Electronic Properties of Graphene

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Solid State II

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OUTLINES

1. Introduction

2. Crystal Structure

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3. Dirac Cones
    (1) theoretical results
    (2) experimental results

4. Conclusions

Introduction

- 1935 L.D. Landau and R.E. Peierls
- 1946 P. R. Wallace

  P.R. Wallace, Physical Review **71**, 622-634 (1947)
- 2004 K.S. Novoselov

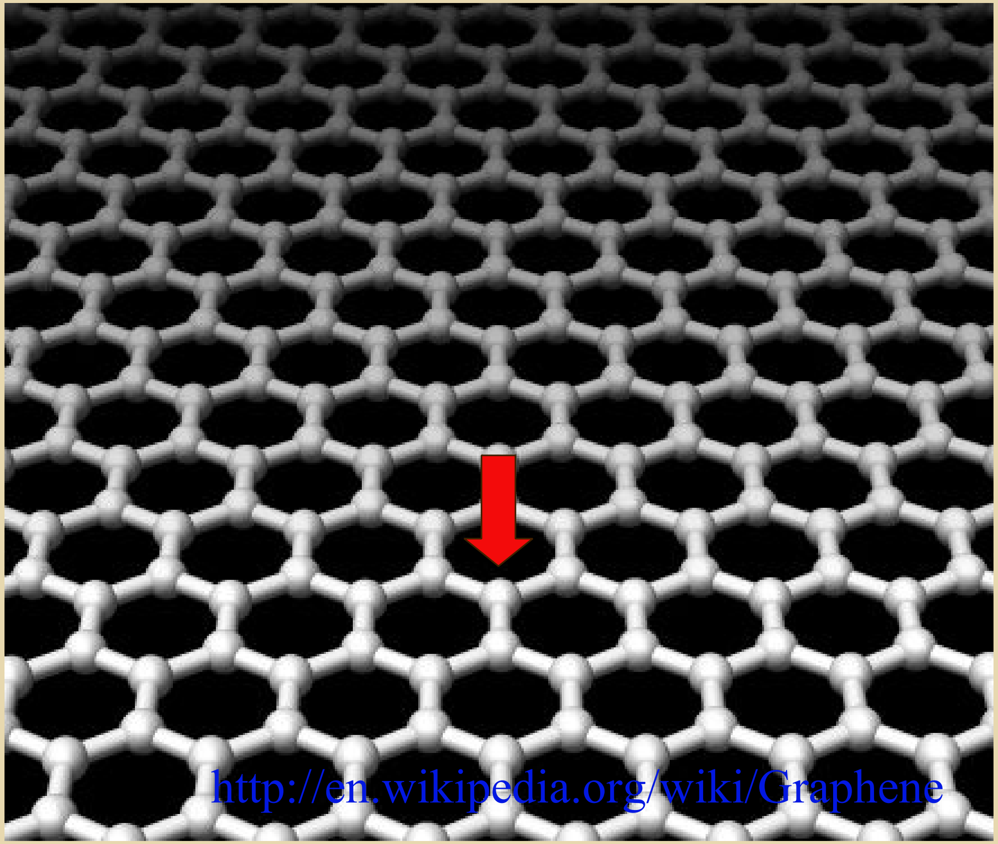
  K.S. Novoselov *et al*, Science **306**, 5696 (2004)
- 2005 K.S. Novoselov

  K.S. Novoselov *et al*, Nature **438**, 197-200 (2005)

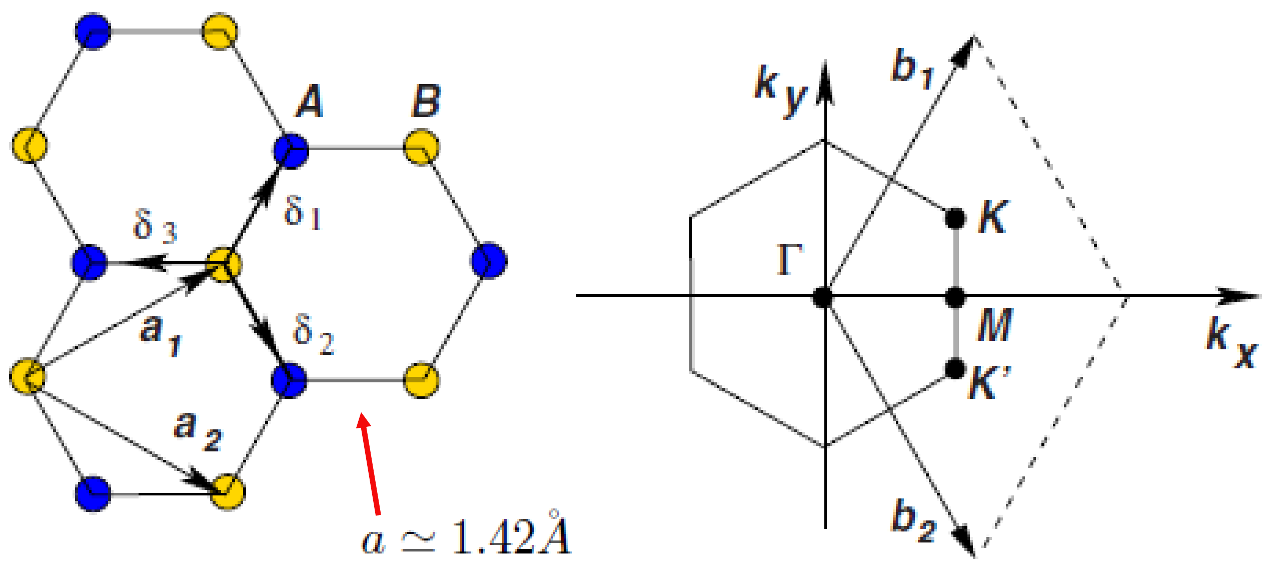
Introduction

- **what is graphene?**

- carbon
- monolayer
- honeycomb



Crystal Structure



- Left: structure lattice
  two triangular sublattices

$$a_1 = \frac{a}{2}(3, \sqrt{3}), \qquad a_2 = \frac{a}{2}(3, -\sqrt{3})$$

$$\delta_1 = \frac{a}{2}(1, \sqrt{3}), \quad \delta_2 = \frac{a}{2}(1, -\sqrt{3}), \quad \delta_3 = -a(1,0)$$

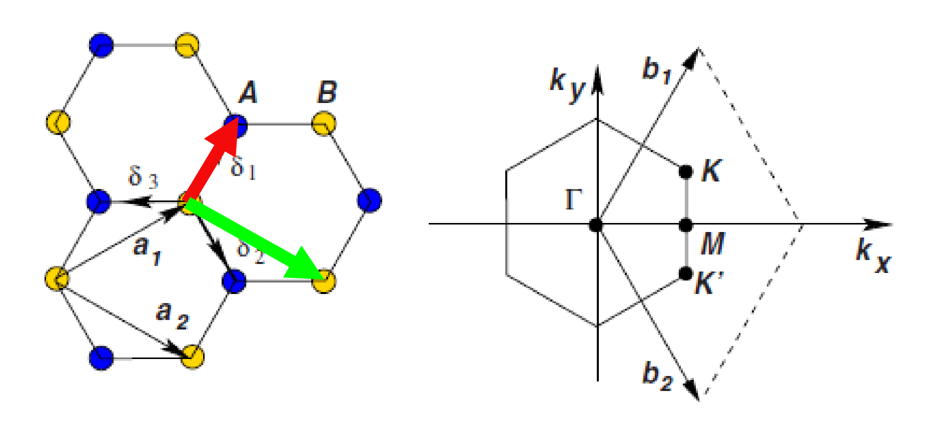
$$\delta'_1 = \pm a_1, \quad \delta'_2 = \pm a_2, \quad \delta'_3 = \pm(a_2 - a_1)$$

- Right: correponding BZ
  Dirac cones are located at:

$$K = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right), \qquad K' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right)$$

A.H. Castro Neto et al, Rev. Mod. Phys **81**, 109-162 (2009)

Dirac cones



$$a_1 = \frac{a}{2}(3, \sqrt{3}), \qquad a_2 = \frac{a}{2}(3, -\sqrt{3})$$

$$\delta_1 = \frac{a}{2}(1, \sqrt{3}), \quad \delta_2 = \frac{a}{2}(1, -\sqrt{3}), \quad \delta_3 = -a(1, 0)$$

$$\delta_1' = \pm a_1, \quad \delta_2' = \pm a_2, \quad \delta_3' = \pm(a_2 - a_1)$$

$$K = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right), \qquad K' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right)$$

- Tight-binding Hamiltonian:

$$H = -t_1 \sum_{<i,j>,\sigma} (a_{i,\sigma}^\dagger b_{j,\sigma} + h.c.) - t_2 \sum_{<<i,j>>,\sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + b_{i,\sigma}^\dagger b_{j,\sigma} + h.c.)$$

NN NNN

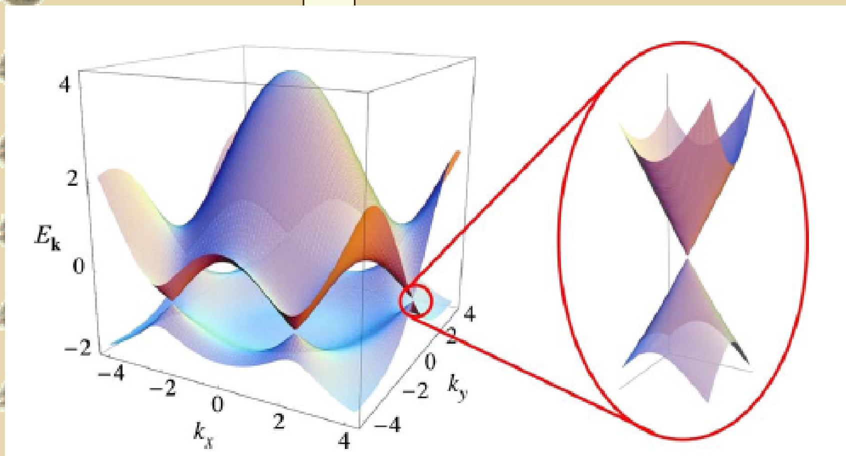
A.H. Castro Neto et al, Rev. Mod. Phys **81**, 109-162 (2009)

Dirac cones

$$H = -t_1 \sum_{<i,j>,\sigma} (a^\dagger_{i,\sigma} b_{j,\sigma} + h.c.) - t_2 \sum_{<<i,j>>,\sigma} (a^\dagger_{i,\sigma} a_{j,\sigma} + b^\dagger_{i,\sigma} b_{j,\sigma} + h.c.)$$

$$H = \sum_{\vec{k},\sigma} (T_1 a^\dagger_{\vec{k},\sigma} b_{\vec{k},\sigma} + T_2 b^\dagger_{\vec{k},\sigma} a_{\vec{k},\sigma} + T_3 (a^\dagger_{\vec{k},\sigma} a_{\vec{k},\sigma} + b^\dagger_{\vec{k},\sigma} b_{\vec{k},\sigma}))$$

$$\begin{aligned} T_1 &= -t_1 (2 e^{i\frac{a}{2}k_x} \cos(\frac{\sqrt{3}}{2} a k_y) + e^{-iak_x}) \\ T_2 &= -t_1 (2 e^{-i\frac{a}{2}k_x} \cos(\frac{\sqrt{3}}{2} a k_y) + e^{iak_x}) \\ T_3 &= -t_2 (4 \cos(\frac{3}{2} a k_x) \cos(\frac{\sqrt{3}}{2} a k_y) + 2\cos(\sqrt{3} a k_y)) \end{aligned}$$



$$E_\pm(\vec{k}) = \pm t_1 \sqrt{3 + f(\vec{k})} - t_2 f(\vec{k})$$

$$f(\vec{k}) = 2\cos(\sqrt{3} a k_y) + 4\cos(\frac{\sqrt{3}}{2} a k_y) \cos(\frac{\sqrt{3}}{2} a k_y)$$

t1=2.7 eV t2=-0.2t1

A.H. Castro Neto et al, Rev. Mod. Phys **81**, 109-162 (2009)

Dirac cones

$$E_\pm(\vec{k}) = \pm t_1\sqrt{3 + f(\vec{k})} - t_2 f(\vec{k}) \qquad t_2 << t_1$$

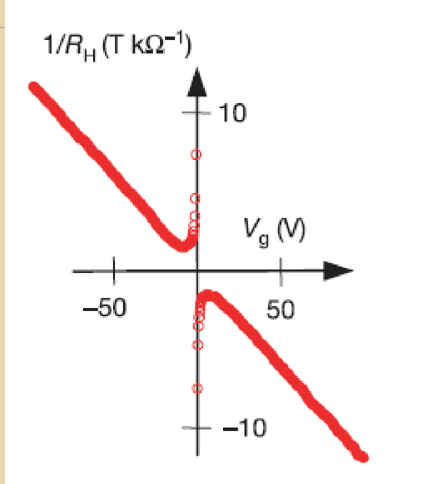
expanding around point $K = (\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a})$ as

with $|\vec{q}| \ll \vec{K}$

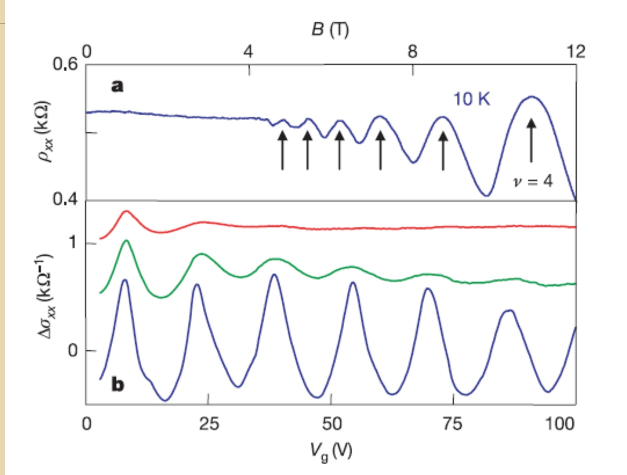
$$E_\pm(\vec{q}) \approx \pm t_1\sqrt{(\frac{3a}{2}q_x)^2 + (\frac{3a}{2}q_x)^2 + O(q_x^3) + O(q_y^3)}$$
$$= \pm v_F|\vec{q}| + O[q^2]$$

$$v_F = \frac{3at_1}{2} \simeq 1 \times 10^6 m/s.$$

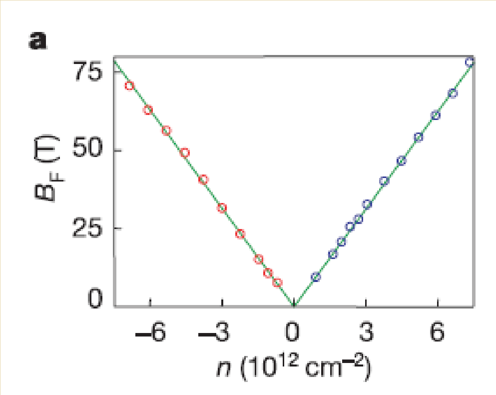
Dirac cones



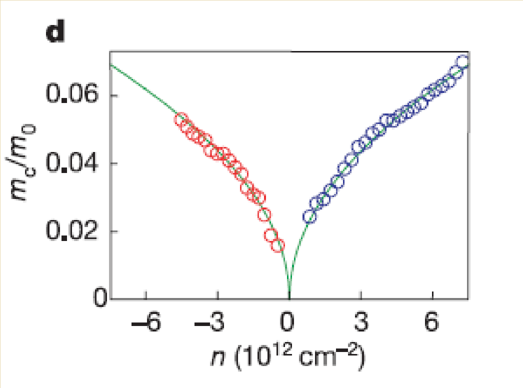
Electric field effect



Shubnikov-de Hass oscillations (SdHOs)



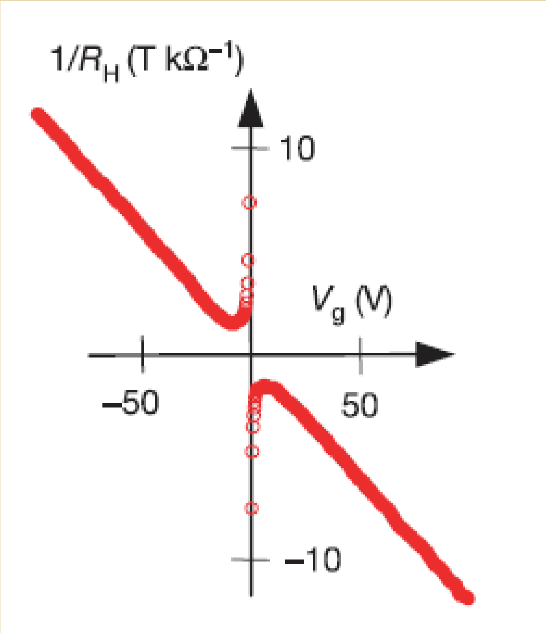
SdHOs frequency vs. carrier concentration



Cyclotron mass vs. carrier concentration

K.S. Novoselov et al, Nature **438**, 197-200 (2005)

Dirac cones

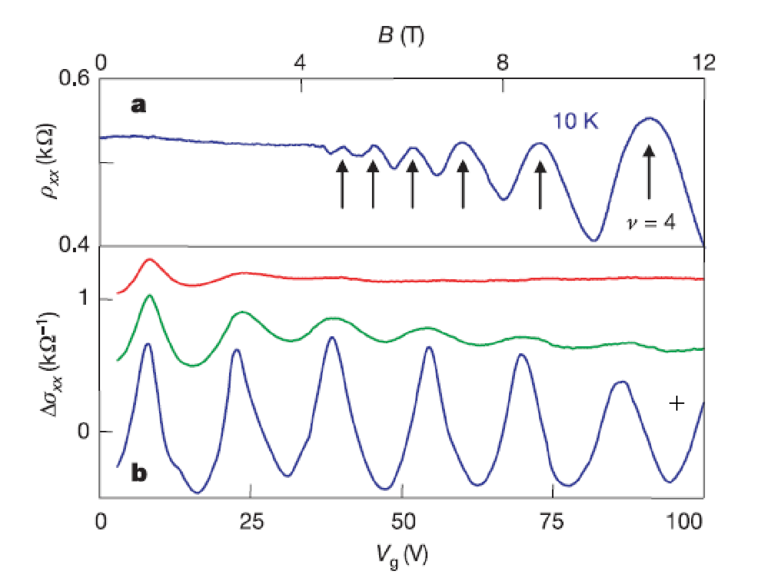


Electric field effect

$$\frac{1}{R_H} \propto V_g \qquad R_H = \frac{1}{ne}$$

$$V_g \propto n$$

Dirac cones



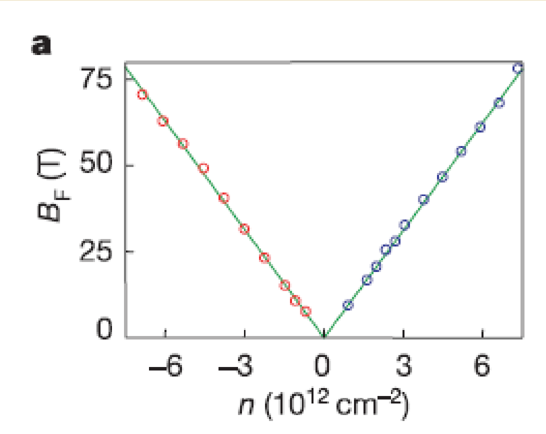
Shubnikov-de Hass oscillations (SdHOs)

- plot the dependence of SdHO frequency B_F on gate voltage V_g by using standard fan diagrams

$$V_g \propto n$$

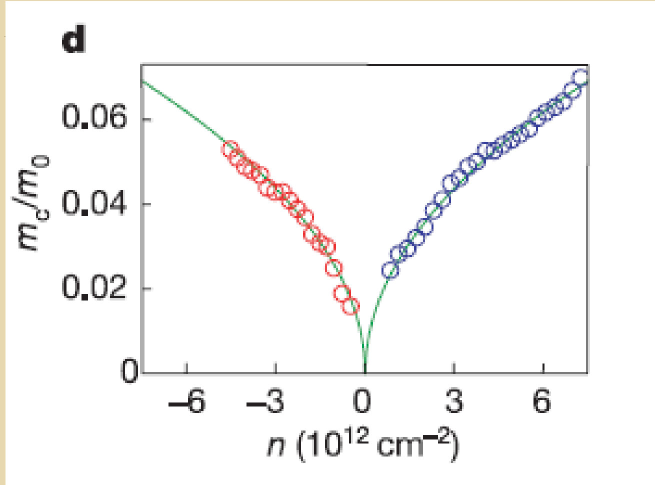
$$B_F = \beta n$$

$$\beta \approx 1.04 \times 10^{-15}\,\mathrm{Tm}^2 \quad (\pm 2\%)$$



SdHOs frequency vs. carrier concentration

Dirac cones



Cyclotron mass vs. carrier concentration

square-root dependence

$$m_c \propto n^{1/2}$$

$$B_F = \beta n$$

$$V_g \propto n$$

mc: cyclotron mass of carrier
(effective mass)

Dirac cones

- Semi-classical expression (Ashcroft & Mermin):

$$B_F = \frac{\hbar}{2\pi e} S(E) \qquad\qquad m_c = \frac{\hbar^2}{2\pi} \frac{\partial S(E)}{\partial E}$$

where $S(E) = \pi k^2$ is the area in k-space of the orbits at the Fermi energy

Dirac cones

$$B_F = \frac{\hbar}{2\pi e} S(E) \quad \xrightarrow{B_F = \beta n} \quad S(E) = \frac{2\pi e}{\hbar} \beta n \propto n$$

$$+$$

$$m_c = \frac{\hbar^2}{2\pi} \frac{\partial S(E)}{\partial E} \quad \xrightarrow{m_c \propto n^{1/2}} \quad \frac{\partial S(E)}{\partial E} \propto n^{1/2}$$

$$\frac{\partial S(E)}{\partial E} \propto \sqrt{S(E)}$$

$$S(E) = \pi k^2 \quad + \quad S(E) \propto E^2$$

$$E \propto k = \hbar c^* k$$

$$c^* \approx 10^6\, m/s$$

Conclusions

- A tight-binding model is investigated to calculate the band dispersion of graphene
- Linear dependence of energy on momentum is deduced from quantum oscillations and electric field effect experiments
- Both calculation and the experiments lead to a linear band dispersion with the same Fermi velocity $v_F \approx 10^6 m/s$

Thank you!

Comments

- The detail information of relativistic theory about graphene can be found in:

  A.H. Castro Neto *et al*, Rev. Mod. Phys **81**, 109-162 (2009)

  and also

  http://en.wikipedia.org/wiki/Graphene