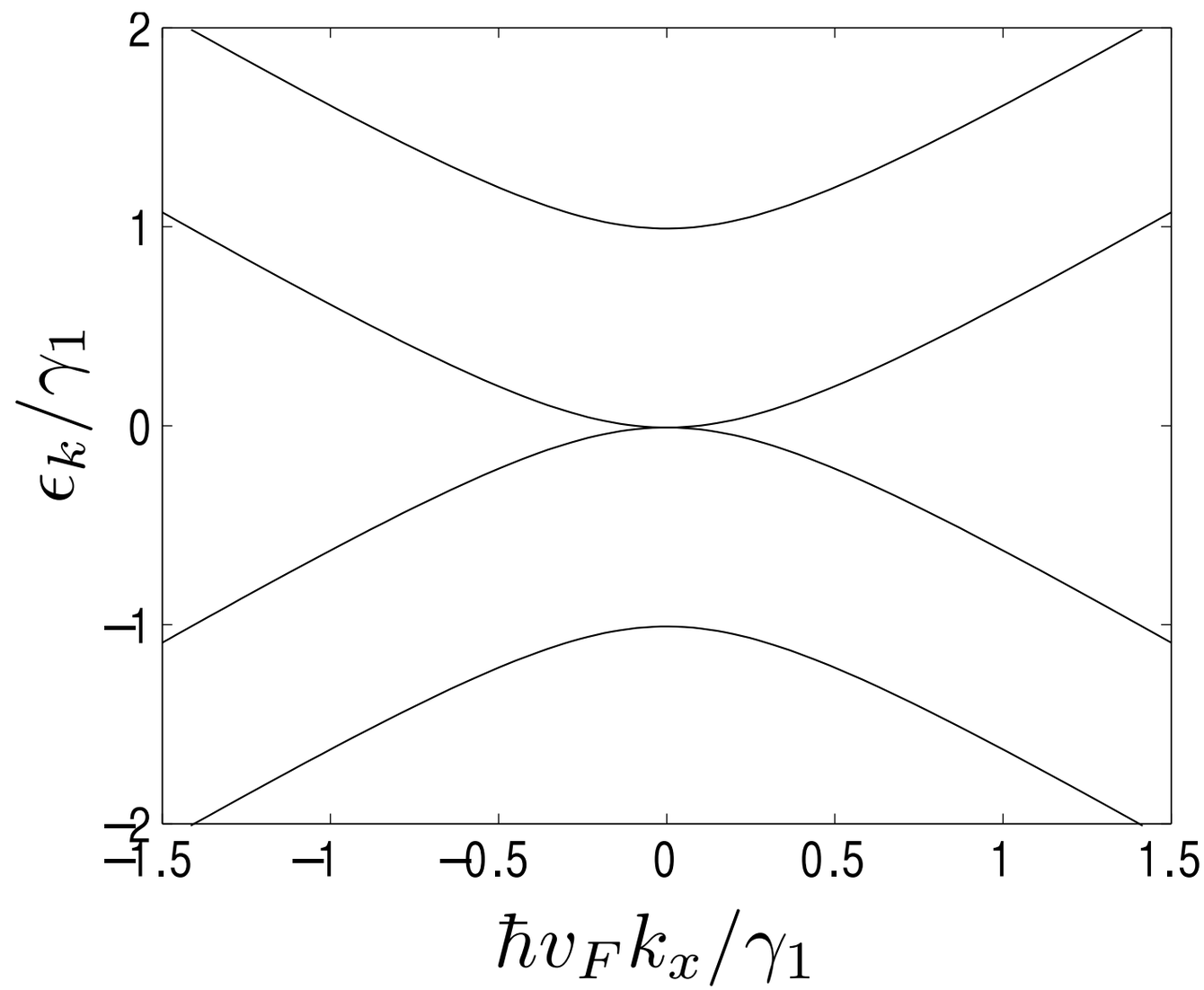


Bilayer graphene

Bernal stacking (non-twisted)



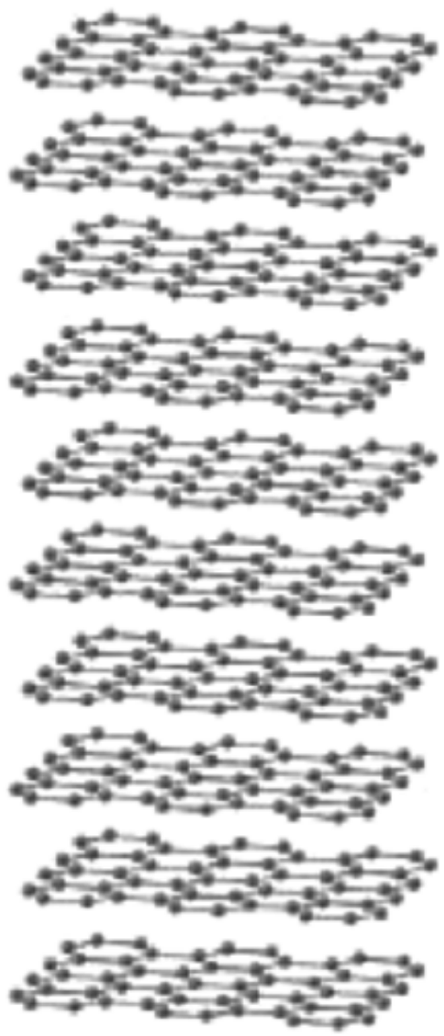
Semimetal with quadratic touching!

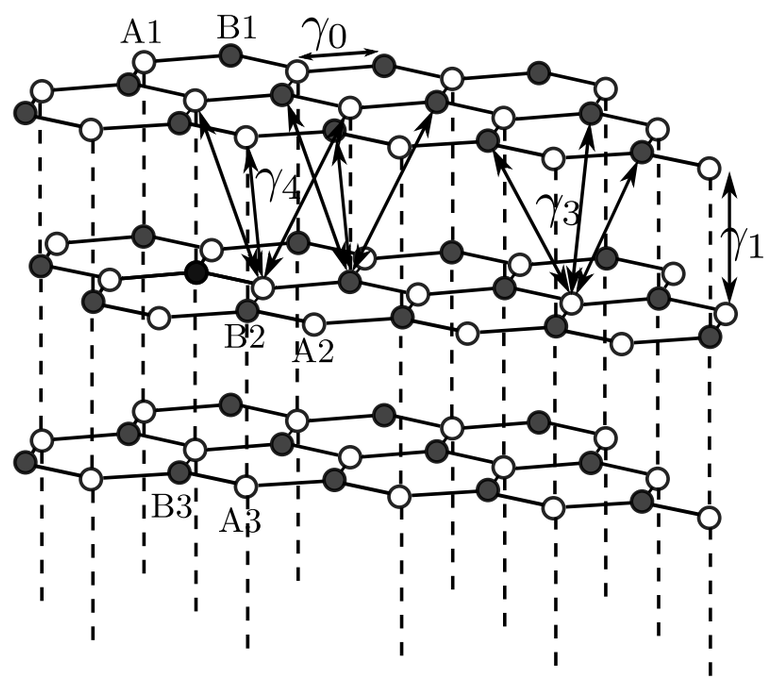


Assume: $\gamma_4 \ll \gamma_1$

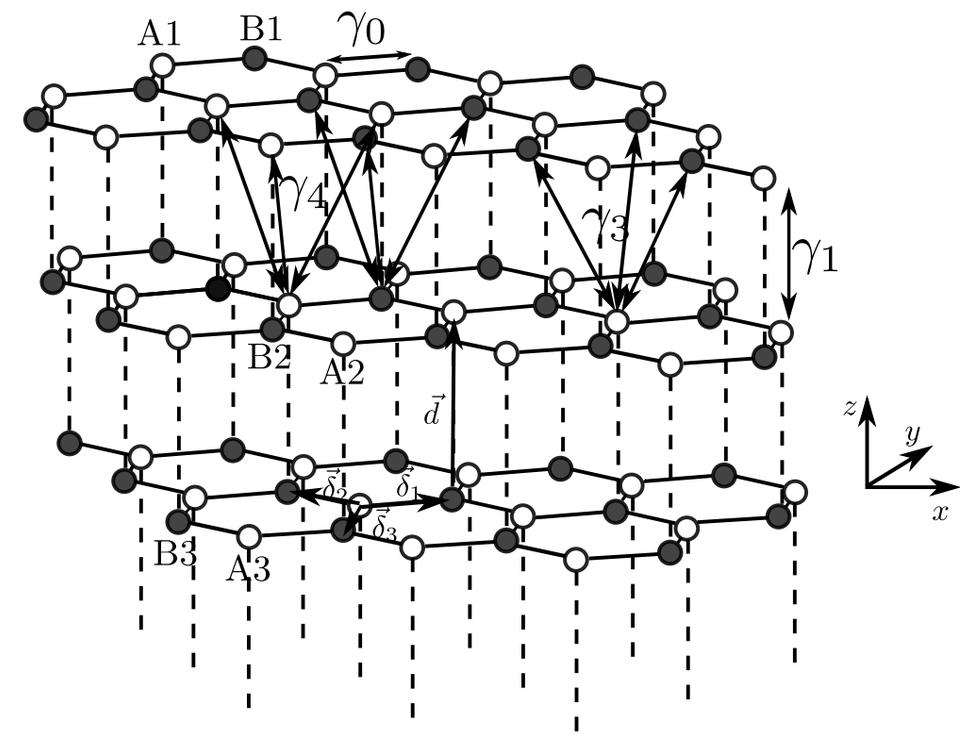
TTH & G.E.Volovik, arXiv:1504.05824

From graphene to graphite

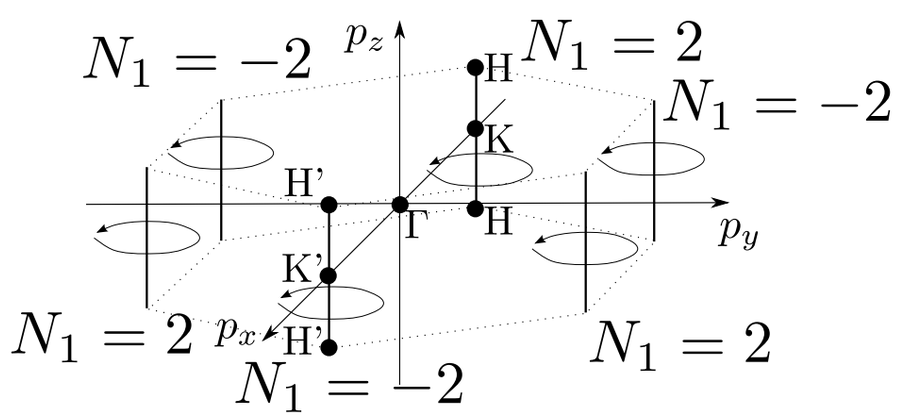


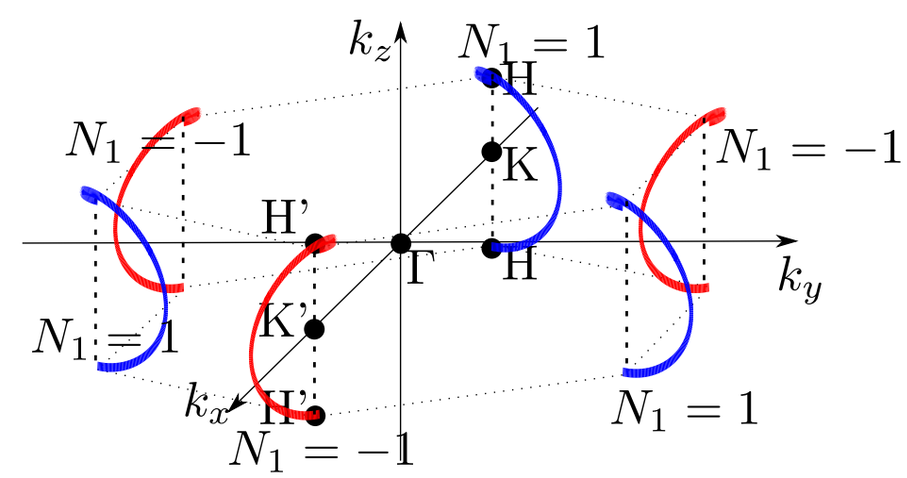


Bernal



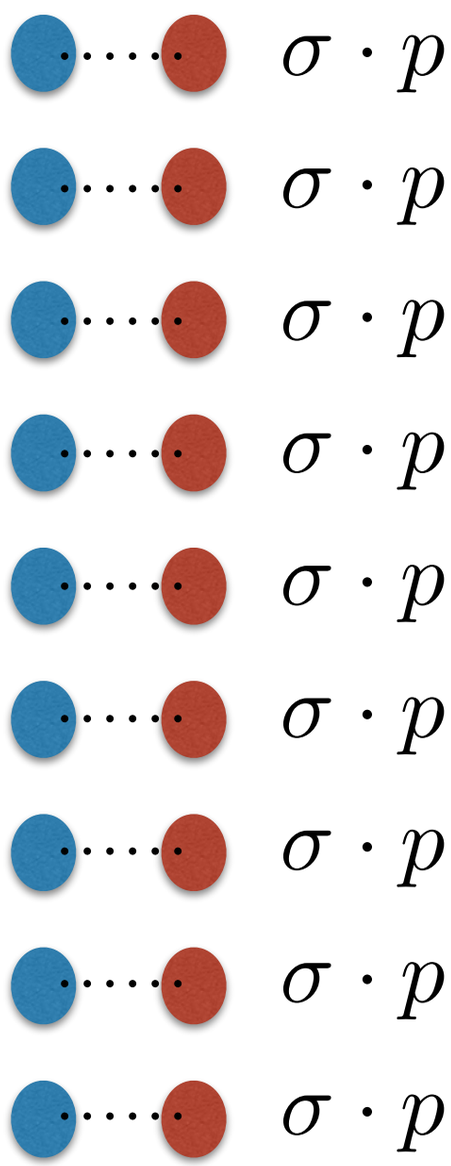
Rhombohedral



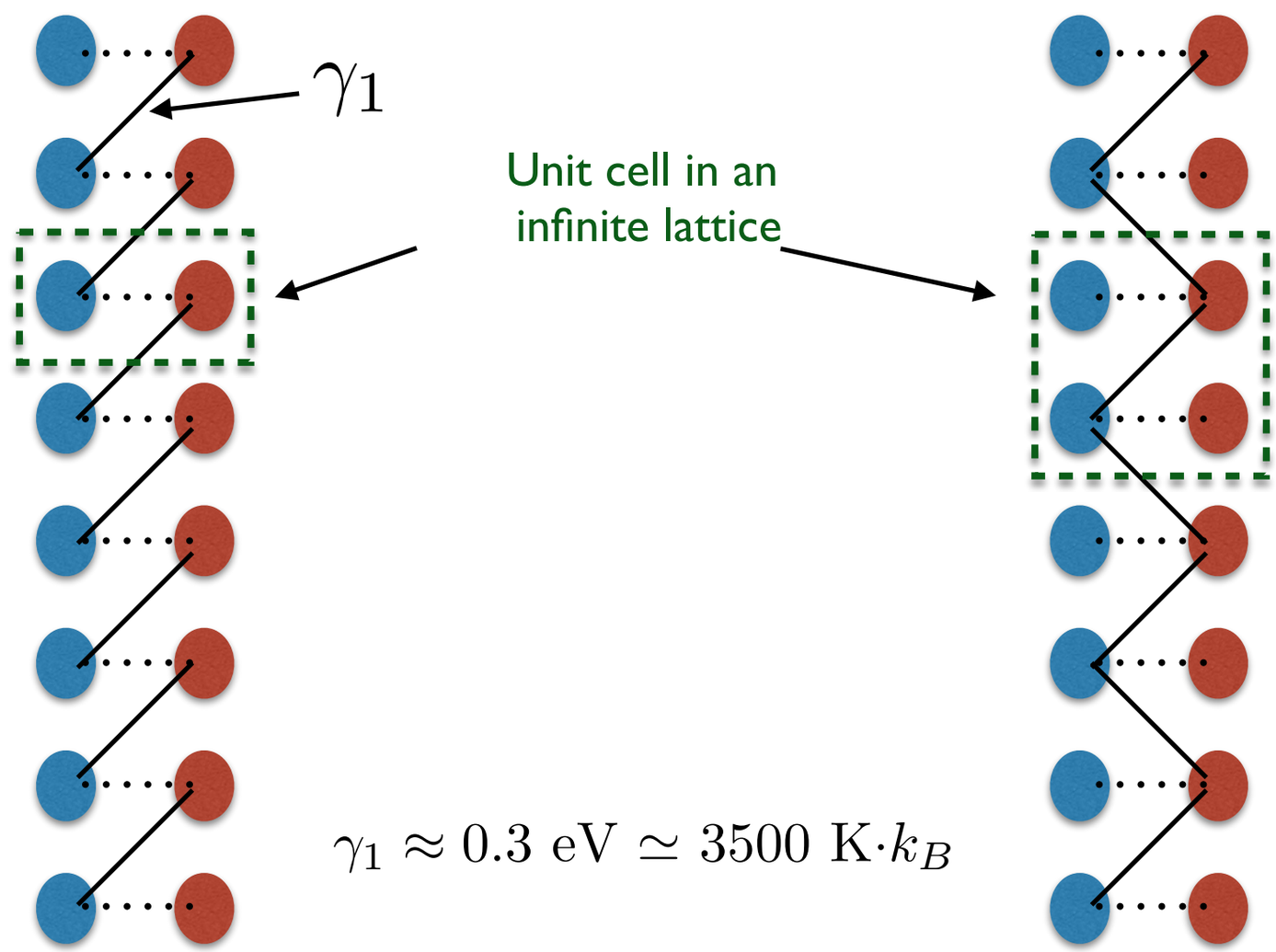


Strongest hopping only

Rule: couple A to B, but not B to A



Two possibilities (and anything in between):

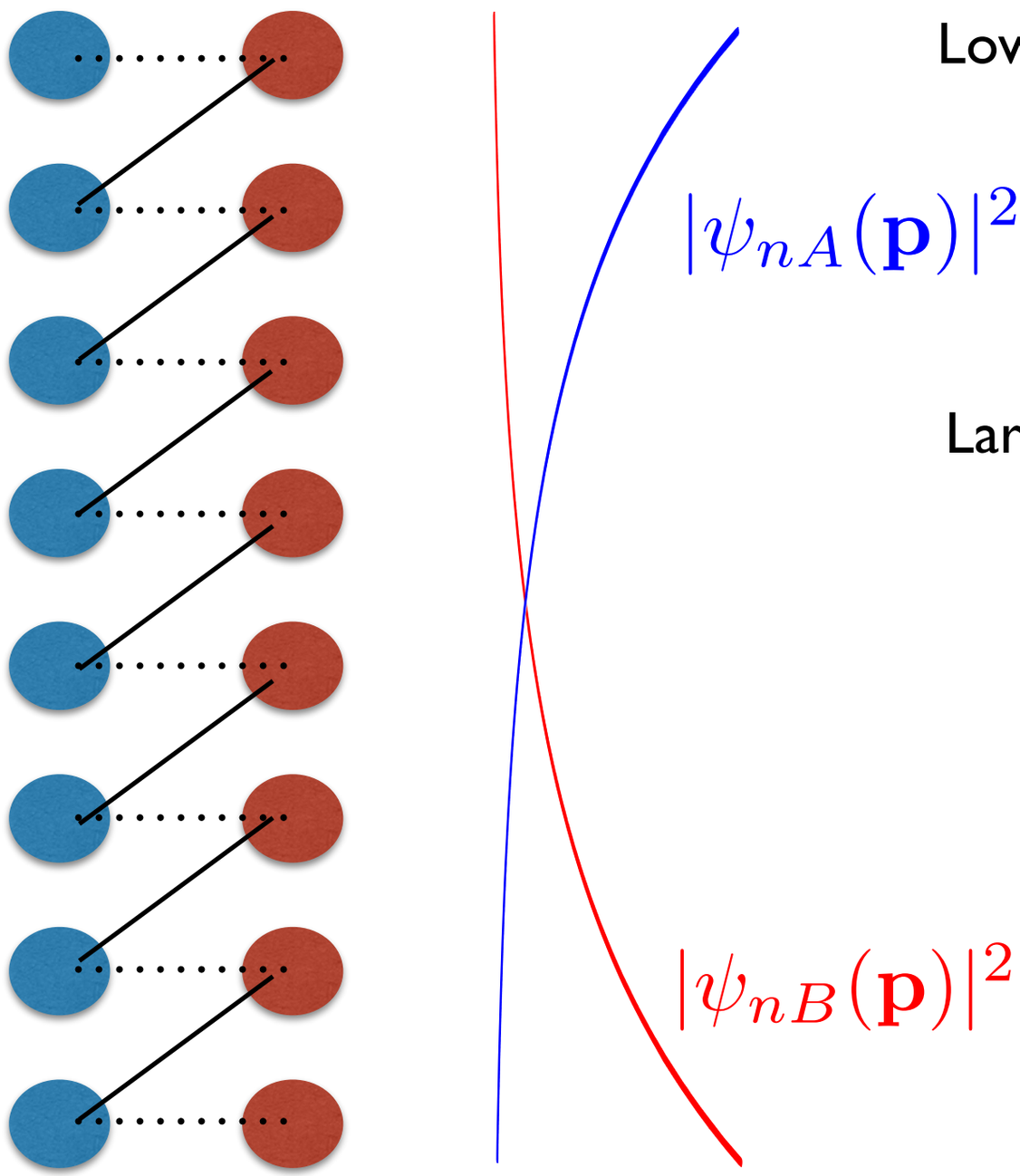


$\gamma_1 \approx 0.3 \text{ eV} \simeq 3500 \text{ K} \cdot k_B$

Rhombohedral

Bernal

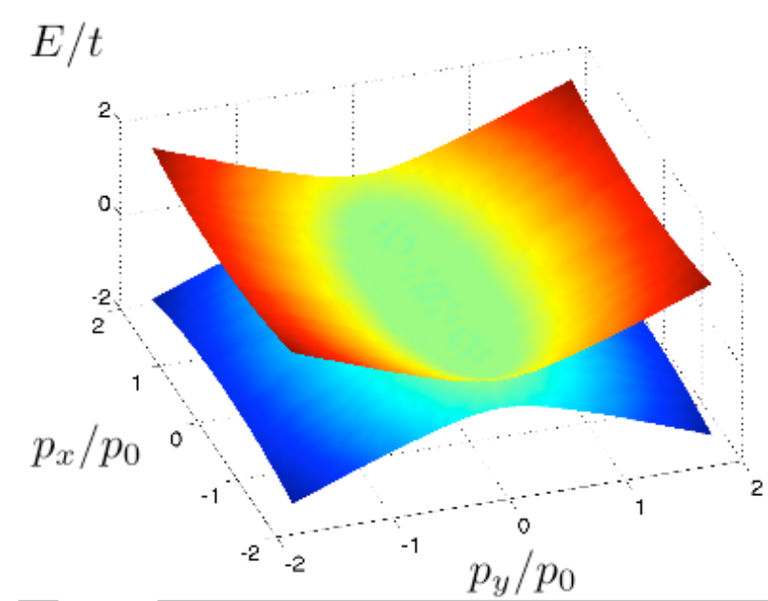
Rhombohedral multilayer



Low-energy spectrum: decaying surface states

$$\epsilon_p \sim \pm p^N$$

Large *N*: flat band!



$$\Omega_{\mathrm{FB}} \sim \pi p_{\mathrm{FB}}^2 = \pi \left(\frac{\gamma_1}{v_F}\right)^2$$

Flat band from nodal lines

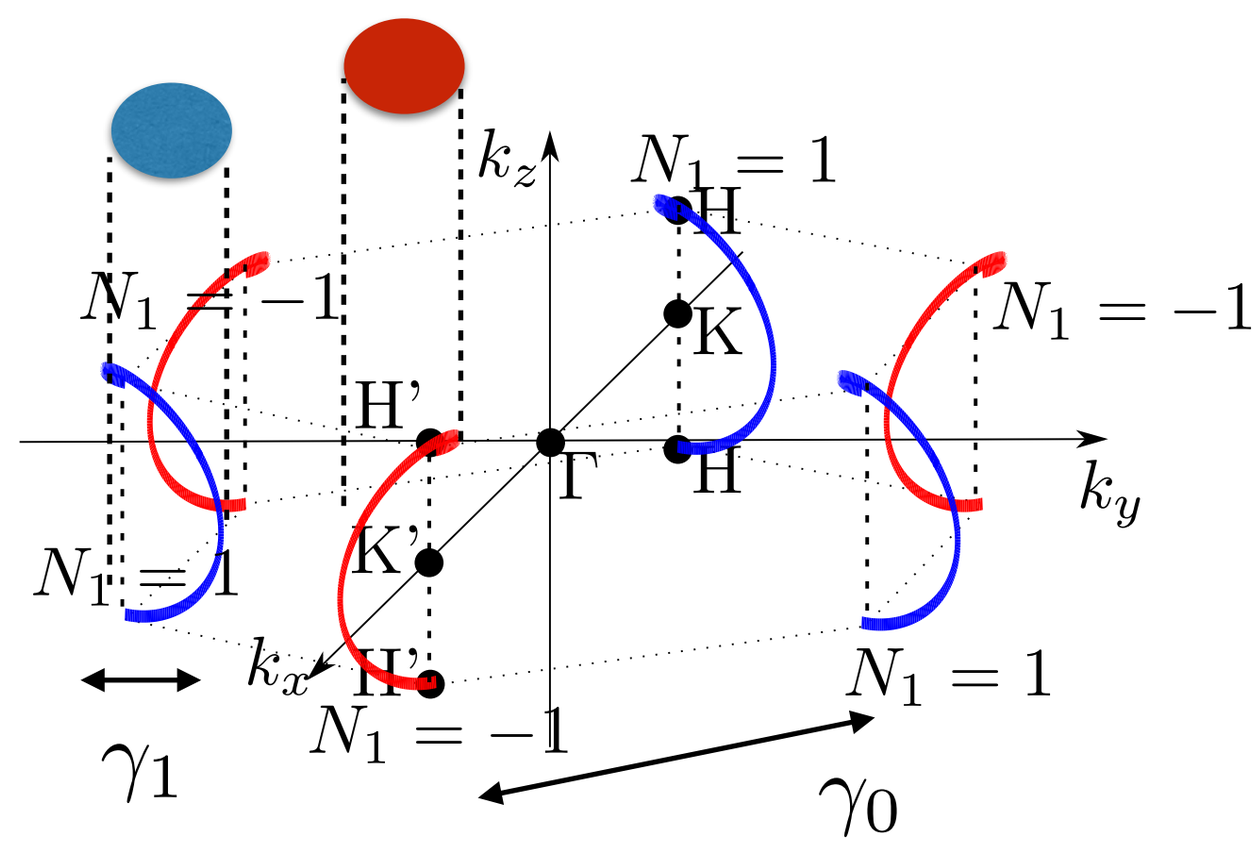
Hamiltonian of bulk rhombohedral graphite:

$$H = \begin{pmatrix} 0 & f \\ f^* & 0 \end{pmatrix}, \quad f = v_F(p_x - ip_y) - \gamma_1 e^{-iap_z}$$

Spiral band touching at

$$p_\perp e^{i\phi} = \frac{\gamma_1}{v_F} e^{-iap_z}$$

Flat bands form at projections of the spirals to the surface:

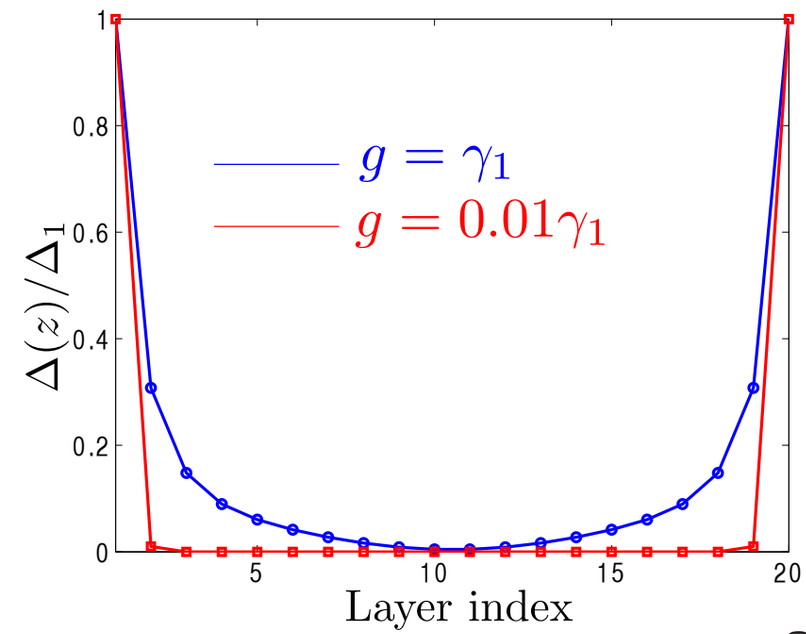


TTH & G.E.Volovik, JETP Lett. **93**, 59 (2011)

Surface superconductivity

Add attractive interaction, self-consistent BdG equations

$\Delta \neq 0$ only on the two surfaces!



Mean field with finite N

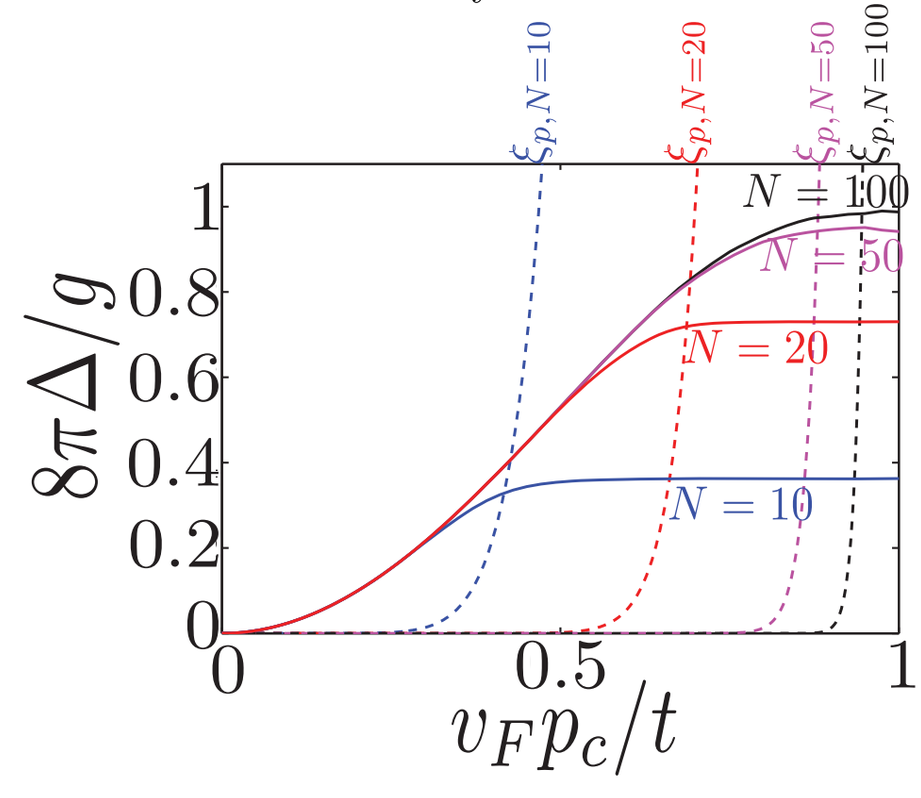
$$\Delta_0 = t\left(\frac{g}{4\pi t}\left[\alpha(N) - \frac{1}{2}(\Delta_0/t)^{\frac{2}{N}}\,\alpha(N/2)\right]\right)^{\frac{N}{N-2}}$$

$$\alpha(N) = \int_0^\infty \frac{x^{\frac{N+2}{N}}dx}{(\sqrt{x^2+1})^3} = \frac{1}{\sqrt{\pi}}\Gamma\left(\frac{N-2}{2N}\right)\Gamma\left(\frac{N+1}{N}\right) \overset{N\to\infty}{\longrightarrow} 1$$

$N \to \infty$:

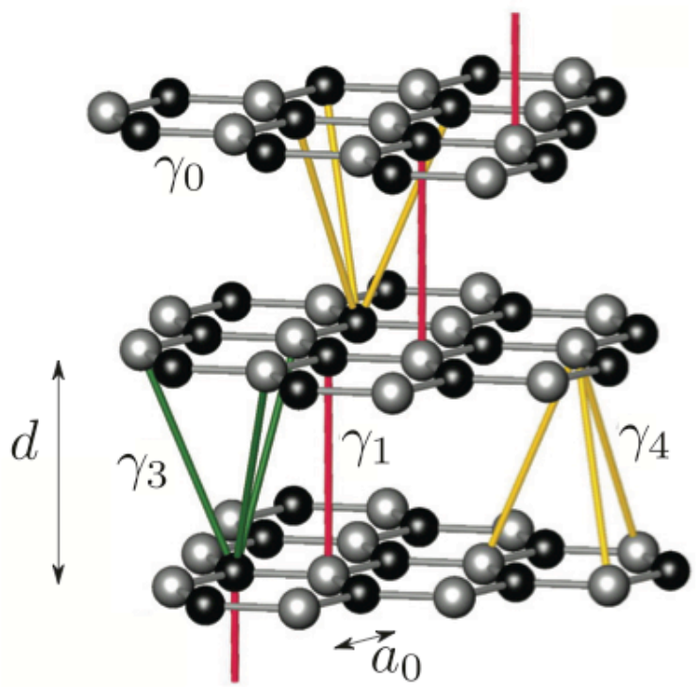
$$\Delta_0 = \frac{g\min(p_c, p_{\rm FB})^2}{8\pi\hbar^2},\ \Delta_0 = 3T_C$$

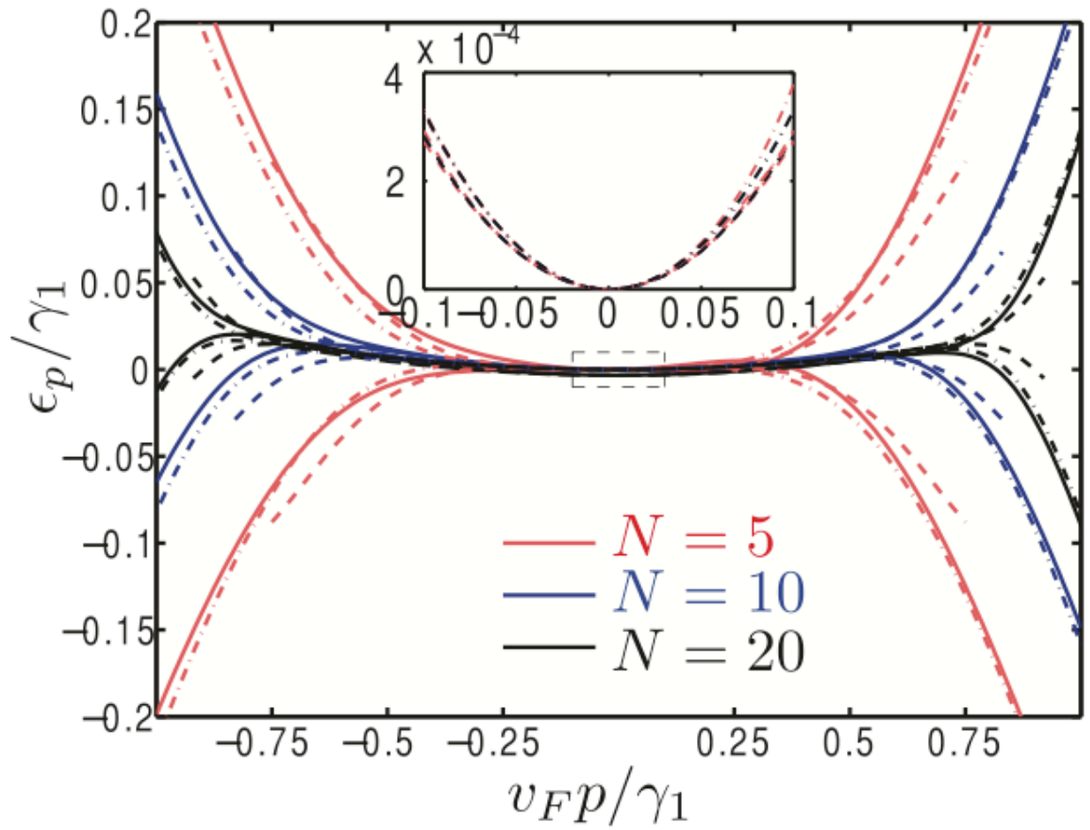
Doping destroys surface superconductivity:
for uniform doping $\mu_C = 2\Delta_0/3$



Kopnin, TTH, G.E. Volovik, PRB **83**, 220503 (R) (2011)
(See also Wang, Yuan, Fu, PRX 2021)

Rhombohedral graphite: higher-order couplings





$$\{H, \sigma_z\} \neq 0$$

"Drumhead"

$$\Rightarrow \text{Quadratic dispersion } \epsilon = 2\gamma_1 \frac{\gamma_4}{\gamma_0} \left(\frac{v_F p}{\gamma_1}\right)^2 \equiv 2\alpha \left(\frac{v_F p}{\gamma_1}\right)^2$$

Still a surface state!

Crossover between "narrow band" and "flat band" limits when $\lambda \sim 4\pi\alpha \sim 0.15$ eV or $T_C^{\mathrm{mf}} \sim 20$ K

N.B. Kopnin, M. Ijäs, A. Harju, and TTH, PRB **87**, 140503(R) (2013)

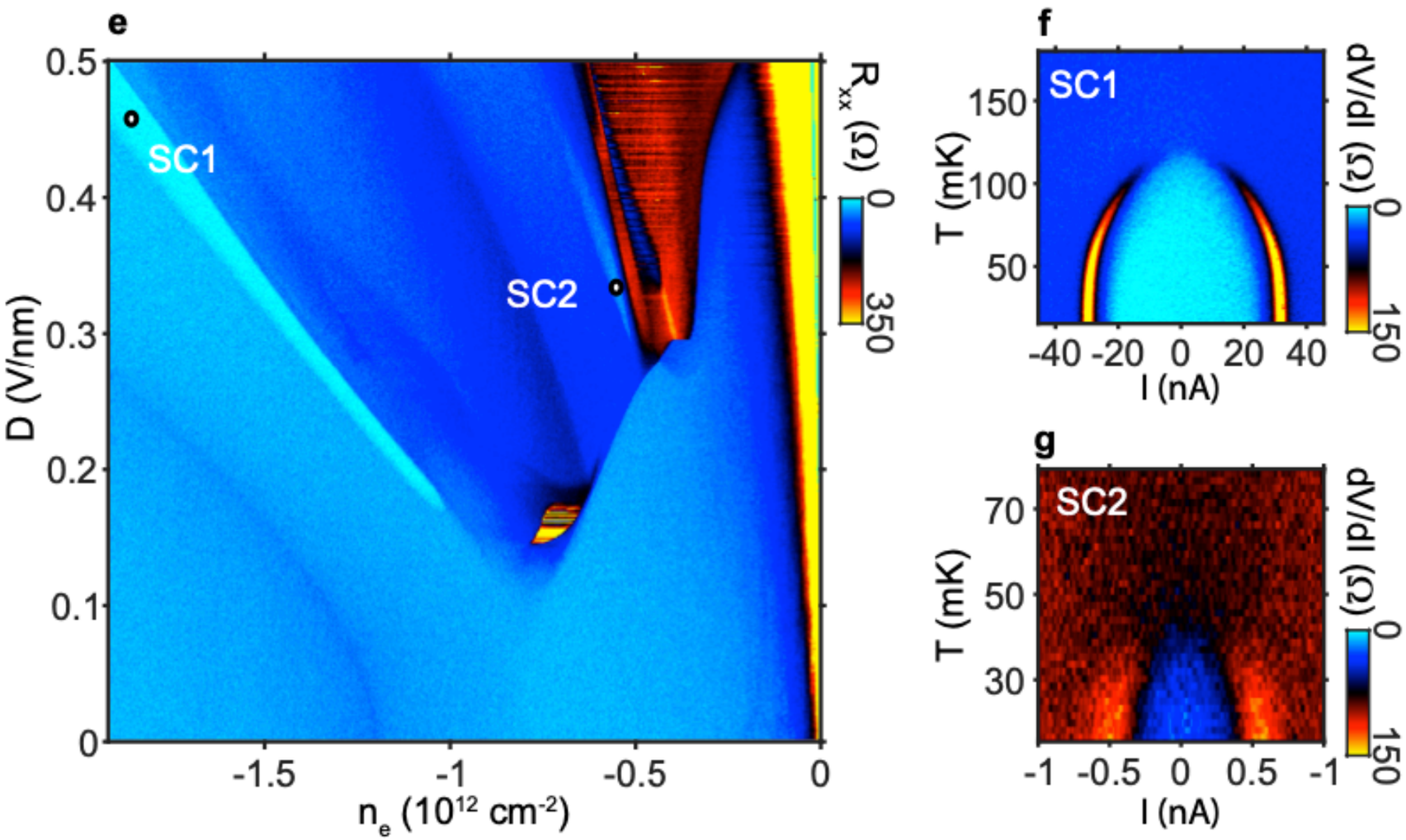
Superconductivity in rhombohedral trilayer graphene

arXiv:2106.07640

Haoxin Zhou,[1] Tian Xie,[1] Takashi Taniguchi,[2] Kenji Watanabe,[3] and Andrea F. Young[1,*]

[1]*Department of Physics, University of California at Santa Barbara, Santa Barbara CA 93106, USA*
[2]*International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
[3]*Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*

(Dated: June 15, 2021)



$T_{\mathrm{BKT}} \sim 100$ mK

Prediction: higher T_c for larger # of layers

Consistent with "surface" superconductivity that depends on potential $\mu_1 = \mu + D$

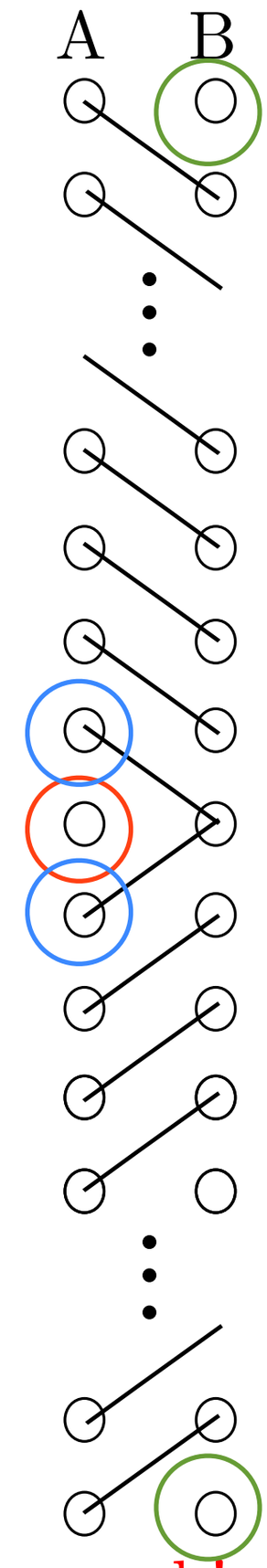
Twin boundaries

Two spatially separated regions with opposite N_2

$N_2 = +1$

$$H = \begin{pmatrix} \sigma\cdot p & g\sigma_\uparrow & 0 & 0 & 0 & 0 & 0 & 0 \\ g^*\sigma_\downarrow & \sigma\cdot p & g\sigma_\uparrow & 0 & 0 & 0 & 0 & 0 \\ 0 & g^*\sigma_\downarrow & \sigma\cdot p & g\sigma_\uparrow & 0 & 0 & 0 & 0 \\ 0 & 0 & g^*\sigma_\downarrow & \sigma\cdot p & g\sigma_\downarrow & 0 & 0 & 0 \\ 0 & 0 & 0 & g^*\sigma_\uparrow & \sigma\cdot p & g\sigma_\downarrow & 0 & 0 \\ 0 & 0 & 0 & 0 & g^*\sigma_\uparrow & \sigma\cdot p & g\sigma_\downarrow & 0 \\ 0 & 0 & 0 & 0 & 0 & g^*\sigma_\uparrow & \sigma\cdot p & g\sigma_\downarrow \\ 0 & 0 & 0 & 0 & 0 & 0 & g^*\sigma_\uparrow & \sigma\cdot p \end{pmatrix}$$

$N_2 = -1$



$\Rightarrow$ flat band at the twinning boundary

$\Rightarrow$ similar surface superconductivity there

Interfaces of differently stacked graphite would also be enough!

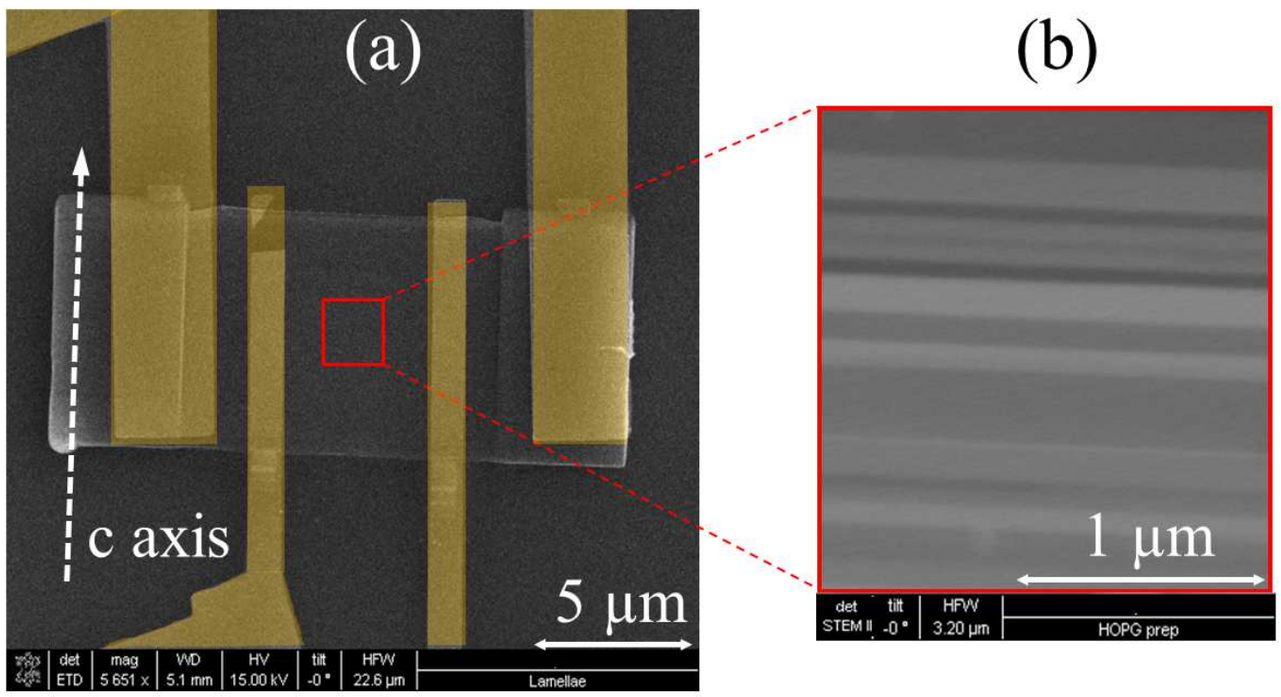
Josephson-coupled superconducting regions embedded at the interfaces of highly oriented pyrolytic graphite

A Ballestar, J Barzola-Quiquia, T Scheike and P Esquinazi[1]
Division of Superconductivity and Magnetism, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany
E-mail: esquin@physik.uni-leipzig.de

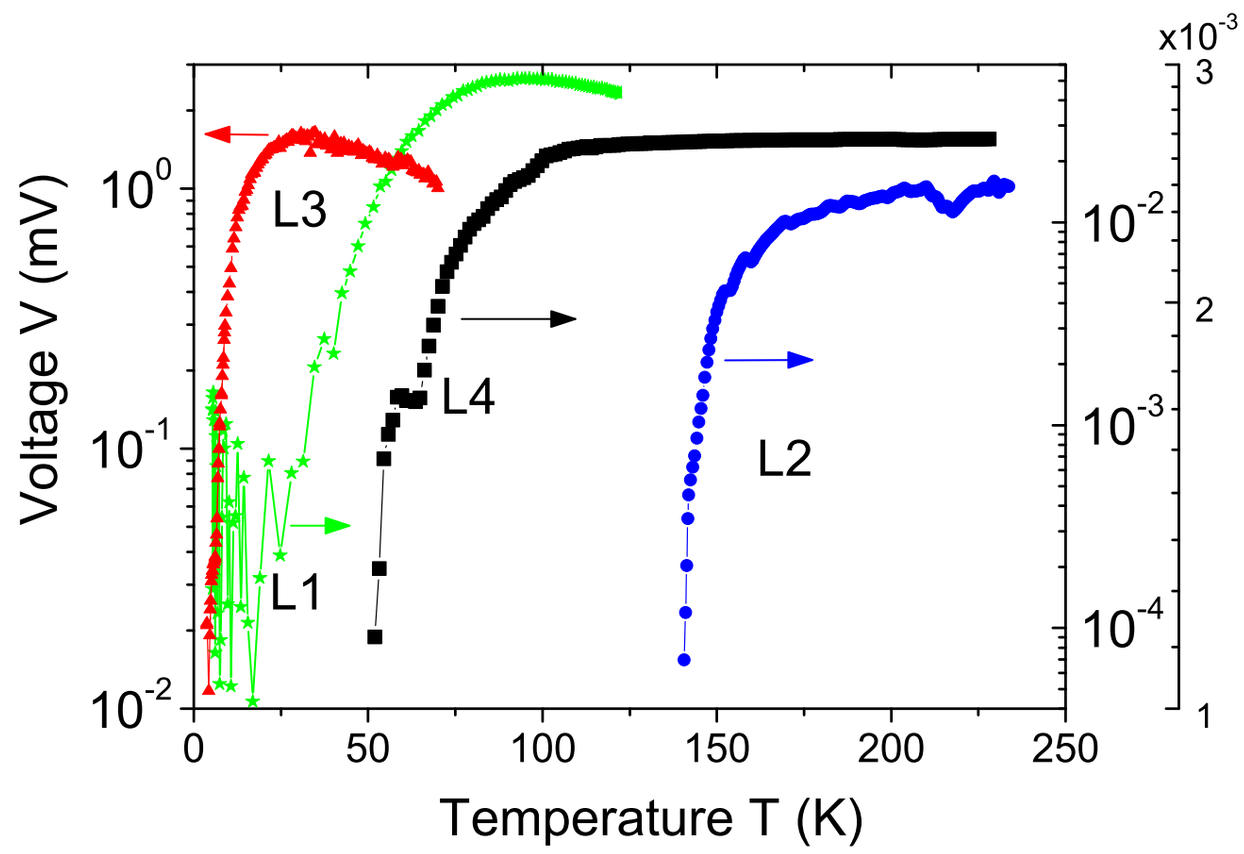
New Journal of Physics **15** (2013) 023024 (15pp)
Received 29 October 2012
Published 15 February 2013

Due to stacking faults?
Problem: Not a very well-defined structure, large sample-to-sample variation

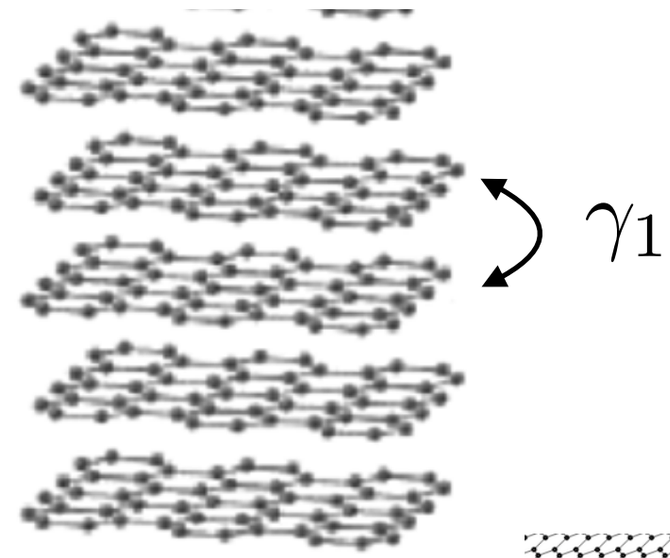
Largest $T_C = 175$ K!



normal to the current direction. (b) Transmission Electron Microscopy (TEM) image of one HOPG lamella. A different brightness corresponds to different orientation within the $a-b$ plane of the crystalline regions of Bernal type with thickness between 30 and 200 nm.

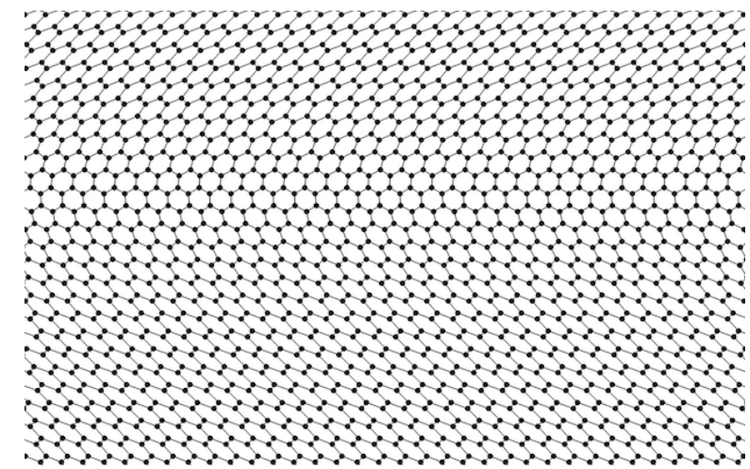


- Stacked graphene

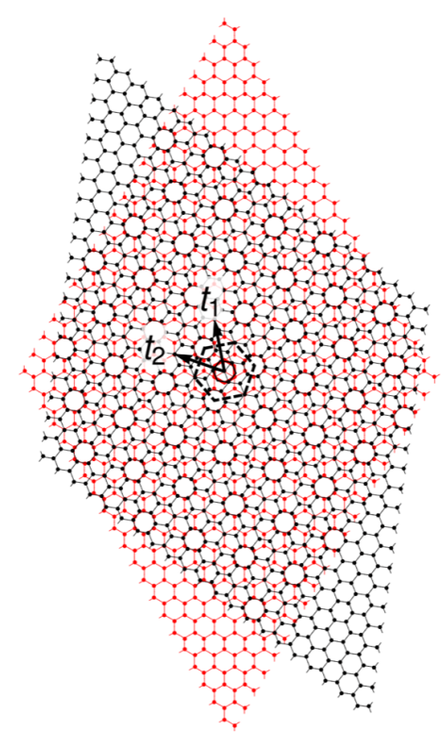


$$\Omega_{\mathrm{FB}} \sim \pi p_{\mathrm{FB}}^2 = \pi \left(\frac{\gamma_1}{v_F} \right)^2$$

- Periodically strained graphene



- Twisted bilayer graphene



Graphene under strain

In-plane strain field (2D vector)

Out-of-plane strain field (scalar h=h(x,y))

$$u_{ij} := \frac{1}{2}(\partial_i u_j + \partial_j u_i) + \frac{1}{2}\partial_i h \partial_j h$$

strain tensor

Pseudo vector potential:

$$\boldsymbol{A} = -\frac{\beta_{\mathrm{G}}}{2a_0}(u_{xx} - u_{yy}, -2u_{xy})$$

Modified Dirac equation:

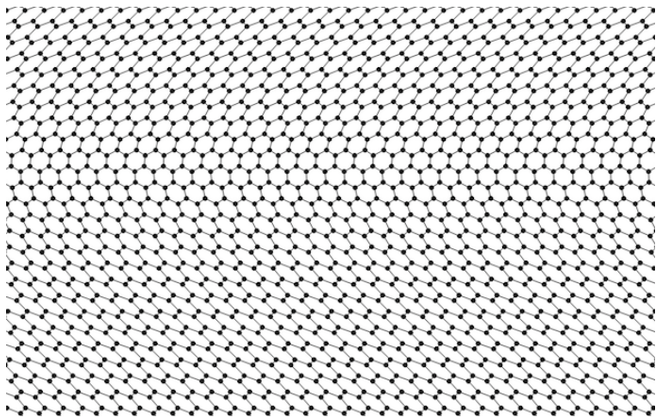
$\rho = \pm 1$ for the two valleys

$$\mathcal{H}^{\rho}(\boldsymbol{r}) := \hbar v_{\mathrm{F}} \boldsymbol{\sigma}^{\rho} \cdot (-\mathrm{i}\nabla + \rho \boldsymbol{A}(\boldsymbol{r})) - \mu$$

Pseudo vector potential: different in the two valleys

M.A.H. Vozmediano, M.I. Katsnelson, F. Guinea, Phys. Rep. **496**, 109 (2010)

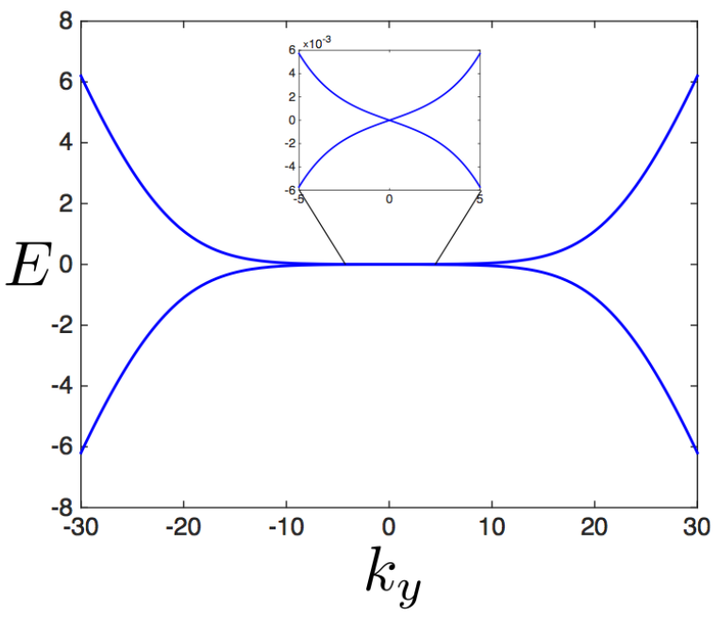
Periodically strained Dirac material



1d strain: $H_0 = \vec{\sigma} \cdot \vec{p} + A_y(x)\sigma_y$

Choose $A_y(x) = \frac{\beta}{L}\cos(2\pi x/L)$ corresponding to (in-plane) strain $u_y(x) = \frac{a\beta}{4\pi}\sin(2\pi x/L)$

$\Rightarrow$ For $\beta \gg 1$ 2D flat band:



$\sim \beta/L$

For low momentum, dispersion is linear:
$\epsilon_p = \pm cp$, $c = v_F/I_0(\beta/\pi)$

$$c \sim \exp(-\beta/\pi) \xrightarrow{\beta\to\infty} 0$$

TTH & G.E. Volovik, arXiv:1504.05824

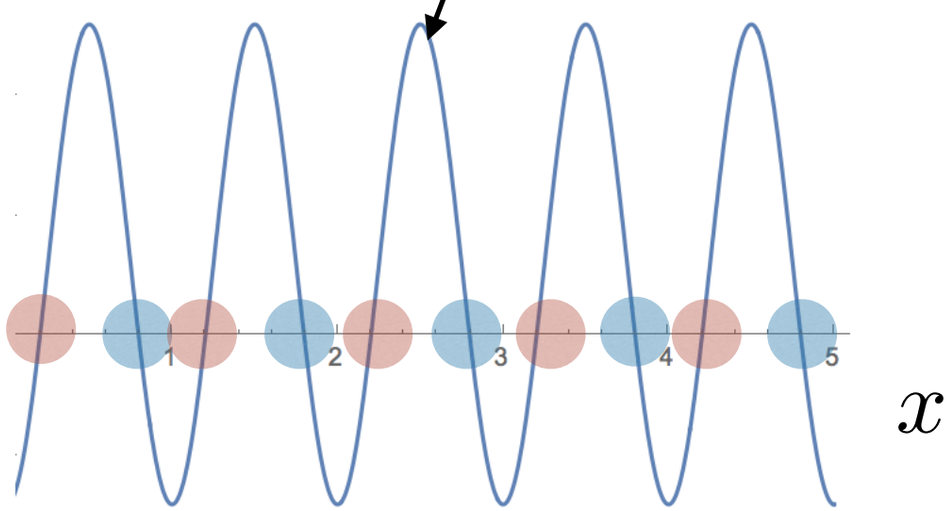
Connection to SSH model

W.P. Su, J.R. Schrieffer, and A.J. Heeger, PRL (1979)

R. Jackiw and C Rebbi, PRD (1976)

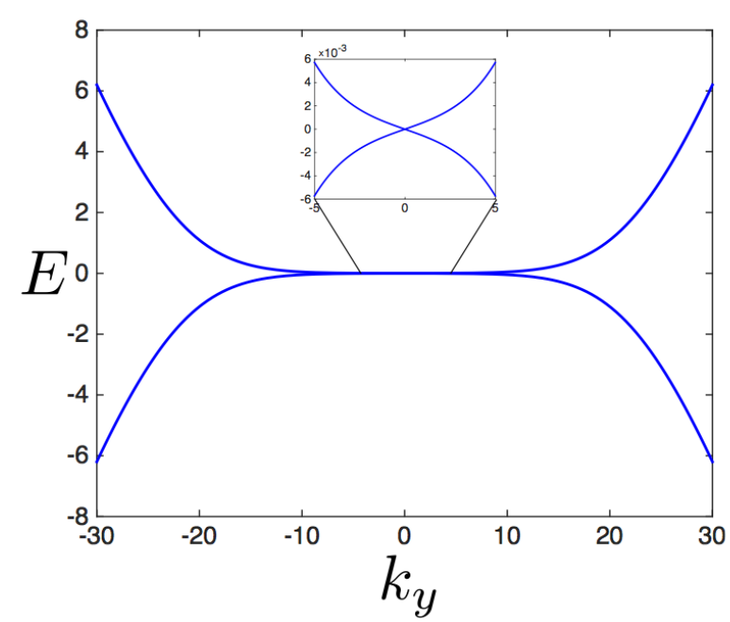
$$H = k_x \sigma_x + [k_y + A(x)]\sigma_y$$

Consider k_y as a parameter: Jackiw-Rebbi model with mass $m(x) = k_y + A(x)$, zero-energy state at each crossing



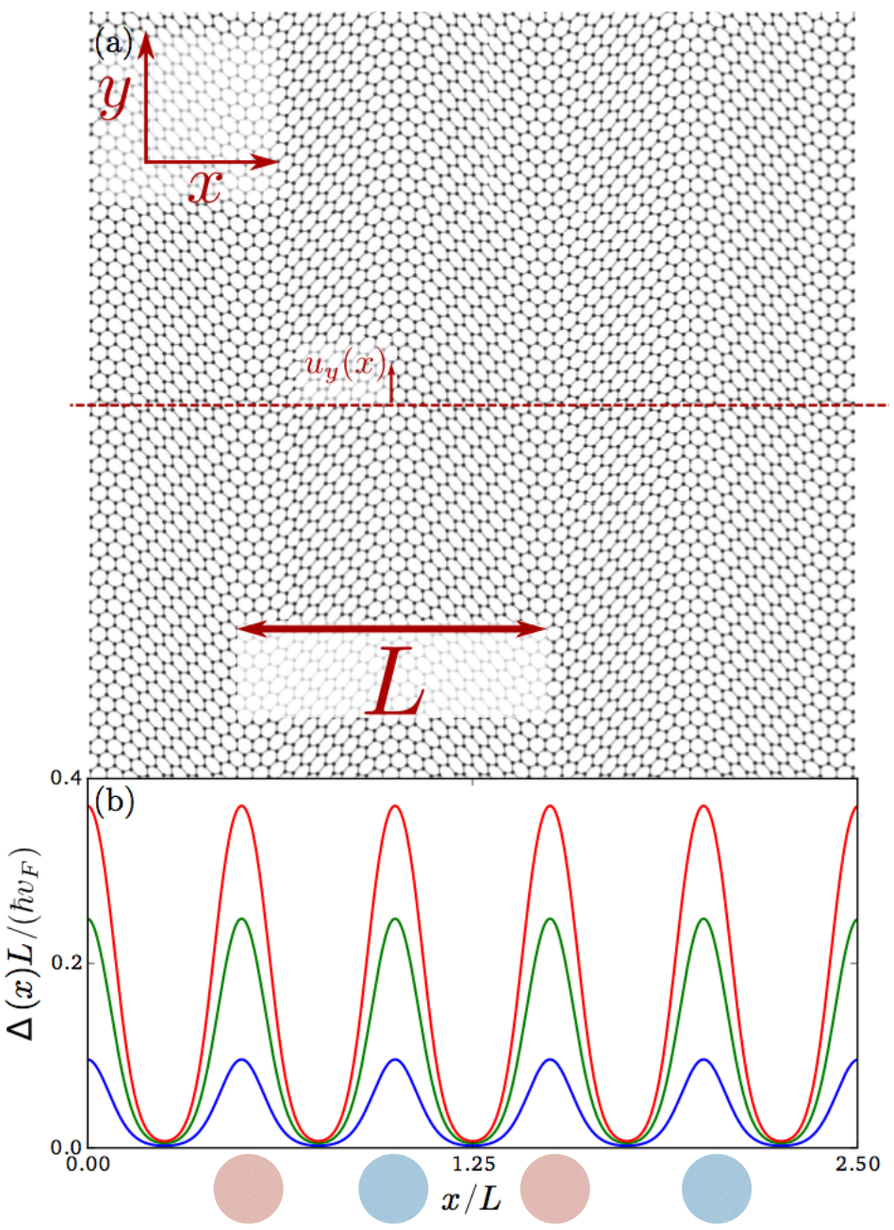
$k_y = 0$: exact, $E = 0$

$k_y \neq 0$: finite overlap energy

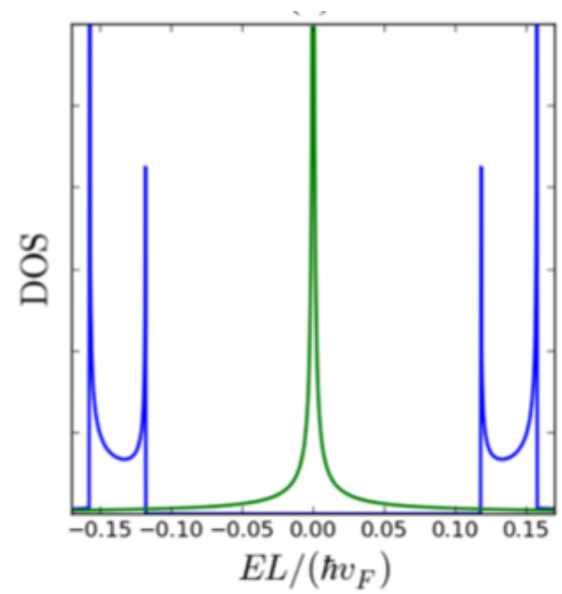


Superconductivity

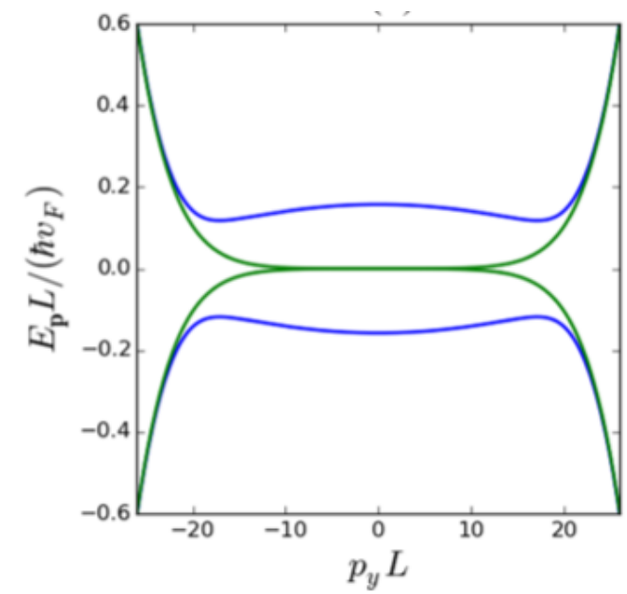
Position dependent Δ



DOS:



Energy dispersion:



Normal state

Superconducting state

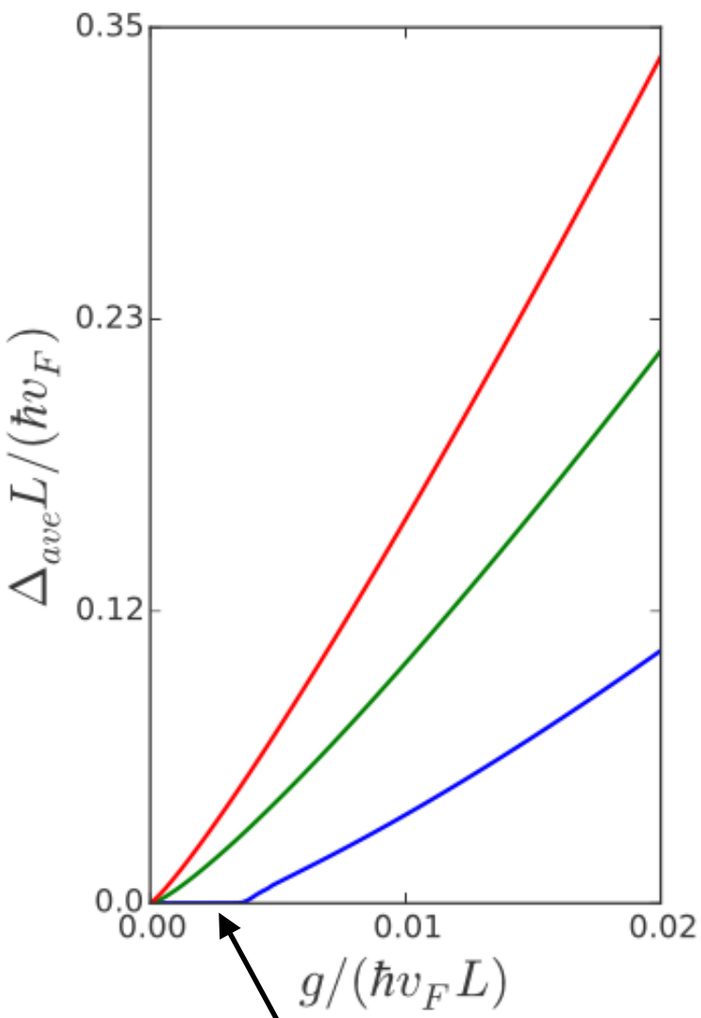
V. Kauppila, F. Aikebaier and TTH, PRB (2016)

(see also Hosseini, EPL (2015))

T. Peltonen and TTH, JPCM 2020

Wang, Yuan, Fu, PRX 2021

Gap vs coupling



$\beta = 40$

$\beta = 30$

$\beta = 20$

$$\Delta \approx \beta g/(2L^2)$$

$$T_c \approx \Delta$$

Can be large!
(Much larger than T_C^{graphene})

$$\Omega_{\text{FB}} \sim \frac{2\pi\beta}{L^2}$$

critical point (linear dispersion)

V. Kauppila, F. Aikebaier and TTH, PRB (2016)

BKT physics: T. Peltonen and TTH, JPCM 2020

Article | Published: 12 August 2020

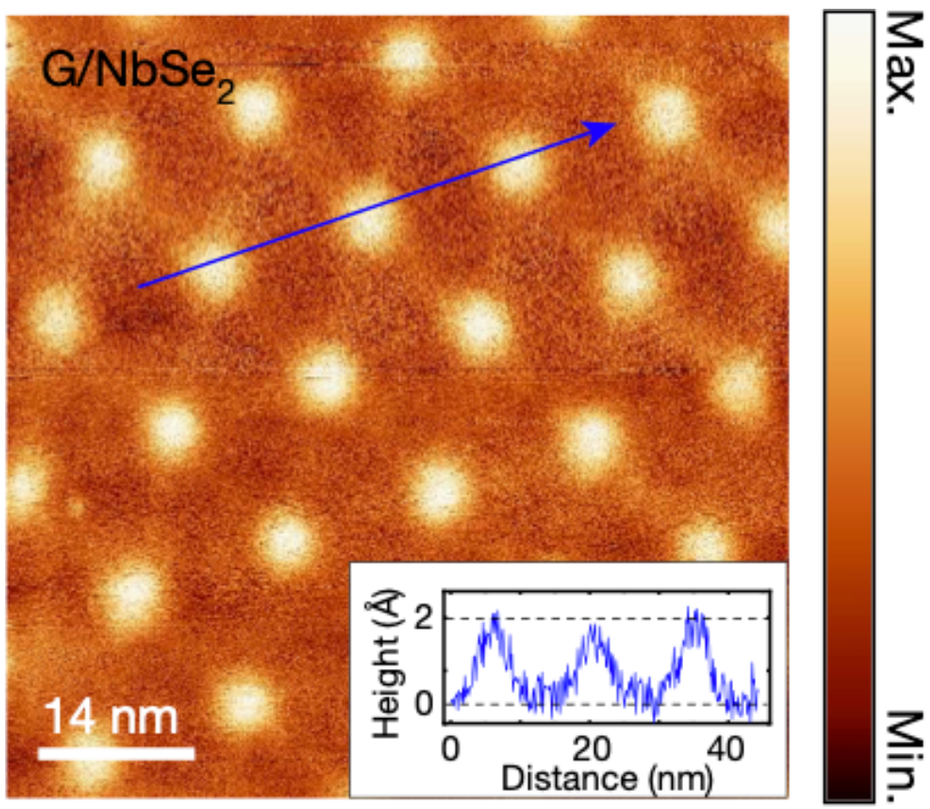
Evidence of flat bands and correlated states in buckled graphene superlattices

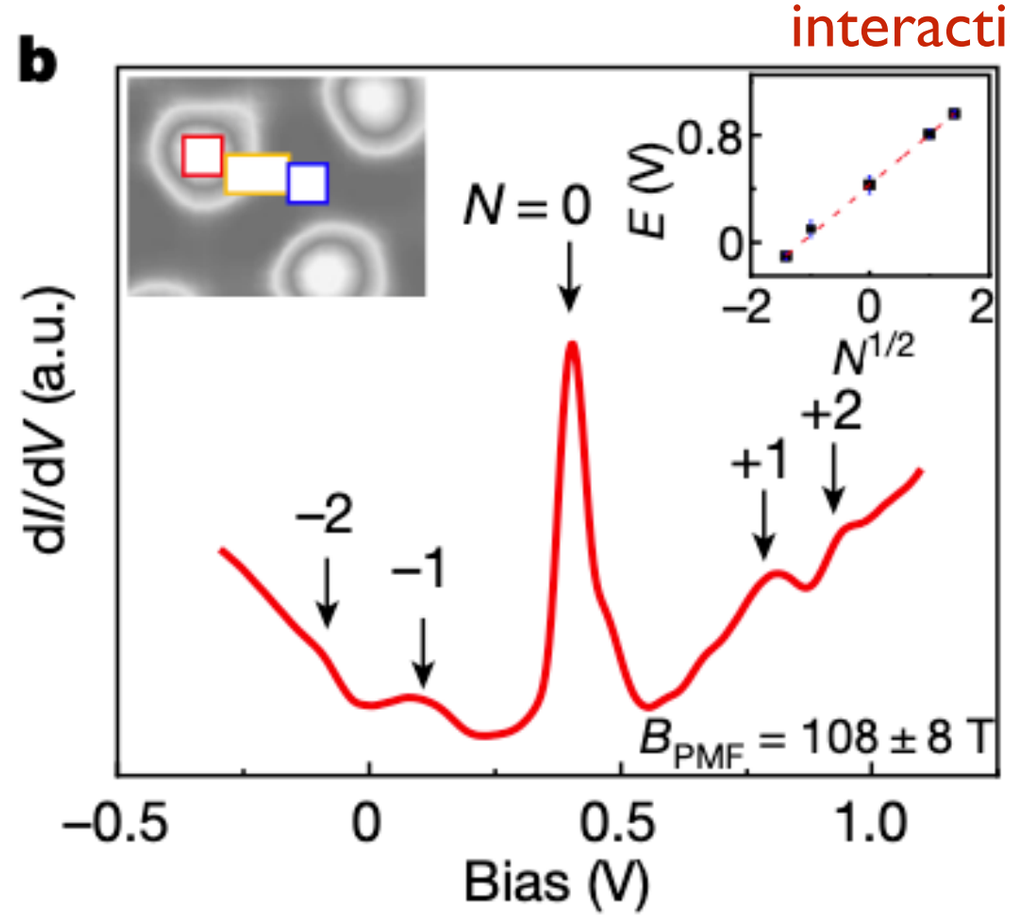
Jinhai Mao, Slaviša P. Milovanović, Miša Anđelković, Xinyuan Lai, Yang Cao, Kenji Watanabe, Takashi Taniguchi, Lucian Covaci, Francois M. Peeters, Andre K. Geim, Yuhang Jiang & Eva Y. Andrei

Nature **584**, 215–220(2020) | Cite this article

Also spectra that depend on the filling indicative of interactions

Buckled structures on graphene membranes

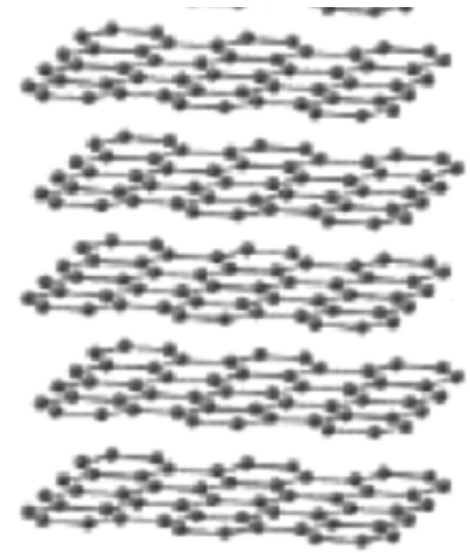




Strain superlattice

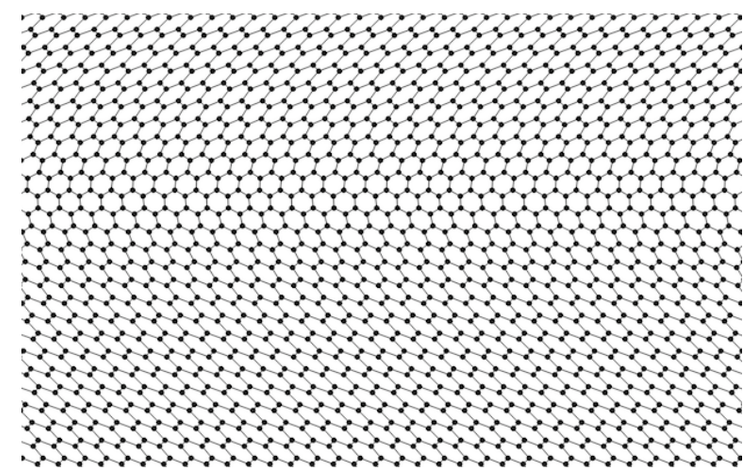
Flat band from pseudo-Landau levels

- Stacked graphene



$$\Omega_{\mathrm{FB}} \sim \pi p_{\mathrm{FB}}^2 = \pi \left(\frac{\gamma_1}{v_F}\right)^2$$

- Periodically strained graphene

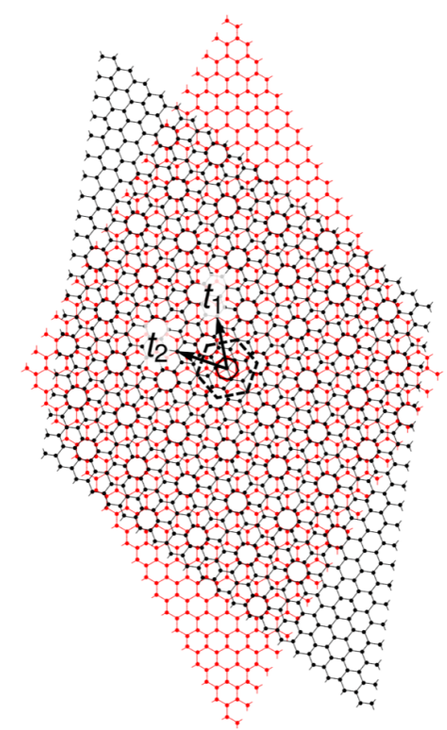


$$\Omega_{\mathrm{FB}} \sim \frac{2\pi\beta}{L^2}$$

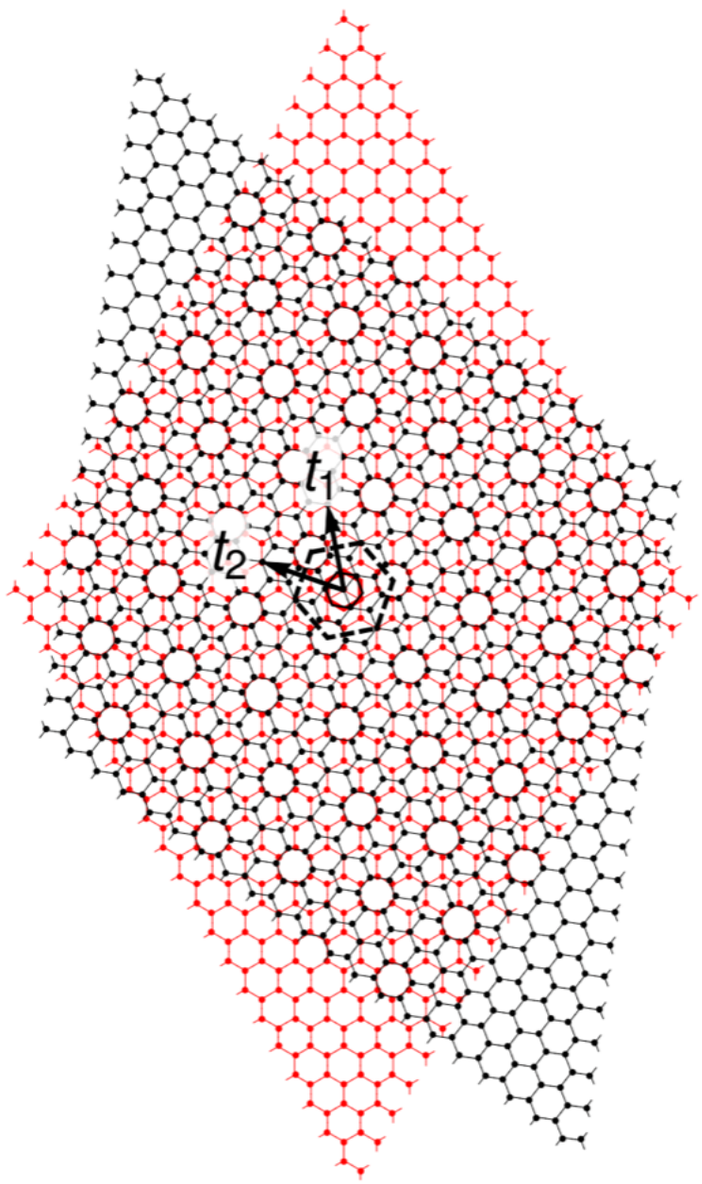
Strain amplitude

Strain period

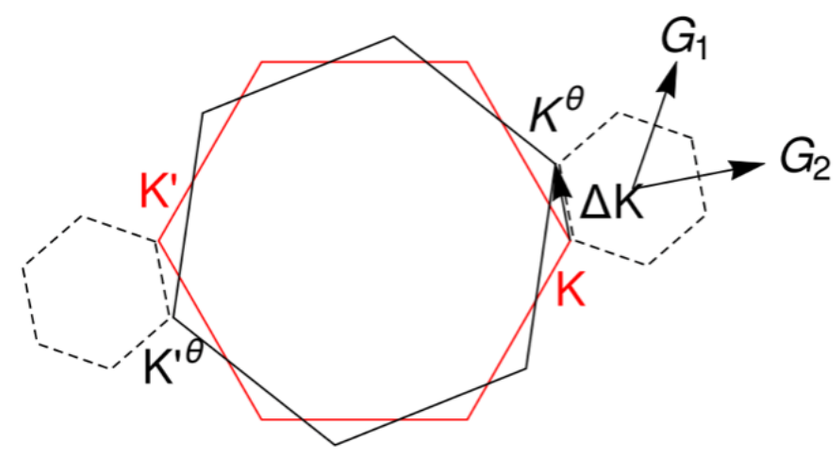
- Twisted bilayer graphene



Twisted bilayer graphene



Moiré superlattice



$$m = 1 \ (\theta = 21.8^\circ)$$

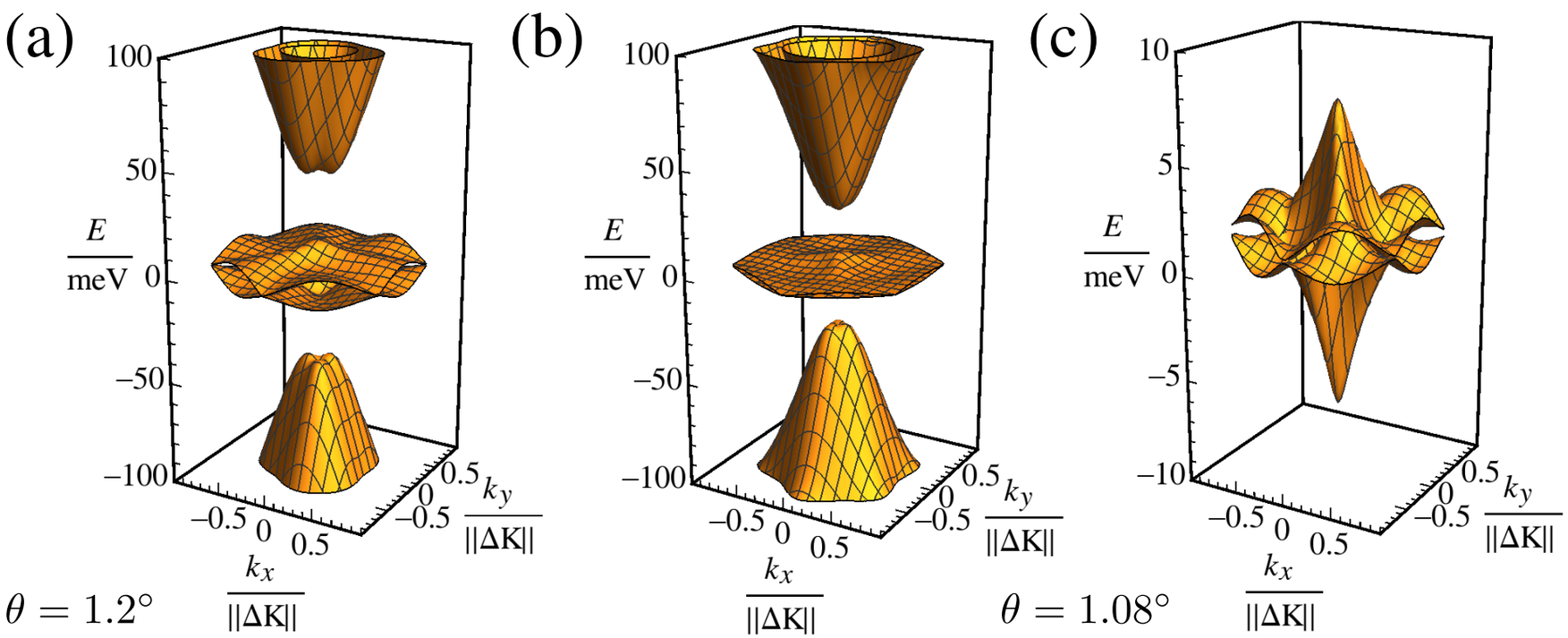
TBG is exactly periodic only for certain angles

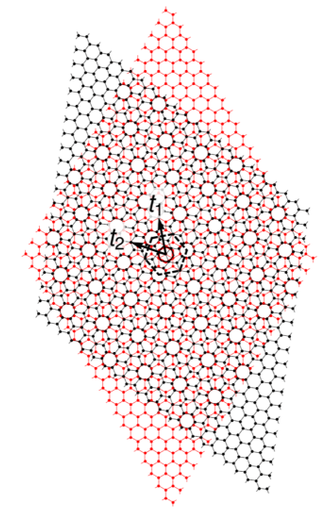
$$\cos(\theta) = \frac{3m^2 + 3mr + r^2/2}{3m^2 + 3mr + r^2} \quad \text{with} \quad m, r \in \mathbb{Z}$$

Exact superlattice = approximate superlattice $\Leftrightarrow r = 1$

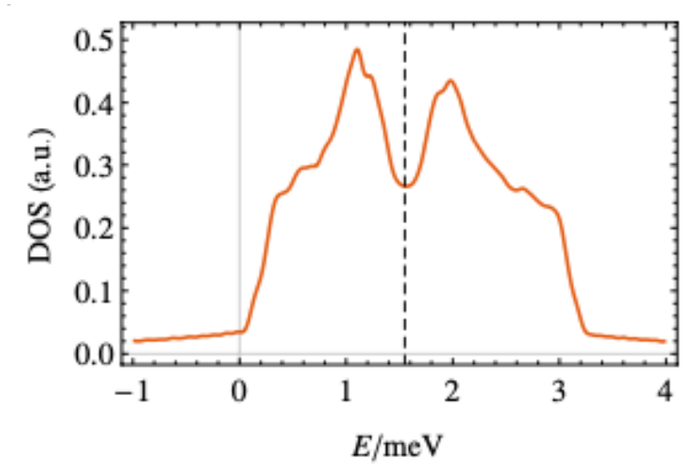
Codes available at
https://gitlab.jyu.fi/jyucmt/psg-and-tbg

"Magic angle"





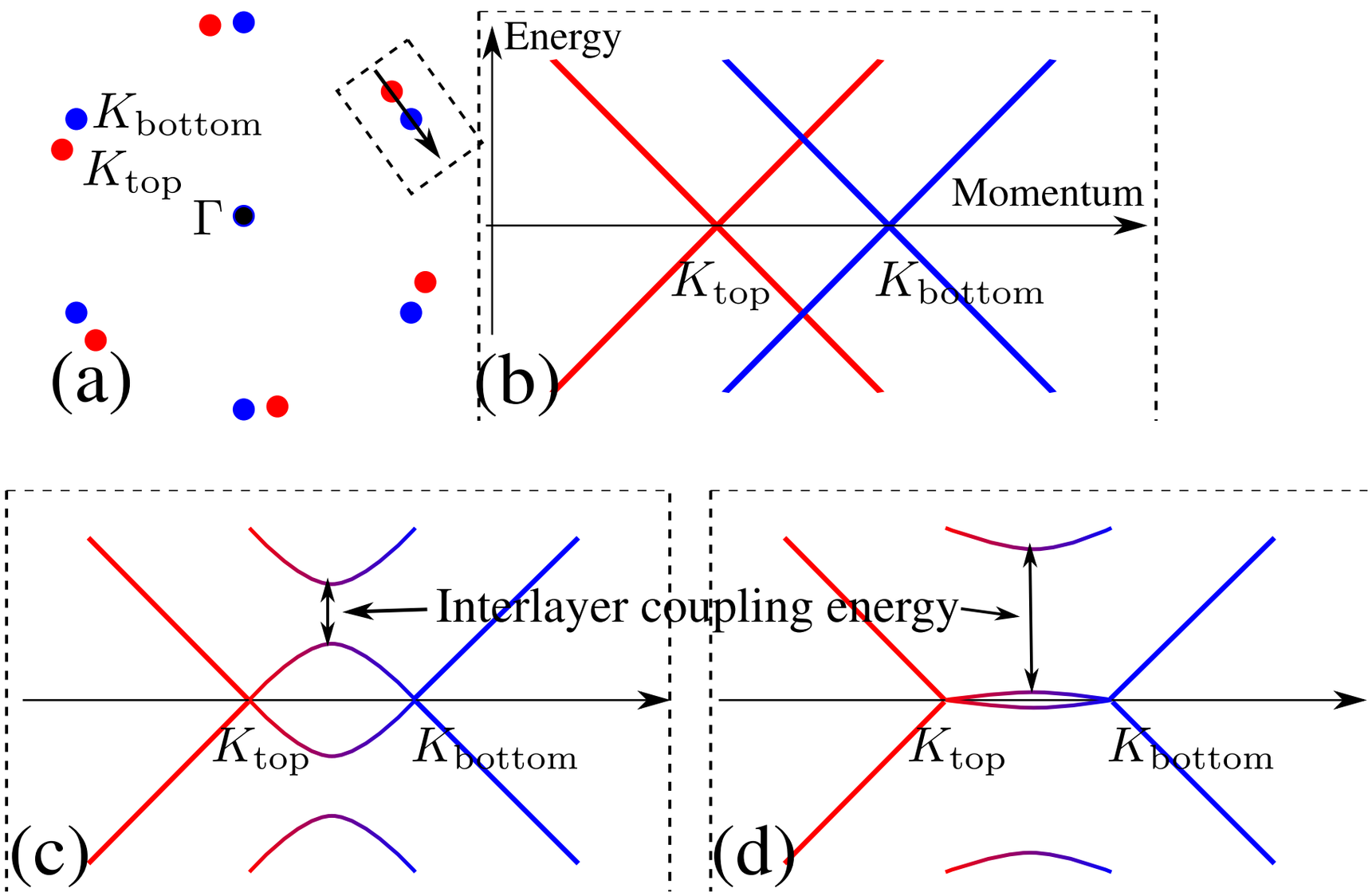
First "magic" angle at $\theta \approx 1.08°$



$\delta E \sim 3$ meV

Lopes dos Santos, Peres, Castro Neto, PRL 2007 and PRB 2012
E. Suarez Morell, et al., PRB (2010)
Bisritzer & MacDonald, PNAS (2011)

Toy model for flat band formation



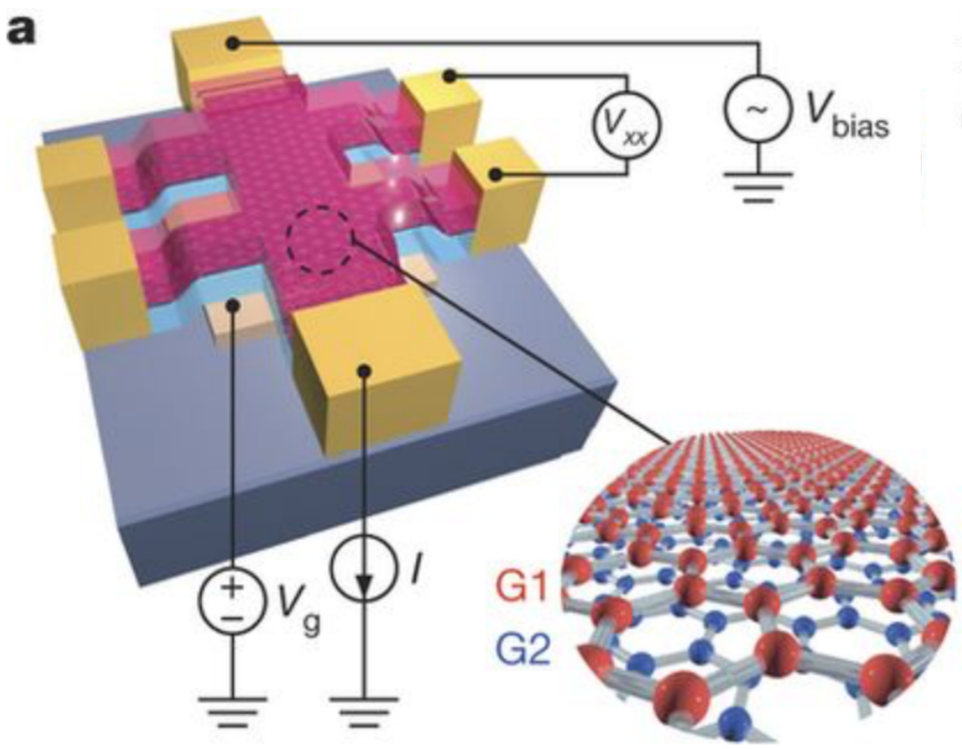
TTH & T. Hyart, Europhys. News **50**, 24 (2019)

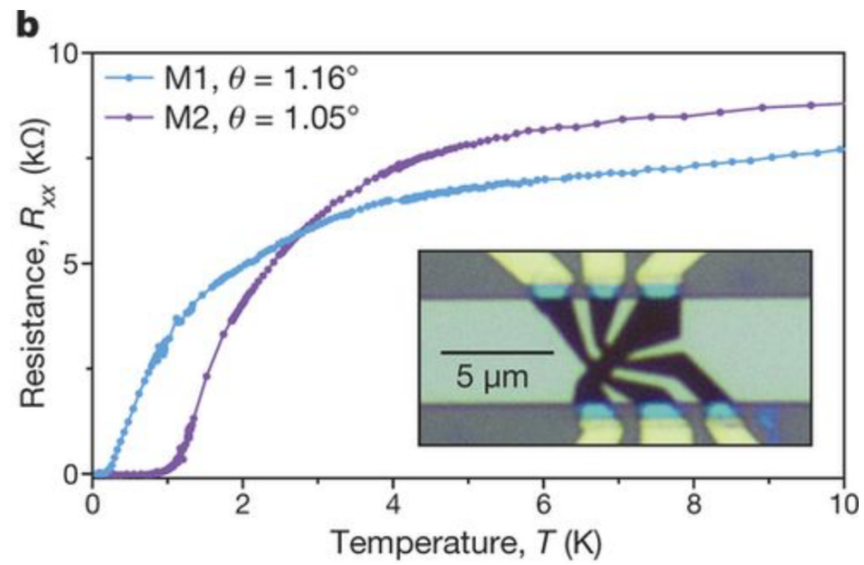
Unconventional superconductivity in magic-angle graphene superlattices

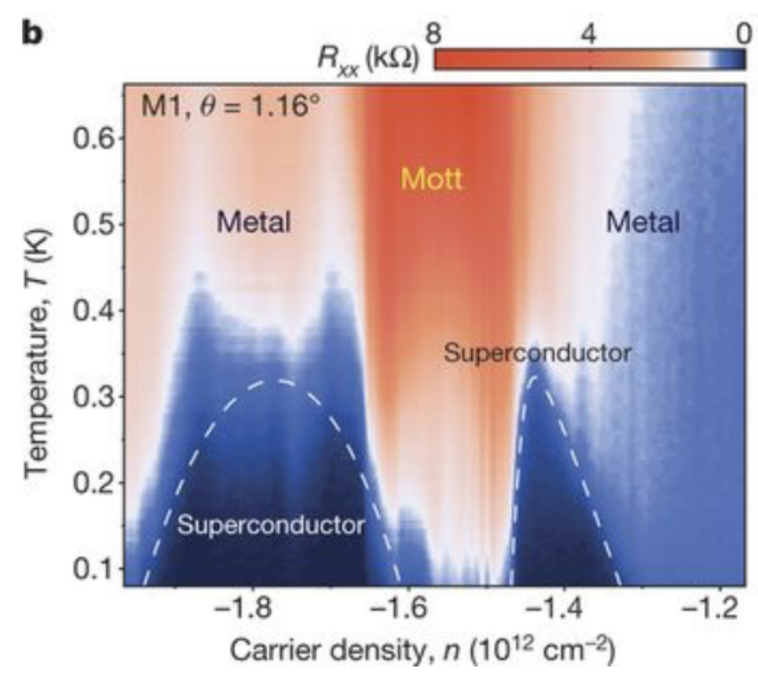
(And many others)

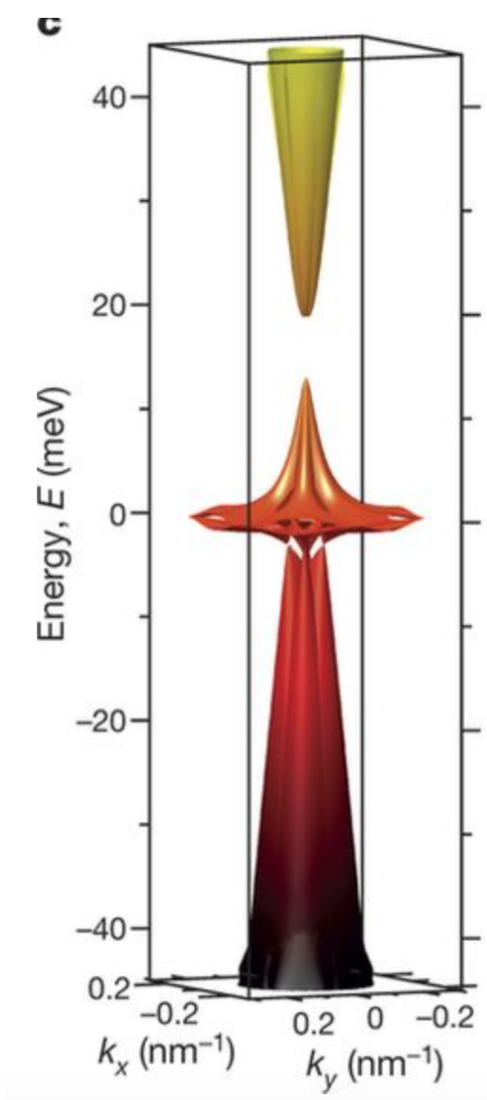
Yuan Cao, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras & Pablo Jarillo-Herrero

Nature **556**, 43–50 (05 April 2018) | Download Citation



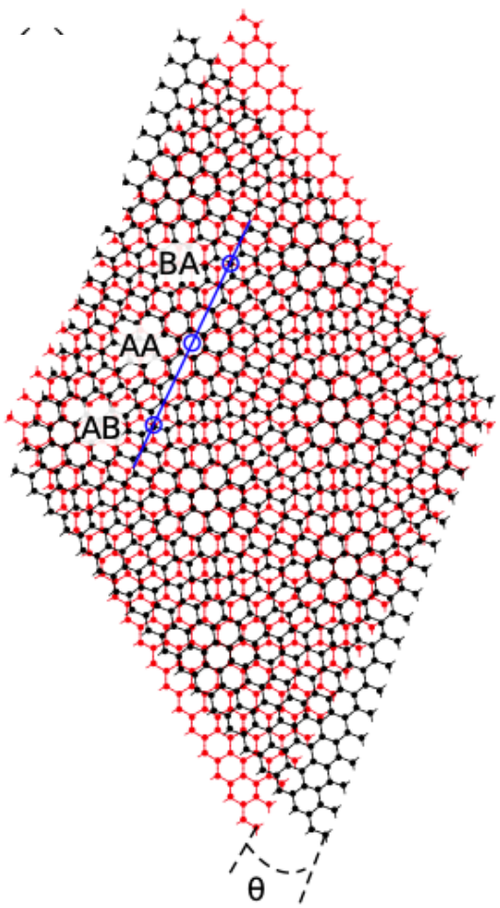


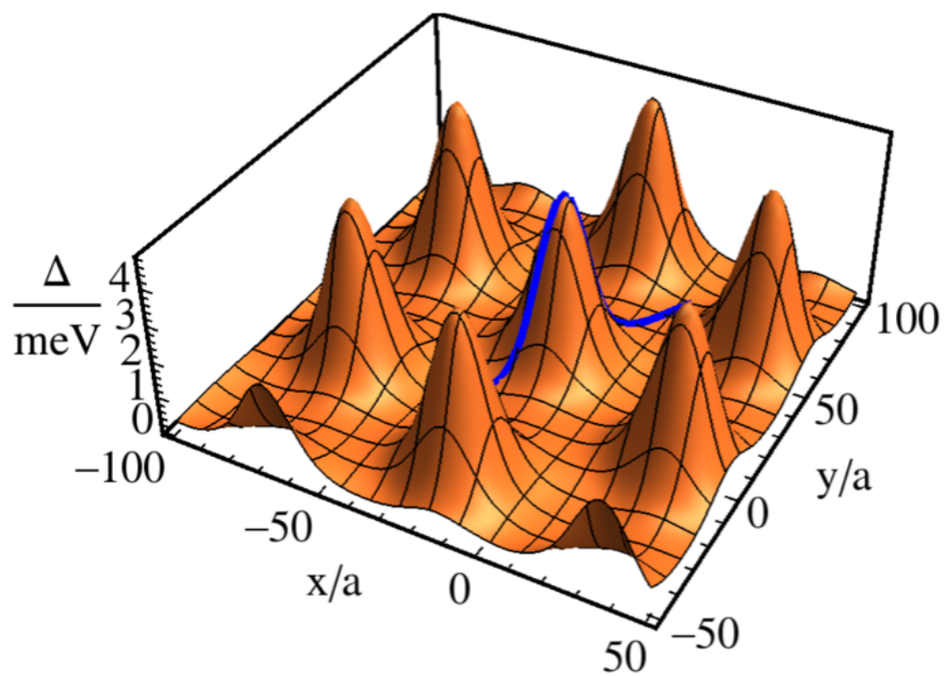




Superconducting state

Inhomogeneous order parameter:

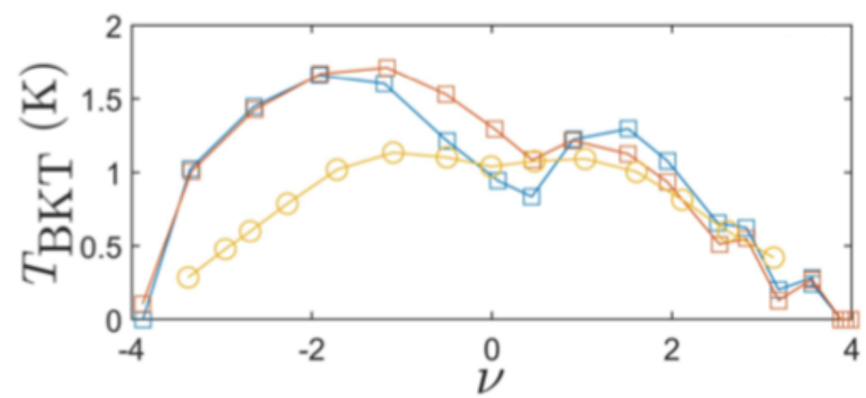




local pairing

Consistent with electron-phonon mediated superconductivity!

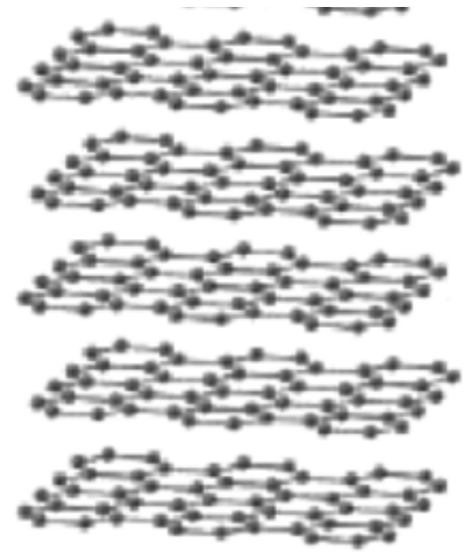
Intermediate between "narrow band" and "flat-band" limits



T. Peltonen, R. Ojajärvi, TTH, Phys. Rev. B **98**, 220504 (2018)
A. Julku, T. Peltonen, L. Liang, TTH, P. Törmä, Phys. Rev. B **101**, 060505 (2020)

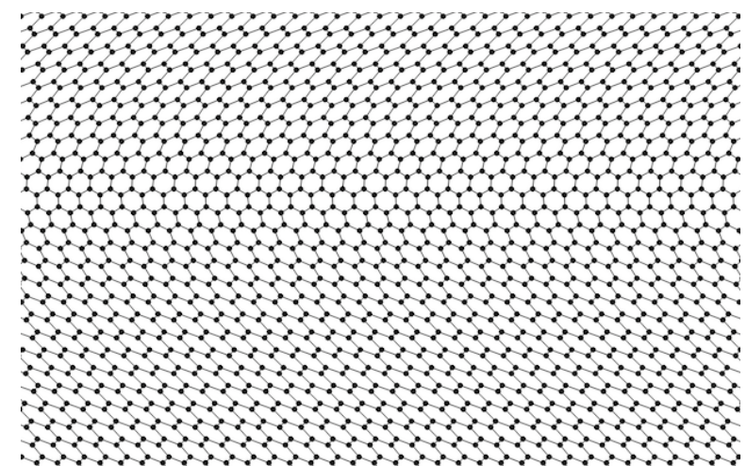
Graphene-based flat bands

- Stacked graphene



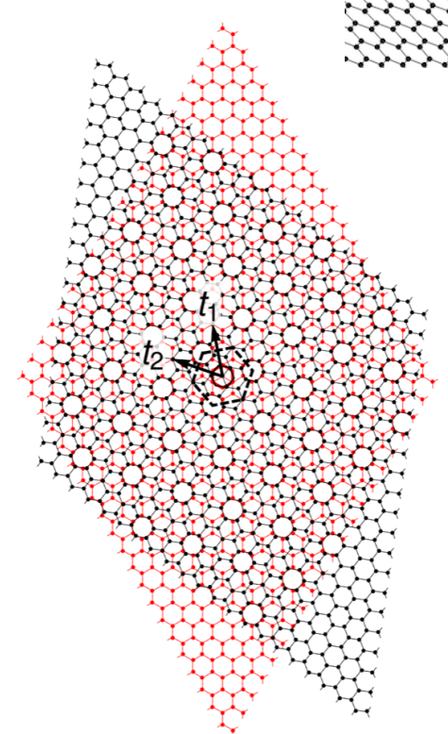
$$\Omega_{\mathrm{FB}} \sim \pi p_{\mathrm{FB}}^2 = \pi \left(\frac{\gamma_1}{v_F}\right)^2$$

- Periodically strained graphene



$$\Omega_{\mathrm{FB}} \sim \frac{2\pi\beta}{L^2}$$

- Twisted bilayer graphene



$$\Omega_{\mathrm{FB}} = \Omega_{\mathrm{BZ}}^{\mathrm{superlattice}} \sim \frac{\Omega_{\mathrm{BZ}}^{\mathrm{graphene}}}{N}$$

$N \sim 10^4$ at $\theta \sim 1.1°$