Graphite. Interactions, transport, and disorder.

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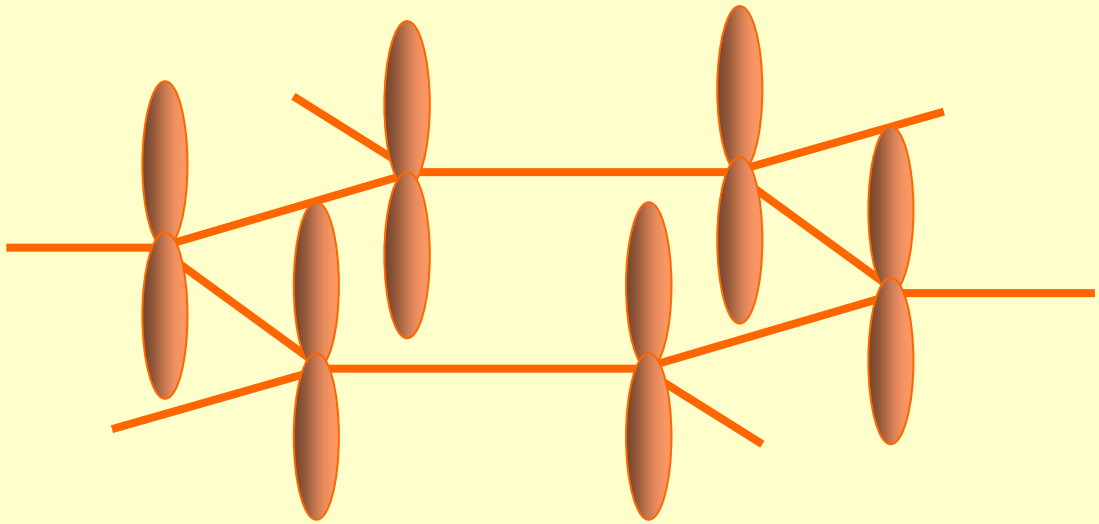
Outline

- **The electronic structure of graphite.**
- **A graphene plane. The Dirac equation.**
- **The electron-electron interaction.**
- **Renormalization.**
- **Related systems and lattice defects.**
- **Disorder. Localized states.**
- **Magnetism, cracks and voids.**
- **Self doping.**
- **Transport properties. Universal conductance.**
- **The quantum Hall effect.**

Electronic band structure

J. W. McClure, Phys. Rev. **108**, 612 (1957)



-The conduction band is built up from the unpaired π orbitals at the C atoms.

-The crystal structure is stabilized by the σ bonds within the plane.

-The hybridization between π orbitals in neighbouring planes cannot be neglected.

Hybridization between in plane nearest neighbours: $\gamma_0 \approx 2.4\text{eV}$

Hybridization between out of plane nearest neighbours: $\gamma_1 \approx 0.3\text{eV}$

Electronic band structure

D. E. Soule, J. W. McClure, and L. B. Smith, Phys. Rev. **134**, A454 (1964).

D. Marchand, C. Frétigny, M. Lagües, F. Batallan, Ch. Simon, I. Roseman, and R. Pinchaux, Phys. Rev. B **30**, 4788 (1984)

The Fermi surface has electron and hole like pockets at the edges of the Brillouin zone.
The effective masses are small, $m_{eff} \approx 0.06 m_0$
The structure is consistent with Shubnikov-de Haas and photoemission experiments.

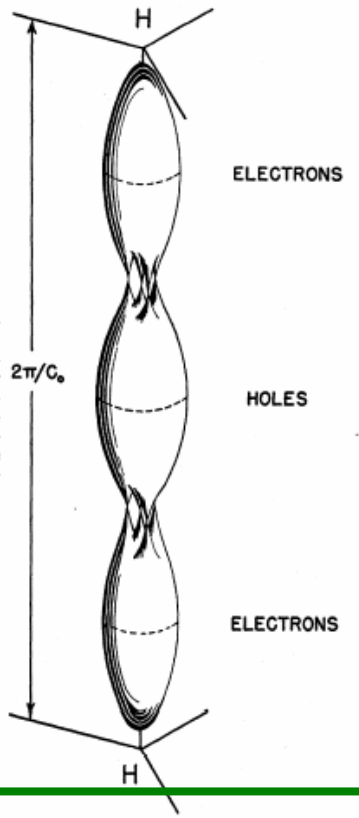
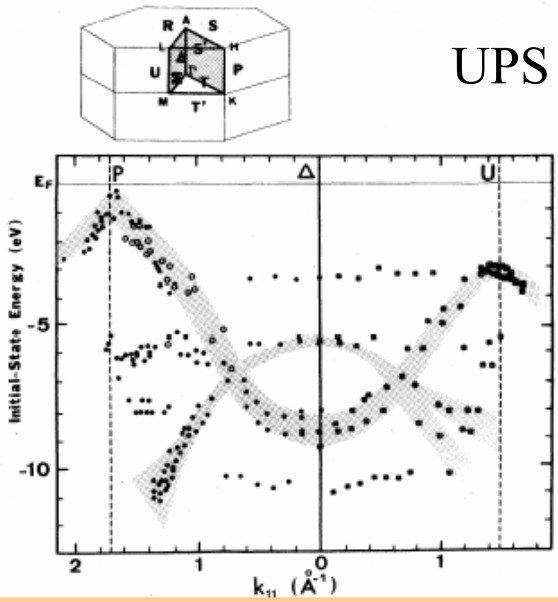
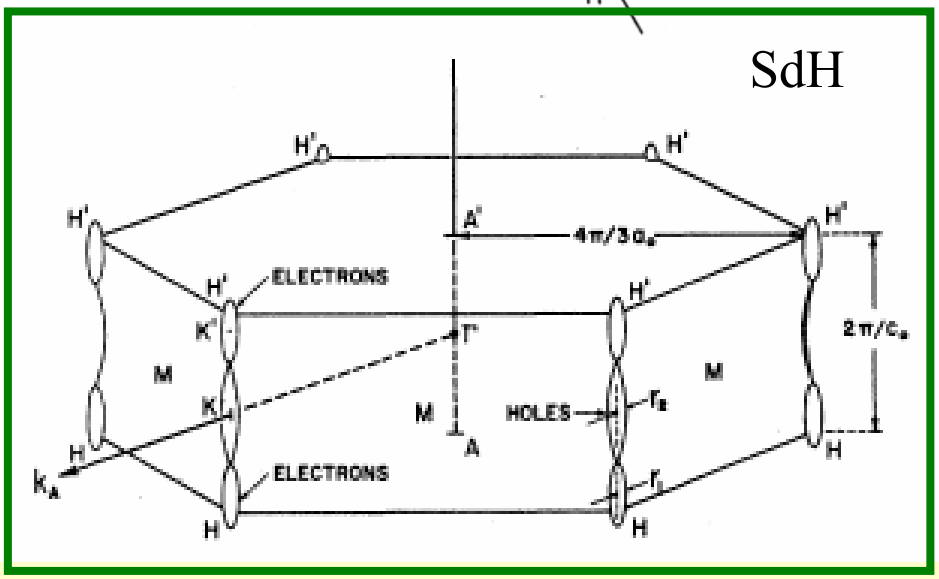


FIG. 4. The Fermi surface for pure graphite. The central surface contains holes and the outer surfaces contain electrons. The length-to-width ratio of each surface is about 13. The trigonal anisotropy is exaggerated for clarity.

UPS

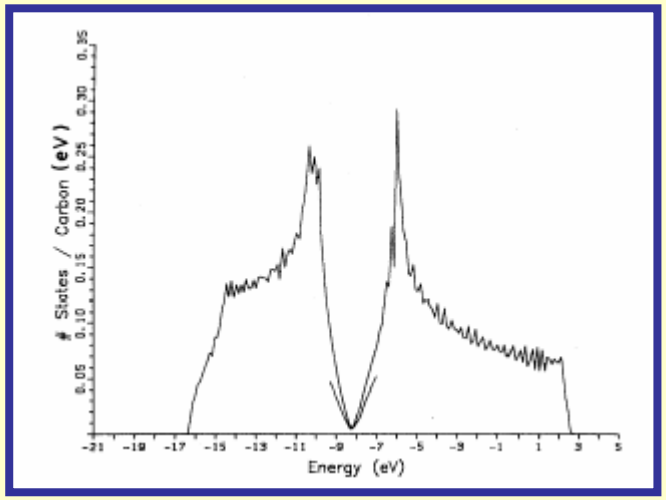


SdH



Electronic band structure

R. C. Tatar, and S. Rabii, Phys. Rev. B **25**, 4126 (1982).
J.-C. Charlier, X. Gonze, and J.-P. Michenaud, Phys. Rev. B **43**, 4579 (1991).



Graphite is a semimetal.

$N(\varepsilon_F) \approx 1.2 \times 10^{-4}$ states/(eV C atom)

$n \approx 2.4 \times 10^{18}\,cm^{-3}$

$\lambda_{FT} \approx 50nm$

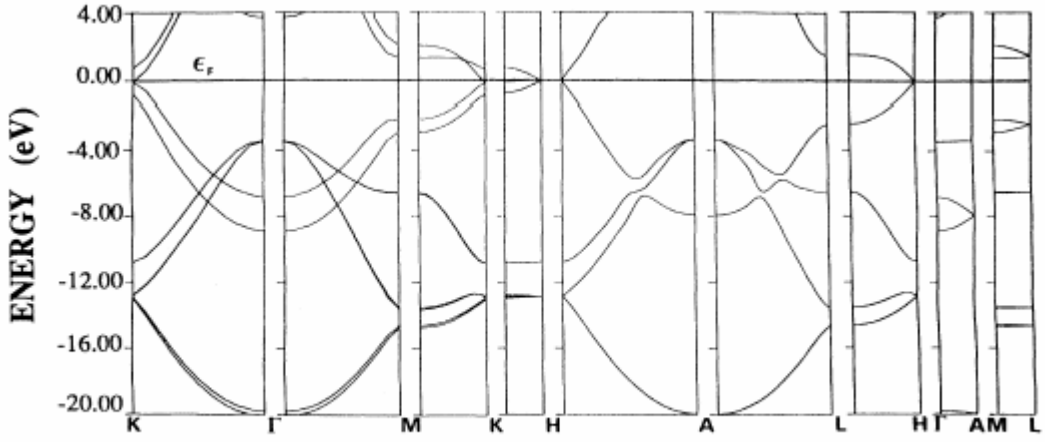


FIG. 3. *Ab initio* band structure of graphite along different lines in the Brillouin zone.

Related materials:

Graphite intercalation compounds:

Doped graphene planes.

Superconducting at low temperatures.

Polyacetylene:

π-bonded chain.

Peierls distortion.

Nanotubes:

superconducting and magnetic instabilities.

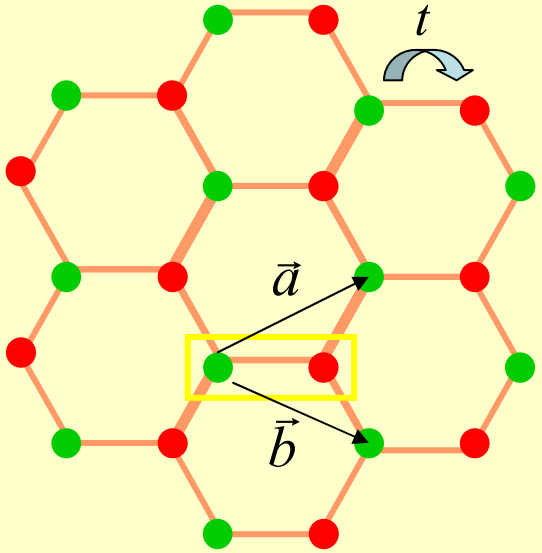
Fullerenes:

superconducting when doped.

Phonons: $\omega_{opt} \approx 0.2\text{eV}$

Electron-phonon coupling: $\dfrac{\partial \gamma_0}{\partial d_{C-C}} \approx 1.4\text{eV}/\overset{0}{\text{A}}$

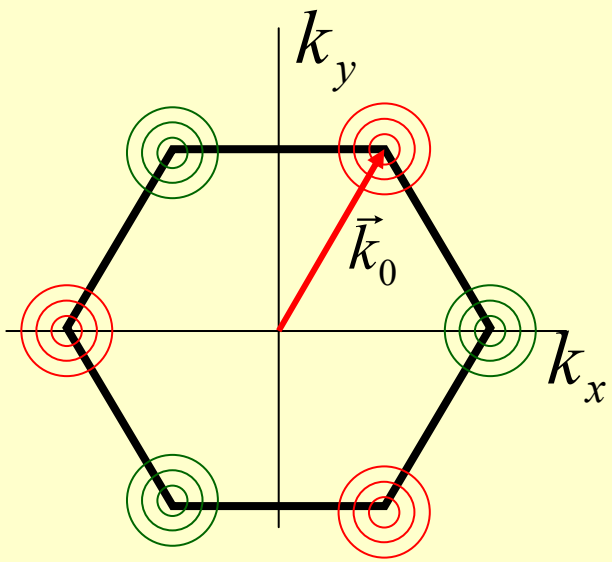
A graphene plane. The Dirac equation.



$$H = t\sum_{n.n.} c_{i,s}^{+} c_{j,s} + h.c.$$

$$H_{\vec{k}} \equiv \begin{pmatrix} 0 & t\left(1+e^{-i\vec{k}\vec{a}}+e^{-i\vec{k}\vec{b}}\right) \\ t\left(1+e^{i\vec{k}\vec{a}}+e^{i\vec{k}\vec{b}}\right) & 0 \end{pmatrix}$$

$$\varepsilon_{\vec{k}} = \pm t\sqrt{3+2\cos\left(\vec{k}\vec{a}\right)+2\cos\left(\vec{k}\vec{b}\right)+2\cos\left[\vec{k}\left(\vec{a}-\vec{b}\right)\right]}$$



$$\vec{k} = \vec{k}_0 + \delta\vec{k}$$

$$\vec{k}_0 = \frac{4\pi}{3\sqrt{3}a}\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right)$$

$$\vec{a} = a\sqrt{3}(1,0)$$

$$\vec{b} = a\sqrt{3}\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right)$$

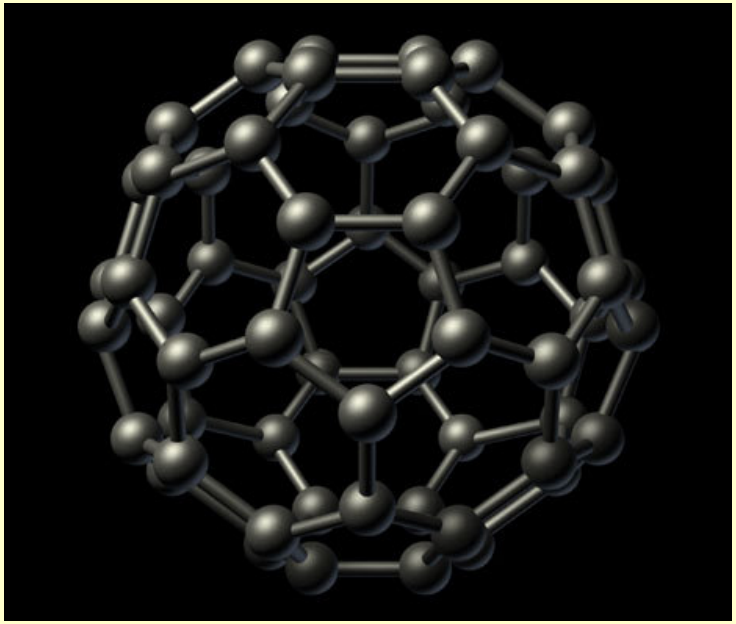
$$e^{i\vec{k}_0\vec{a}} = -\frac{1}{2}+i\frac{\sqrt{3}}{2}$$

$$e^{i\vec{k}_0\vec{b}} = -\frac{1}{2}-i\frac{\sqrt{3}}{2}$$

Dirac equation:

$$H \cong \frac{3ta}{2}\begin{pmatrix} 0 & k_x+ik_y \\ k_x-ik_y & 0 \end{pmatrix}$$

Related systems. C_{60}

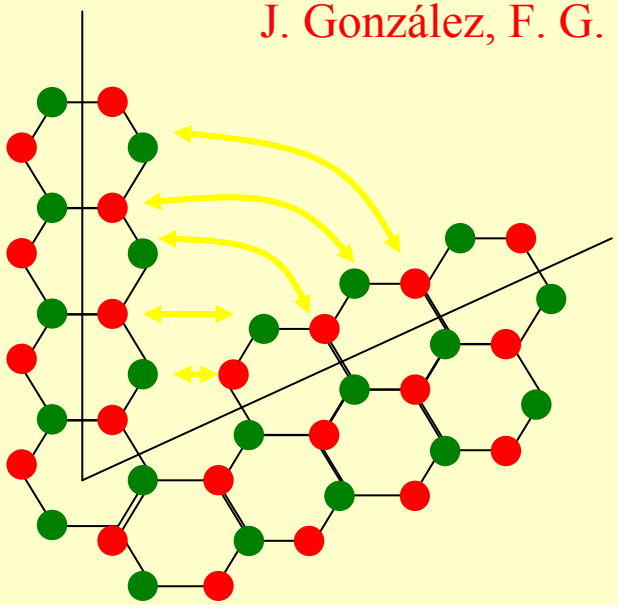


- **Threefold coordination**
- **The curvature is induced by five-fold rings**
- **There is a family of quasispherical compounds**
- **The valence orbitals are derived from π atomic orbitals.**

The Dirac equation on a sphere?

Lattice frustration as a gauge potential.

J. González, F. G. and M. A. H. Vozmediano, Phys. Rev. Lett. **69**, 172 (1992)



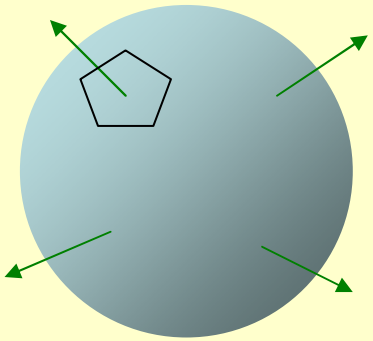
- **A fivefold ring defines a disclination.**
- **The sublattices are interchanged.**
- **The Fermi points are also interchanged.**
- **These transformations can be achieved by means of a gauge potential.**

$$i\vec{\nabla} \rightarrow i\vec{\nabla} - \vec{A}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\Phi = \int \vec{A}\, d\vec{l}$$

The flux Φ is determined by the total rotation induced by the defect.

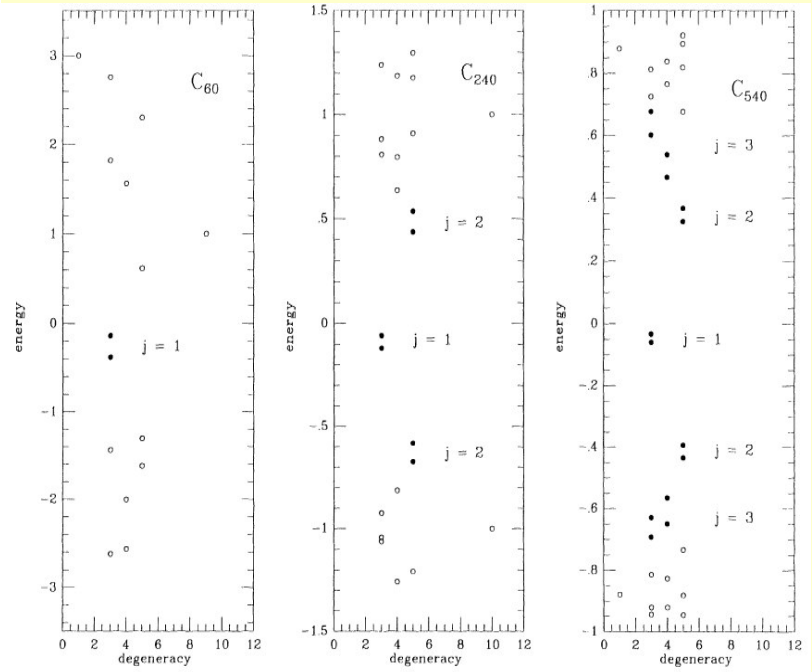
Continuum model of the fullerenes.



- Dirac equation on a spherical surface.
- Constant magnetic field (Dirac monopole).

$$\frac{\hbar v_F}{R}\left[i\partial_\theta - \frac{1}{sin(\theta)}\partial_\phi + \frac{i(1+l)cos(\theta)}{2\,sin(\theta)}\right]\Psi_a = \varepsilon\Psi_b$$

$$\frac{\hbar v_F}{R}\left[i\partial_\theta + \frac{1}{sin(\theta)}\partial_\phi + \frac{i(1-l)cos(\theta)}{2\,sin(\theta)}\right]\Psi_b = \varepsilon\Psi_a$$



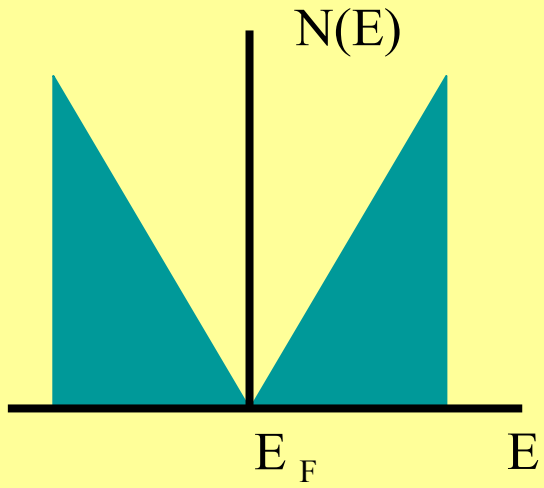
$$\varepsilon_J = \frac{\hbar v_F}{R}\sqrt{\left[J(J+1)\right] - l(l+1)} \qquad J \geq l$$

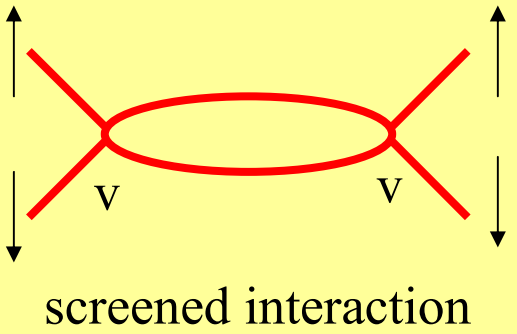
Coulomb interactions

Non Fermi liquid behavior of quasiparticle lifetimes.

Expts: S. Yu, J. Cao, C. C. Miller, D. A. Mantell, R. J. D. Miller, and Y. Gao, Phys. Rev. Lett. **76**, 483 (1996).

Theory: J. González, F. G., and M. A. H. Vozmediano Phys. Rev. Lett. **77**, 3589 (1996)





screened interaction

Single graphene planes:

- Absence of screening.
- Perturbation theory leads to logarithmic divergences.
- The expansion has similar properties to that for 1D metallic systems (Luttinger liquids).
- Large coupling constant: e^2/v_F=2-5
- Deviations from Fermi liquid behavior.

Limits of validity:

High energies > 0.3eV.

Neglects electron-phonon interaction.

Renormalization of the Coulomb interaction.

$$H = iv_F \int d^2\vec{r}\,\Psi^+(\vec{r})\vec{\sigma}\vec{\nabla}\Psi(\vec{r}) + \\ + \frac{e^2}{8\pi}\iint d^2\vec{r}_1 d^2\vec{r}_2 \Psi^+(\vec{r}_1)\Psi(\vec{r}_1)\frac{1}{|\vec{r}_1 - \vec{r}_2|}\Psi^+(\vec{r}_2)\Psi(\vec{r}_2)$$

Dimensional analysis:

$$[l] \equiv [t]$$

$$[H_K] \equiv [H_{int}] \equiv \frac{1}{l}$$

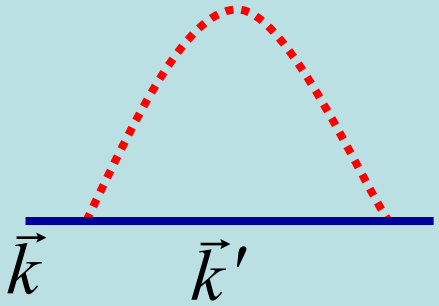
$$[\Psi] \equiv \frac{1}{l^{D/2}}$$

$$[e^2] \equiv l^0$$

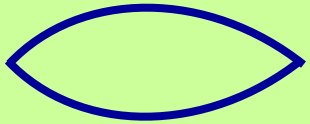
- The interaction is marginal in any dimension (as in QED).
- The interaction is mediated by photons in three dimensional space.
- The interaction breaks the Lorentz invariance of the Dirac equation.

Renormalization of the Coulomb interaction.

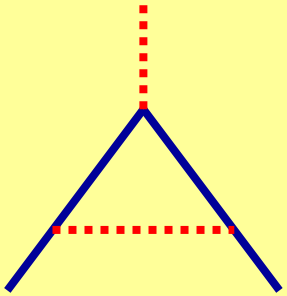
J. González, F. G. and M. A. H. Vozmediano., Nucl. Phys. B **424**, 595 (1994)



Hartree Fock selfenergy: $\Sigma(\vec{k}) \approx \frac{e^2}{8\pi}\vec{\sigma}\,\vec{k}\log\left(\frac{\Lambda}{|\vec{k}|}\right)$

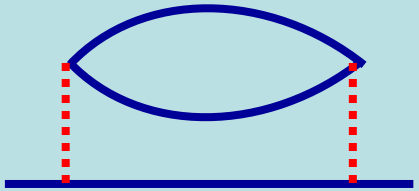


Bare polarizability: $\Pi_0(\vec{k},\omega) = i\frac{e^2}{8}\frac{\vec{k}^2}{\sqrt{v_F^2\vec{k}^2-\omega^2}}$



The vortex corrections are finite (to all orders).

Renormalization of the Coulomb interaction.



One loop calculation:
Renormalization of the particle residue.

$$\Psi_R = Z^{-1/2}\Psi_0$$

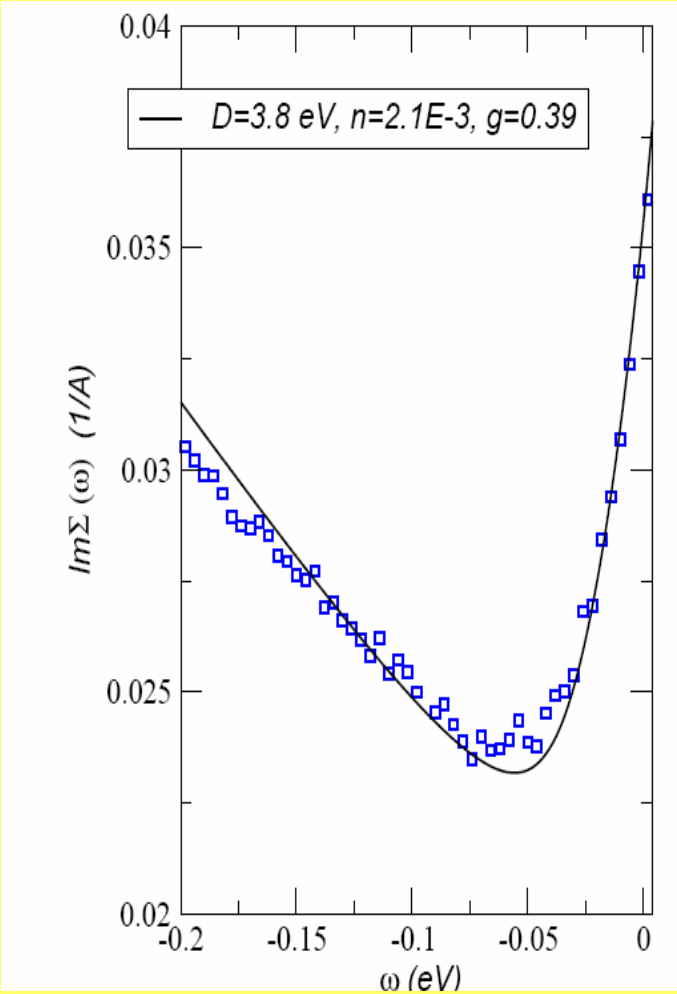
$$Z^{-1} = \frac{\partial \Sigma}{\partial \omega}$$

$$Im\,\Sigma(\omega) \propto |\omega|$$

Lowest order RG flow: $$\Lambda \frac{\partial}{\partial \Lambda} \frac{e^2}{v_F} = \frac{8}{\pi^2} \frac{e^2}{v_F}$$

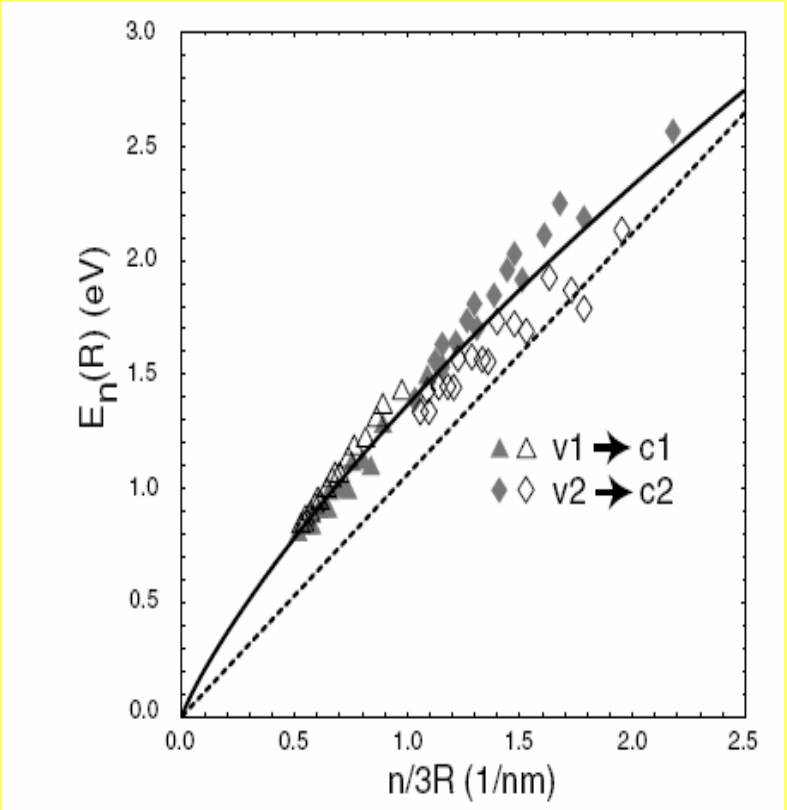
The coupling constant goes to zero at low energies.

Experimental consequences?



A. Lanzara *et al*, unpublished.

The combined effects of disorder and electron-electron interactions lead to a non monotonous dependence of the quasiparticle lifetime on disorder.



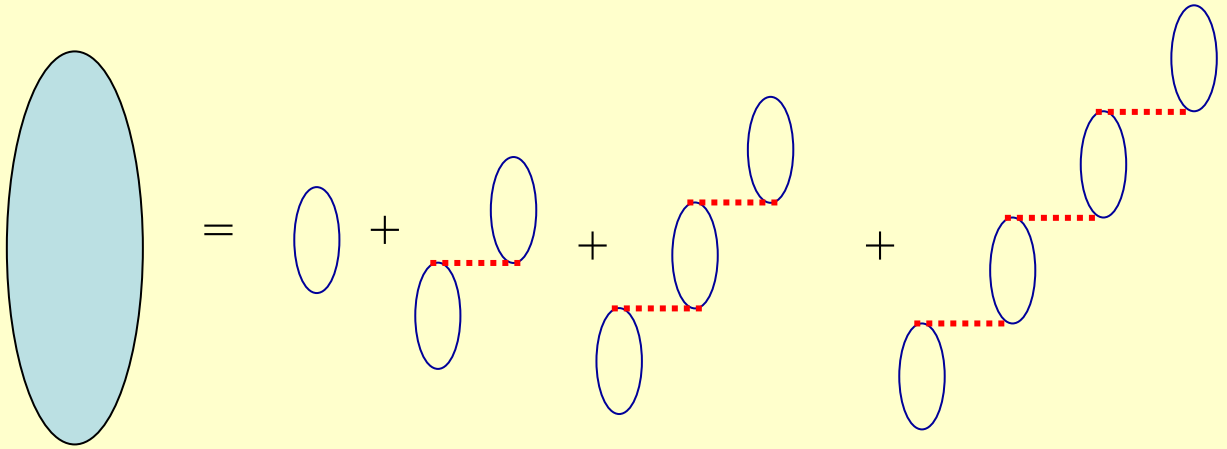
C. L. Kane and E. J. Mele, Phys. Rev. Lett. **93**, 197402 (2004)

The electronic self energy due to the long range Coulomb interaction modifies the dependence of the gap on the radius in semiconducting nanotubes.

Renormalization of the Coulomb interaction.

J. González, F. G. and M. A. H. Vozmediano, Phys. Rev. B **59**, R2474 (1999)

RPA summation:



RG flow equation:
(which can be analytically extended to g > 1)

$$\Lambda \frac{\partial}{\partial \Lambda} g = \frac{8}{\pi^2}\left(g + \frac{\arccos g}{\sqrt{1-g^2}} \right) - \frac{4}{\pi}$$

The coupling constant always flows to zero at low energies.

Non perturbative phase transitions.

D.V. Khveshchenko, Phys. Rev. Lett. **87**, 246802 (2001).

Compensation between low density of states and unscreened interaction

Stoner criterium:

$$U_c N(E_F) = 1 \quad \leftrightarrow \quad N_f \frac{e^2}{|\vec{q}|} \frac{|\vec{q}|}{v_F} = 1$$

For sufficiently large couplings, a charge density wave phase is induced

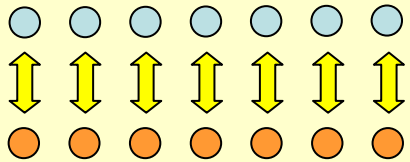
Interlayer hopping

M. A. H. Vozmediano, M. P. López-Sancho, and F. G., Phys. Rev. Lett. **89**, 166401 (2002); *ibid,* Phys. Rev. B **68**, 195122 (2003).

In plane interactions reduce the interlayer coupling.
Similar effect as in the cuprate superconductors.

Interchain hopping in Luttinger liquids

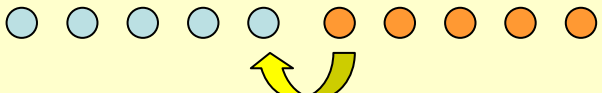
Extended hopping



X.G. Wen, Phys. Rev. B **42**, 6623 (1990).
F. G. and G. Zimanyi, Phys. Rev. B **47**, 501 (1993).
S. Chakravarty and P.W. Anderson, Phys. Rev. Lett. **72**, 3859 (1994).
J.M.P. Carmelo, P.D. Sacramento, and F. G., Phys. Rev. B **55**, 7565 (1987)
A.H. Castro-Neto and F. G., Phys. Rev. Lett. **80**, 4040 (1998).

See also:

Local hopping

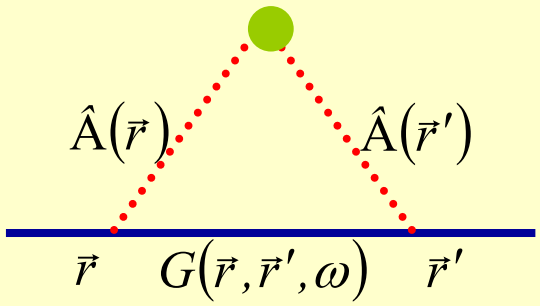


C.L. Kane and M.P.A. Fisher, Phys. Rev. Lett. **68**, 1220 (1992).

Disorder effects.

F. G., J. González, and M. A. H. Vozmediano, Phys. Rev. B **59**, 134421 (2001)

Disorder can be modeled as a gauge field



$$H = iv_F \int d^2\vec{r}\,\Psi^+(\vec{r})\left[\vec{\sigma}\vec{\nabla} - i\hat{A}(\vec{r})\right]\Psi(\vec{r})$$

$$\left\langle \hat{A}(\vec{r})\hat{A}(\vec{r}')\right\rangle = \hat{\Delta}\delta^{(2)}(\vec{r}-\vec{r}')$$

$$\left[\hat{A}\right] \equiv \frac{1}{l}$$

$$\left[\hat{\Delta}\right] \equiv l^0$$

$$\left\langle G(\vec{r},\vec{r}',\omega)\right\rangle = \left\langle G_0(\vec{r},\vec{r}',\omega)\right\rangle + \left\langle G_0(\vec{r},\vec{r}',\omega)\vec{A}(\vec{r})G_0(\vec{r},\vec{r}',\omega)\vec{A}(\vec{r}')G_0(\vec{r},\vec{r}',\omega)\right\rangle + \ldots$$

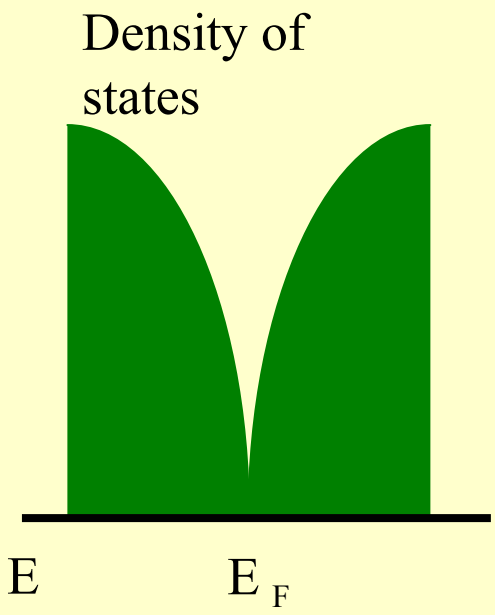
$$\Sigma(\vec{r},\vec{r}',\omega) = \left\langle \vec{A}(\vec{r})G_0(\vec{r},\vec{r}',\omega)\vec{A}(\vec{r}')\right\rangle + \ldots$$

Disorder effects.

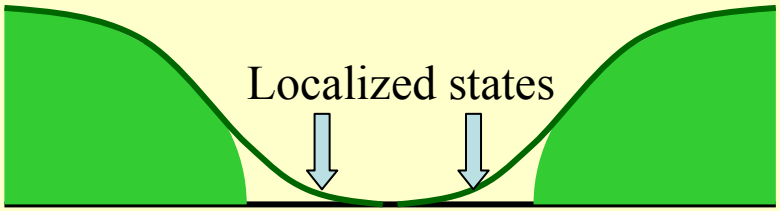
See also H. E. Castillo, C. de C. Chamon, E. Fradkin, P. M. Goldbart and C. Mudry, Phys. Rev. B **56**, 10668 (1997)

$$\Sigma(\omega) = c\Delta\omega \log\left(\frac{\Lambda}{\omega}\right)$$ Selfenergy

$$D(\omega) \propto \frac{\omega + \Sigma(\omega)}{\Lambda^2} \approx \frac{\omega^{1-c\Delta}}{\Lambda^2}$$ Density of states (sum of leading logarithms)

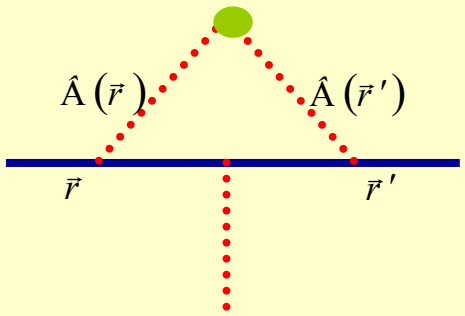


- The density of states is enhanced near the Fermi level.
- Similar effects take place at band edges.
- Local interactions become less irrelevant (their scaling dimension increases)

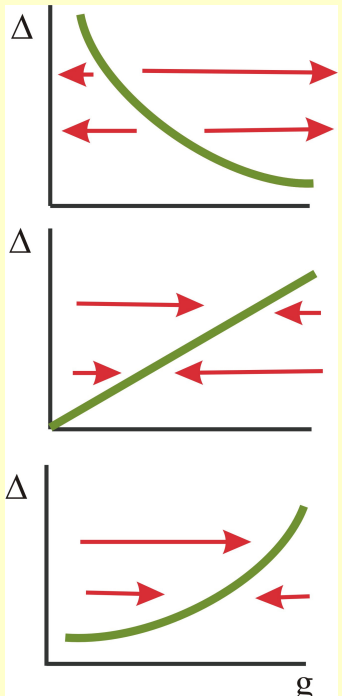


Electrostatic interactions and disorder.

T. Stauber, F. G. and M. A. H. Vozmediano, Phys. Rev. B **71**, 041406 (2005).
J. Ye, Phys. Rev. B **60**, 8290 (1999).



- There are selfenergy and vortex corrections.
- The selfenergy induces wavefunction renormalization.
- The vortex corrections depend on the type of disorder.
- The wavefunction renormalization changes the flow of the coupling constant.



Smooth random potential

Coarse grained lattice defects

Smooth staggered potential

Electrostatic interactions and disorder.

$$\Delta \approx c\left(\frac{V}{\hbar v_F}\right)^2$$

Random concentration (c) of defects of strength V.

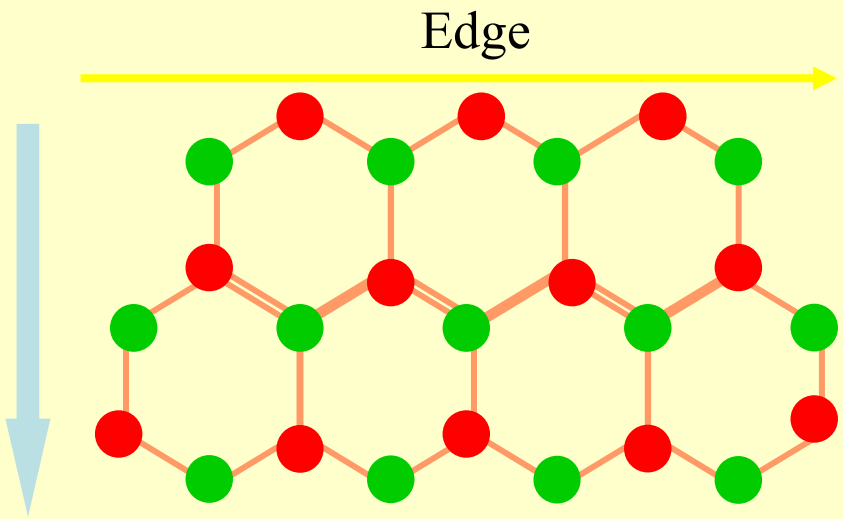
$$\Delta \approx cb^2$$

Random concentration (c) of dislocations with Burgers vector b.

- Line of fixed points (the critical exponents depend on the interactions).
- Non Fermi liquid behavior.
- New features due to higher order corrections?

Localized states. Continuum approximation.

$$H \cong \hbar v_F \left(i\sigma_x \frac{\partial}{\partial x} + i\sigma_y \frac{\partial}{\partial y} \right) + \ldots$$



Edge states

K. Wakabayashi, M. Fujita, H. Ajiki, and M. Sigrist, Phys. Rev. B **59**, 8271 (1999)

$$H\,|\Psi_k\rangle = 0 \Rightarrow \Psi_k \propto \begin{pmatrix} e^{ika} e^{-ka} \\ 0 \end{pmatrix}$$

Midgap surface states.
The edge sites belongs to the same sublattice.

Other types of defects.

Localized states at zero energy:

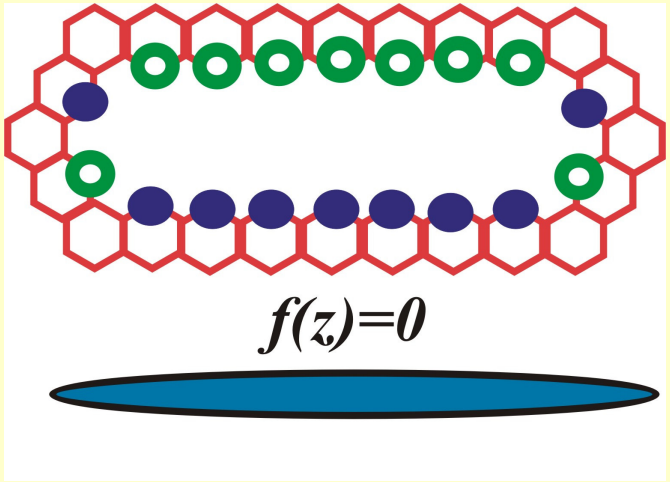
$$H \equiv i\hbar v_F \begin{pmatrix} 0 & \partial_z \\ \partial_{\bar{z}} & 0 \end{pmatrix}$$

$$H\left|\Psi(z,\bar{z})\right\rangle = 0 \Rightarrow \Psi(z,\bar{z}) = \begin{cases} \begin{pmatrix} 0 \\ f(z) \end{pmatrix} \\ \begin{pmatrix} f(\bar{z}) \\ 0 \end{pmatrix} \end{cases}$$

Other types of defects.

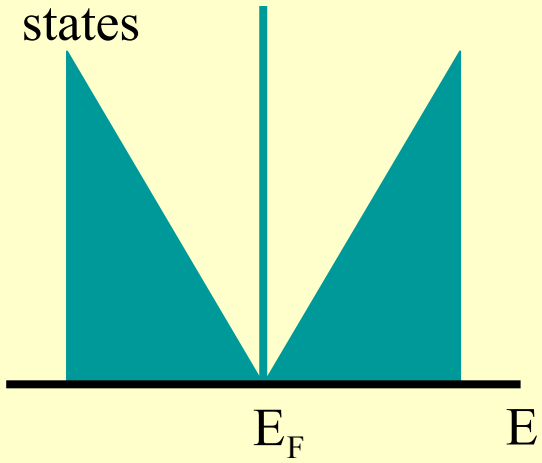
M. A. H. Vozmediano, M. P. López Sancho, T. Stauber and F. G., Phys. Rev. B **72**, 155121 (2005).

Localized states near a crack:



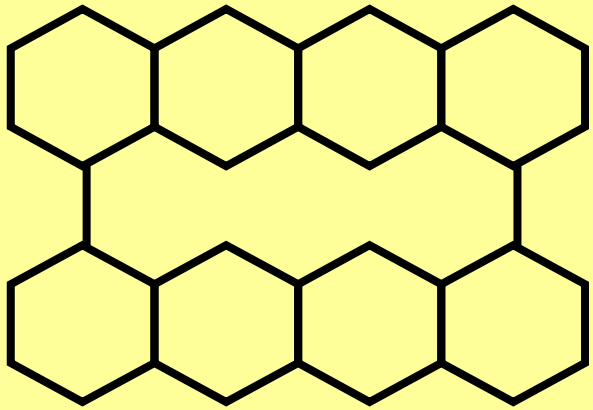
$$\Psi_n(z,\bar{z}) \equiv \begin{pmatrix} 0 \\ Re\left[\dfrac{A}{z^n\sqrt{z^2-a^2}}\right] \end{pmatrix}$$

Density of states

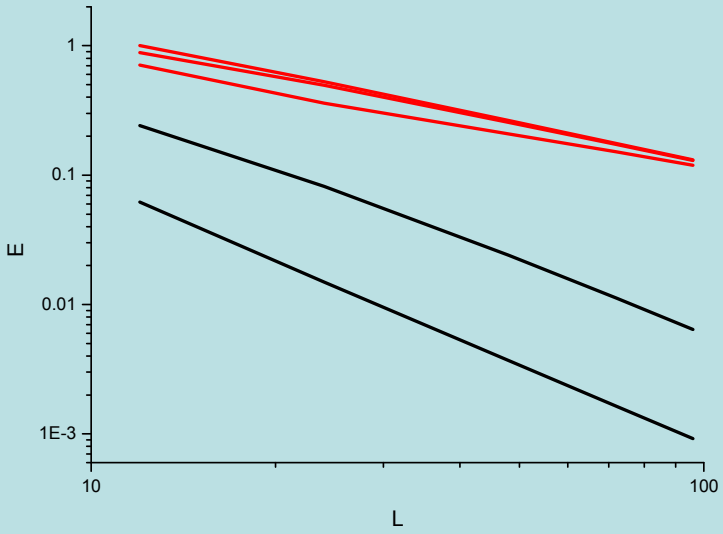


Exchange effects polarize these states.

Other types of defects.



Tight binding model



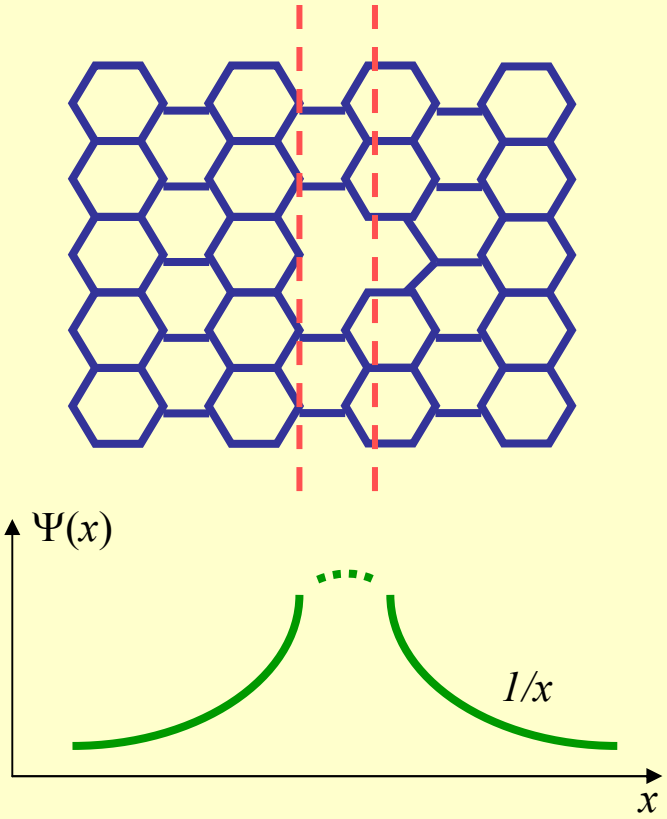
Scaling of eigenenergies close to zero

Interaction between local moments: $J_{RKKY}(\vec{r}) \approx (Ua^2)^2 \int d^2\vec{k}\, e^{i\vec{k}\vec{r}}\, \chi(\vec{k}) \approx \frac{(Ua^2)^2}{\hbar v_F |\vec{r}|^3}$

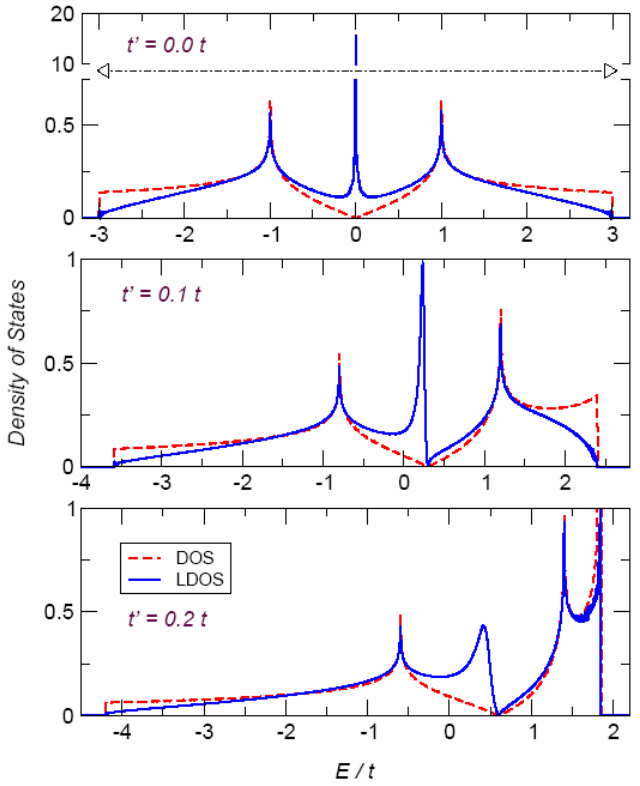
The RKKY coupling does not change sign.

(Half) localized states near vacancies.

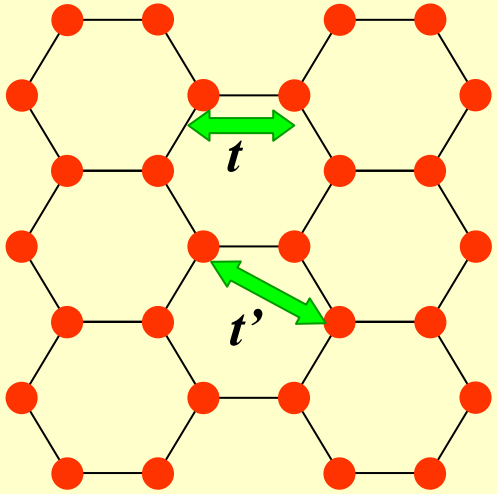
V. M. Pereira, F. G., J. M. P. Lopes dos Santos, N. M. R. Peres, and A. H. Castro Neto, cond-mat/0508530, Phys. Rev. Lett., in press



A single vacancy induces a slowly decaying state in the π band near zero energy,



Deviations from electron-hole symmetry

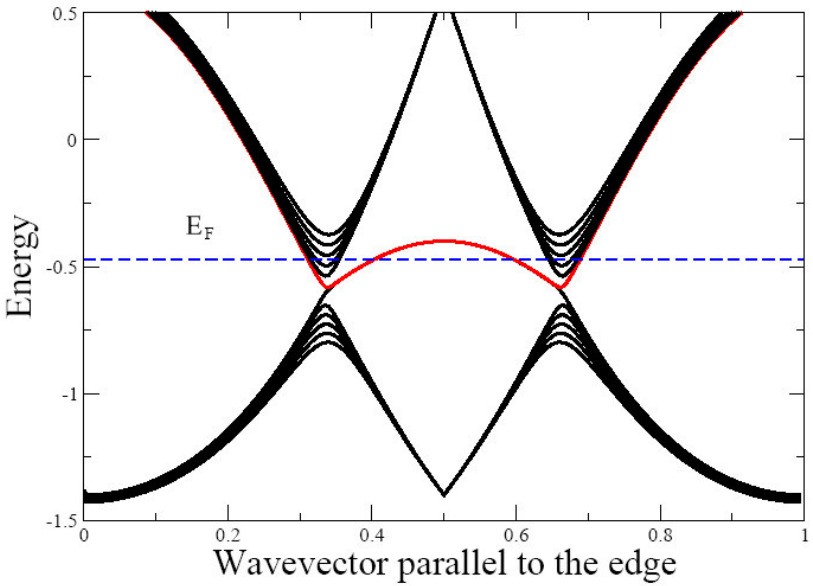


N. M. R. Peres, F. G. and A. H. Castro Neto, cond-mat/0506709

Hoppings between π orbitals:

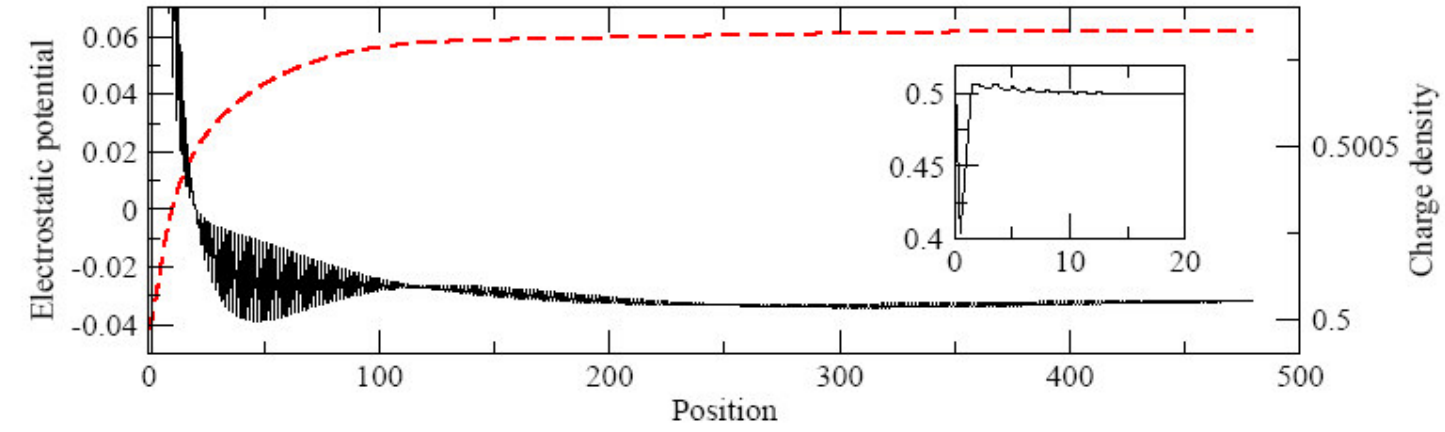
$t = 3\text{eV}$

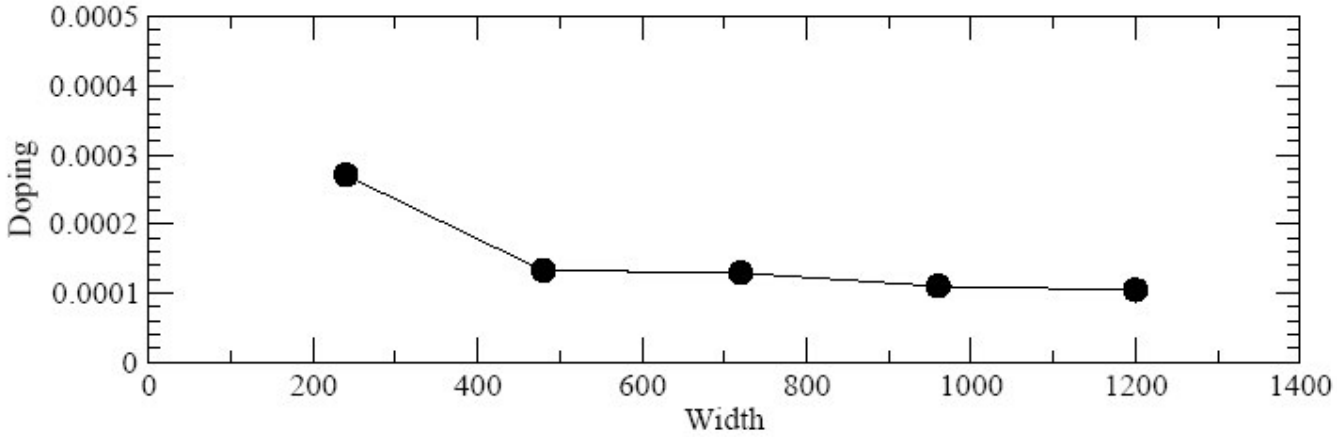
$t' \sim 0.2t = 0.5\text{eV}$



Charge is transferred between states localized near defects and extended states

Self doping effects

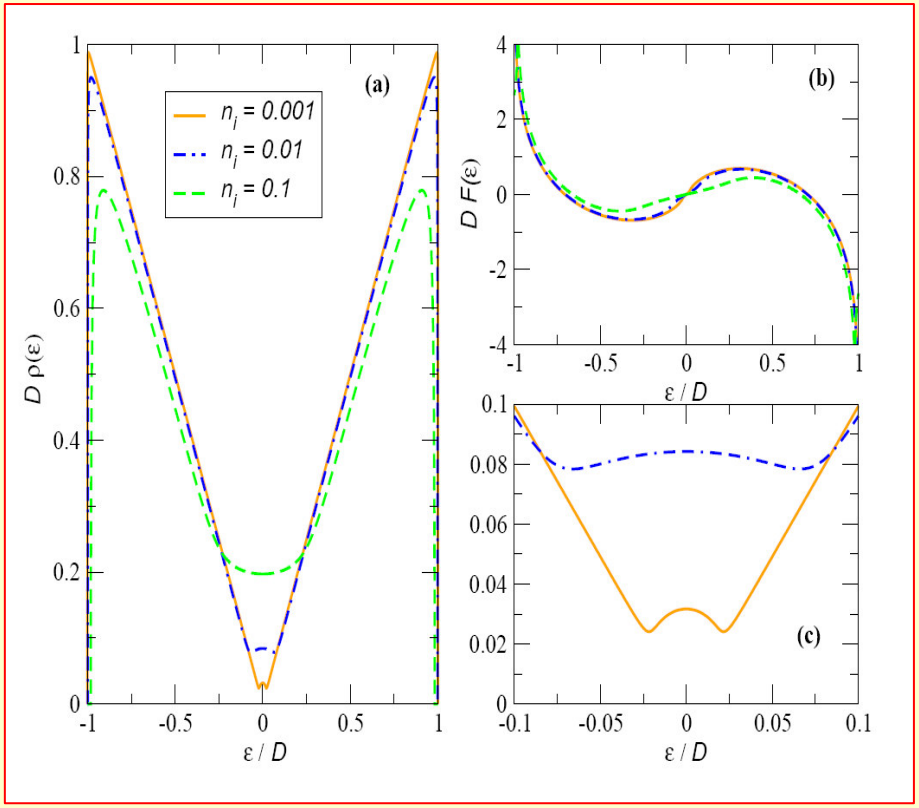




Distance between boundaries: 100 – 1000 nm
Doping (e per unit cell): 10^{-4} - 10^{-5}

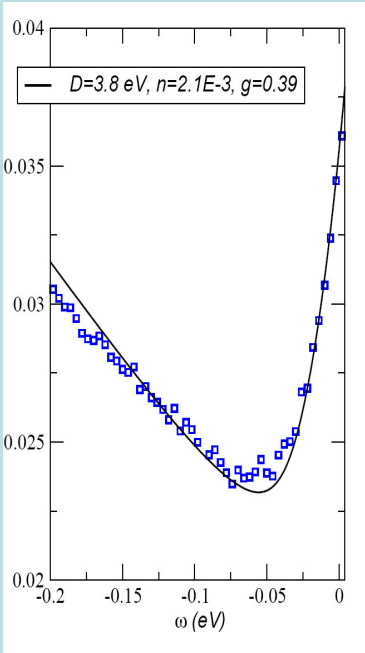
The bulk of the system remains in the clean limit

Local defects. Vacancies.



Density of states

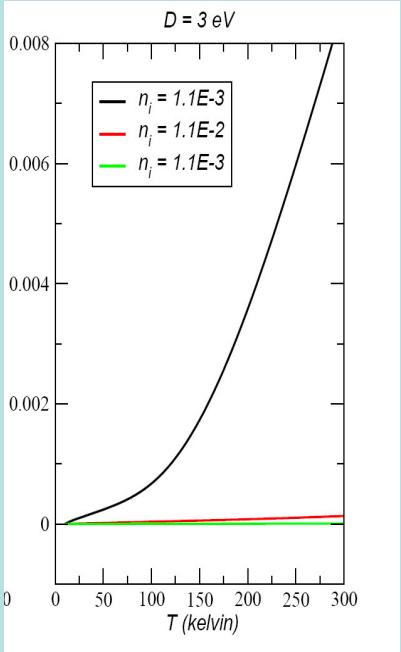
Selfenergy.
Elastic lifetime.



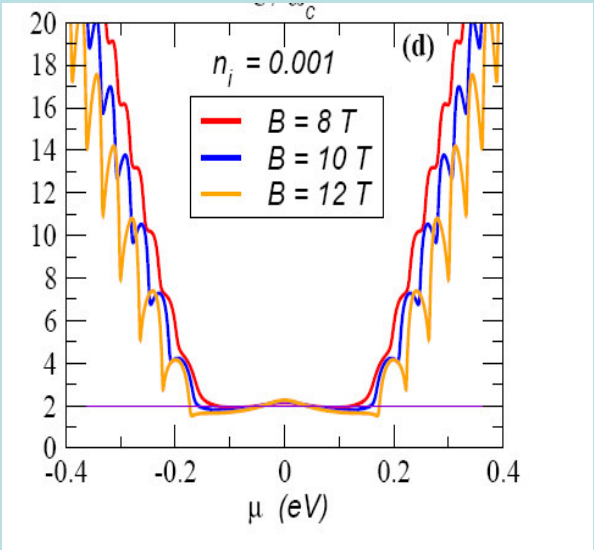
Elastic and inelastic lifetime.
Fit to ARPES data (A. Lanzara, *et al*, unpublished)

- Vacancies induce a finite density of states at the Fermi level.
- The elastic lifetime has a peak at zero frequency.

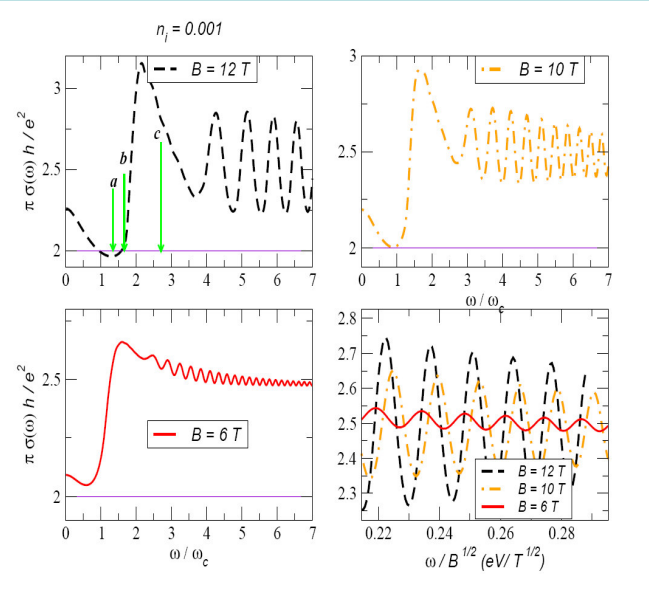
Conductivity.



Temperature dependence



Dependence on chemical potential.



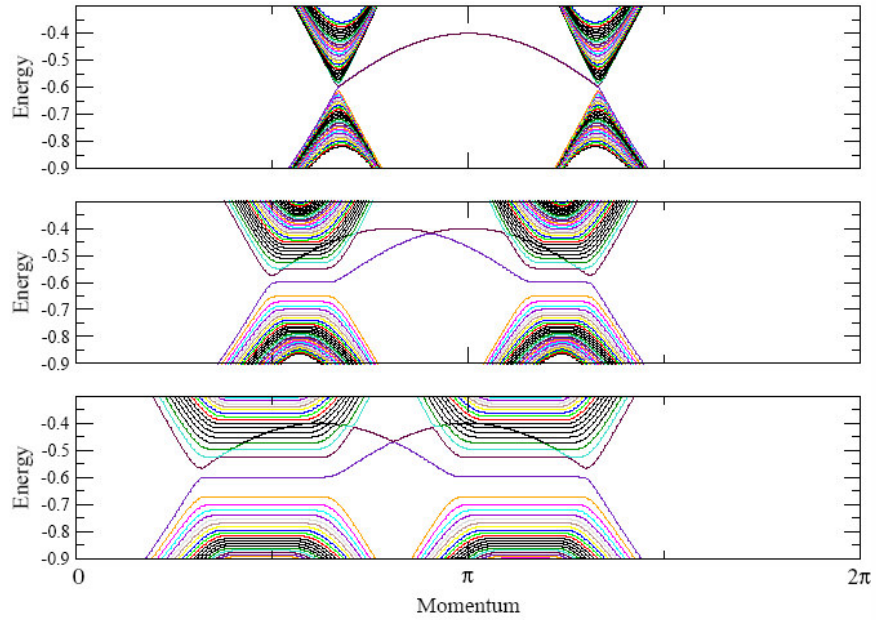
Frequency and magnetic field dependence.

- Universal conductivity at zero frequency and zero temperature.
- The conductivity increases with temperature.

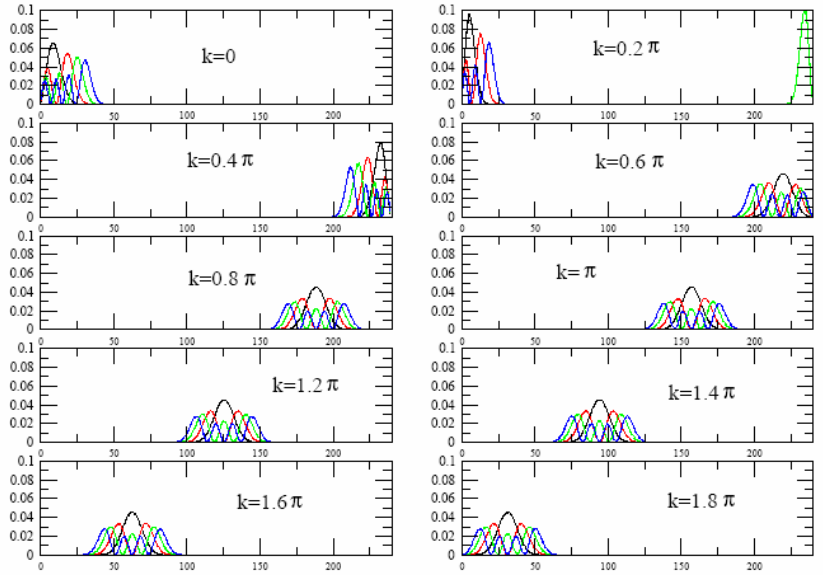
$$\lim_{T\to 0}\sigma_{DC} = \frac{4e^2}{\pi h}$$

E. Fradkin, Phys. Rev. B **33**, 3257 (1986)
P. A. Lee, Phys. Rev. Lett. **71**, 1887 (1993).

Quantum Hall effect



Energy bands as function of magnetic field.
Landau levels and surface states.

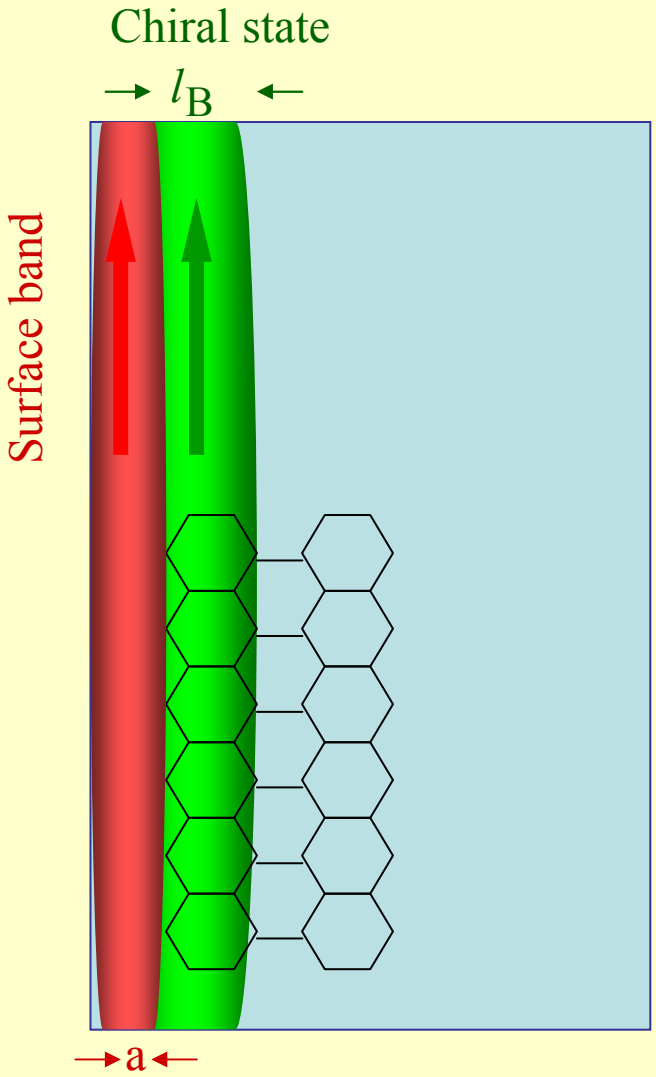


Spatial extension of Landau levels and
surface states

$$\sigma_{xy} = \frac{2e^2}{\hbar}(2n+1)$$

Fractional Quantum Hall effect.

A. H. Castro Neto, F. G., and N. M. R. Peres, cond-mat/0509709

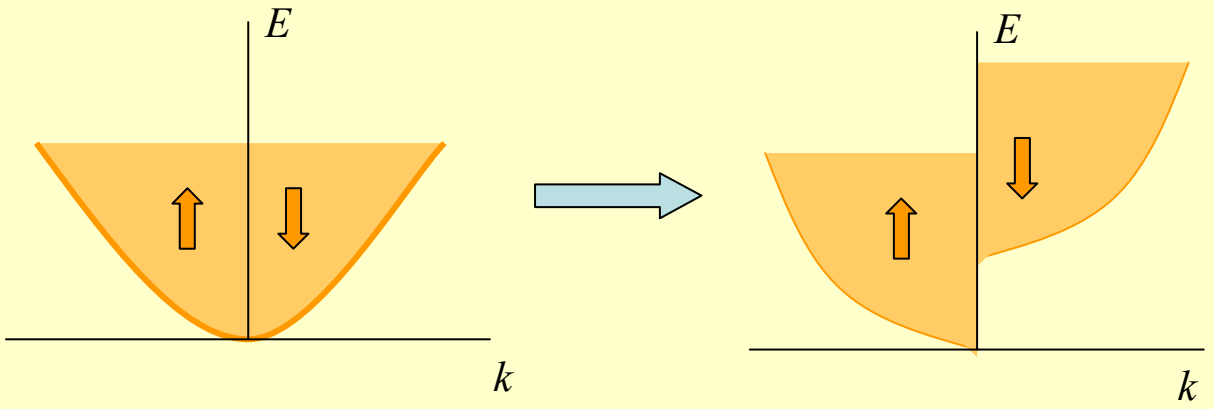


- Total Hall current due to edge Landau levels and surface states.
- Deviations from universal values.
- Finite longitudinal resistance.
- Luttinger liquid features
- The electrons in the surface band are dragged by the field induced chiral states..

C. C. Chamon and X.-G. Wen, Phys. Rev. B **49**, 8227 (1994)

Exchange instability in graphene.

N. M. R. Peres, F. G. and A. H. Castro Neto, Phys. Rev. B **72**, 174406 (2005)



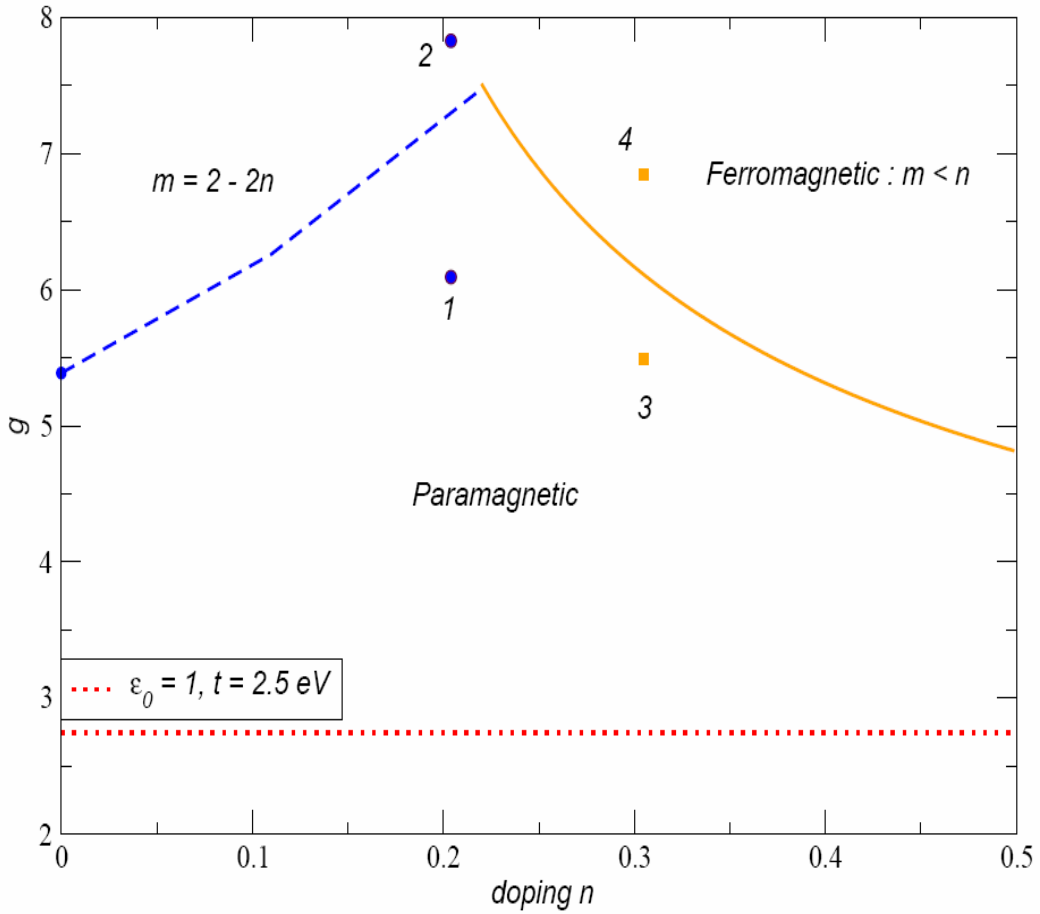
$$E(k_\uparrow, k_\downarrow) = \frac{A}{4\pi}\frac{\hbar^2}{2m}(k_\uparrow^4 + k_\downarrow^4) + \frac{A}{4\pi^2}\frac{e^2}{2\epsilon_0}\frac{8}{3}(k_\uparrow^3 + k_\downarrow^3)$$

Kinetic energy

Exchange energy

The exchange energy favors a ferromagnetic ground state.
This instability is expected in a low density 2DEG.

Exchange instability in graphene.



The instability requires too high coupling values.

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

The instability is enhanced in the presence of disorder (neglecting localized states).

$$g_c \approx 3.8$$

What next?

- **Bilayers, multiple layers.**

E. McCann and V. I. Fal'ko, cond-mat/0510237.
A. K. Geim, *et at*, unpublished.

- **Nanostructures.**

C. Berger, Z. M. Song, T. B. Li, A. Y. Oabazghi, R. Feng, Z. T. Dai, A. N. Marchenkov, E. H. Conrad, P. N. First, and W. A. de Heer, J. Phys. Chem. B **108**. 19912 (2004).
J. S. Bunch, Y. Yaish, M. Brink, K. Bolotin, and P. L. McEuen, Nano Lett. **5**, 287 (2005).

- **Magnetism in graphite and related structures.**

Carbon Based Magnetism: an Overview of metal free carbon-based compounds and materials T. Makarova and F. Palacios eds. Elsevier, Amsterdam (2005).

- **(Strong) disorder, interactions.**
- **Nature of clean, 3D, graphite.**

N. B. Brandt, S. M. Chudinov, and Ya. G. Ponomarev, in **Modern Problems in Condensed Matter Sciences,** V. M. Agranovich and A. A. Maradudin, North Holland, Amsterdam (1988).
I. A. Luk'yanchuk and Y. Kopelevich, Phys. Rev. Lett. **93**, 166402 (2004).