Stacking faults in crystalline graphite

bound states and Landau levels

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F. Guinea, CSIC Madrid

Phys. Rev. B **78**, 245416 (2008)

Benasque, 2009

Brief outline

1. Stacking and graphitic structures

2. Bernal hexagonal vs. rhombohedral graphite

3. Landau levels, surface states, possible 3DQHE

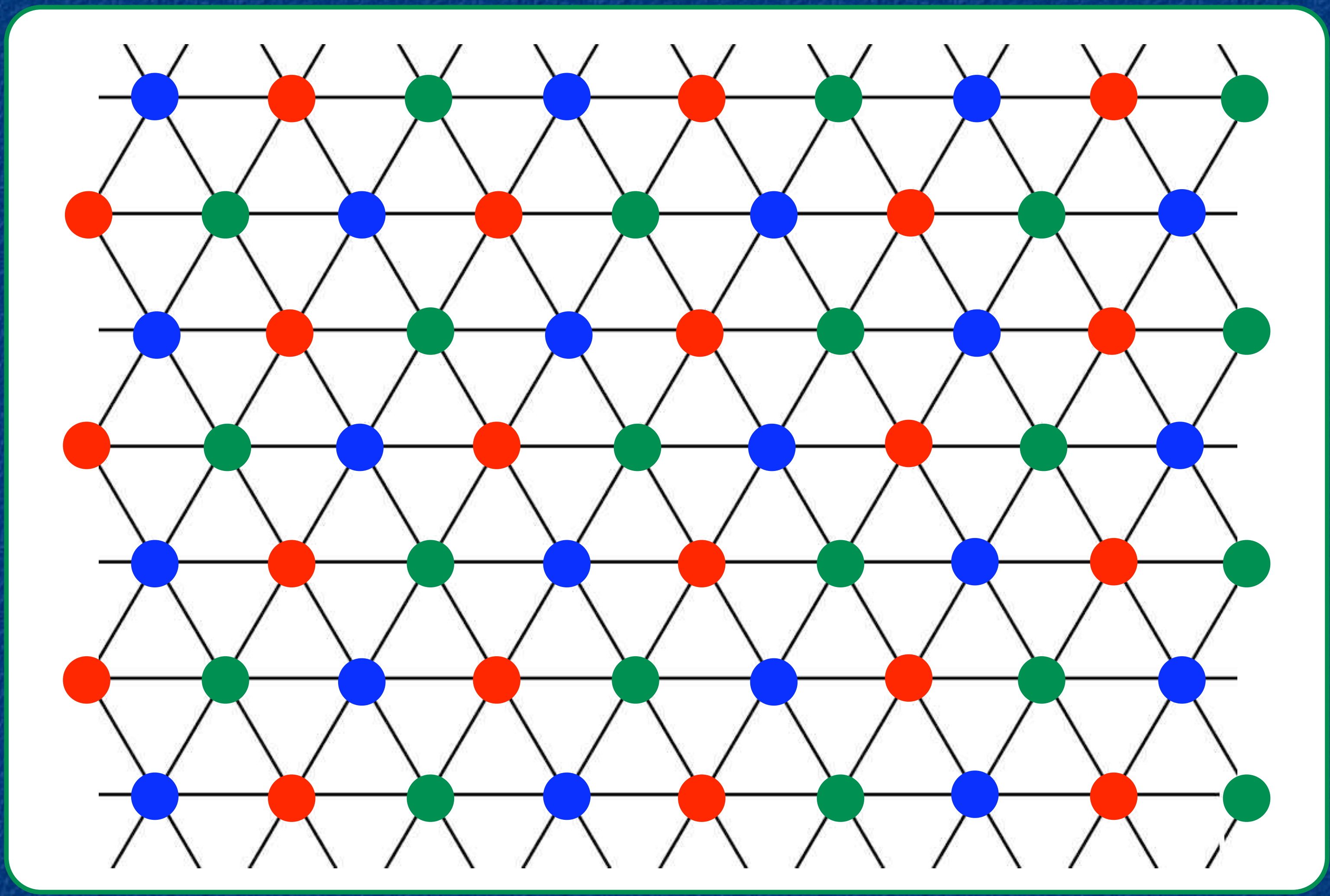
4. Simple model of a stacking fault:
   S-matrix, bound states, Landau levels

5. Surface spectroscopy of buried faults

6. Full SWMc treatment of a stacking fault

Graphene stacks : from triangular lattice

A / **B** / **C** sublattices (tripartite)



Graphitic structures

1. Bernal stacking : ABAB...

- hexagonal Bravais lattice $a_0 = 2.46$ Å ; $c_0 = 2d = 6.74$ Å

2. rhombohedral : ABCABC...

- ab initio calculations → 0.11 meV / atom more total energy than BHG

  J. C. Charlier, X. Gonze, and J.-P. Michenaud, *Carbon* **32**, 289 (1994)
- exists only in combination with Bernal hexagonal phase (as high as 40%)

  S. Chehab, K. Guerin, J. Amiell, and S. Flandrois, *Eur. Phys. J. B* **13**, 235 (2000)

3. disordered ("turbostratic")

- disordered stacking plus some orientational disorder

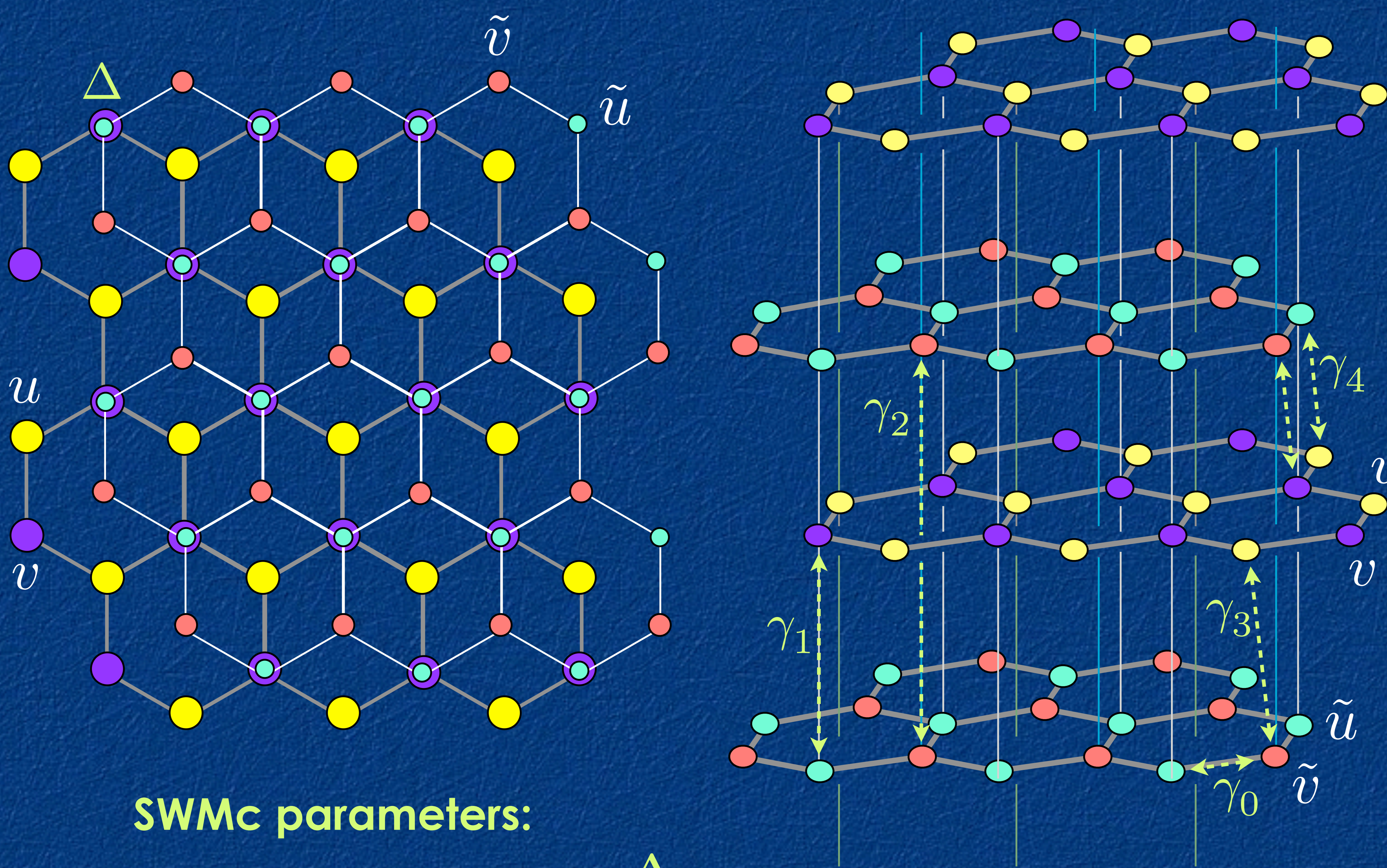
  A. Marchand, in *Les Carbones*, A. Pacault, ed. (Masson, Paris, 1965), T. 1, Part III, p. 232

  J. C. Charlier, J.-P. Michenaud, and Ph. Lambin, *Phys. Rev. B* **46**, 4540 (1992)

4. hexagonal : AAA...

- e.g. in Li - intercalated graphite

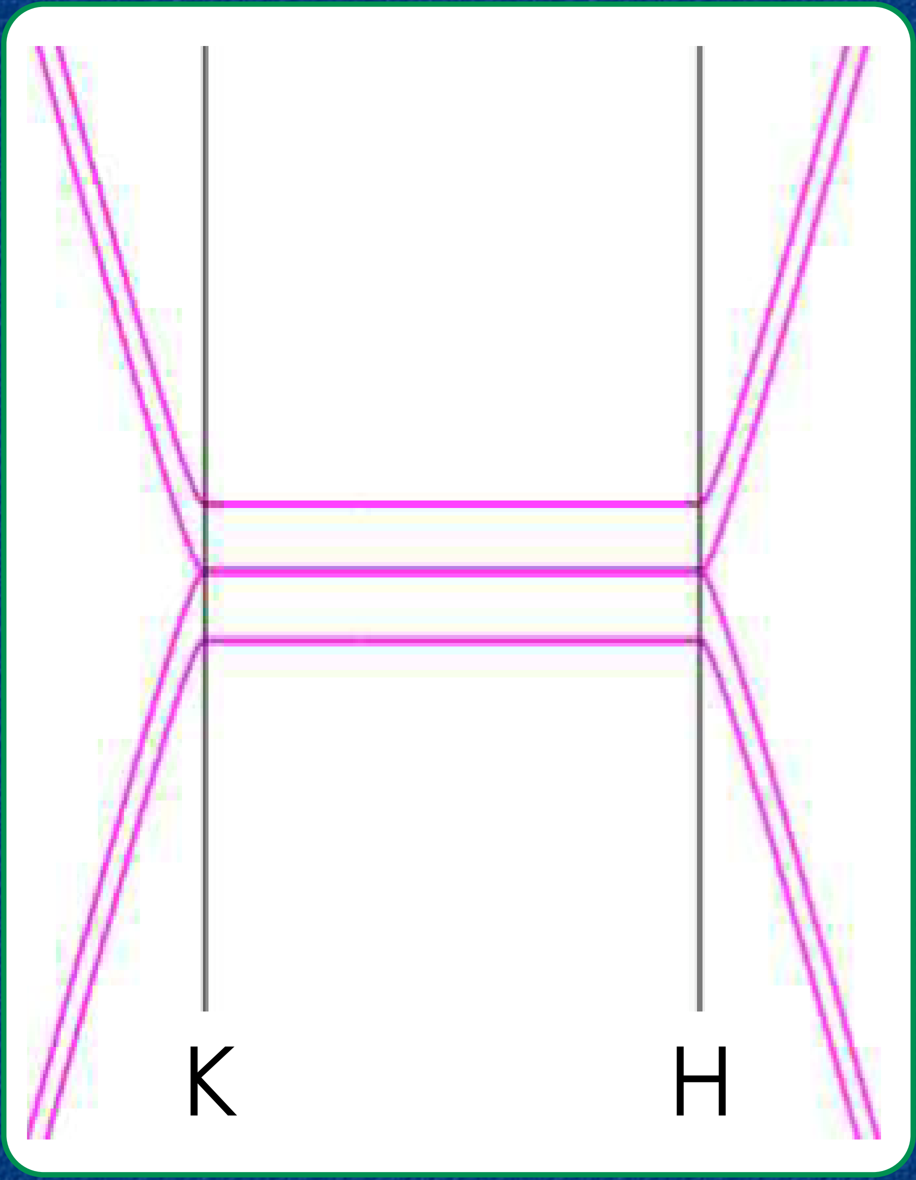
Bernal stacking ABAB...



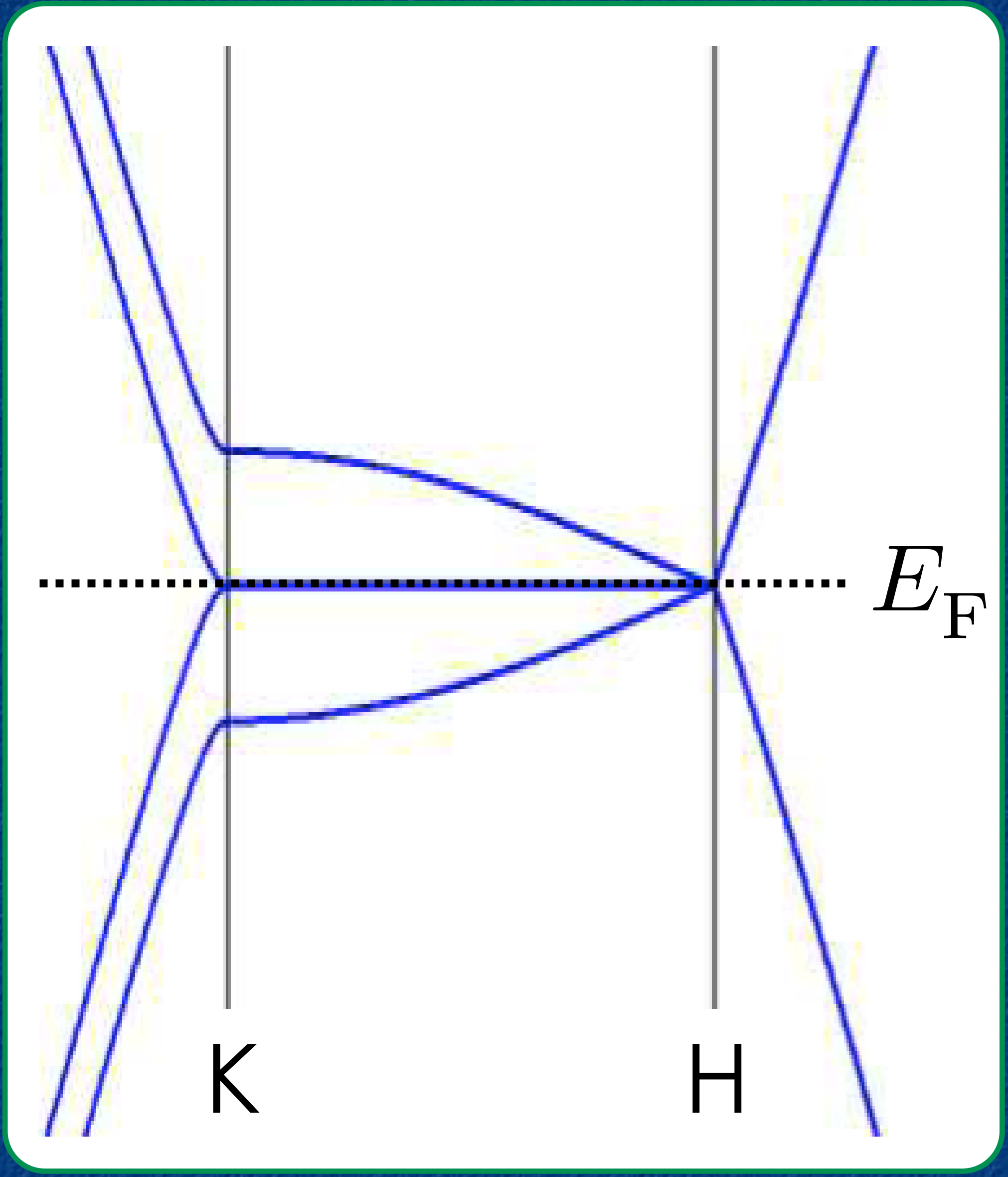
SWMc parameters:

$$\gamma_0\,,\gamma_1\,,\gamma_2\,,\gamma_3\,,\gamma_4\,,\gamma_5\,,\Delta$$

Predictions of nearest-neighbor tight-binding model : *zero-gap semiconductor*



graphene bilayer

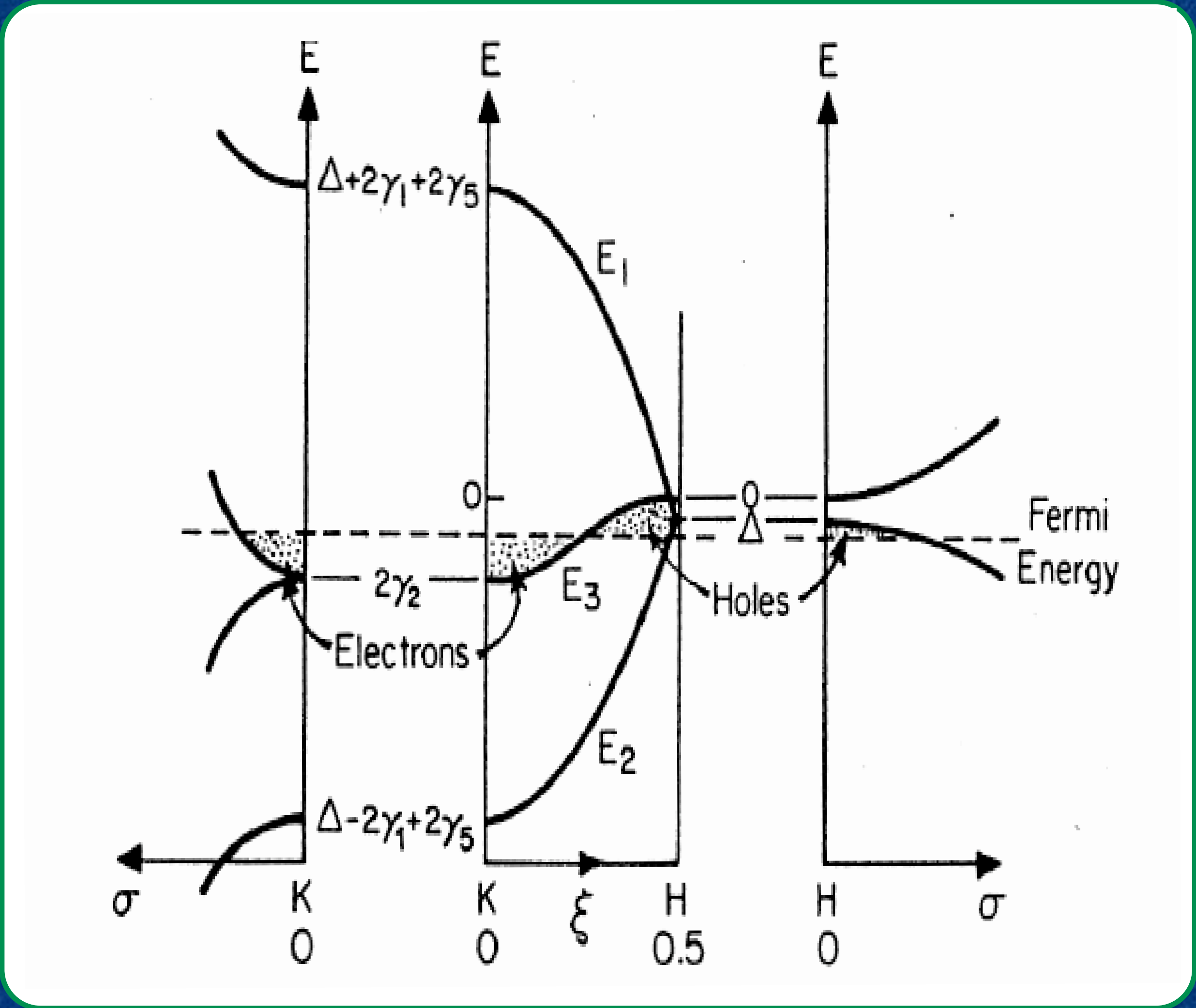


Bernal hexagonal graphite

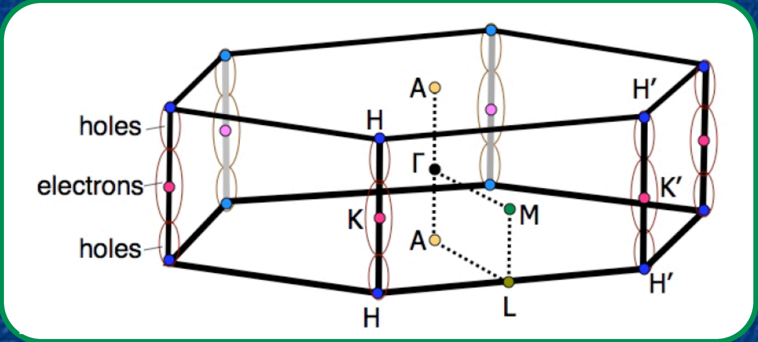
F. Guinea, A. H. Castro Neto, and N. M. R. Peres, *PRB* **73**, 245426 (2006)

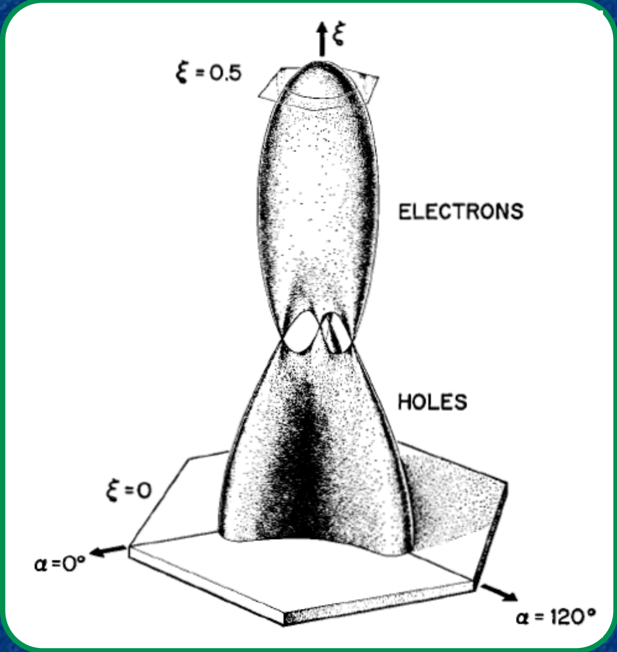
Degeneracy along KH lifted by γ_2 hopping

Bernal graphite is a semi-metal



M. S. Dresselhaus and G. Dresselhaus, *Adv. Phys.* **51**, 1 (2002)

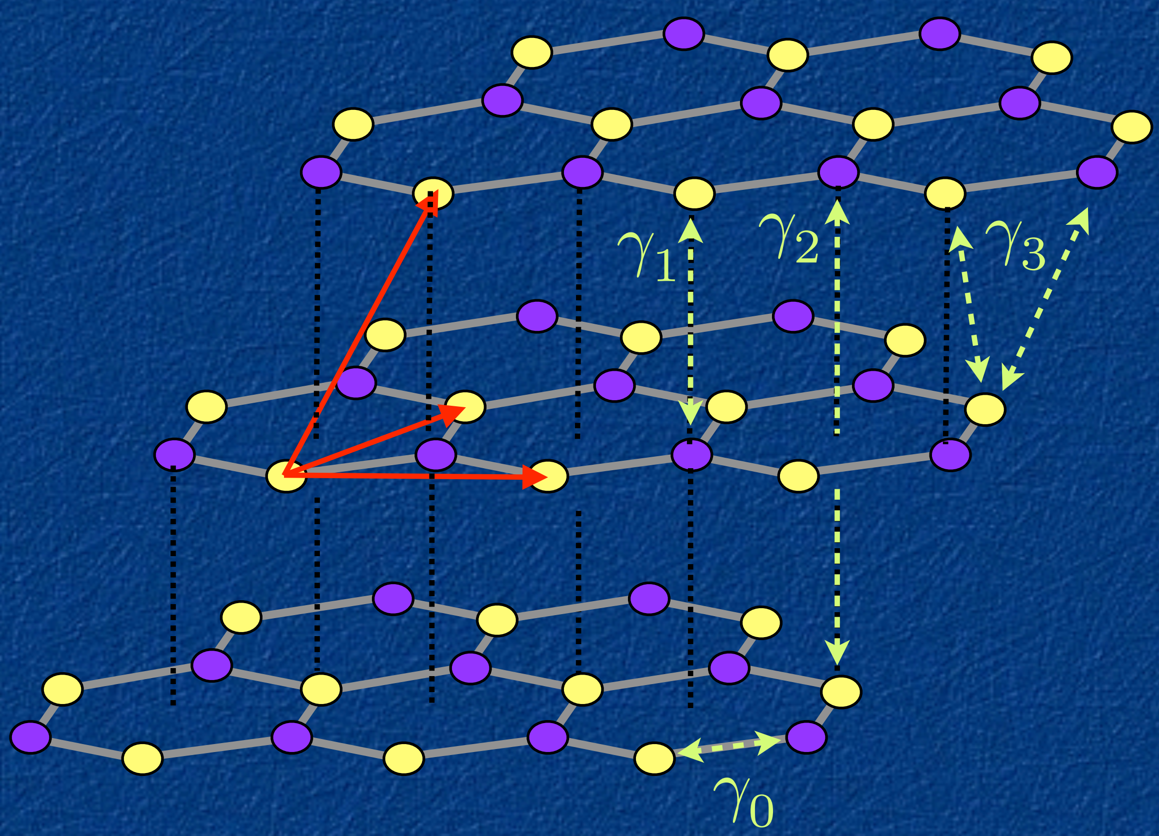


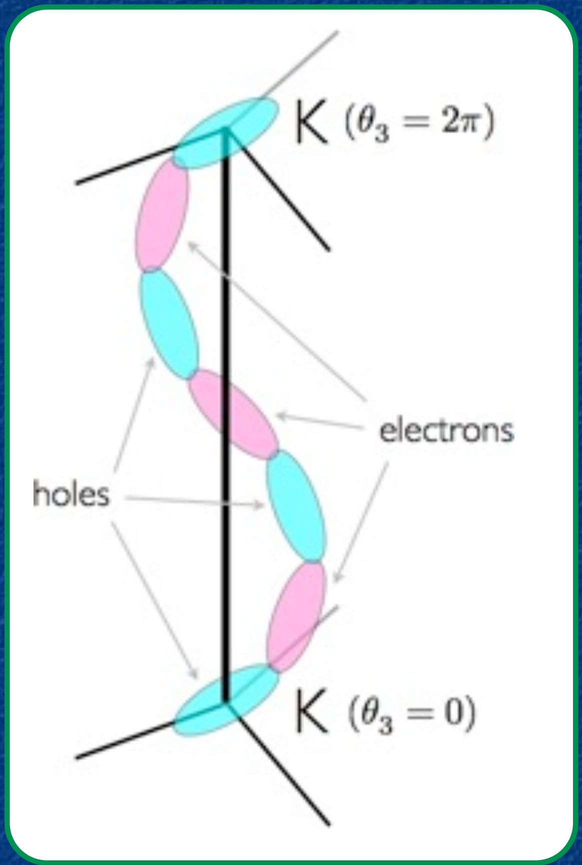


M. S. Dresselhaus and J. G. Mavroides, *IBM Res. Jour.* **8**, 262 (1964)

Rhombohedral graphite

- ABCABC stacking (but 2-atom unit cell)
- "sausage link" Fermi surface -- almost graphene (McClure 1969)
- DOS ≈ 10^{-4} states / eV·atom·spin (RG), 3×10^{-3} eV·atom·spin (BHG)
- LLs : $E_n = -\Gamma\cos(3\theta_3) \pm \gamma_0\sqrt{nB/B_0}$ with $\Gamma \approx 6.5\,\mathrm{meV}$ and $B_0 \approx 7300\,\mathrm{T}$





J. W. McClure, *Carbon* **7**, 425 (1969)

Landau levels

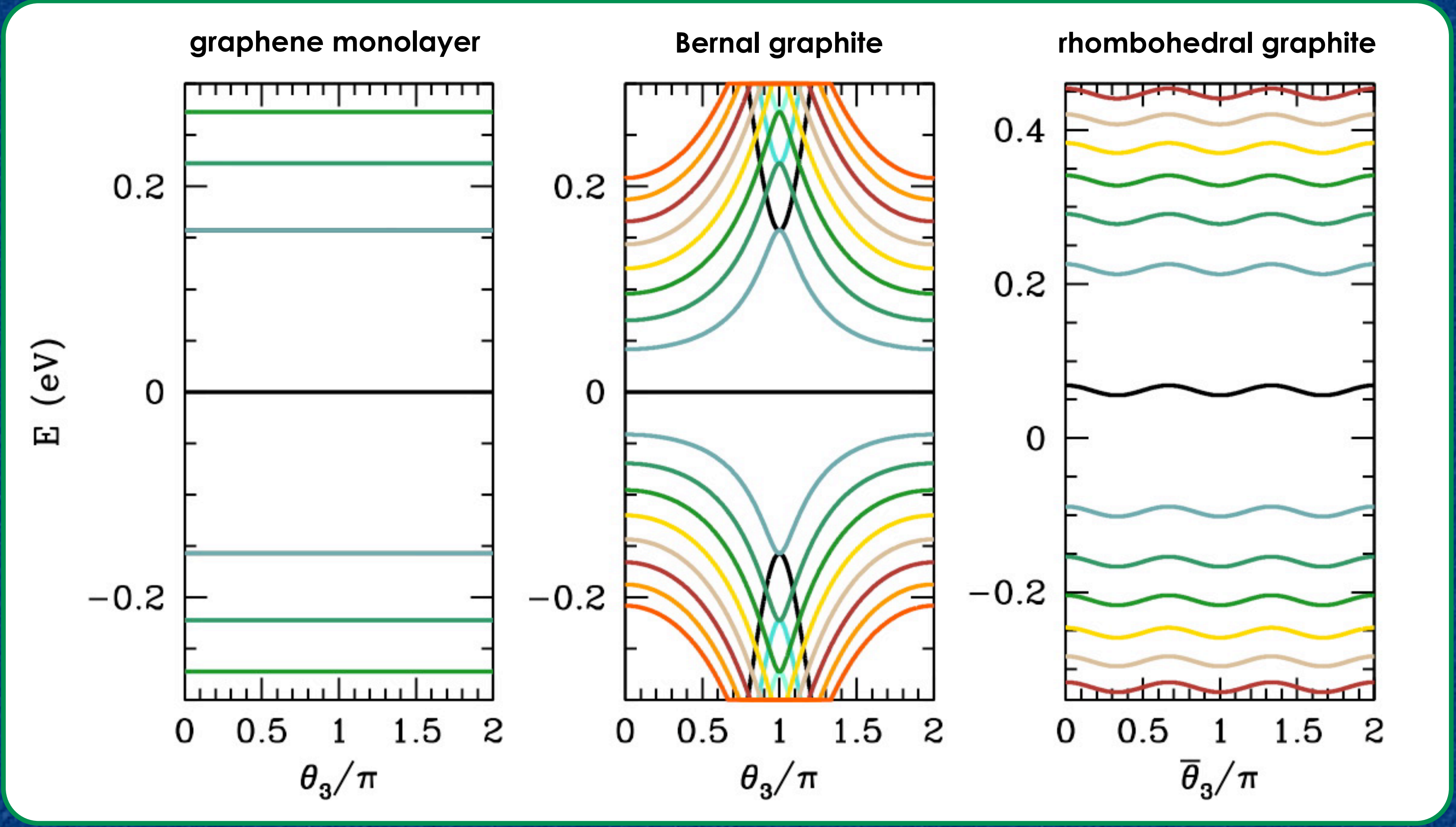
$\epsilon \equiv \sqrt{B/B_0}$, $B_0 = \frac{hc/e}{3\pi a^2} \approx 7300\,\mathrm{T}$

$$E_n^{\mathrm{BHG}} = \pm\left[(n+\tfrac{1}{2})\,\epsilon^2\,\gamma_0^2 + 2\gamma_1^2\cos^2\!\left(\tfrac{\theta_3}{2}\right) \pm 2\sqrt{\left(\tfrac{1}{2}\,\epsilon\,\gamma_0\right)^4 + (n+\tfrac{1}{2})\,\epsilon^2\,\gamma_0^2\,\gamma_1^2\,\cos^2\!\left(\tfrac{\theta_3}{2}\right) + \gamma_1^4\cos^4\!\left(\tfrac{\theta_3}{2}\right)}\right]^{1/2}$$

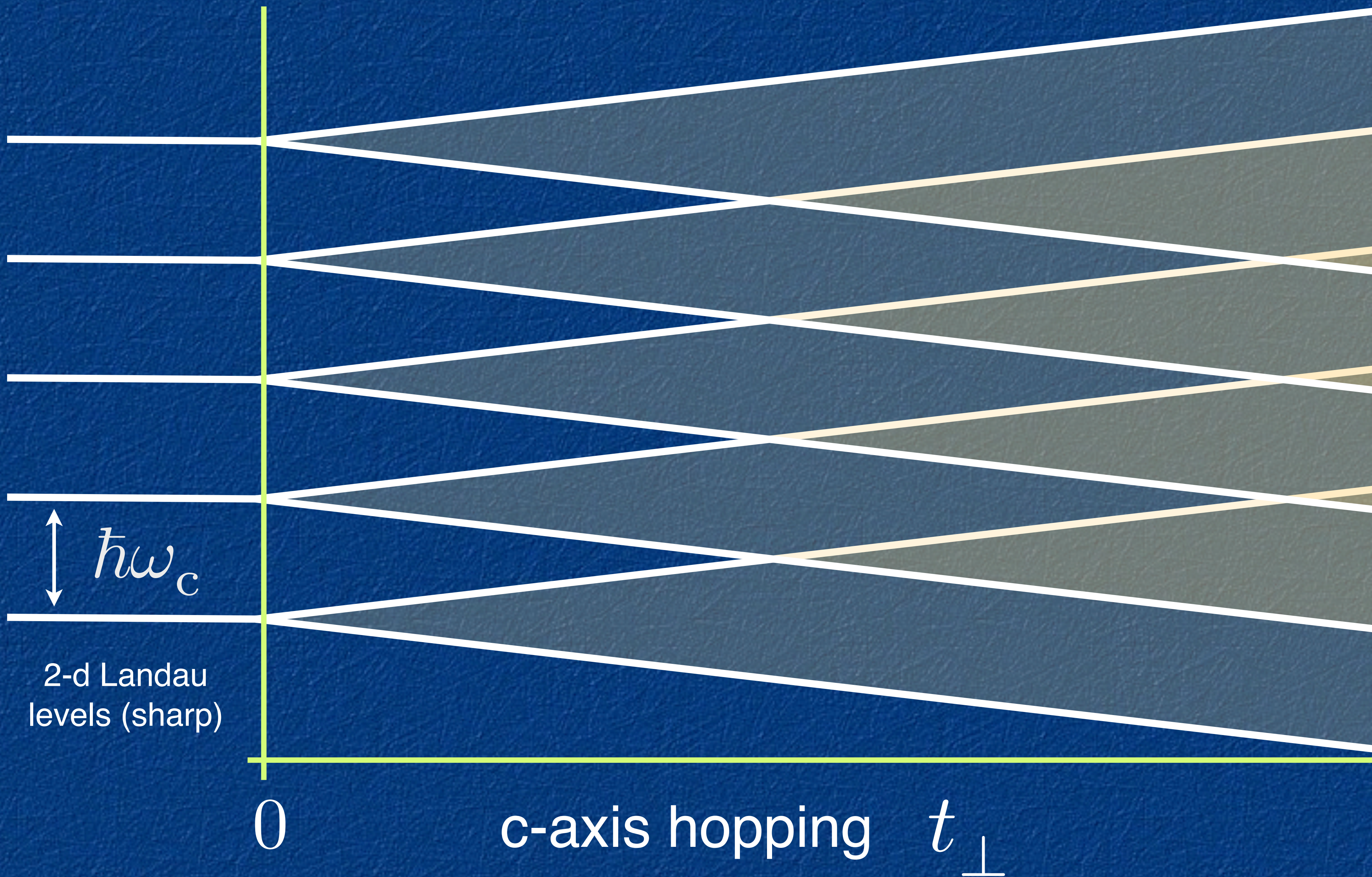
$$\mathcal{E}_0 = \left(\frac{\gamma_0\gamma_1 + \gamma_2\gamma_3}{\gamma_0^2 - \gamma_3^2}\right)\cdot 2\gamma_3 = 62\,\mathrm{meV}$$

$$E_n^{\mathrm{RG}} = \mathcal{E}_0 + W\cos(3\bar{\theta}_3) \pm \epsilon\,\gamma_0\sqrt{n}$$

$$W = \left(\frac{\gamma_1\gamma_3 + \gamma_0\gamma_2}{\gamma_0^2 - \gamma_3^2}\right)\cdot 2\gamma_3 = 6.5\,\mathrm{meV}$$

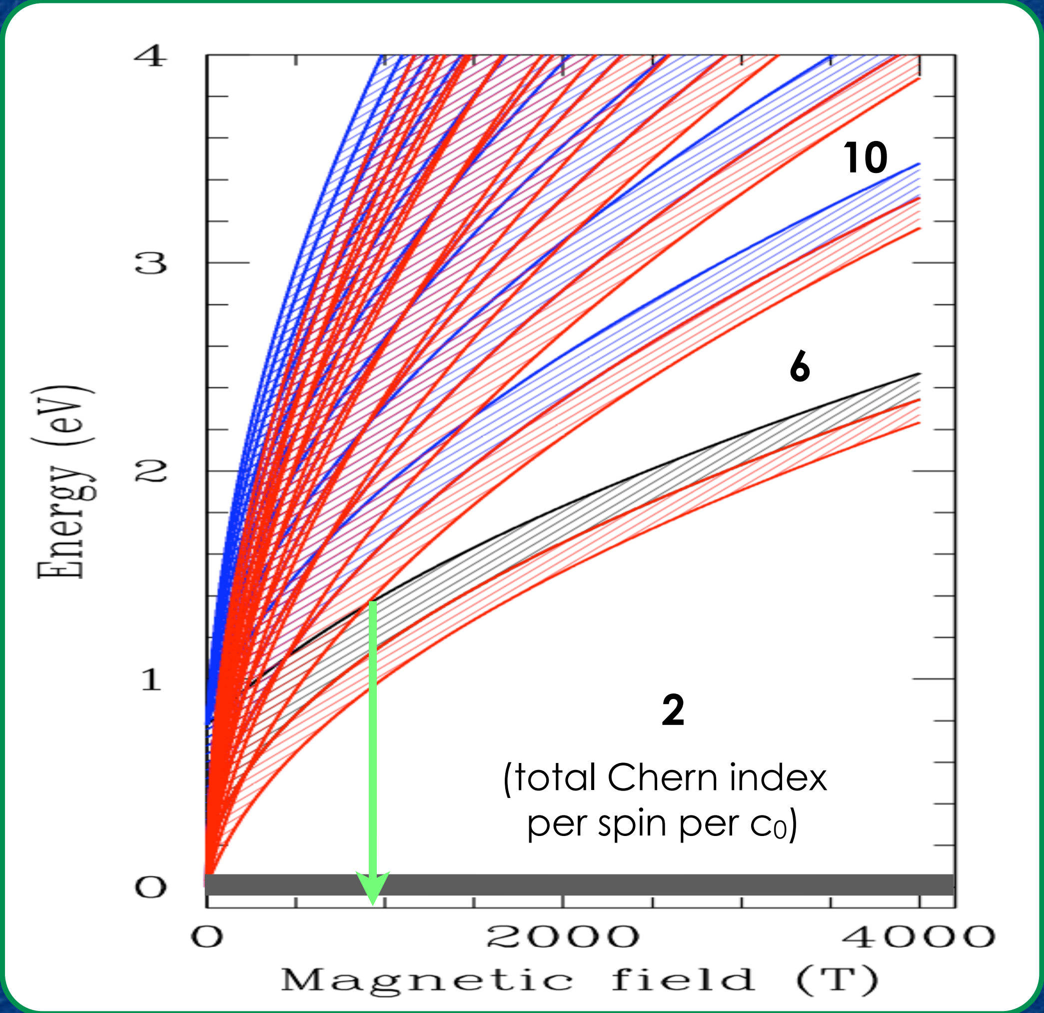


Collapse of cyclotron gaps by c-axis hopping

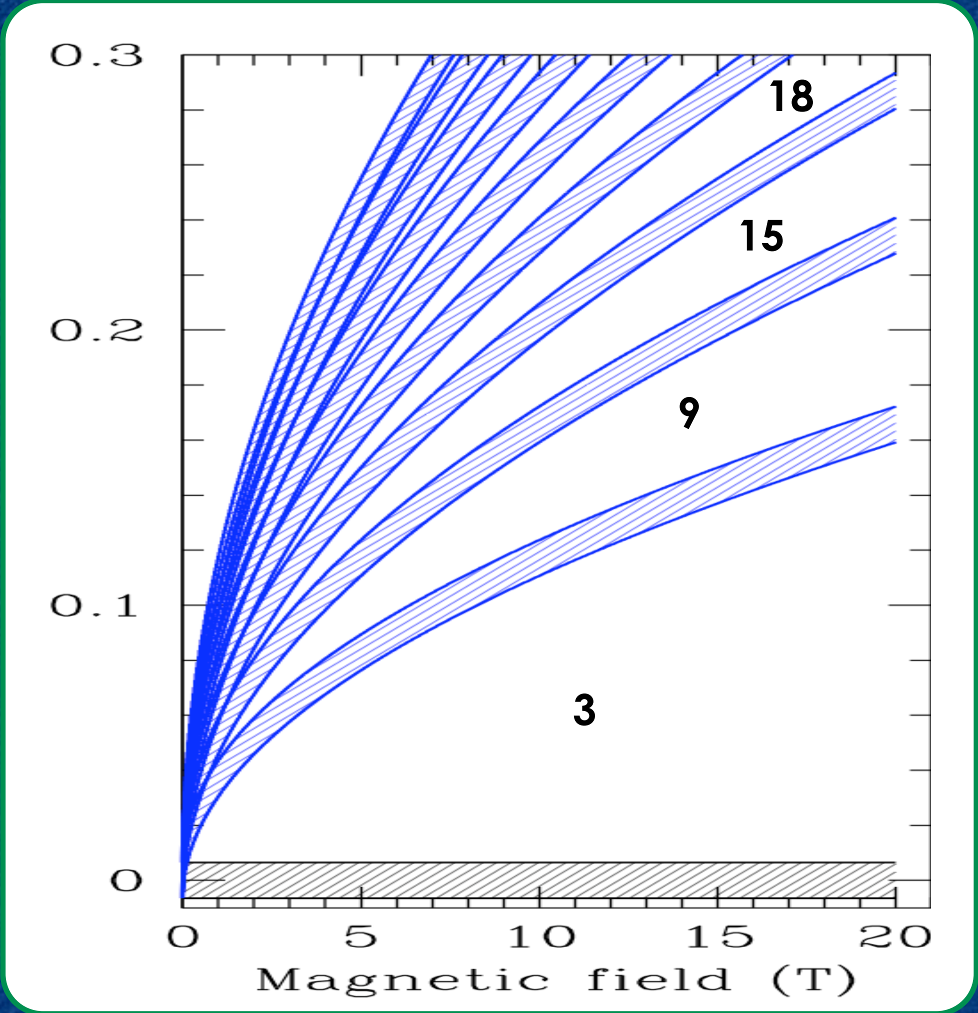


Energy bands *vs.* magnetic field

Bernal stacking



rhombohedral

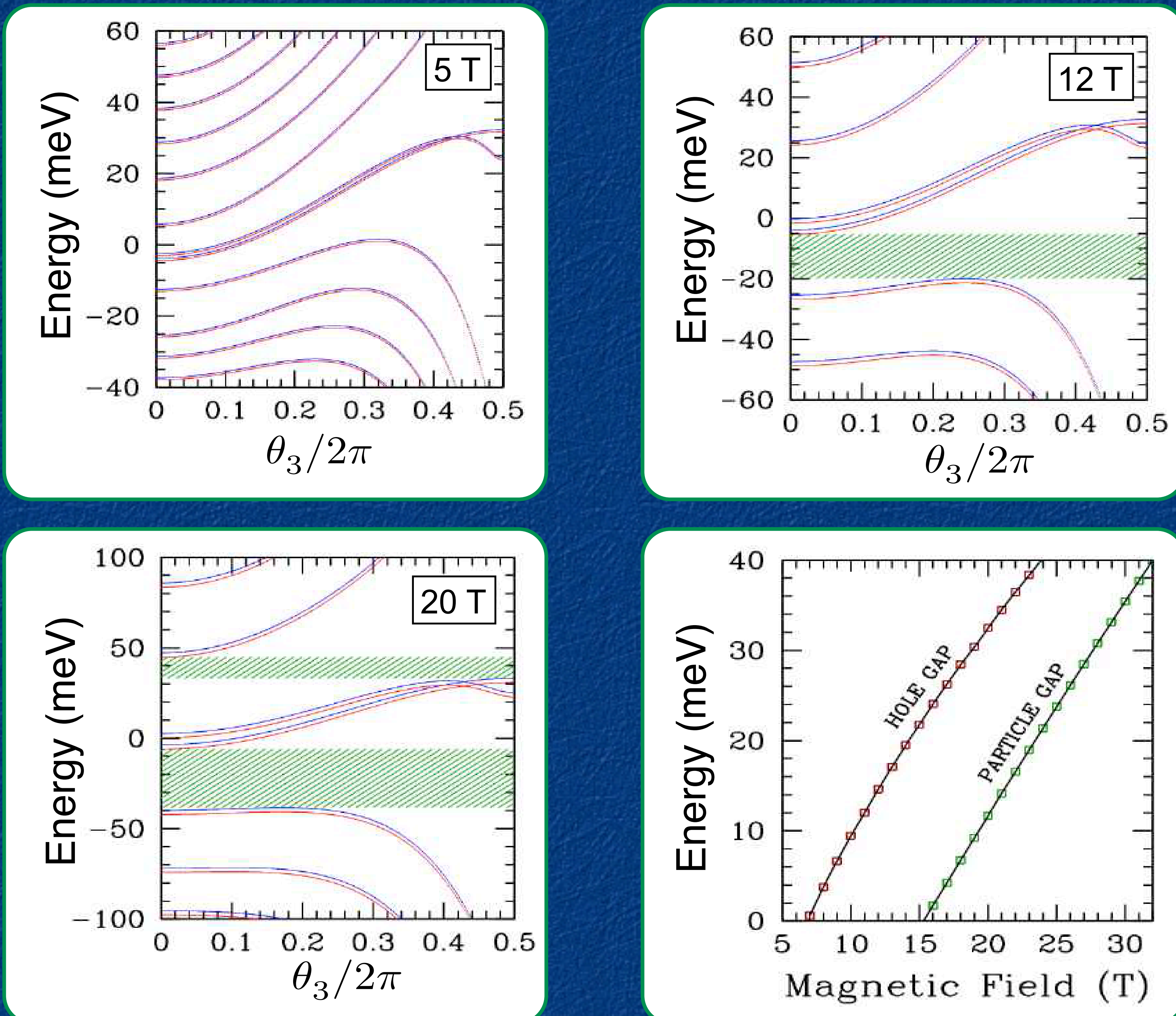


simple hexagonal (AAA) :

$$E_n(B,\boldsymbol{k}) = 2\gamma_1 \cos(k_z c) + \mathrm{sgn}(n)\,\gamma_0\sqrt{nB/B_0}$$

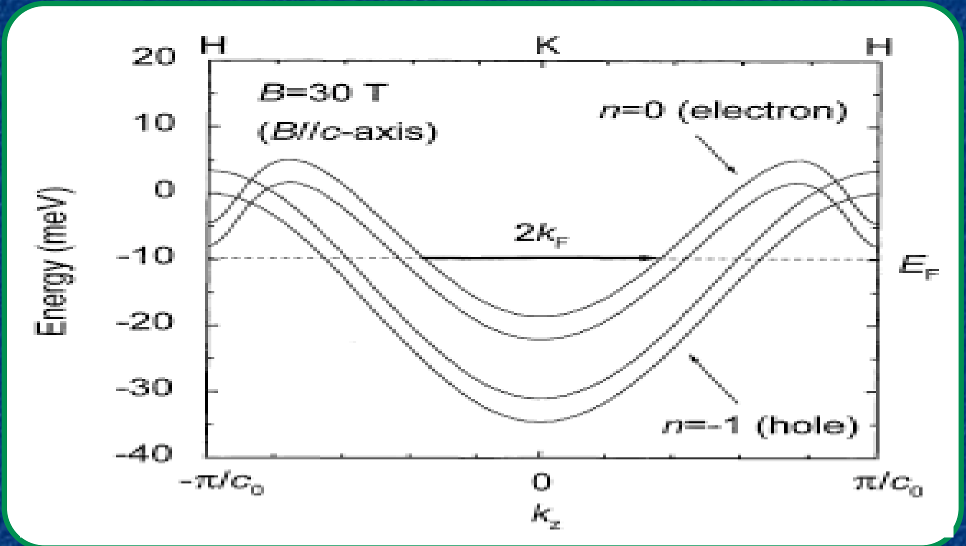
$$B_0 = \frac{hc/e}{3\pi a^2} \approx 7300\,\mathrm{T}$$

$$B_n^* = \left(\frac{4\gamma_1}{\gamma_0}\right)^2 \cdot \frac{B_0}{(\sqrt{n+1}-\sqrt{n})^2} \approx 1800\,\mathrm{T}\ \ (n=1)$$



B. A. Bernevig *et al.*, *Phys. Rev. Lett.* **99**, 146804 (2007)

Undoped Case : CDW Transition



D. Yoshioka and H. Fukuyama, *J. Phys. Soc. Japan* **50**, 725 (1981)

- One-dimensional dispersion : $Q=2k_F$ instability

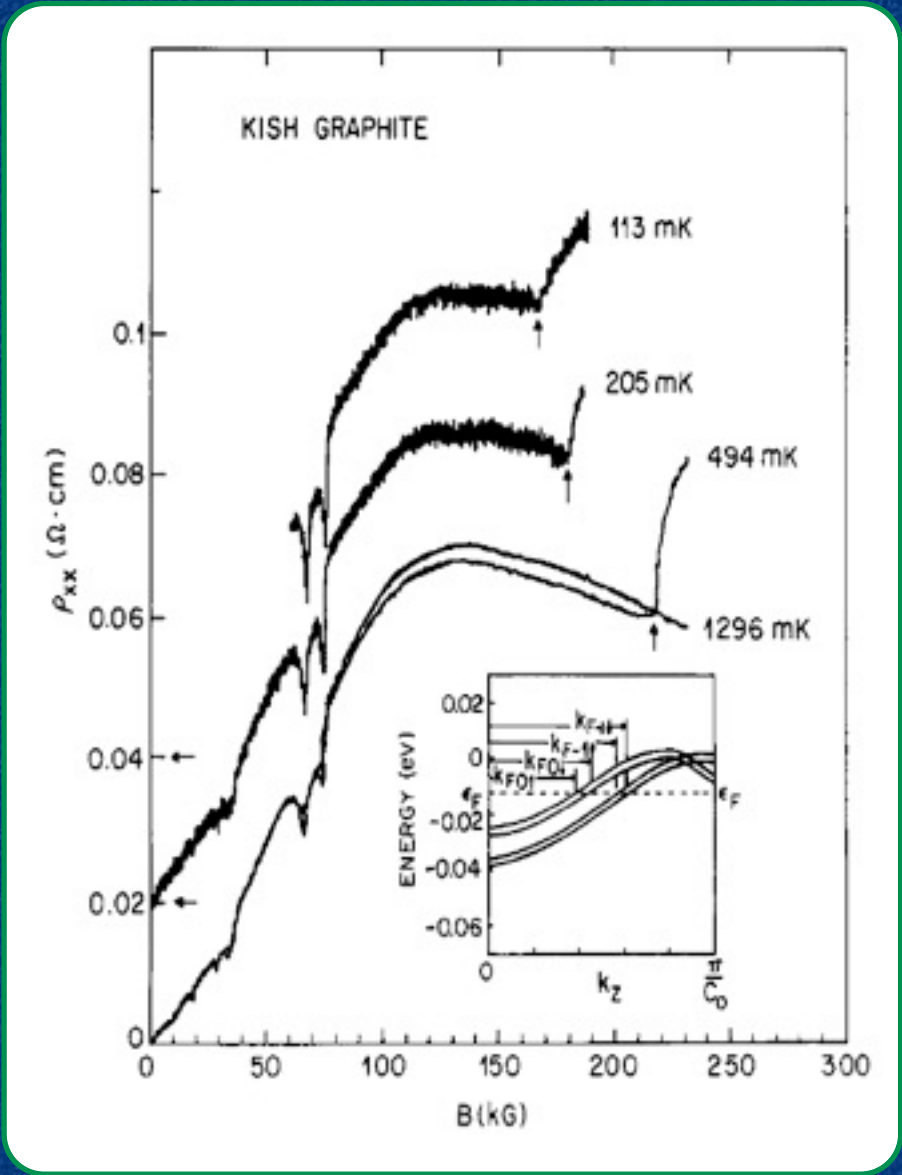
$$\rho(z) = \rho_Q \cos(Qz)$$

- Two central LLs (from A/B graphene planes) are spin-split and valley degenerate: 8 bands

- Highest T_c from (n = 0 , σ = ↑) subband

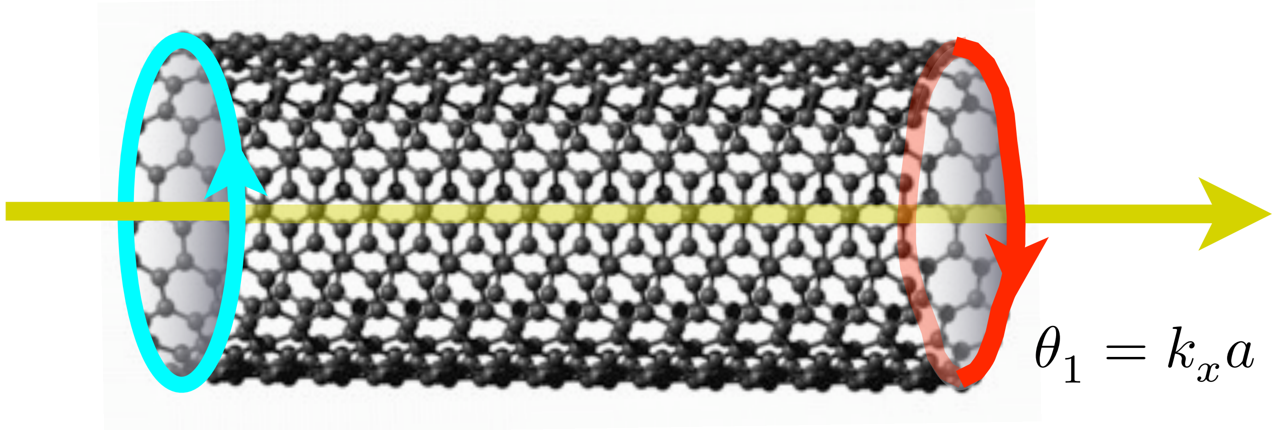
$$T_c(B) = T^* e^{-B^*/B}$$

$$T^* = 100\,\mathrm{K} \quad , \quad B^* = 1\,\mathrm{kG}$$



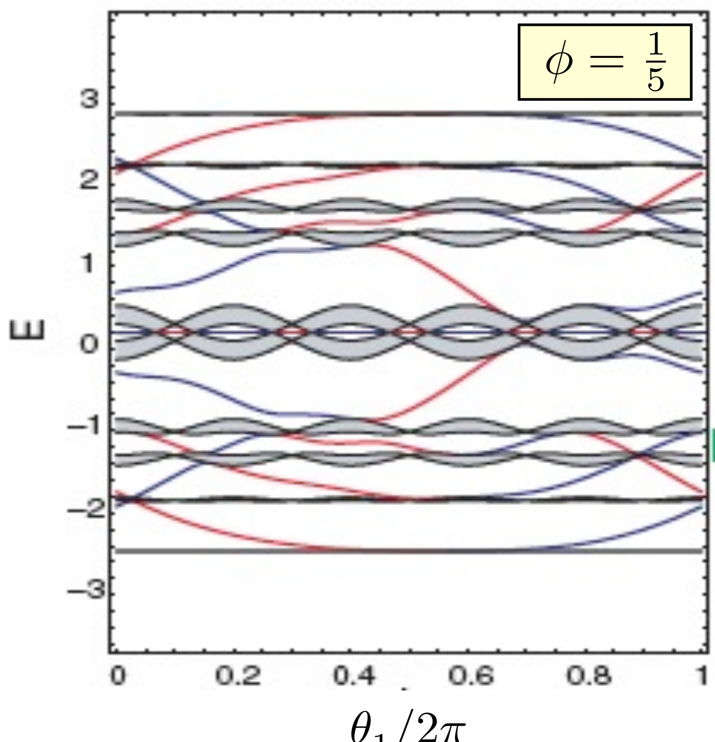
Y. Iye, P. E. Berglund, and L. E. McNeil, *Sol. St. Comm.* **52**, 975 (1984)

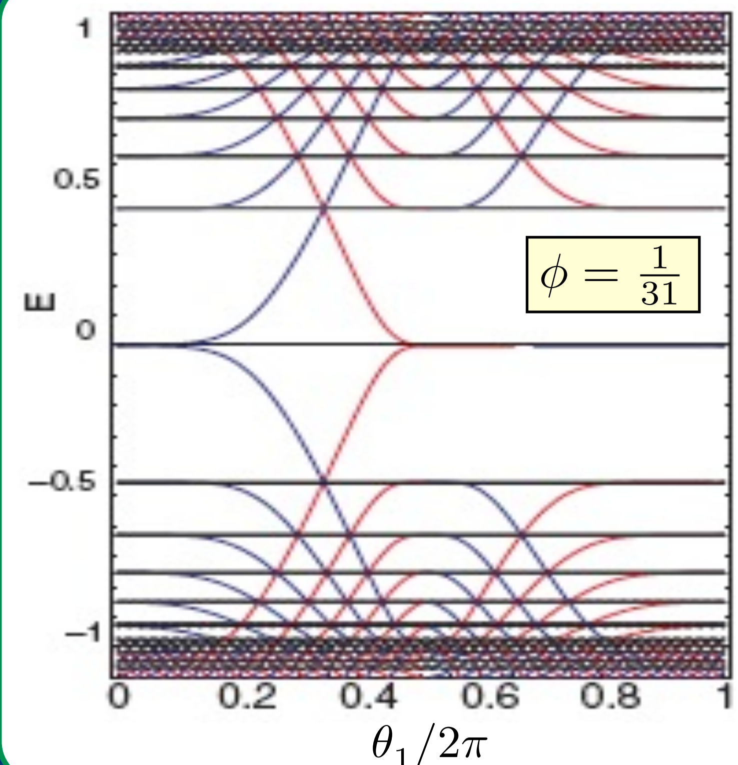
Chiral edge states in graphene



$$E = E(k_x)$$

$$v(k_x) = \frac{1}{\hbar}\frac{\partial E}{\partial k_x}$$



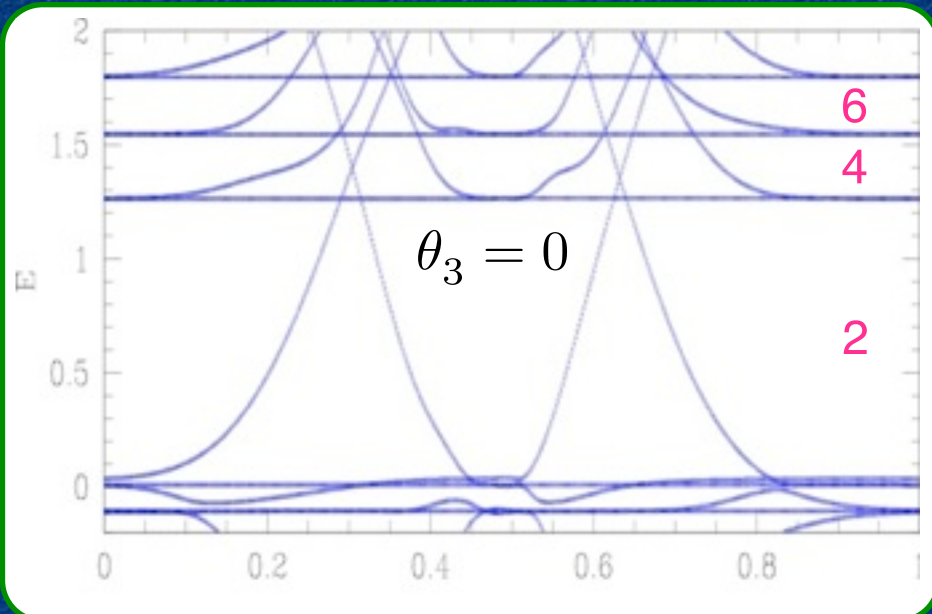


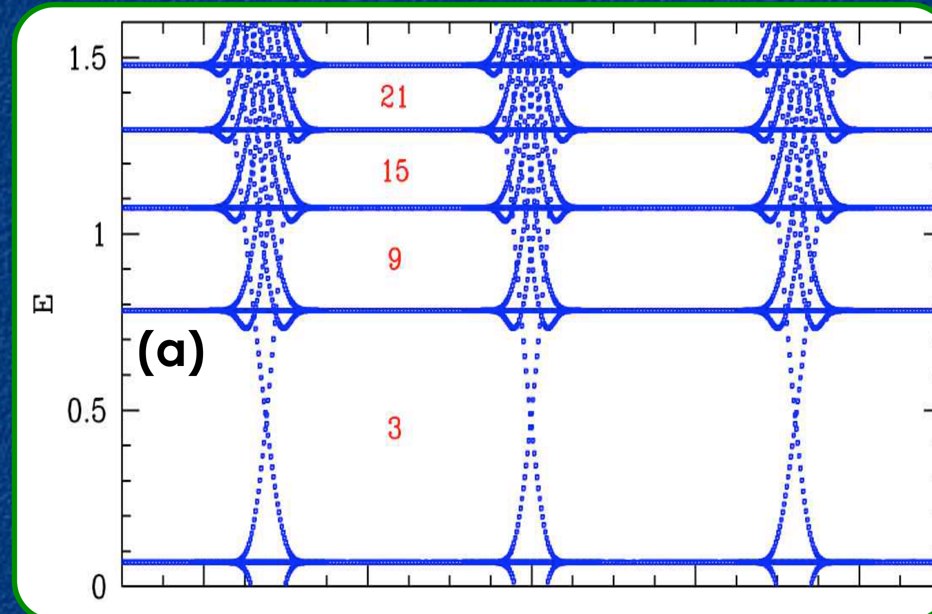
Y. Hatsugai, T. Fukui, and H. Aoki, *Eur. Phys. J. Special Topics* **148**, 133 (2007)

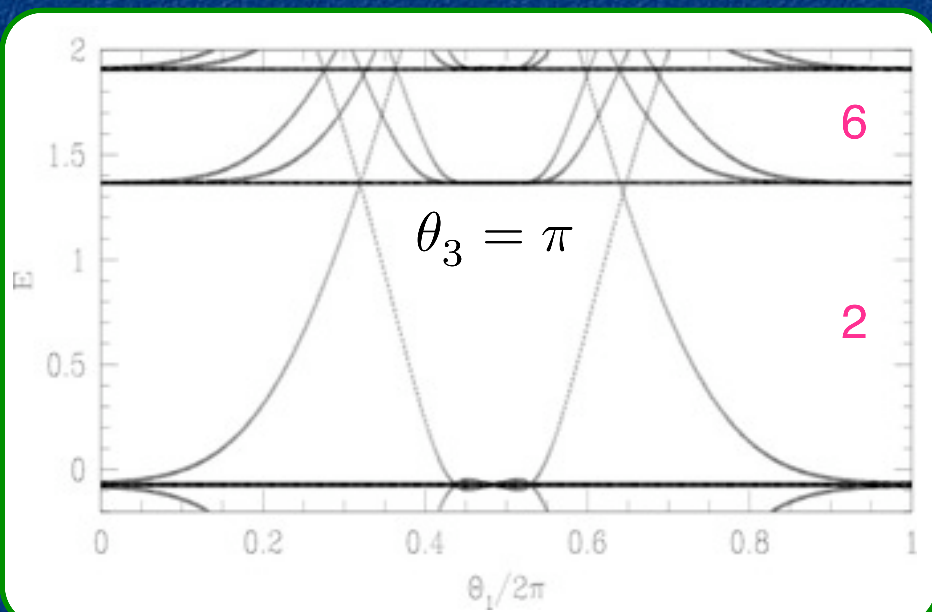
Spectral flow of graphite surface states

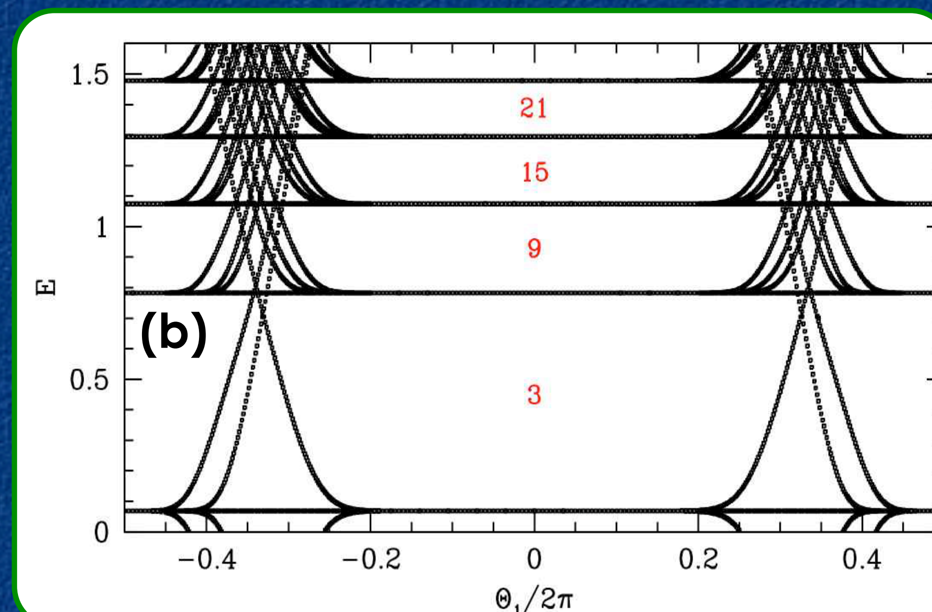
Bernal stacking

rhombohdral

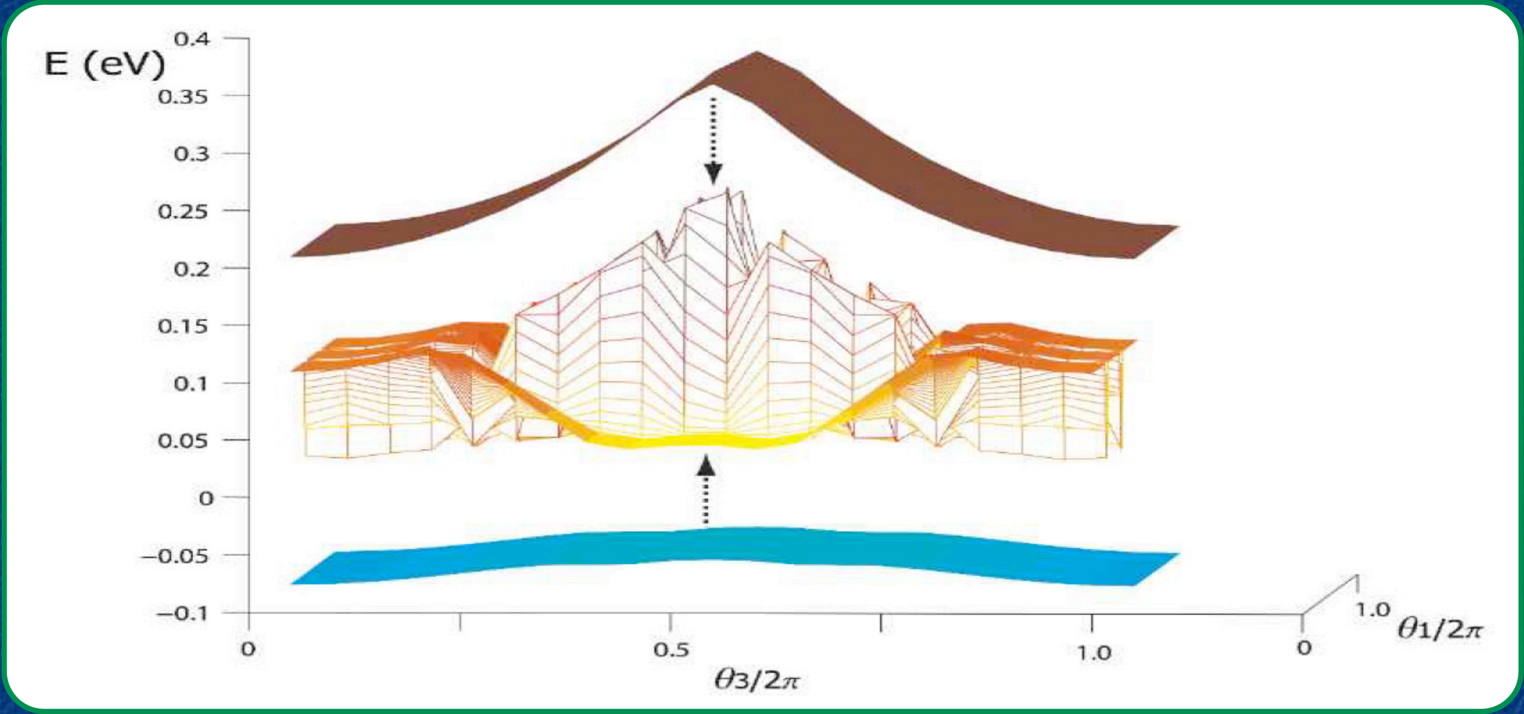


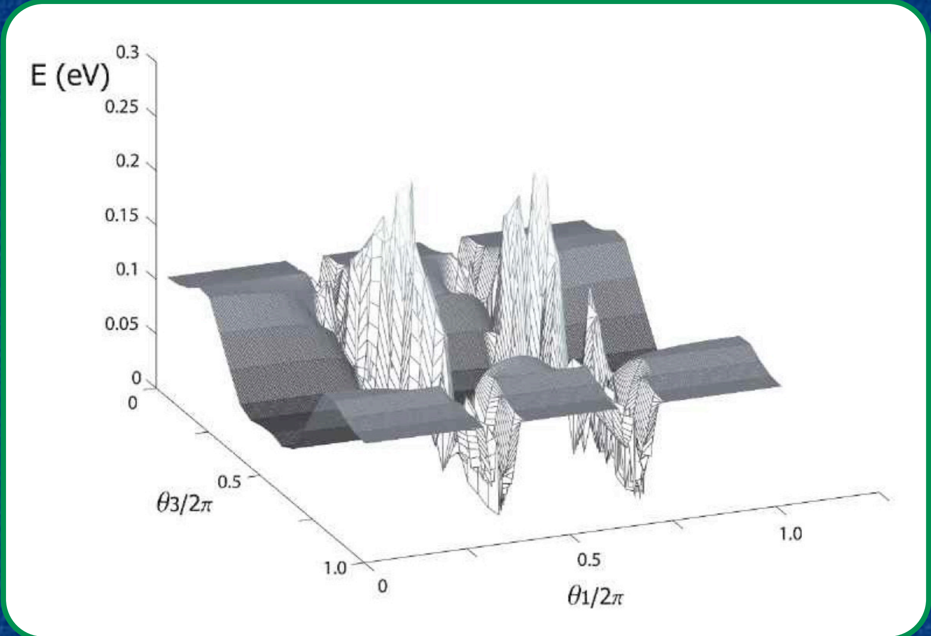


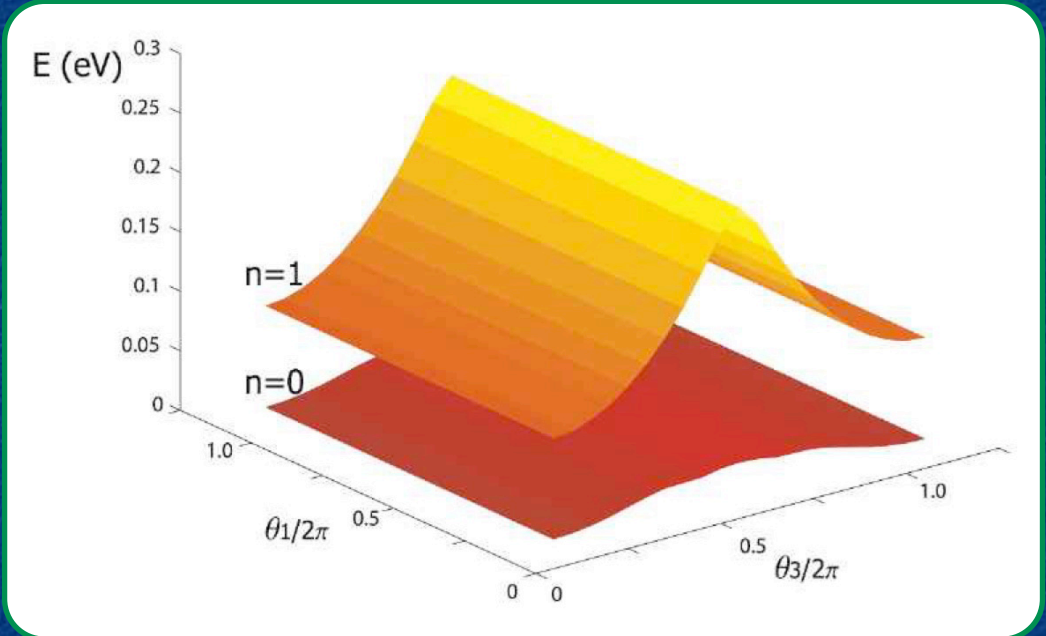




Three-dimensional BHG surface state plots







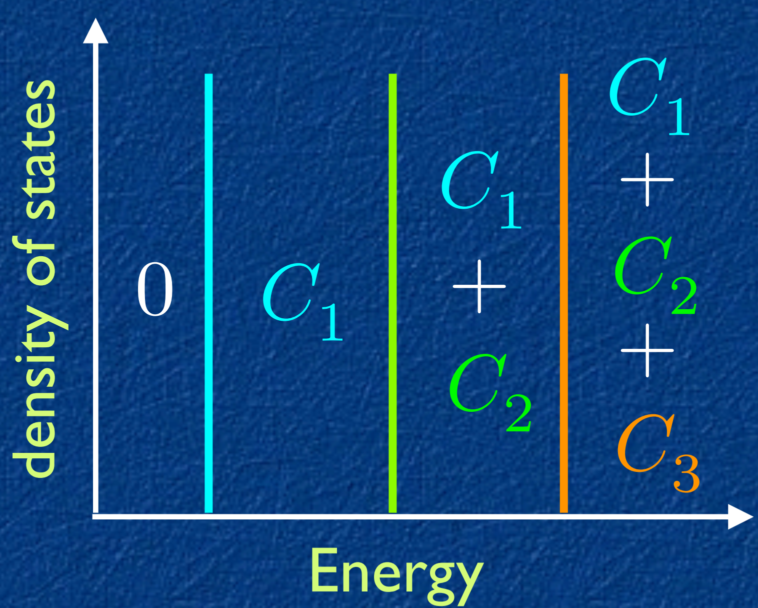
Quantum Hall Effect

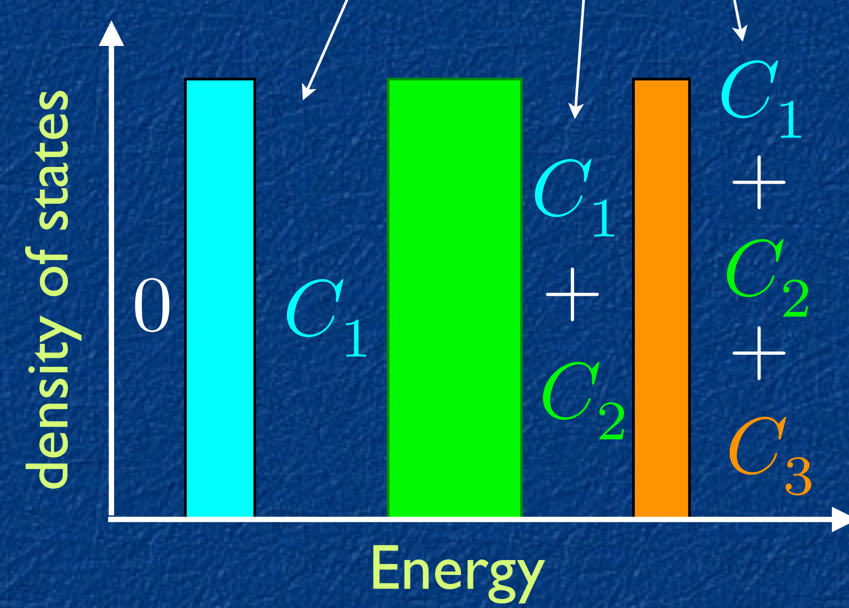
TKNN formula : $\sigma_{xy} = \frac{e^2}{h} \sum_{\text{filled bands}} C_i$

integer "Chern number"

D. J. Thouless *et al.*, *PRL* **49**, 405 (1982)

edge state transport inside energy gaps





$B \ll B_0$: sharp Landau levels

$B \gtrsim B_0$: Landau subbands

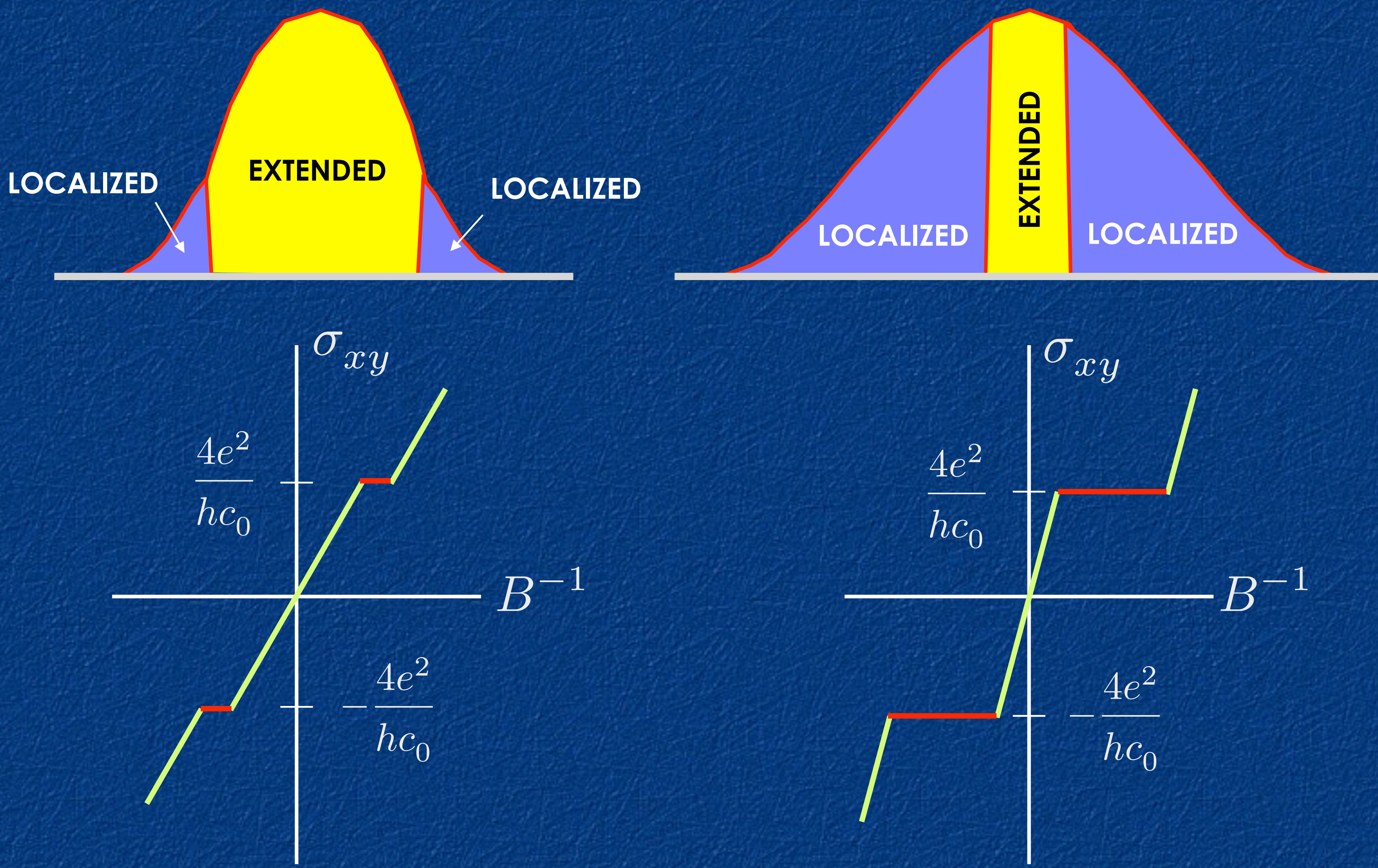
$$B_0 \simeq \frac{hc/e}{\Omega}$$

Dirac flux quantum $\phi_0 = 4.13 \times 10^5 \, \mathrm{T\,Å}^2$

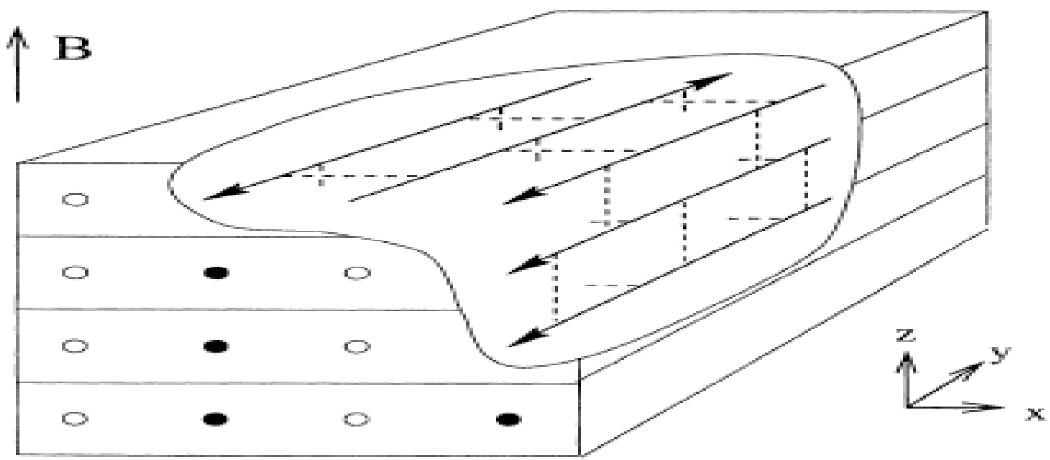
unit cell area

Qualitative effect of disorder (cartoon)

J. T. Chalker and A. Dohmen, *PRL* **75**, 4496 (1995)

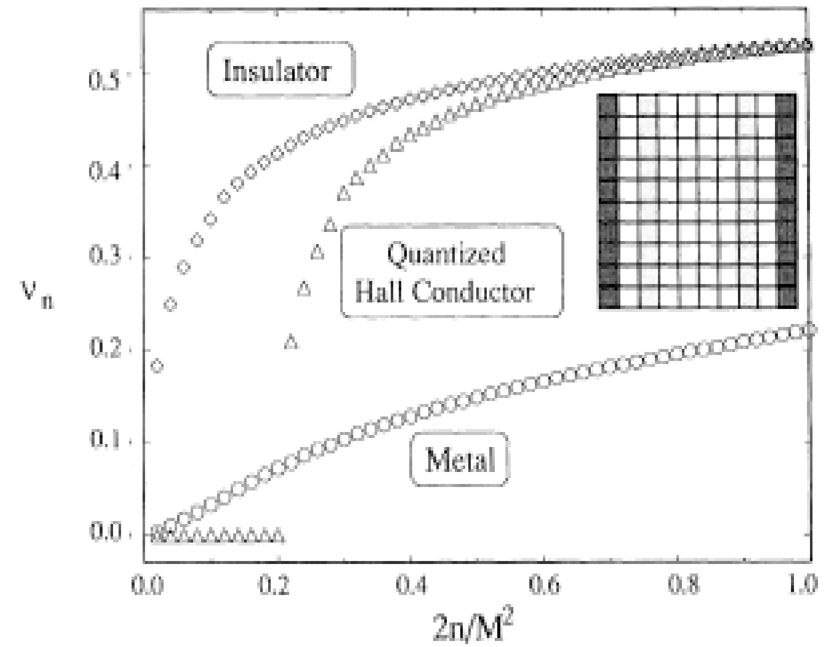


3D Quantum Percolation
Network Model

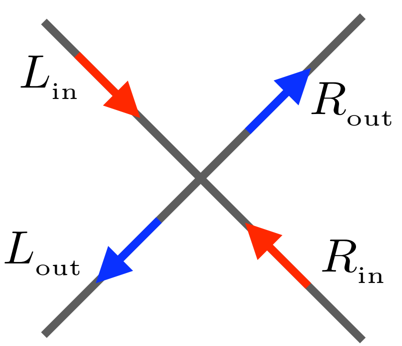


J. T. Chalker and A. Dohmen, *PRL* **75**, 4496 (1995)

positive Lyapunov exponents



quantum scattering at vertices described by transfer or S-matrix



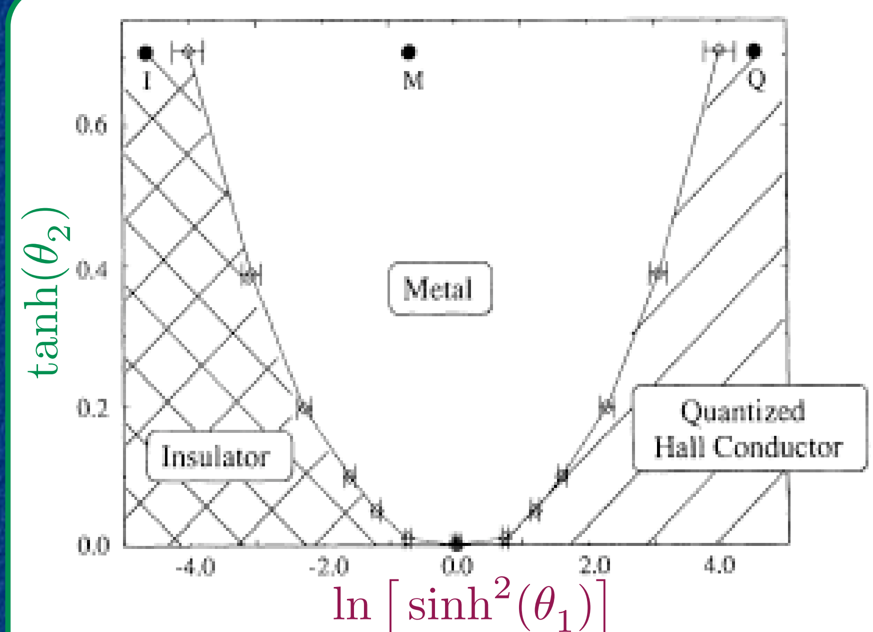
random phases accrued along links

$$\Psi'_{in} = \Psi_{out}\, e^{iA}$$

$$\begin{pmatrix} R_{in} \\ R_{out} \end{pmatrix} = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix} \begin{pmatrix} L_{in} \\ L_{out} \end{pmatrix}$$

interlayer : θ_1

intralayer : θ_2



Surface State Properties

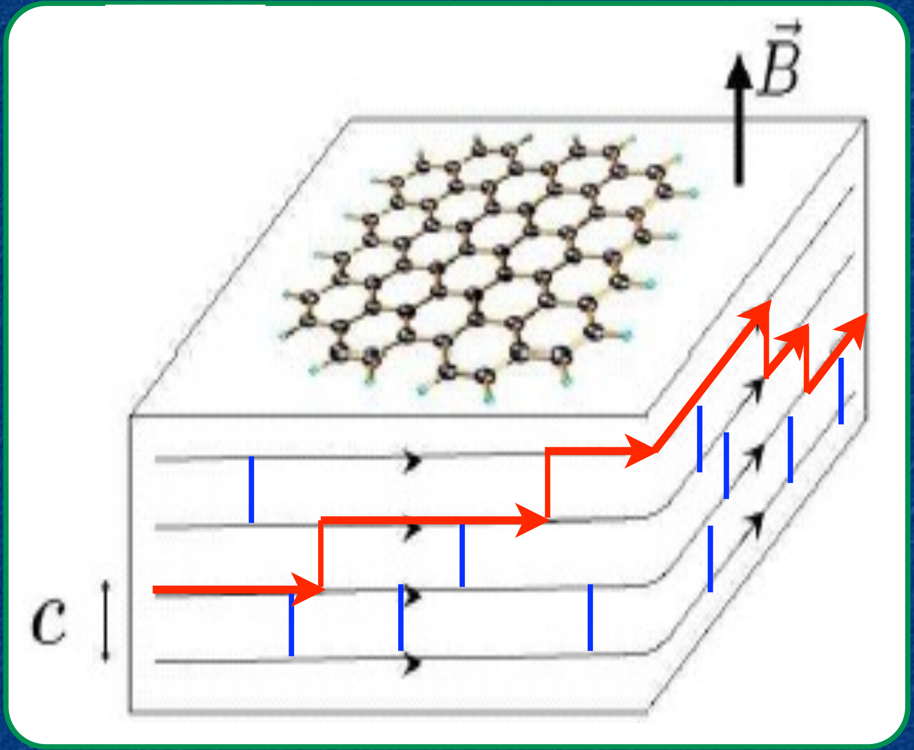
L. Balents and M. P. A. Fisher, PRL 76, 1996

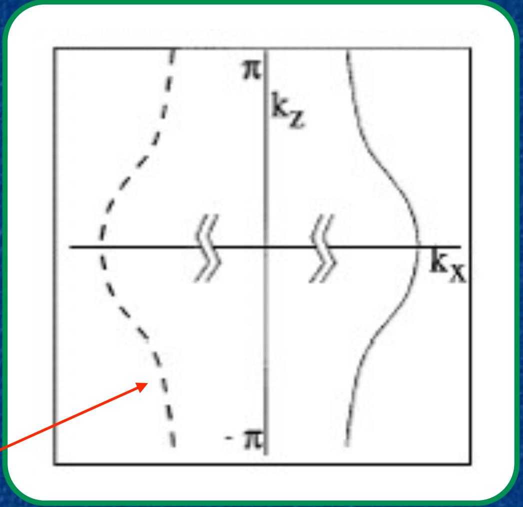
Integer 3DQHE chiral surface states are **always diffusive** in **z**-direction

$$\langle |G(k_x, k_z, \omega)|^2 \rangle \approx \frac{1}{i\omega - ivk_x - Dk_z^2}$$

Different scaling than for non-chiral Fermi liquid leads to a stable metallic phase with surface disorder.

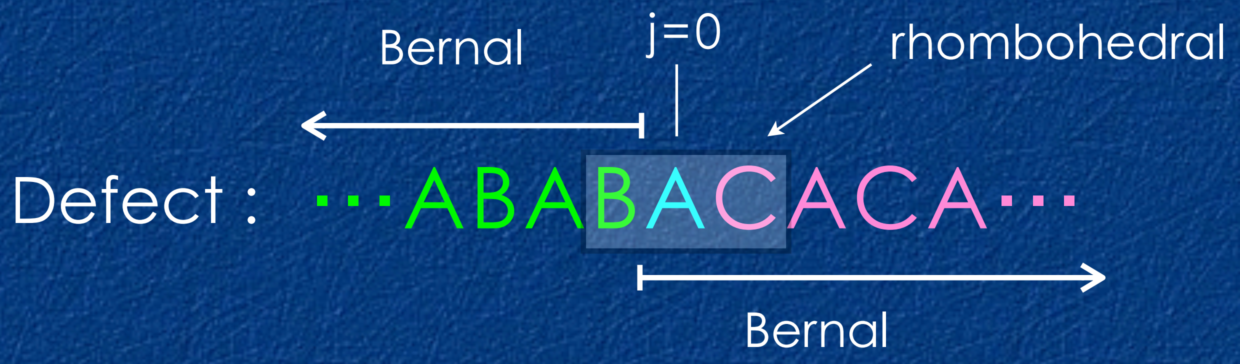
Strong bulk disorder “floats up” 3DQHE.





missing!

Simple model of a graphite stacking fault



A stacking pattern can be written as a sequence of **+** and **–** symbols :

$$\cdots A + B - A + B - A - C + A - C + A \cdots$$

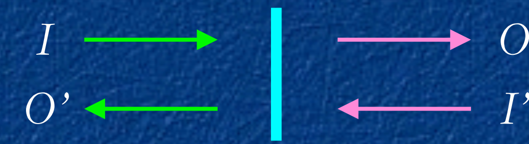
$$\psi_j(\boldsymbol{k}) = \begin{pmatrix} U_j(\boldsymbol{k}) \\ V_j(\boldsymbol{k}) \end{pmatrix} \quad ; \quad M\psi_j - \gamma_1 {}^t\Sigma^{\sigma_{j-\frac{1}{2}}}\psi_{j-1} - \gamma_1 \Sigma^{\sigma_{j+\frac{1}{2}}}\psi_{j+1} = 0$$

$$M = \begin{pmatrix} E & \gamma_0 S_{\boldsymbol{k}} \\ \gamma_0 S^*_{\boldsymbol{k}} & E \end{pmatrix} \quad ; \quad \Sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad ; \quad \Sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Here *E* is the bulk dispersion in any of the four graphite bands.

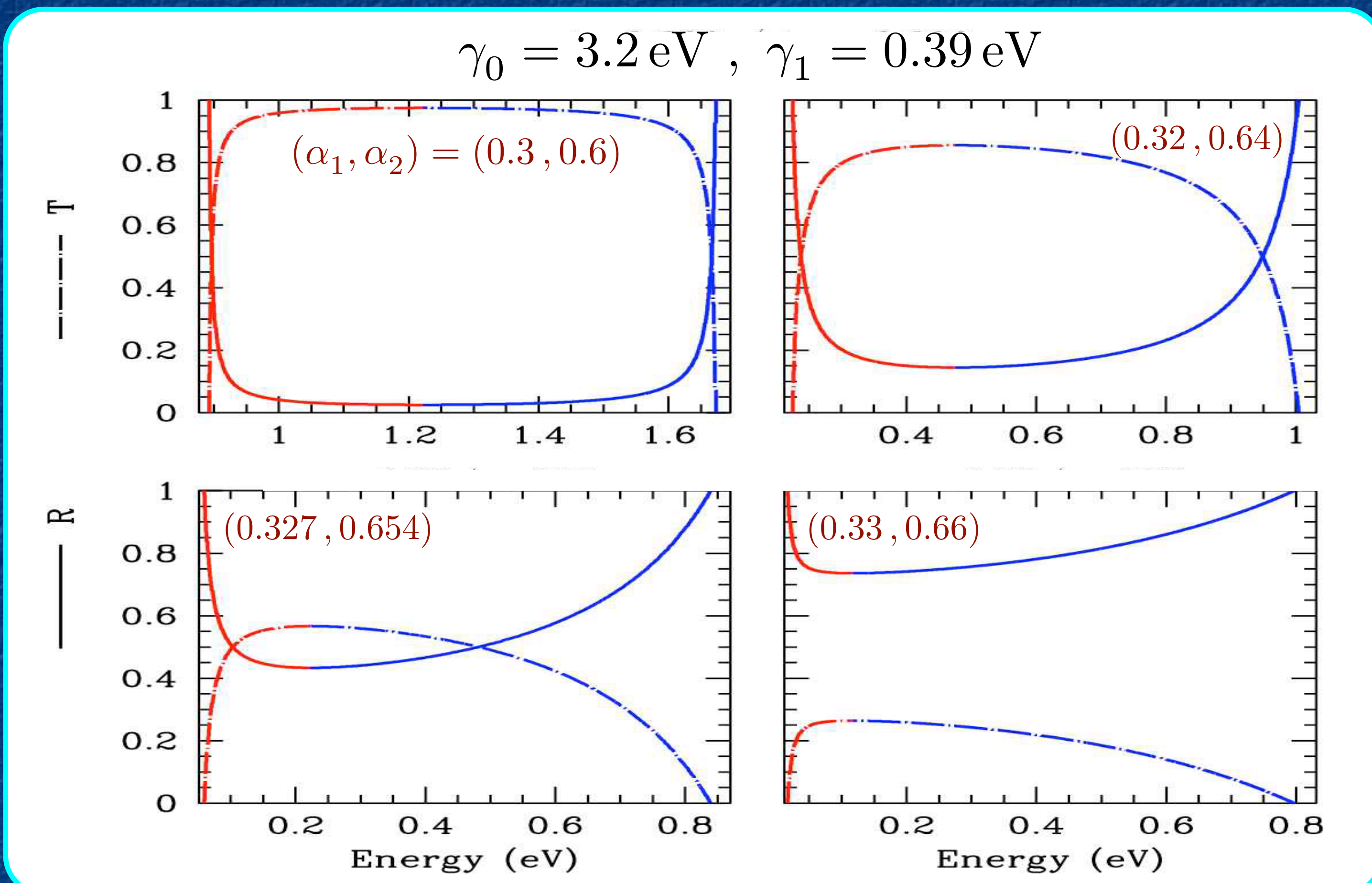
Stacking fault : *S*-matrix

defect : ⋯ABABACACA⋯

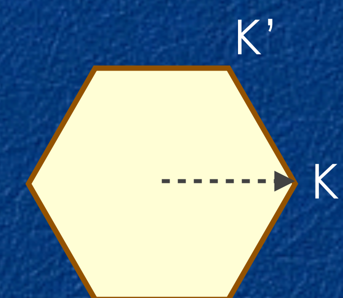


$$\begin{pmatrix} O \\ O' \end{pmatrix} = \overbrace{\begin{pmatrix} t & r' \\ r & t' \end{pmatrix}}^{S-\mathrm{matrix}} \begin{pmatrix} I \\ I' \end{pmatrix}$$

$$R = |r|^2 = \frac{\gamma_1^2}{\gamma_1^2 + 4\,\gamma_0^2\,|S_{\boldsymbol{k}}|^2 \sin^2(\theta_3/2)}$$



$$S_{\boldsymbol{k}} = \sum_{\boldsymbol{\delta}} e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}}$$



$$\boldsymbol{k} = \alpha_1\,\boldsymbol{b}_1 + \alpha_2\,\boldsymbol{b}_2$$

Stacking fault : sublattice configuration

j	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6
layer	A	B	A	B	A	B	A	C	A	C	A	C	A
A		$\tilde{v}$		$\tilde{v}$		$\tilde{v}$		$\tilde{u}$		$\tilde{u}$		$\tilde{u}$	
B	u		u		u		u	$\tilde{v}$	u	$\tilde{v}$	u	$\tilde{v}$	u
C	v	$\tilde{u}$	v	$\tilde{u}$	v	$\tilde{u}$	v		v		v		v

RHOMBOHEDRAL

BERNAL HEXAGONAL

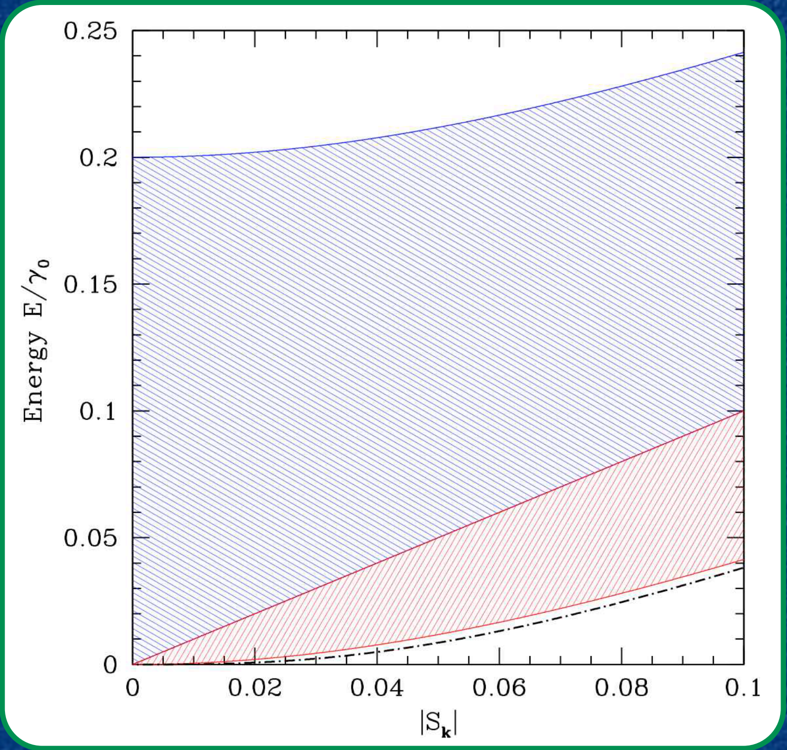
BERNAL HEXAGONAL

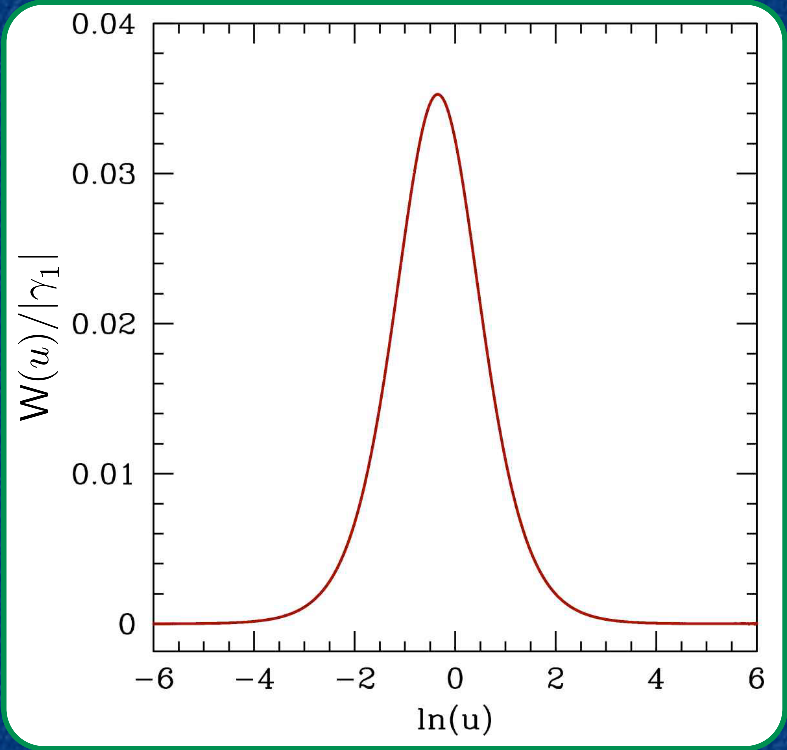
Stacking fault : bound states $\psi_j(\boldsymbol{k}) \propto e^{-\kappa|j|}$

dispersion: $$E_\mathrm{B} = |\gamma_1| \left(u + \frac{1}{2u} - \sqrt{1+u^2} \right) = \frac{\gamma_0^3\,|S_{\boldsymbol{k}}|^3}{\gamma_1^2} + \mathcal{O}(u^{-5})$$

$$u \equiv \sinh(\kappa) = |\gamma_1|/2\gamma_0\,|S_{\boldsymbol{k}}| \qquad \propto |\boldsymbol{k}|^3$$

binding energy: $$\frac{\mathrm{W}(u)}{|\gamma_1|} = \frac{1}{2u}\left(\sqrt{1+4u^2} - 1\right) + \sqrt{1+u^2} - 1 - u$$





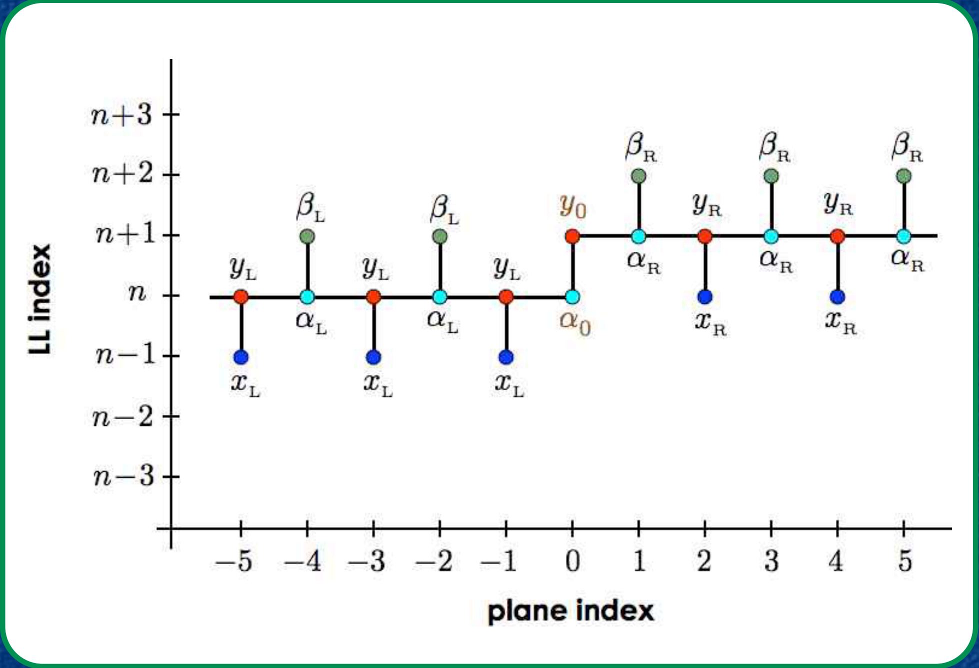
Stacking fault : Landau levels

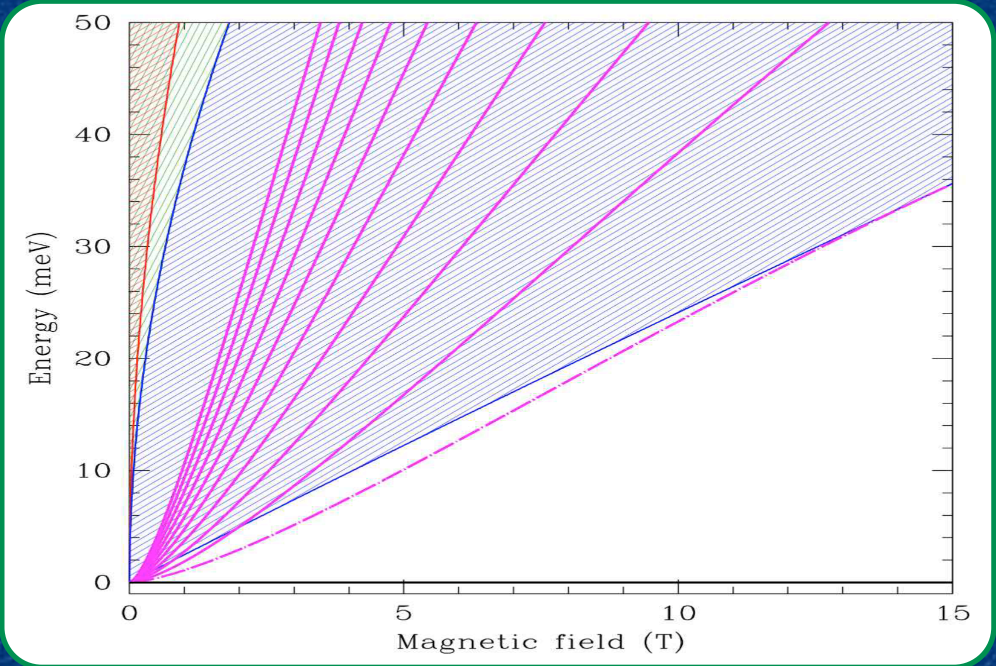
Condition for bound state: $\det \mathcal{M}(E) = 0$

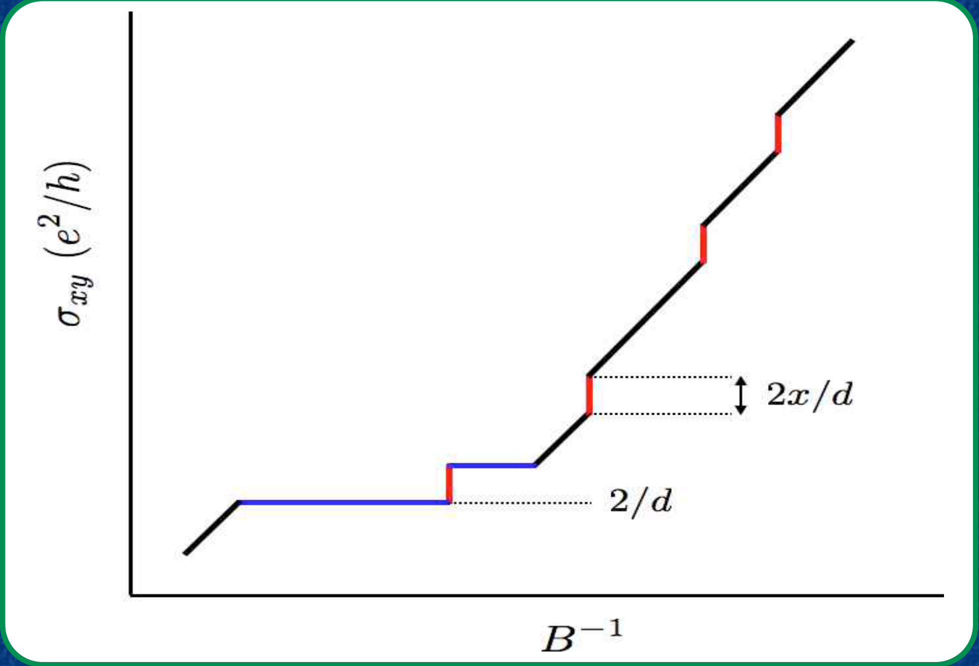
$$\det \mathcal{M}(E) \approx \gamma_1^2 - (n+1)^2(n+2)\,\frac{\epsilon^6\,\gamma_0^6}{\gamma_1^2\,E^2}$$

$$E_{\rm B} = \pm(n+1)(n+2)^{1/2}\,\frac{\epsilon^3\,\gamma_0^3}{\gamma_1^2}$$

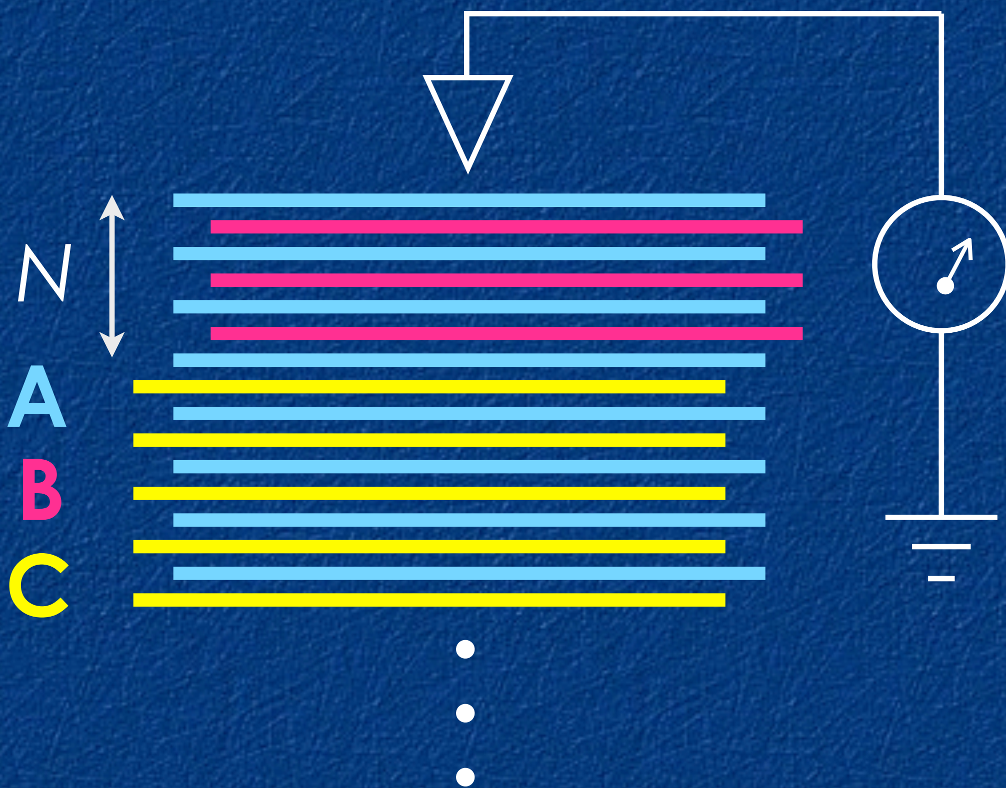
The energy of the bound state Landau level behaves as $\boldsymbol{B^{3/2}}$ rather than $\boldsymbol{B^{1/2}}$

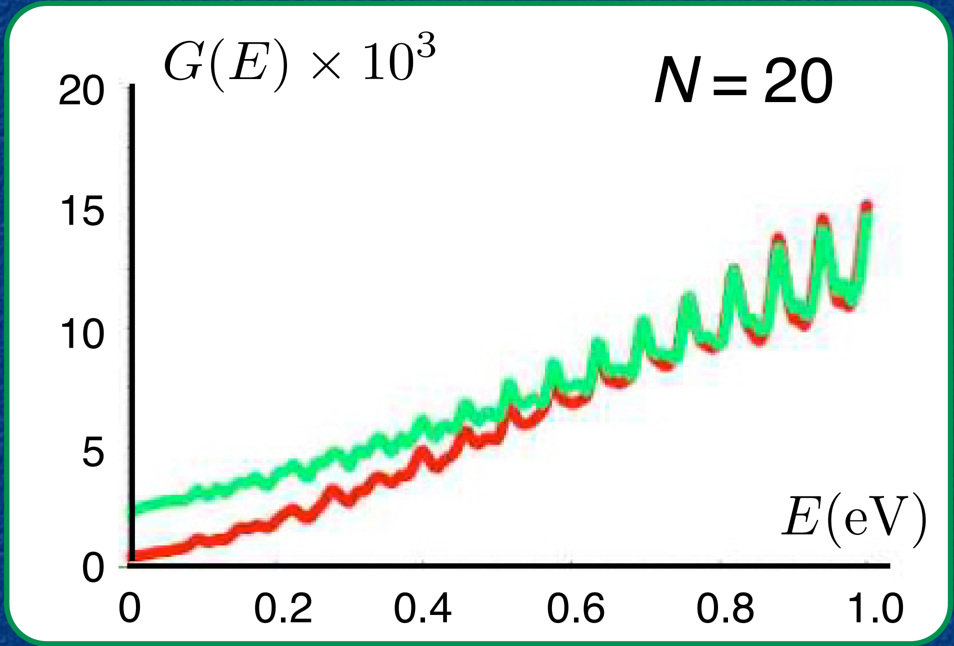


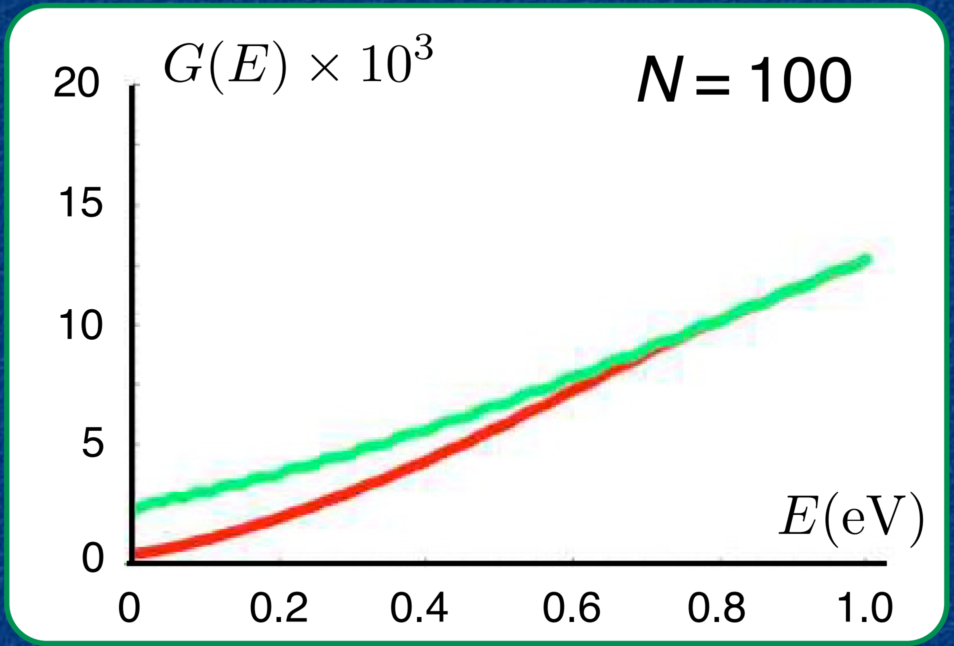




Surface spectroscopy of buried faults







Compute $G_{uu}^{l=1}(\omega)$ and $G_{vv}^{l=1}(\omega)$

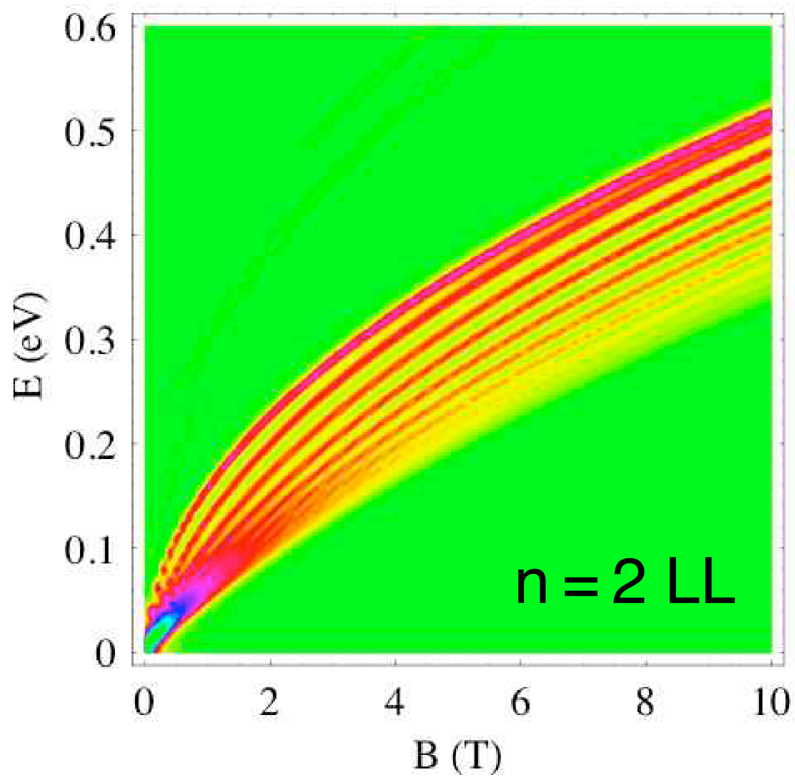
using hierarchy for $\Sigma_l(\omega)$

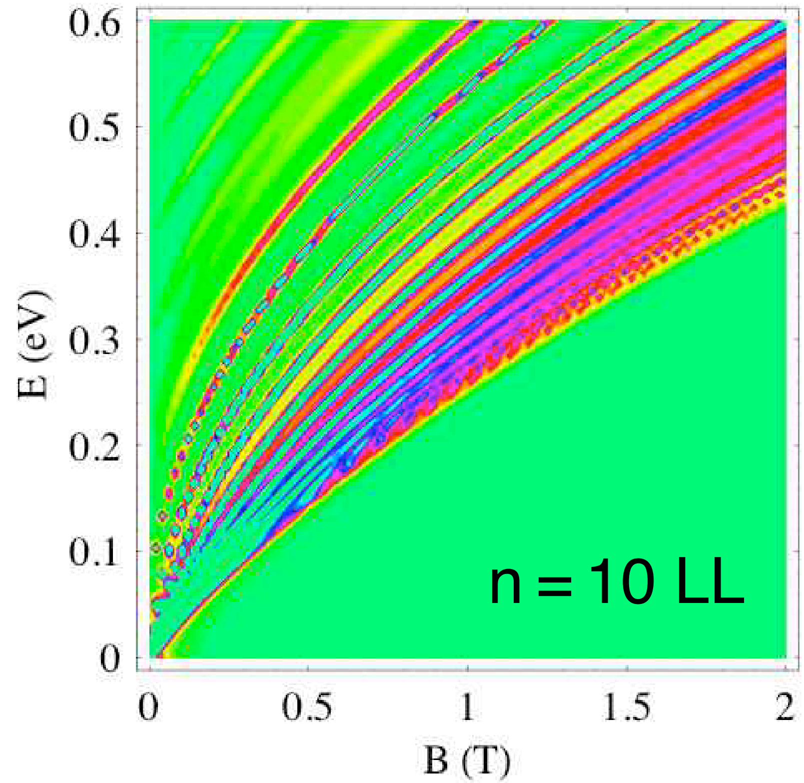
$$\Sigma_{l-1}(\omega) = \frac{|\gamma_0\, S_{\boldsymbol{k}}|^2}{\omega} + \frac{\gamma_1^2}{\omega - \Sigma_l(\omega)}$$

Surface spectroscopy in a field

Landau level index shifts in consecutive layers :

$$\Sigma_l(\omega) = \frac{n\, v_{\rm F}^2\, \ell_B^{-2}}{\omega} + \frac{\gamma_1^2}{\omega - \Sigma_{l+1}(\omega)} \quad , \quad \Sigma_{l-1}(\omega) = \frac{(n-1)\, v_{\rm F}^2\, \ell_B^{-2}}{\omega} + \frac{\gamma_1^2}{\omega - \Sigma_l(\omega)}$$





Full SWMc treatment of a stacking fault

- scattering states (no band overlap) :

$$n < 0 \;:\quad \psi_n = \mathcal{I}\, e^{ikn}\, \chi_1 + \mathcal{O}'\, e^{-ikn}\, \chi_5 + A_2\, z_2^n\, \chi_3 + A_3^n\, z_3^n\, \chi_3 + A_4\, z_4^n\, \chi_4$$

$$n > 0 \;:\quad \phi_n = \mathcal{I}'\, e^{-ikn}\, \chi_1^* + \mathcal{O}\, e^{ikn}\, \chi_5^* + A_6\, z_6^{*\,n}\, \chi_6^* + A_7\, z_7^{*\,n}\, \chi_7^* + A_8\, z_8^{*\,n}\, \chi_8^*$$

- bound states :

$$n < 0 \;:\quad \psi_n = A_1\, z_1^n\, \chi_1 + A_2\, z_2^n\, \chi_2 + A_3^n\, z_3\, \chi_3 + A_4\, z_4^n\, \chi_4$$

$$n > 0 \;:\quad \phi_n = A_5\, z_5^{*\,n}\, \chi_5^* + A_6\, z_6^{*\,n}\, \chi_6^* + A_7\, z_7^{*\,n}\, \chi_7^* + A_8\, z_8^{*\,n}\, \chi_8^*$$

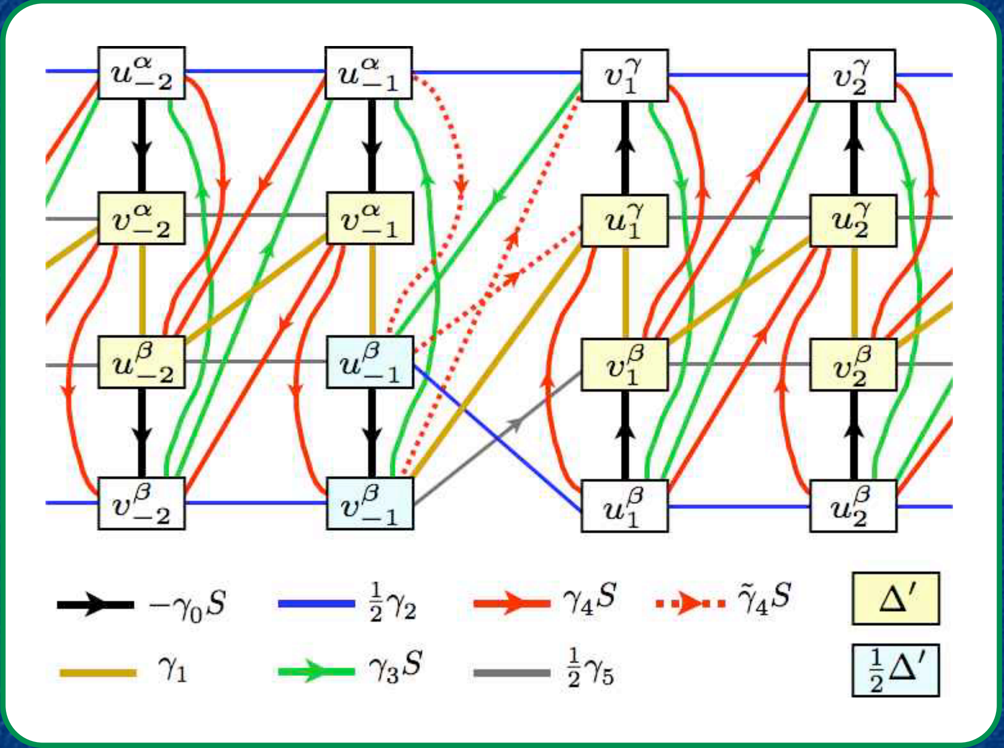
$$\big|z_{1,2,3,4}\big| > 1 \quad , \quad \big|z_{5,6,7,8}\big| < 1 \quad , \quad z_k^* = z_{k+4}^{-1}$$

- scattering equations :

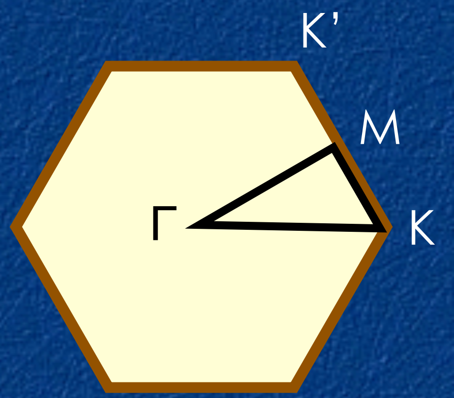
$$M\psi_{-2} + K\psi_{-1} + F^\dagger\phi_1 = 0$$

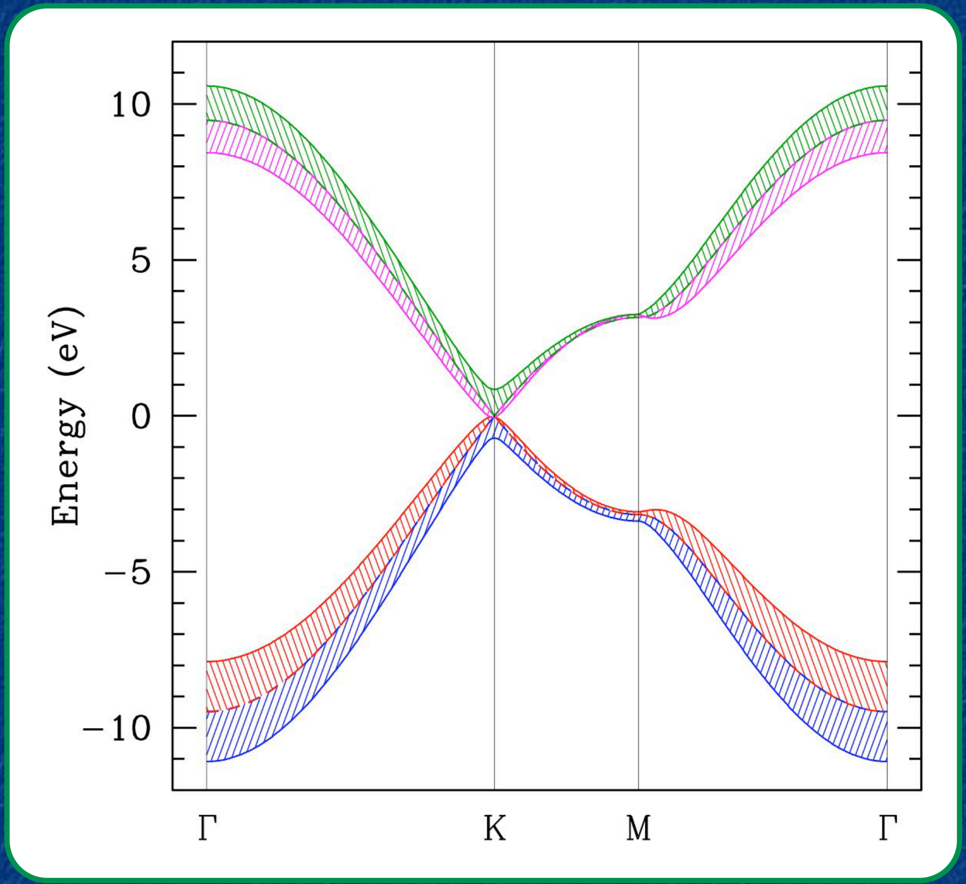
$$F\psi_{-1} + K^*\phi_1 + M^{\mathrm{t}}\phi_2 = 0$$

- solve these to obtain *S*-matrix and/or bound state energies

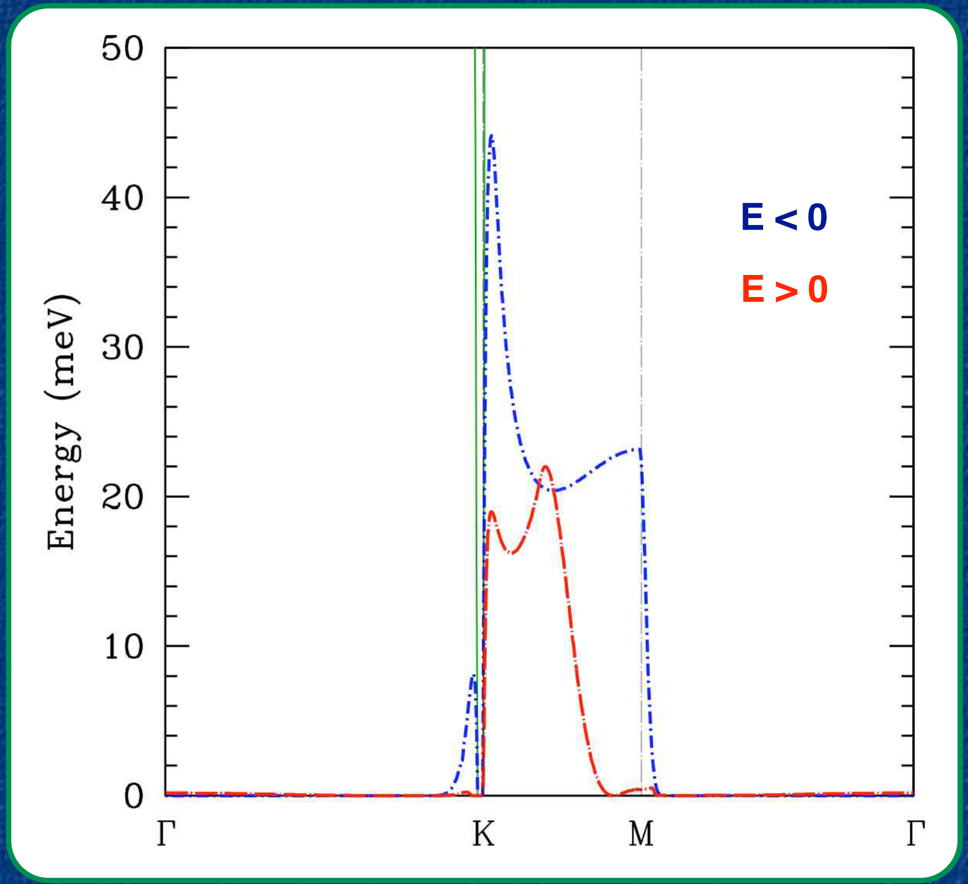


- Find bound states within gap along KM segment in basal Brillouin zone
- Maximum binding energy ~45 meV (compare 14 meV for γ_0-γ_1 model)
- SWMc parameterization suspect away from K-H segment (e.g. it fails to accurately reproduce full graphite π-band





SWMc bands for graphite



bound state binding energies

Brief outline

1. Stacking and graphitic structures

2. Bernal hexagonal vs. rhombohedral graphite

3. Landau levels, surface states, possible 3DQHE

4. Simple model of a stacking fault:
   S-matrix, bound states, Landau levels

5. Surface spectroscopy of buried faults

6. Full SWMc treatment of a stacking fault