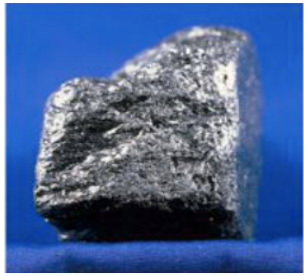
Carbon materials…

Karyn Le Hur, Yale University

Šiber, 2003.

Boulder 2008, Lecture III

History of carbon



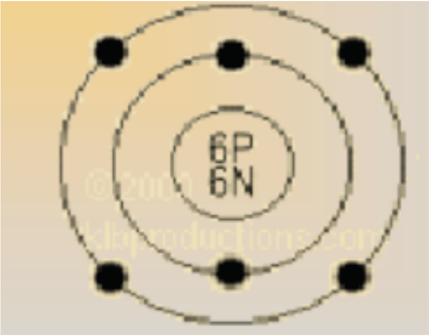
- Carbon is a prehistoric knowledge as diamond as well as graphite. Diamonds were known at least as early as 1200B.C (Hindu writings)

diamond derives from adamas ``The invincible'' in greek

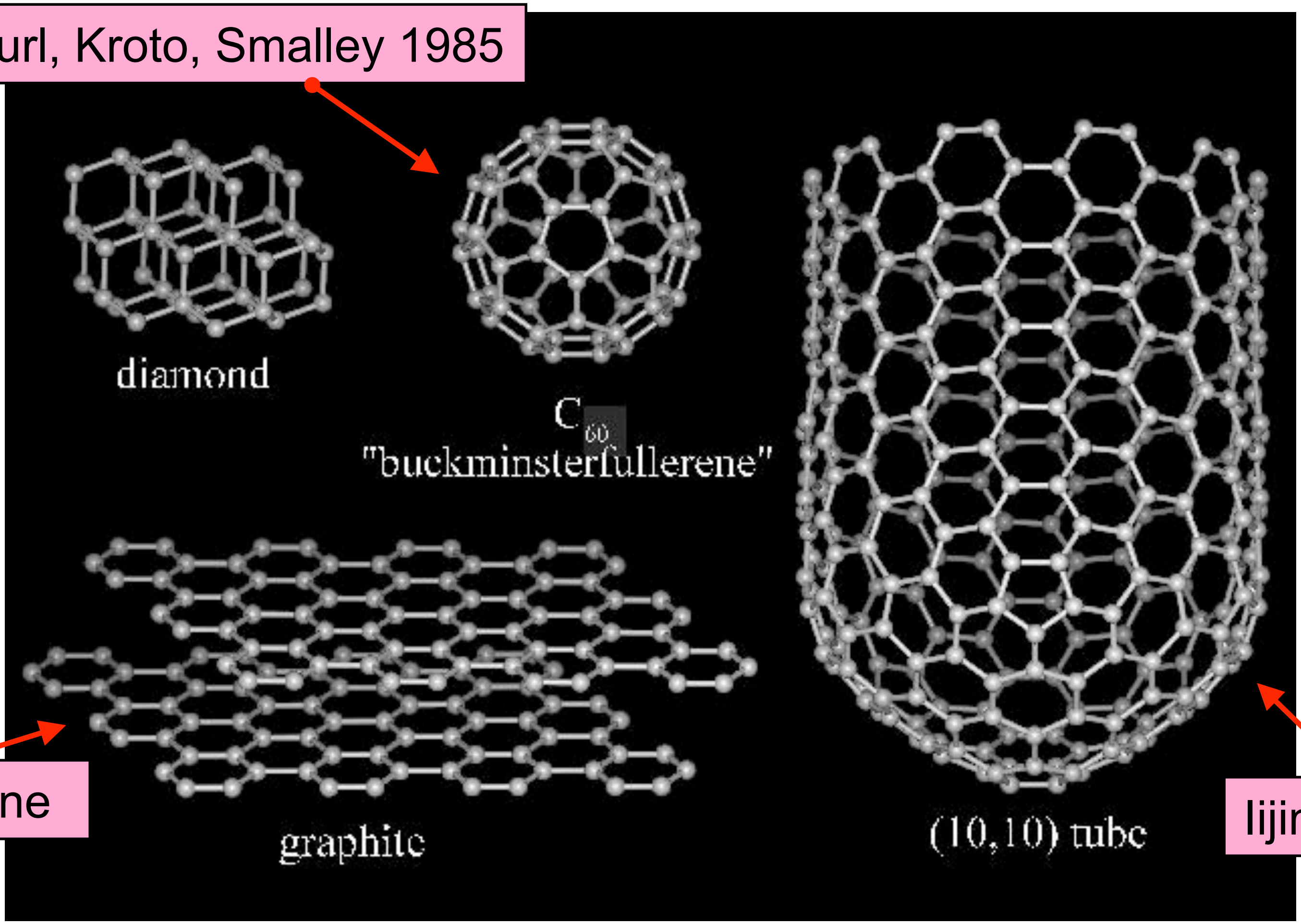
4th most abundant element in Nature…

$1s^2, \underline{2s^2, 2p^2}$

Very close in energy



Carbon: Various Forms in nature



Curl, Kroto, Smalley 1985

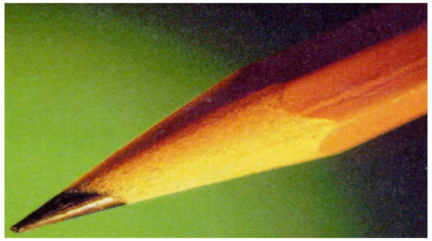
graphene

Iijima 1991

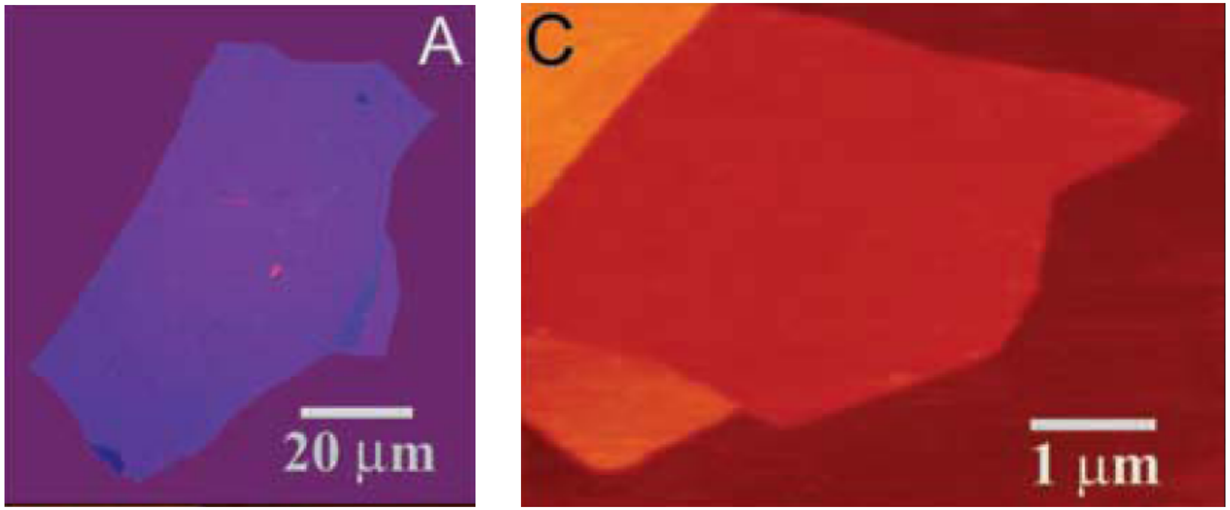
A. K. Geim & K. S. Novoselov, Nature Materials **6**, 183 (2007)
P. L. McEuen, Physics World **13**, 31 (2000)

ULTRATHIN graphitic films

Ultra-thin graphitic films: from flakes to micro-devices



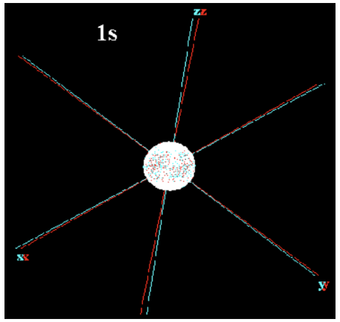
Novoselov *et al* -
Science 306, 666 (2004)

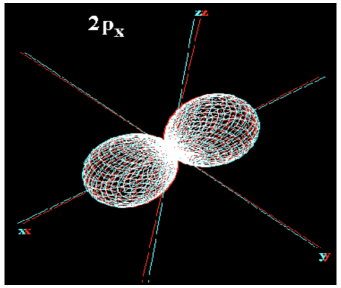


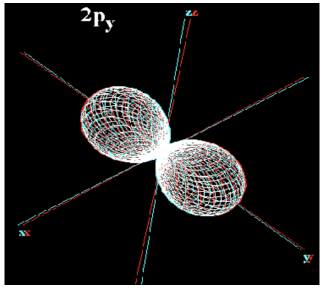
<u>Geim’s group at Manchester</u>
Novoselov *et al* - Nature 438, 197 (2005)
Novoselov *et al* - Nature Physics 2, 177 (2006)

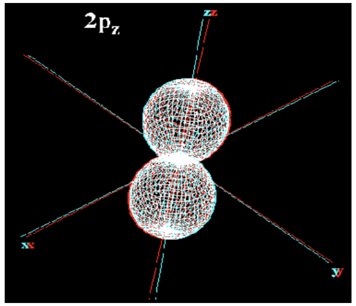
<u>Kim-Stormer group at Columbia University</u>
Zhang *et al* - PRL 94, 176803 (2005)
Zhang *et al* - Nature 438, 201

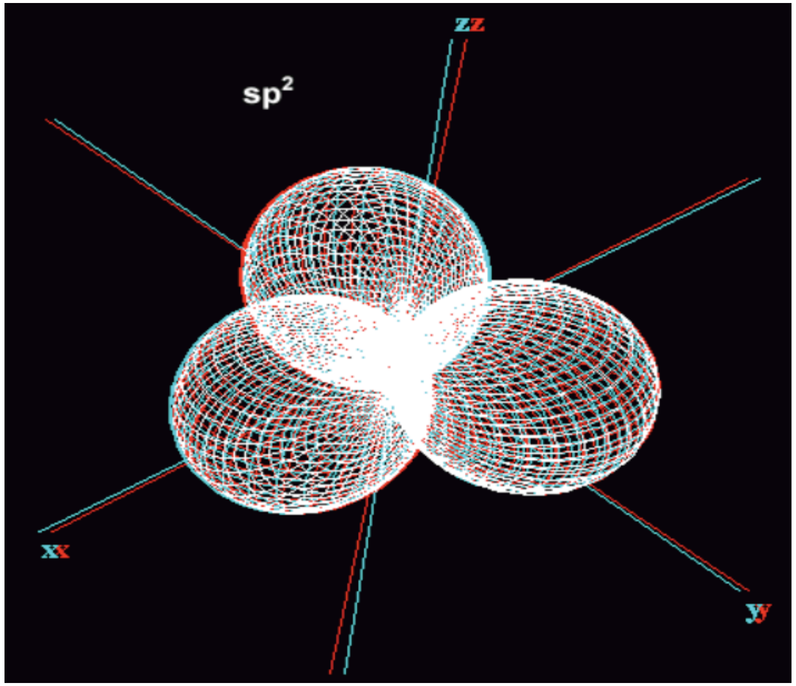
sp2 hybridization in graphene





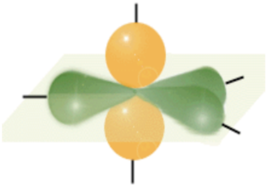






Within graphite, 2s and 2p orbitals undergo a sp2 hybridization

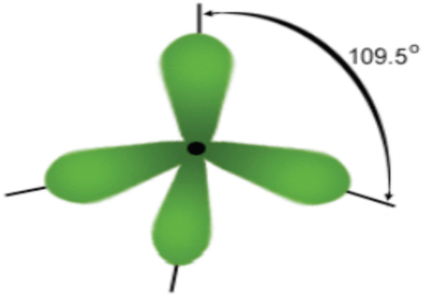
The geometry of the hybridized orbital is trigonal planar:
3 nearest neighbors



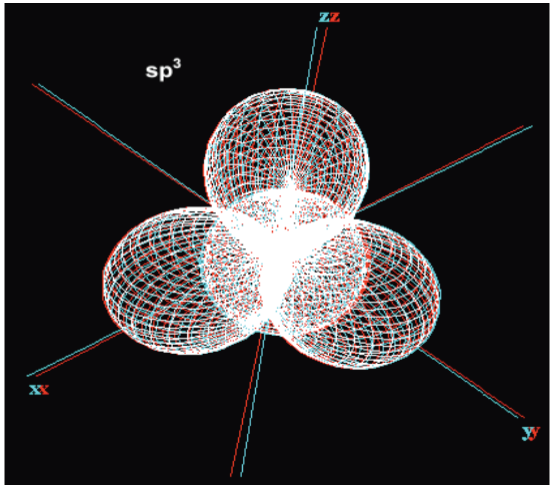
The last p-orbital forms the π-orbital

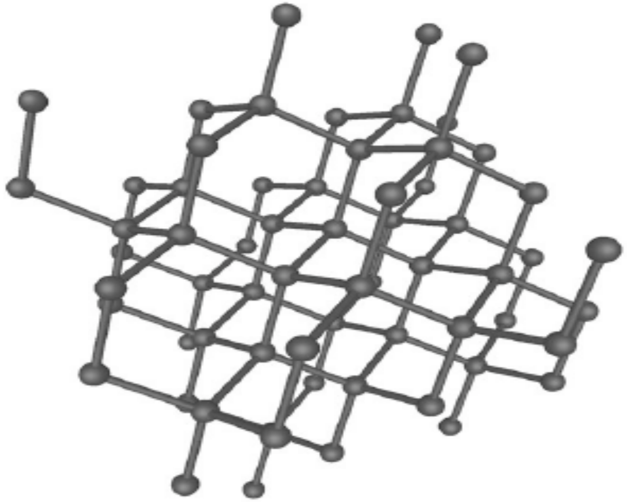
Diamond is different…

- Within diamond, 1s2 and the 3p orbitals undergo a sp3 hybridization



- Tetrahedral symmetry





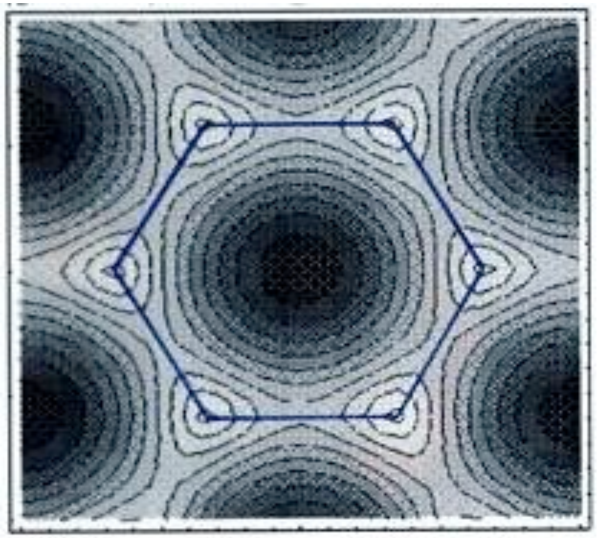
Slater and Koster (1954), Hall (1958)

Band Structure of Graphene I

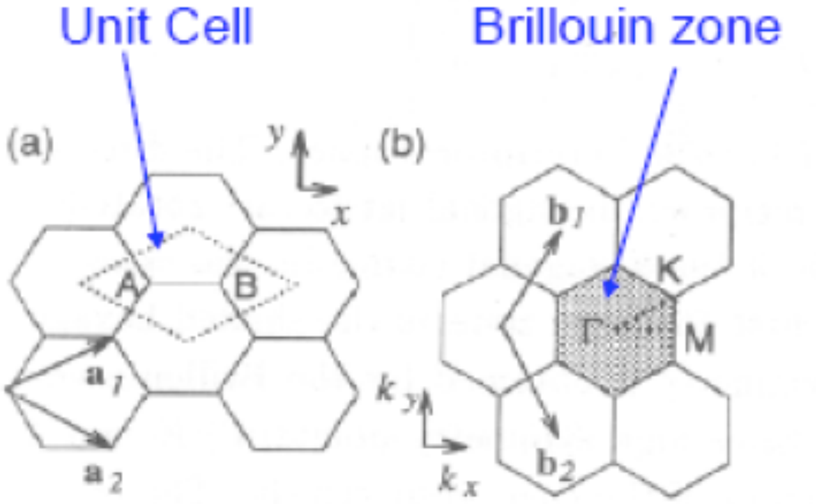
- Tight-binding model on hexagonal lattice

t~2.8eV
$a_{C\text{-}C}$~1.42Å

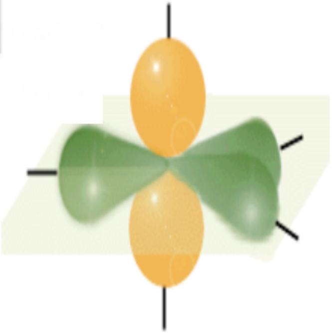
-two atoms in unit cell



Wallace, 1947

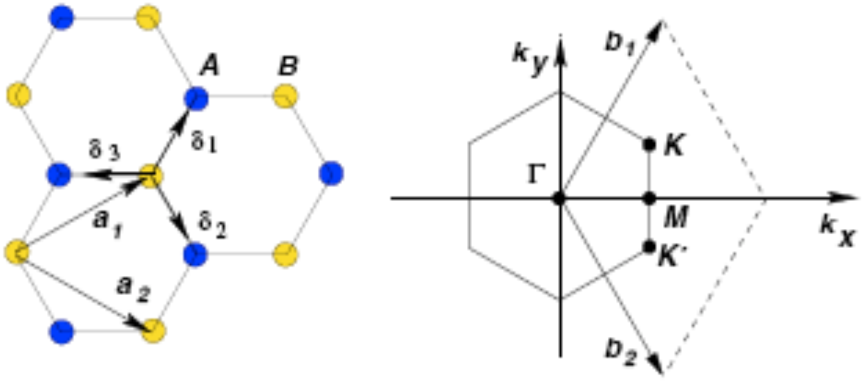


-hexagonal Brillouin zone



Details

A.H. Castro Neto et al (RMP)



$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(a^{\dagger}_{\sigma,i} b_{\sigma,j} + \text{h.c.} \right) - t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} \left(a^{\dagger}_{\sigma,i} a_{\sigma,j} + b^{\dagger}_{\sigma,i} b_{\sigma,j} + \text{h.c.} \right)$$

$$E_{\pm}(\mathbf{k}) = \pm t\sqrt{3 + f(\mathbf{k})} - t' f(\mathbf{k}) ,$$

$$f(\mathbf{k}) = 2\cos\left(\sqrt{3}k_y a\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_x a\right) ,$$

$E_{\pm}(\mathbf{q}) \approx \pm v_F|\mathbf{q}| + \mathcal{O}((q/K)^2)$ for k=K+q

ab-initio calculations

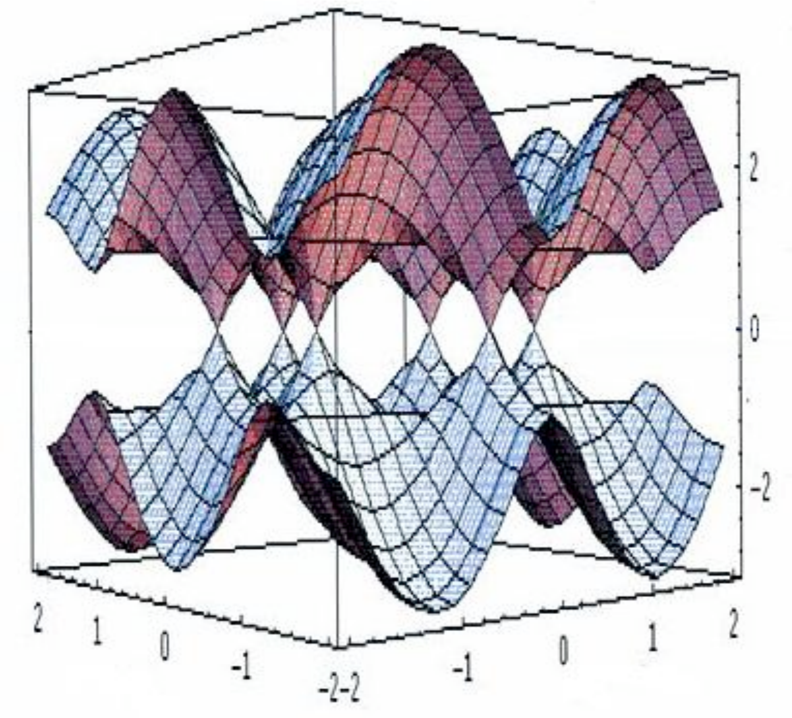
$$0.02t \leq t' \leq 0.2t$$

Dirac fermions close to K and K' points

Band Structure of Graphene II

$v_F \sim 3ta/2 \sim 10^6 m/s = c/300$

Π* band



Π band

- [Tight-binding model]

  Valence and conduction bands touch at E=0
  At half-filling Fermi energy is zero
  (particle-hole symmetry): no Fermi surface,
  six isolated points, only two inequivalent

- [Near Fermi points]

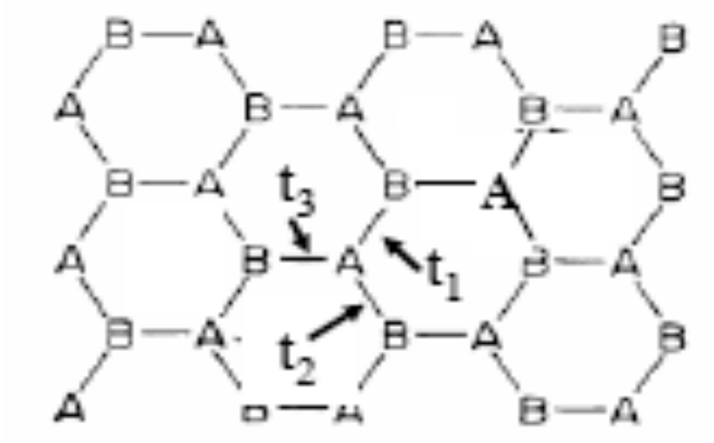
  Relativistic dispersion relation
  (neglect corrections in q^2)

- Graphene: zero gap semiconductor

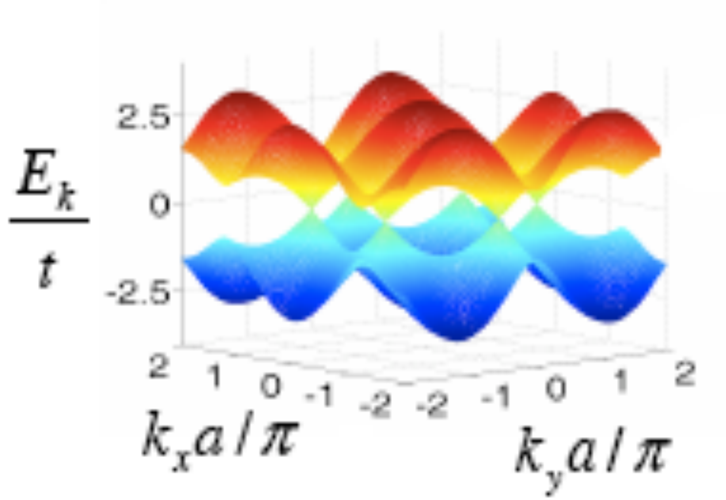
Band Structure of Graphene III

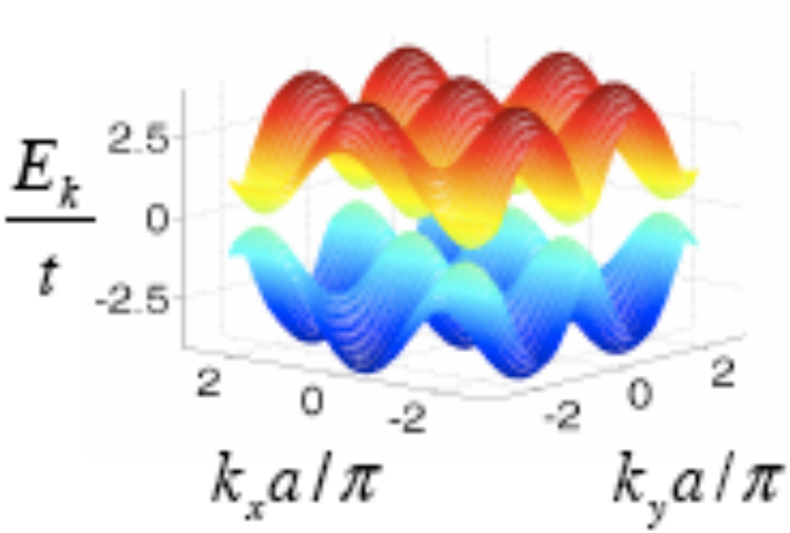
Robustness of Dirac points…

$$t_1 = t_2 = t \text{ and } t_3 = \beta t$$

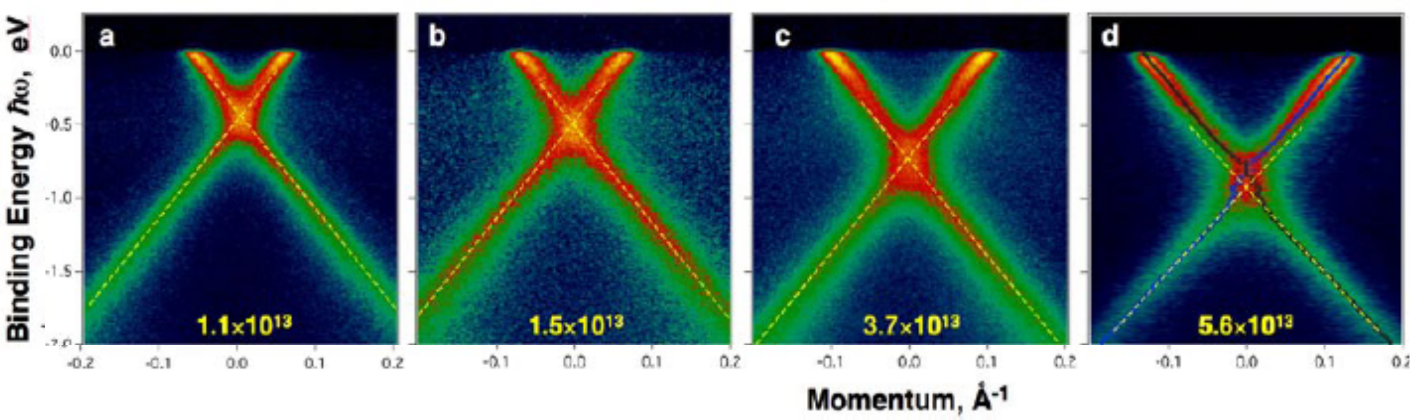


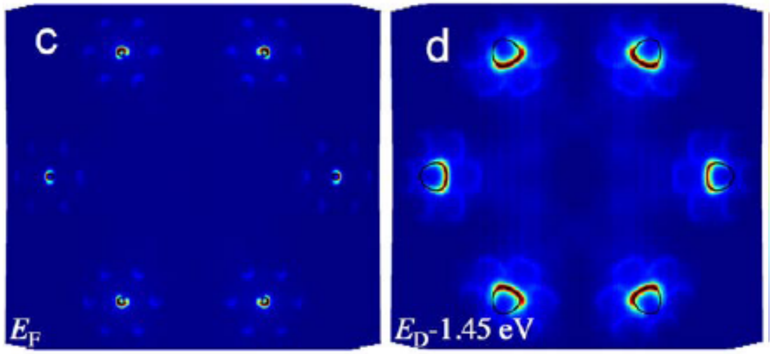
Presence of Dirac points: β<2





ARPES measurements





ARPES: heavily doped graphene synthesized on silicon carbide

A. Bostwick *et al* – Nature Physics, 3, 36 (2007)

Relativistic description in 2D

Review: A.H. Castro Neto et al. cond-mat/0709.1163 (RMP)

2 inequivalent valleys: the quasiparticles in each valley are described by a Dirac type Hamiltonian

$$-iv_F\boldsymbol{\sigma}\cdot\nabla\psi(\mathbf{r})=E\psi(\mathbf{r})$$

The isospin σ acts on each branch (sublattice)

Quantum mechanical operator for helicity

$$\hat{h}=\frac{1}{2}\boldsymbol{\sigma}\cdot\frac{\mathbf{p}}{|\mathbf{p}|}$$

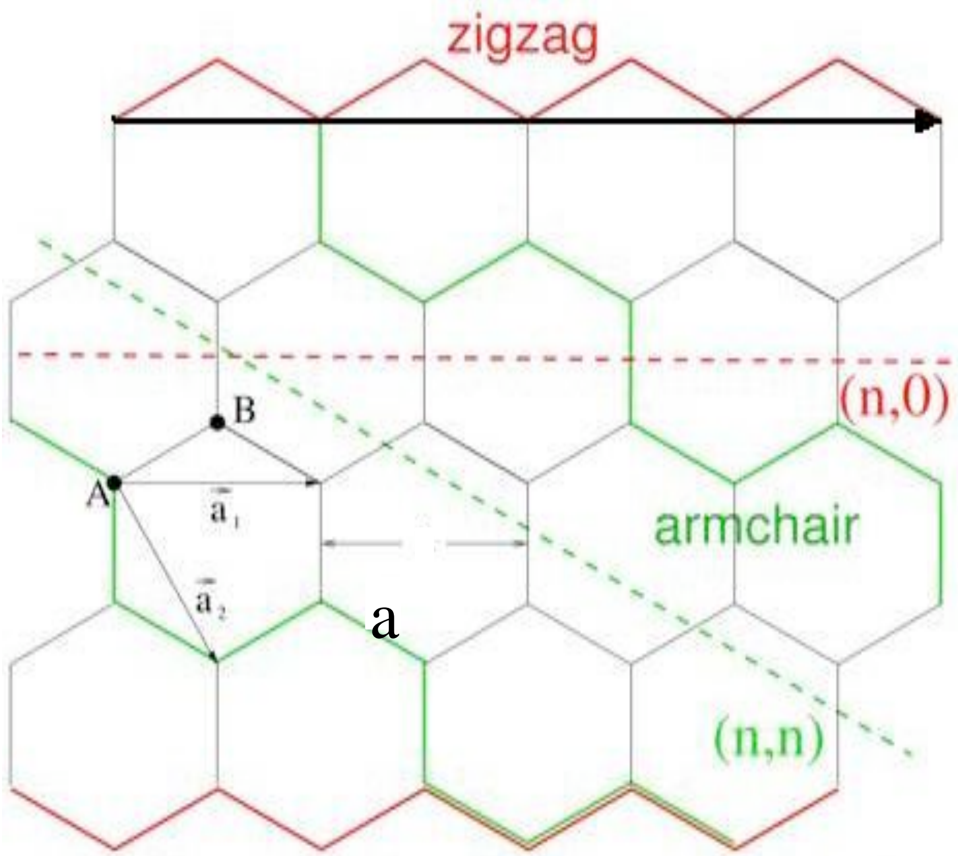
Cyclotron mass

$$m^*=\frac{\sqrt{\pi}}{v_F}\sqrt{n}$$

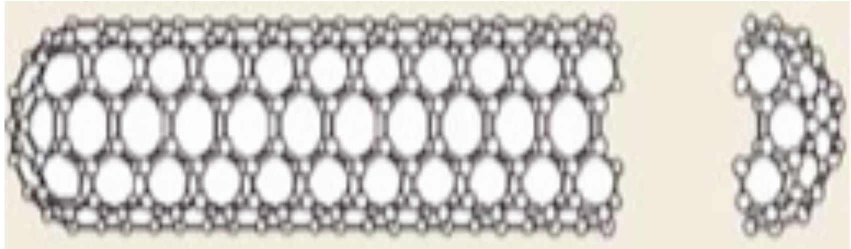
Deacon et al PRB 76, 081406 (2007)
Jing et al, PRL 98, 197403 (2007),…

Nanotubes

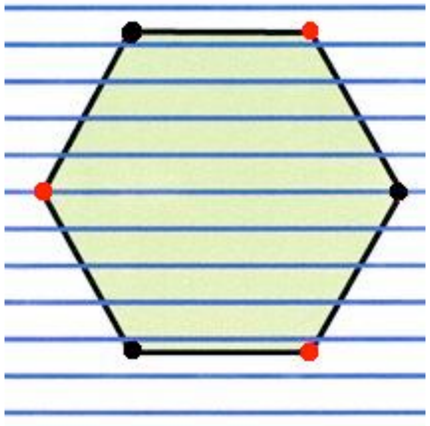
http://www.lassp.cornell.edu/lassp_data/mceuen/homepage/welcome.html



- necessary condition: (2n+m)/3 = integer



(n,n) armchair tube



1/3 of the tubes are metallic

Density of States

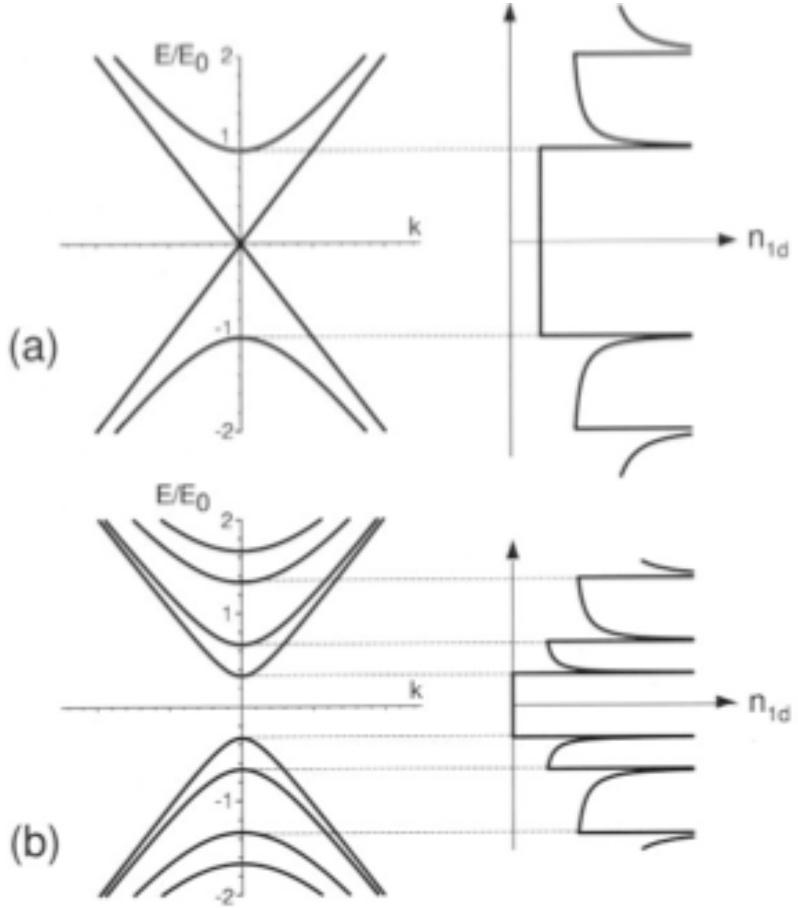
- Metallic tubes (SWMNTs):
  - constant DOS around E=0
  - van Hove singularities when opening new bands

- Semiconducting tubes:

  Gap around E=0

Energy scale ~ 1eV

Effective theory valid at room T



Outline

- SWMNT ideal one-dimensional conductor with two bands in its excitation spectrum: Luttinger physics at room temperature

Two bands should bring new physics?
Exotic Superconductivity?

- Graphene:

Klein Paradox
Interactions, Disorder, Transport
Bilayer graphene
Topological Insulator and zero energy modes
Dirac fermions in 3 dimensions…

Conductance of ballistic SWMNTs

Landauer formula: for good contacts to reservoirs conductance is

$$G = N_{bands} \frac{2e^2}{h} = \frac{4e^2}{h}$$

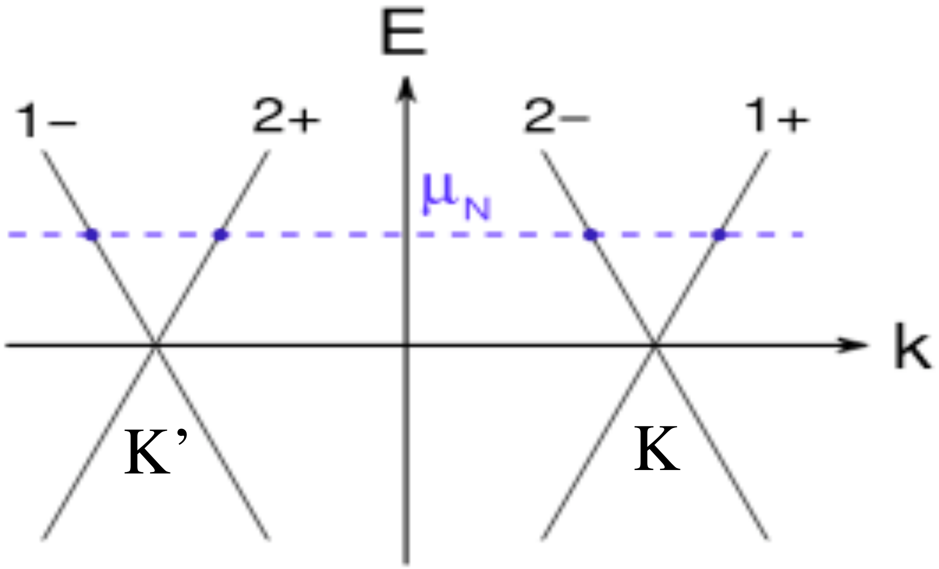
Stanford group: PRL 87, 106801 (2001)

Long mean free path (≥1μm), no Peierls instability, SWMNT conducting at very low Temperatures ⇒ Ideal system to study Interactions

Interactions ?

Two band spectrum

Analogy to Hubbard ladder!



Notations: $\psi_{ir\alpha}$

i = band index

r = chirality

α = spin

Two Fermi points K and K'

Two sublattices A & B combine to give 2 bands:

Band 1, symmetric combination & Band 2, anti-symmetric combination

Effect of Interactions in the SWMNT

Kane, Balents, Fisher, 1997

Low-energy theory: 4 modes (3 neutral & total charge mode)

$$H_{int} = e^2 \ln(R_s/R) \int dx\, \rho_{tot}^2(x)$$

R is the tube radius & R_s is the screening length

The total charge mode is described by a Luttinger theory & the Luttinger parameter is given by:

$$g = (1+ (8e^2/(v_F \pi \hbar))\ln(R_s/R))^{-1/2}$$

Long-range Coulomb forces result in $g << 1$

Tunneling DOS

Review: R. Egger, P. McEuen, et al. cond-mat/0008008

Suppression of tunneling DoS:

$$\boxed{\rho(x,E) \propto E^{\alpha}}$$

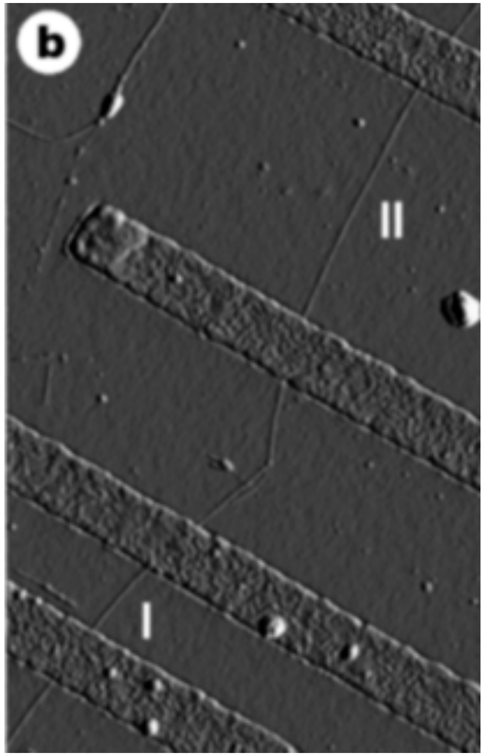
geometry dependent exponent: $\alpha_{bulk} = (g + 1/g - 2)/8$

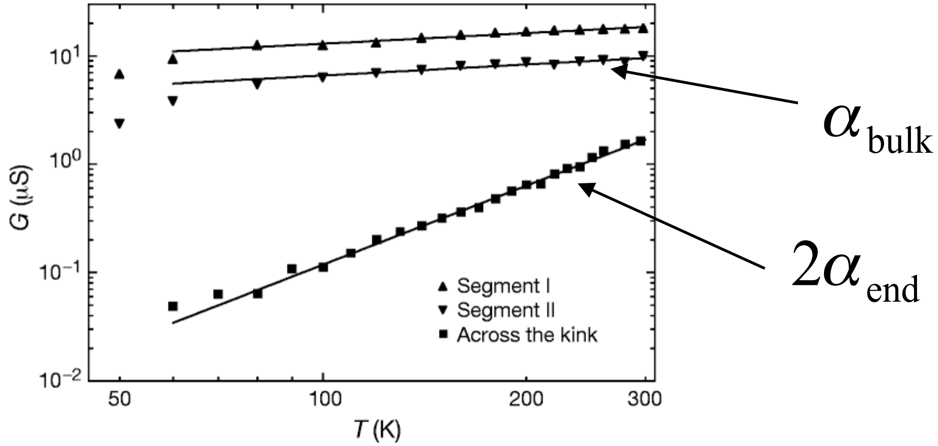
$\alpha_{end} = (1/g - 1)/4$

Linear conductance across an impurity: $\boxed{G(T) \propto T^{2\alpha_{end}}}$

Universal Scaling in eV/k_BT

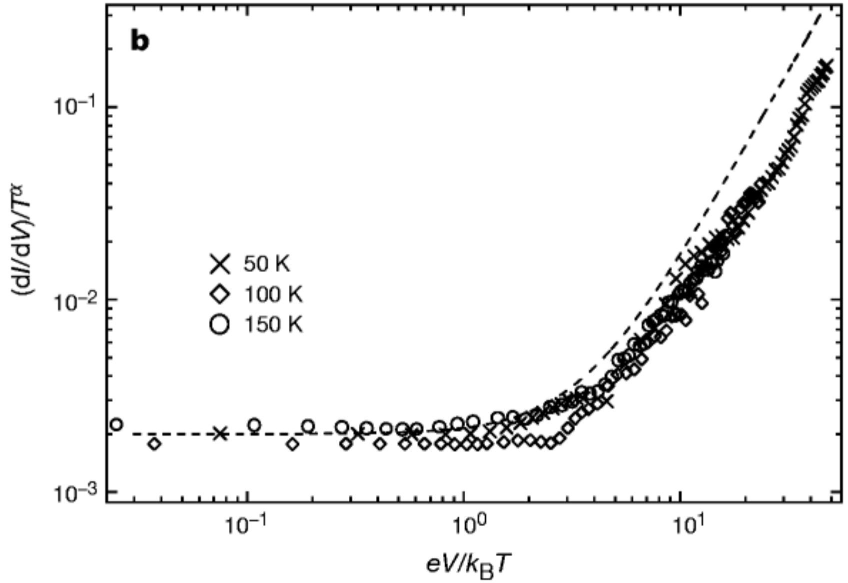
Observation of Luttinger liquid





α_{bulk}

$2\alpha_{\text{end}}$



gives $g \approx 0.22$

(Yao et al., Nature 1999)

Other Short-range Interactions

R. Egger and A. O. Gogolin, 1997-98

Momentum exchange

Coupling constant

$$b / a = 0.1e^2 / R$$

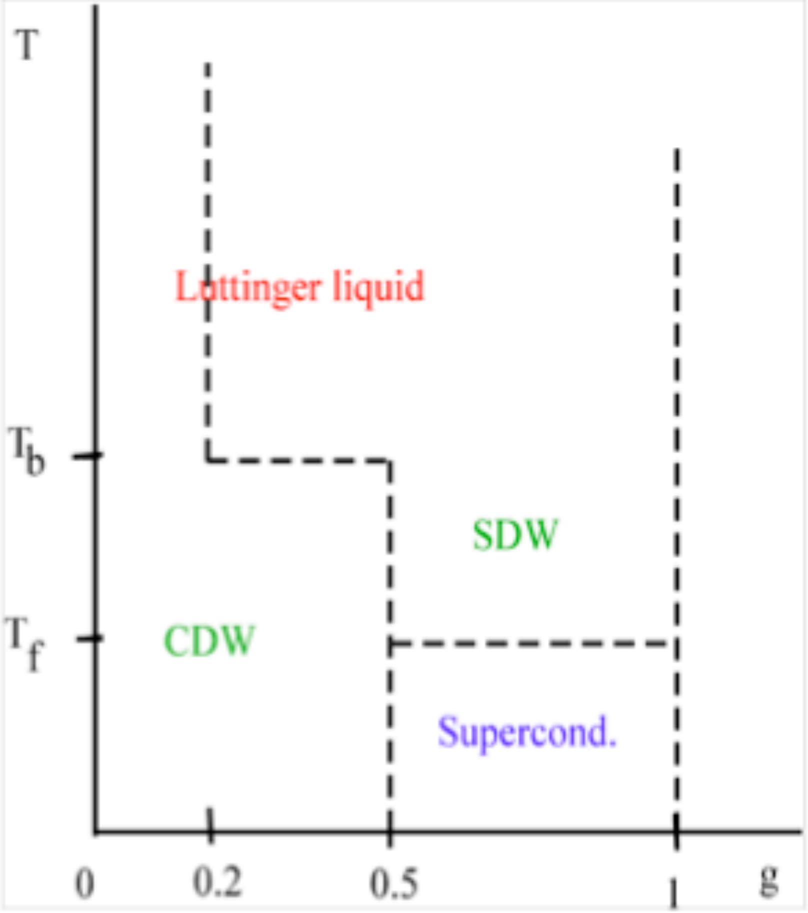
$$f / a = 0.05e^2 / R$$

Phase diagram of Isolated tube

- Effective field theory can be solved in practically exact way
- Low temperature phases matter only for ultrathin tubes or in sub-mKelvin regime

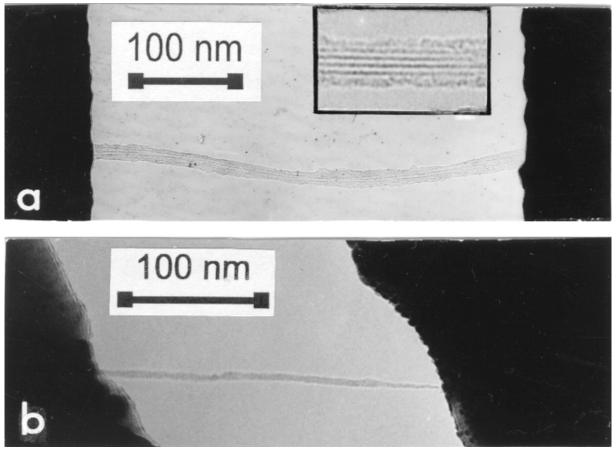
$$T_f = (f/b)T_b$$

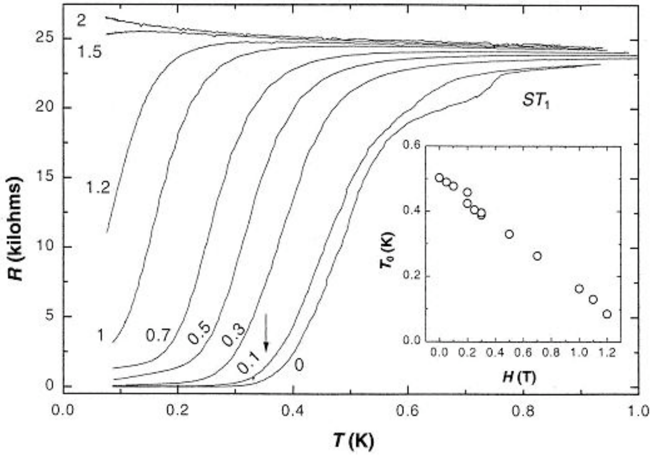
$$k_B T_b = De^{-v_F/b} \propto e^{-R/R_b}$$

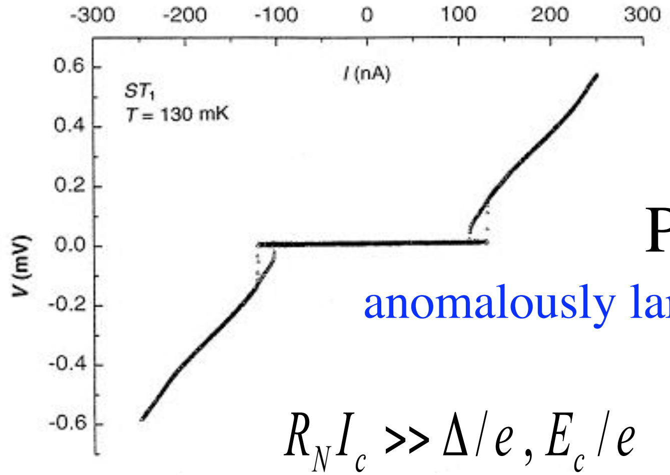


Proximity-Induced SC…

Kasumov et al. Science 1999, Morpurgo et al. Science 1999



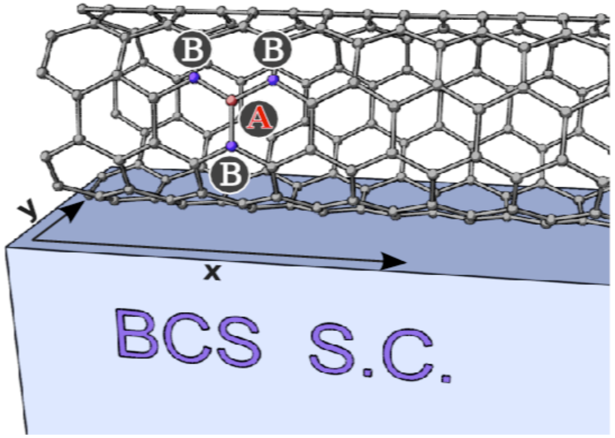




$R_N I_c >> \Delta / e , E_c / e$

Phonons?

anomalously large critical current

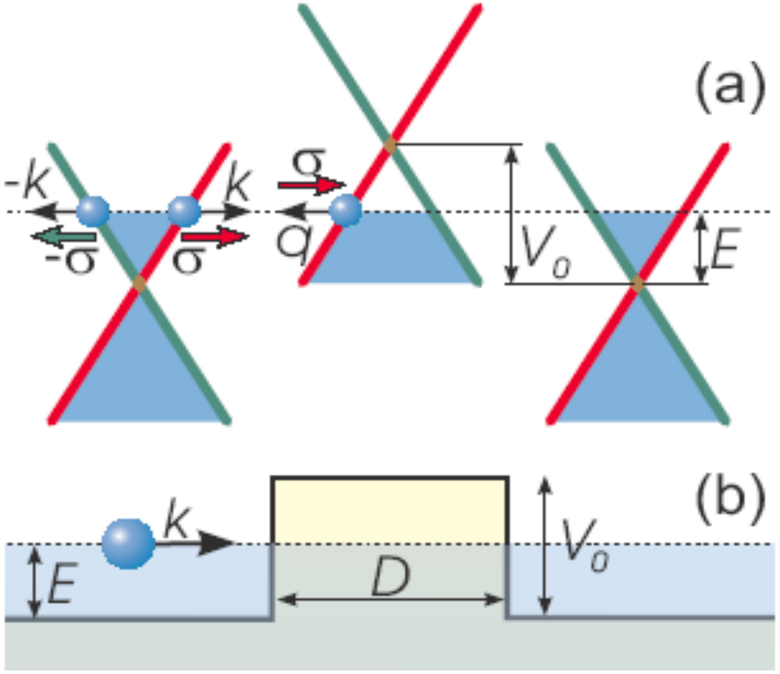


K. Le Hur, S. Vishveshwara, C. Bena, 2007

Klein Paradox for graphene:

Perfect transmission through a classically forbidden region

Katsnelson, Novoselov, Geim, Nature Physics 2006



A slowly varying barrier is more efficient:
See Cheianov & Falko, PRB 2006

Dirac equation

$$-iv_F\boldsymbol{\sigma}\cdot\nabla\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

The transmission probability
T is directionally-dependent.

For high barriers ($V_0 >> E$)

$$T(\phi) \simeq \frac{\cos^2\phi}{1-\cos^2(Dq_x)\sin^2\phi}$$

$$q_x = \sqrt{(V_0 - E)^2/(v_F^2) - k_y^2}$$

If V's are different for different spin orientations (magnetic gates): spin-polarized currents

Graphene: Interactions?

Thomas-Fermi screening length diverges:

$$\lambda_{TF} \approx \frac{1}{4\alpha}\frac{1}{k_F} = \frac{1}{4\alpha}\frac{1}{\sqrt{\pi n}}$$

$$\alpha = \frac{e^2}{\epsilon_0 v_F}$$

fine structure constant

bare value ~ 1 (strong)

Gonzalez, Guinea,
Vozmediano 1994,96

$k_B T >> 0$: non-Fermi liquid (similar to 1D!)

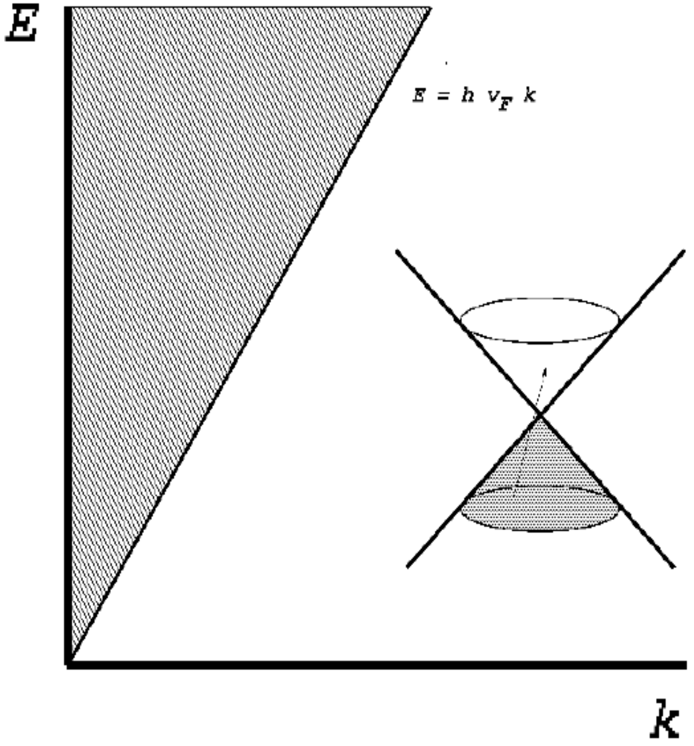
Fermi velocity acquires αlnT corrections…

Inverse Quasiparticle lifetime ~ $\alpha^2 T$

$$\Lambda \frac{\partial \alpha}{\partial \Lambda} = -\frac{\alpha^2}{4}$$

Interactions marginally IRRELEVANT
at low temperatures…

Graphene: Interactions II



$$\prod(k, E) \approx \frac{k^2}{\sqrt{v_F^2 k^2 - E^2}}$$

Quasiparticle lifetime requires $\omega > v_F p$: dimensional reduction

Divergence of the density
of electron/hole pairs at $\omega = v_F p$

$$\lim_{\omega \to \epsilon_p + 0^+} \Im m \Sigma(\omega, \vec{p}) = \frac{1}{48} \left(\frac{e^2}{\epsilon_0 v_F} \right)^2 v_F |\vec{p}|$$

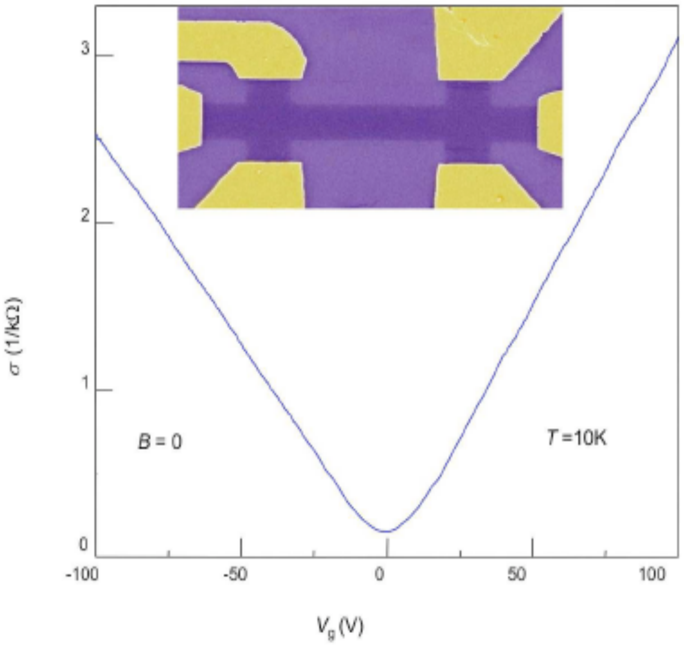
Transport

Doped graphene

$$-\boldsymbol{v_k}\cdot\boldsymbol{\nabla_r} f(\epsilon_{\boldsymbol{k}}) - e(\boldsymbol{E}+\boldsymbol{v_k}\times H)\cdot\nabla_{\boldsymbol{k}} f(\epsilon_{\boldsymbol{k}}) = -\left.\frac{\partial f_{\boldsymbol{k}}}{\partial t}\right|_{scatt.}$$

Boltzmann distribution: $f_k = f_k^0 + g_k$

$$-\left.\frac{\partial f_{\boldsymbol{k}}}{\partial t}\right|_{scatt.} \rightarrow \frac{g_{\boldsymbol{k}}}{\tau_{\boldsymbol{k}}}$$



Novoselov et al. (2005)

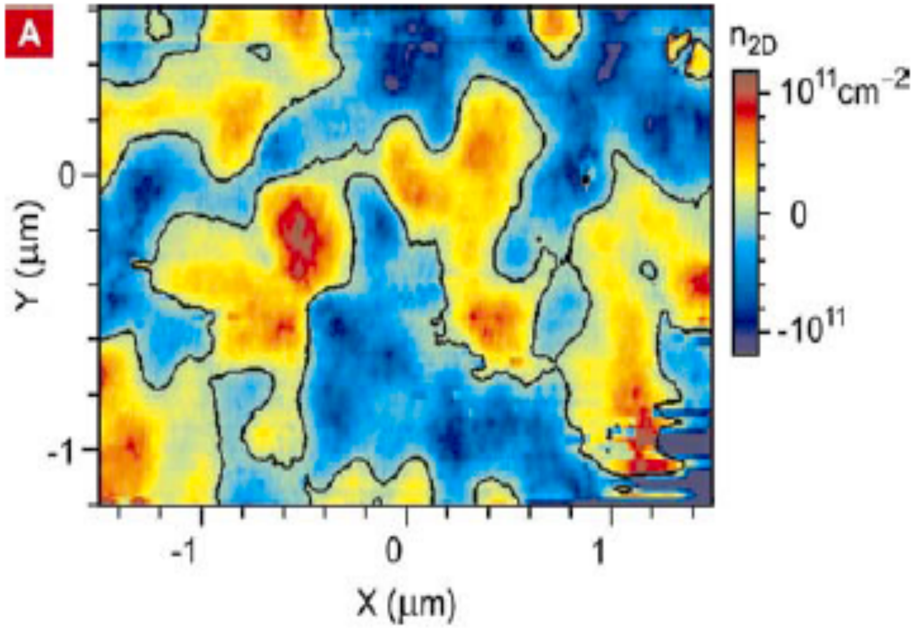
δ-Potential: τ_k varies as 1/k, σ~const
(Shon and Ando, 1998)

Charged impurities: τ_k varies as k, σ ~ n
(Ando; Nomura and MacDonald, 2006)

Residual conductivity at n=0?

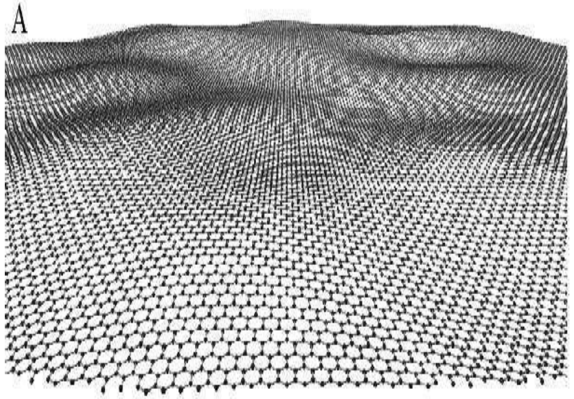
STM measurements: dirty…

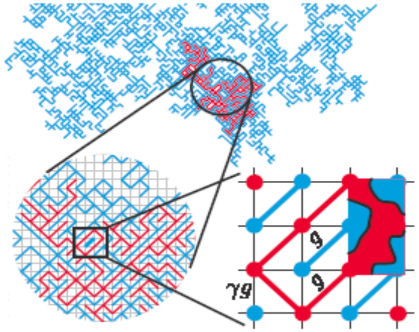
(Martin et al, 2006)



A color map of the spatial density variations in the graphene flake

Blue regions are holes, gold regions are electrons. black contour – zero density. About 100 particles/puddle.





Random resistor network
Cheianov et al., 2007

$$\sigma_{\min} \sim \frac{e^2}{\hbar}\left(a^2\delta n\right)^{0.41}$$

Single Layer

•Main problem: Manufacturing clean samples…

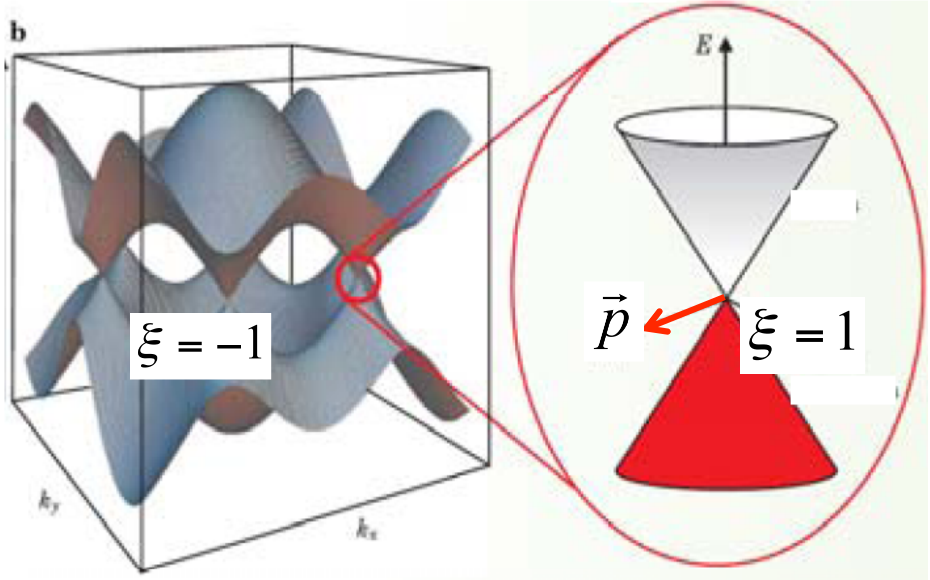
•Beyond single-particle physics in graphene…

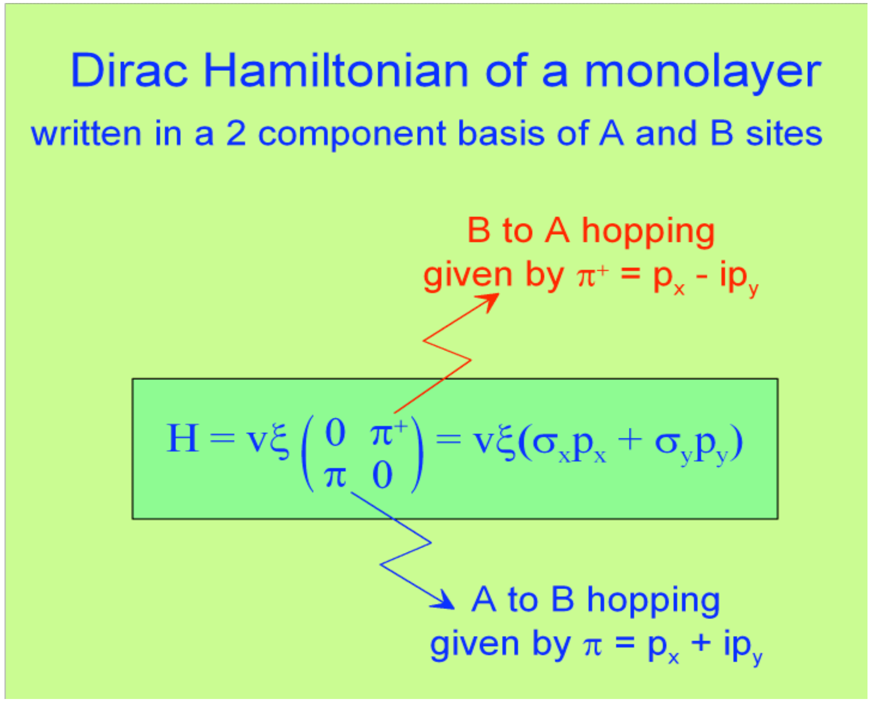
$\mathrm{Im}\Sigma \sim T$ observed in graphite at 0.3-4 eV (S. Yu et al. PRL 76, 483 (1996))
graphene (ARPES, Rotenberg et al.)

Quantum Hall effect

•Role of bending fluctuations: theory needs to be pushed further
Coupling between geometry and electron propagation: interesting

Compact description





Dirac Hamiltonian of a monolayer

written in a 2 component basis of A and B sites

B to A hopping
given by $\pi^+ = p_x - ip_y$

$$H = v\xi \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} = v\xi(\sigma_x p_x + \sigma_y p_y)$$

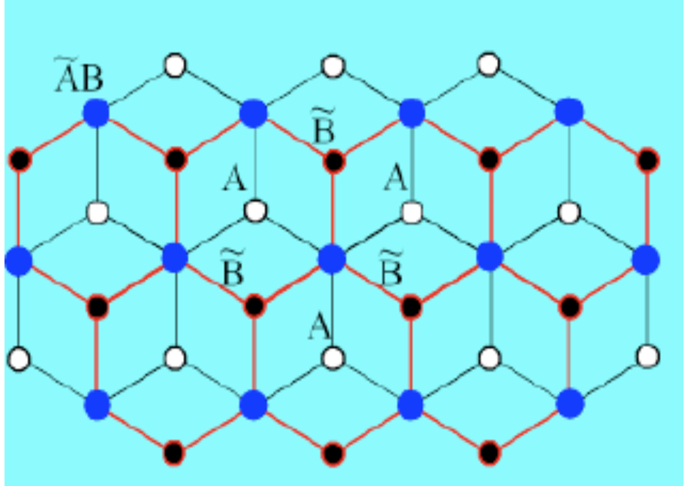
A to B hopping
given by $\pi = p_x + ip_y$

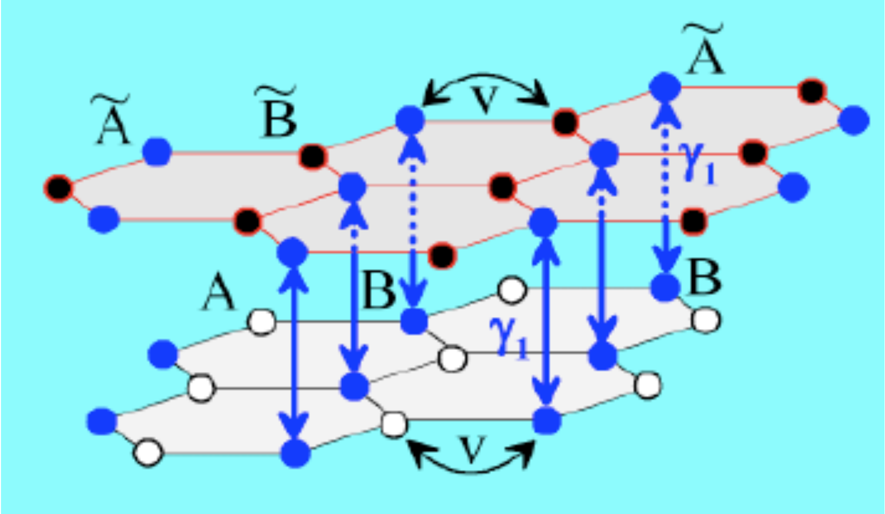
More than one…

Bernal Stacking

McCann & Falko, 2006

$\gamma_1 \sim 0.3\text{-}0.4\text{eV}$



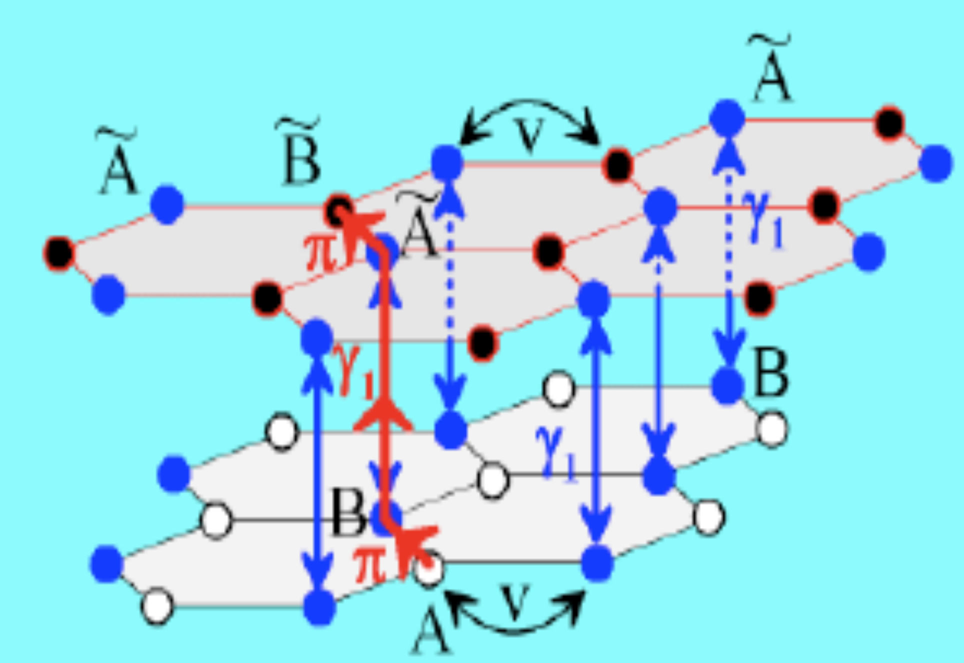


Bilayer Hamiltonian

$$H = \begin{array}{cc} \begin{array}{cccc} A & \tilde{B} & \tilde{A} & B \end{array} & \\ \left(\begin{array}{cccc} 0 & 0 & 0 & v\pi^{+} \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^{+} & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{array}\right) & \begin{array}{c} A \\ \tilde{B} \\ \tilde{A} \\ B \end{array} \end{array}$$

$$\pi = p_x + ip_y$$

Hamiltonian for bilayer



$$m \sim 0.05 m_e$$

$$H = \frac{-1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix}$$

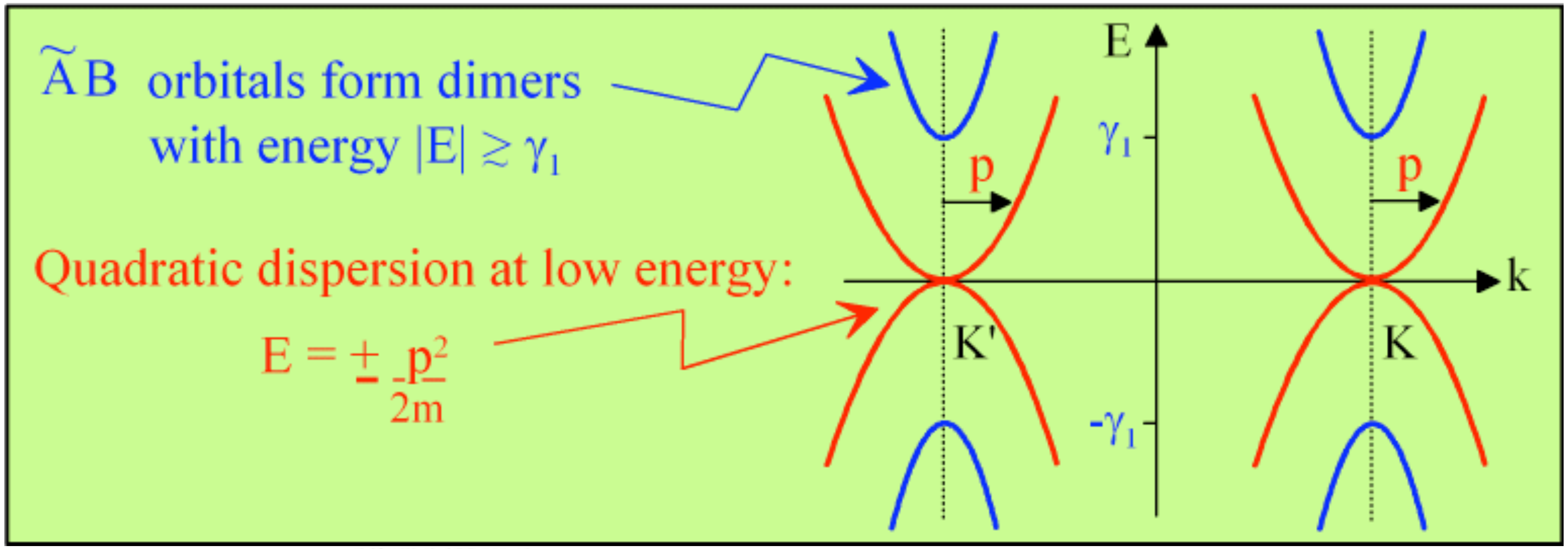
mass
$m = \gamma_1 / v^2$

A to $\tilde{B}$ hopping

- bottom layer A → B (factor π)
- switch layers via dimer B$\tilde{A}$ (γ_1^{-1})
- top layer $\tilde{A}$ → $\tilde{B}$ (factor π)

$$\pi = p_x + i p_y$$

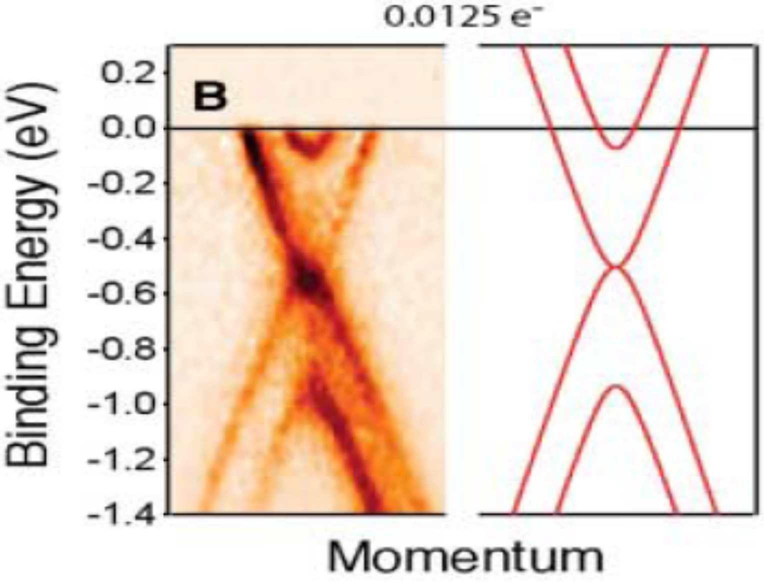
Band Structure



$\tilde{A}B$ orbitals form dimers with energy $|E| \gtrsim \gamma_1$

Quadratic dispersion at low energy:

$$E = \pm \frac{p^2}{2m}$$



T. Ohta *et al* – Science 313, 951 (2006)
(Rotenberg's group at Berkeley NL)

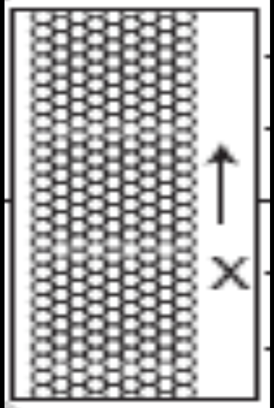
Heavily doped bilayer

Topological Insulator

Kane and Mele (2005) showed zero mode edge states exist in a (bulk) gapped insulating state in a model on the honeycomb lattice with spin-orbit coupling

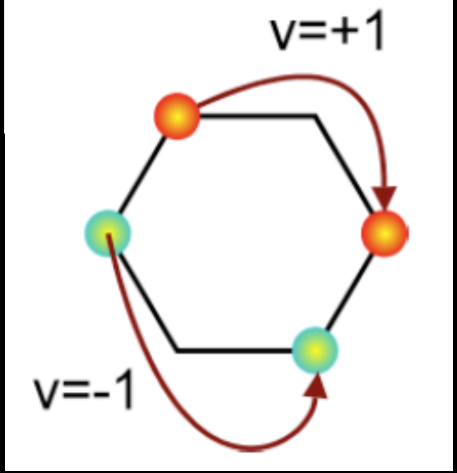
$$\mathcal{H} = -t \sum_{\langle ij \rangle \alpha} f^{\dagger}_{i\alpha} f_{j\alpha} + i\Delta_{SO} \sum_{\langle\langle ij \rangle\rangle \alpha\beta} \nu_{ij} \sigma^{z}_{\alpha\beta} f^{\dagger}_{i\alpha} f_{j\alpha}$$

Description of Haldane (1988)



Strip geometry and zigzag edges

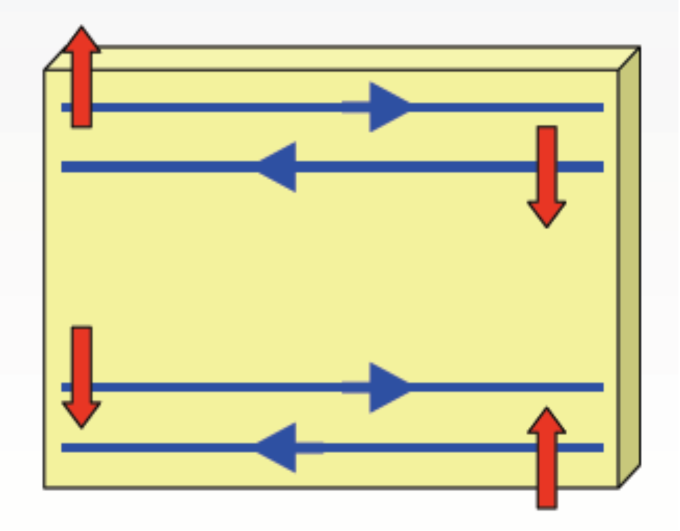
Zero energy states at the edges subsist until $\Delta_{SO} \sim 0$



Insulator with Zero energy modes at the edges…

here σ = spin !!!

Graphene is light, Bi is heavy



<u>Zero energy modes on honeycomb lattice:</u>

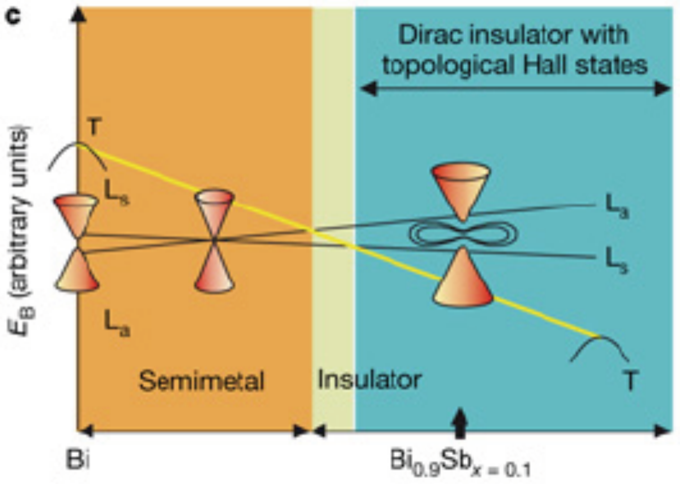
* superconducting phases
P. Ghaemi and F. Wilczek, 2007
D. Bergman and K. Le Hur, 2008

* Kekule distortion model
Chamon et al.

* Kitaev spin model,…

Spin Hall effect: $E=\sigma vq>0$

BiSb: studied in the 60s
no Dirac particle



Nature ***452*, 970-974 (24 April 2008)**
Topological insulator in 3D
Cava, Hasan, et al.

Berry Phase

Monolayer:

$$H = v\xi \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix}$$

Bilayer:

$$H = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix}$$

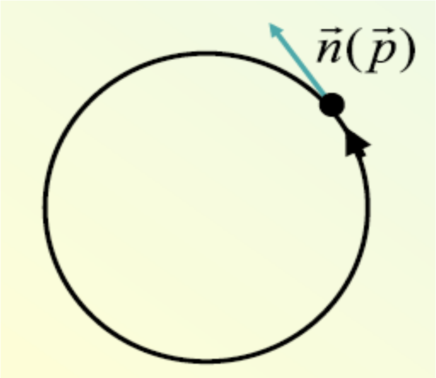
$$\pi = p_x + ip_y = pe^{i\varphi} \qquad \pi^+ = p_x - ip_y = pe^{-i\varphi}$$

$$H = g\,|p|^J \begin{pmatrix} 0 & e^{-iJ\varphi} \\ e^{iJ\varphi} & 0 \end{pmatrix} = g\,|p|^J\,(\sigma_x \cos J\varphi + \sigma_y \sin J\varphi)$$

$$H = g|p|^J\,(\sigma . n)$$

$$\sigma = (\sigma_x, \sigma_y)$$

$$n = (\cos J\varphi, \sin J\varphi)$$



$$\psi \;\rightarrow\; e^{J 2\pi \frac{i}{2}\sigma_3}\psi = e^{iJ\pi}\psi$$

Conclusion of these lectures:

- 1D: liquid phase is Luttinger

  Rigorous treatment of Mott/Luttinger transition

  New experimental tools: momentum-resolved tunneling

  cold atomic fermions: non-equilibrium phenomena,…

  Rich quasi-1D physics: doped Mott insulator and exotic SC

- 2D: Half-filled case, Mott phase with AF ordering

  Doped Mott insulator: truncated Fermi surface and SC

- Carbon materials; a route to Dirac fermions in 1D and 2D…

  3d materials with Dirac fermions: BiSb