2. Bandstructure of monolayer graphene

Why graphene ?



graphene is **2D**, "relativistic", chiral and won a flagship !



appond "the future in a trace of a pencil"

- thin, but strong
- best thermal conductor
- excellent electrical conductor
- transparent
- flat 2.3% light absorption
- applications ...



Graphene Press Seminar – October 10, 2013

Graphene is 2D

dimensional dependence of electronic properties

when do metals exists ?

- 0d "insulator"
- 1d (infinite long wire) insulator for $T \rightarrow 0$
- 2d **?**
- 3d there are materials that stay metals at all temperatures



Graphene



Sheldon in Big Bang Theory





I follow the manuscript "Bandstructure of Graphene and Carbon Nanotubes: An Exercise in Condensed Matter Physics". I abbreviate this with BG

3 · sp² orbitals/bonding,
4th valence electron →
"bonding" and "antibonding" states

 π and π^* bands



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goal: calculate the energy of the eigenstates in tight-binding approximation (LCAO). Further, derive a simplified (effective) Hamiltonian.

Bandstructure of graphene, see BG-2 to 15

Ansatz of the wavefunction (Bloch function)

R is a lattice vector and ϕ_1 , ϕ_2 are p_z orbitals of the A(1) and B(2) sites

$$\psi_{\vec{k}} = \sum_{\vec{R} \in G} e^{i\vec{k} \cdot \vec{R}} \phi(\vec{x} - \vec{R}) \,,$$

$$\phi(\vec{x}) = b_1 \phi_1(\vec{x}) + b_2 \phi_2(\vec{x}) = \sum_n b_n \phi_n$$

Hamiltonian:

 $\gamma_1 \begin{pmatrix} 0 & \alpha \\ \alpha^* \end{pmatrix}$

$$H = \frac{\vec{p}^2}{2m} + \sum_{\vec{R} \in G} \left(V_{at}(\vec{x} - \vec{x}_1 - \vec{R}) + V_{at}(\vec{x} - \vec{x}_2 - \vec{R}) \right)$$

Note: in this problem there are only two unknowns, b_1 and b_2 . Hence 2 equations need to be derived. These can be obtained by using expectation values of the Schrödinger equation:

$$H\psi_{k} = E(k)\psi_{k} - \begin{bmatrix} \langle \phi_{1} | H | \psi_{k} \rangle = E\langle \phi_{1} | \psi_{k} \rangle \longrightarrow \langle \phi_{1} | \Delta U | \psi_{k} \rangle \cong Eb_{1} \longrightarrow \gamma_{1}\alpha \cdot b_{2} \cong Eb_{1} \\ \langle \phi_{2} | H | \psi_{k} \rangle = E\langle \phi_{2} | \psi_{k} \rangle \longrightarrow \langle \phi_{2} | \Delta U | \psi_{k} \rangle \cong Eb_{2} \longrightarrow \gamma_{1}\alpha^{*} \cdot b_{1} \cong Eb_{2} \end{bmatrix}$$

where $\gamma_1 = \langle \phi_1 | \Delta U | \phi_2 \rangle$ is the nearest neighbor overlap, which has three contributions captured by α $\alpha(\vec{k}) = 1 + e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2}$

$$= E \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$
 note: this is already a (a further assumption is

 b_2 note: this is already a bit more simplified than equation BG-15 (a further assumption is that the energy of the atomic p_z orbital is set to zero)

$$\gamma_{1}\begin{pmatrix} 0 & \alpha \\ \alpha^{*} & \end{pmatrix} \begin{pmatrix} b_{1} \\ b_{2} \end{pmatrix} = E \begin{pmatrix} b_{1} \\ b_{2} \end{pmatrix} \longrightarrow E (\vec{k}) = \pm \gamma_{1} |\alpha(\vec{k})|$$
$$E(k_{x}, k_{y}) = \pm \gamma_{1} \sqrt{1 + 4\cos\left(\frac{\sqrt{3}ak_{y}}{2}\right)\cos\left(\frac{ak_{x}}{2}\right) + 4\cos^{2}\left(\frac{ak_{x}}{2}\right)}$$
(18)

a is the lattice constant, i.e. $a = \sqrt{3}a_0$. Note: Tero's a is my a_0



reciprocal lattice











$$\gamma_1 \begin{pmatrix} 0 & \alpha \\ \alpha * & \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = E \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

linearize around e.g. K-point: $\vec{k} = \vec{K} + \vec{\kappa}$

$$\varepsilon(\vec{\kappa}) = E(\vec{k}) - E(\vec{K})$$

$$\mathcal{E}(\vec{\kappa}) = \pm \hbar v_F \left| \vec{\kappa} \right|$$

(note, one gets in addition an expression forthe Fermi velocity)

$$\widetilde{H} = \hbar v_F \begin{pmatrix} 0 & \mp \kappa_x - i\kappa_y \\ \mp \kappa_x + i\kappa_y & 0 \end{pmatrix} = \hbar v_F (\mp \kappa_x \sigma_x + \kappa_y \sigma_y)$$

The two signs correspond to **the two valleys**, see Heikkilä equ. (10.10) Note: the **Pauli matrices** operate on **"pseudo-spin"** (b1,b2). The real spin is conserved in the Hamiltonian. Note further that for one sign the equation is exactly the **massless Dirac equation** in 2D

$$H_D = c\vec{\sigma}\cdot\vec{p} + \beta mc^2$$

the velocity of light c is replaced by v_F

$$\begin{pmatrix} \mu_g & \hbar v_F \left(\pm i \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \\ \hbar v_F \left(\pm i \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) & \mu_g \end{pmatrix} \begin{pmatrix} \psi_A(x, y) \\ \psi_B(x, y) \end{pmatrix} = E \begin{pmatrix} \psi_A(x, y) \\ \psi_B(x, y) \end{pmatrix}$$
(10.11)
$$\Psi(x, y) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{\mp i \phi/2} \\ s e^{\pm i \phi/2} \end{pmatrix} e^{i(\pm k_x x + k_y y)} \qquad E(\vec{k}) = \mu_g \pm \hbar v_F \Big| \vec{k} dx$$

+/- corresponds to the two valleys

Note: Tero uses again E and k. Also s=sign(E) further:

$$\phi = \arctan(k_x / k_y)$$

→ graphene is chiral



Chirality in graphene (and CNT)

one can define a helicity as:





Paul Mc Euen et al. Phys. Rev. Lett. 83, p5098 (1999)

3. Bandstructure of carbon nanotubes and graphene nanoribbons

Bandstructure of carbon nanotubes

chiral vector $\vec{w} = n_1 \vec{a}_1 + n_2 \vec{a}_2$



example: armchair CNT



example: armchair CNT



how ballistic can it be?

VOLUME 87, NUMBER 10

PHYSICAL REVIEW LETTERS

3 September 2001

Quantum Interference and Ballistic Transmission in Nanotube Electron Waveguides

Jing Kong, Erhan Yenilmez, Thomas W. Tombler, Woong Kim, and Hongjie Dai Department of Chemistry and Laboratory for Advanced Materials, Stanford University, Stanford, California 94305

> Robert B. Laughlin Department of Physics, Stanford University, Stanford, California 94305

Lei Liu, C. S. Jayanthi, and S. Y. Wu Department of Physics, University of Louisville, Louisville, Kentucky 40292

(Received 27 February 2001; published 16 August 2001)

The electron transport properties of well-contacted individual single-walled carbon nanotubes are investigated in the ballistic regime. Phase coherent transport and electron interference manifest as conductance fluctuations as a function of Fermi energy. Resonance with standing waves in finite-length tubes and localized states due to imperfections are observed for various Fermi energies. Two units of quantum conductance $2G_0 = 4e^2/h$ are measured for the first time, corresponding to the maximum conductance limit for ballistic transport in two channels of a nanotube.



Data CNT from our own lab



Minkyung Jung et al.

general CNT (chiral)



Graphene:

hexagonal lattice of carbon atoms



Atomically resolved STM image of a single-wall carbon nanotube.



Wildöer et al, Nature **391**, 59 (1998)

general CNT (chiral)

- Armchair = All metallic
- The rest are metallic only when (m - n) = multiple of 3











simplified band structure



Graphene nanoribbons



GNR band structure for zig-zag type (in CNT notation, this is armchair). Tight binding calculations predict that zigzag type is always metallic

GNR band structure for armchair type. Tight binding calculations show that armchair type can be semiconducting or metallic depending on width.

4. Bandstructure of bilayer (multilayer) graphene



 $H = \begin{pmatrix} 0 & v\pi^{+} & 0 & 0 \\ v\pi & 0 & \gamma_{1} & 0 \\ 0 & \gamma_{1} & 0 & v\pi^{+} \\ 0 & 0 & v\pi & 0 \end{pmatrix}$ in the basis A_1, B_1, A_2, B_2

left: band structure for u=0 (no interlayer electric field). Bands have massive, but still they are chiral)



Figure 2. (a) Plan and (b) side view of the crystal structure of bilayer graphene. Atoms A1 and B1 on the lower layer are shown as white and black circles, A2, B2 on the upper layer are black and grey, respectively. The shaded rhombus in (a) indicates the conventional unit cell.



Figure 2. (a) Plan and (b) side view of the crystal structure of bilayer graphene. Atoms A1 and B1 on the lower layer are shown as white and black circles, A2, B2 on the upper layer are black and grey, respectively. The shaded rhombus in (a) indicates the conventional unit cell.

v₃ term can close the gap again. Effect known as trigonal warping and results into a so called **Lifshitz transition**

McCann Rep. Prog. Phys. 76, 056503 (2013)

5. Charaterization





locate flakes in optical microscope...

... and identify the number of layer with Raman spectroscopy.(also reveals chemical doping and contaminations)

Quantum Hall effect in monolayer graphene



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

Quantum Hall effect in bilayer graphene



zero-energy LL has 8-fold degeneracy

 \rightarrow expect also broken symmetry states in clean samples

Feldman et al. Nature Phys. 5, p889 (2009) Zhao et al. Phys. Rev.Lett. 104, p066801 (2010)



from our lab (very recent)



L. Wang, et al., Science, 342, 614 (2013);



3 B (T) 5

6

2

-20

-30

0

-> SLG (single layer)

C. Handschin, B. Fülöp, P. Makk et al.

6. Electron optics in ballistic graphene



Conservation of transverse momentum Snell's law

$$\vec{k}_l \sin \theta_l = \vec{k}_r \sin \theta_r$$

Bipolar interface (nn' or pp')



Conservation of transverse momentum **anomalous** Snell's law

 $\vec{k}_l \sin \theta_l = -\vec{k}_r \sin \theta_r$

reason: velocity is opposite to wavevector in p-doped regions



wavefunctions at the two sides of a sharp potential step:



solution chosen so that helicity is correct on the right side

electron diffraction



PHYSICAL REVIEW B 74, 041403(R) (2006)

Selective transmission of Dirac electrons and ballistic magnetoresistance of *n-p* junctions in graphene

Vadim V. Cheianov and Vladimir I. Fal'ko Department of Physics, Lancaster University, Lancaster, LA1 4YB, United Kingdom (Received 23 March 2006; revised manuscript received 21 May 2006; published 17 July 2006)

We show that an electrostatically created n-p junction separating the electron and hole gas regions in a graphene monolayer transmits only those quasiparticles that approach it almost perpendicularly to the n-p interface. Such a selective transmission of carriers by a single n-p junction would manifest itself in nonlocal magnetoresistance effect in arrays of such junctions and determines the unusual Fano factor in the current noise universal for the n-p junctions in graphene.

angle-filtering at sharp p-n interface: $w_{\text{step}}(\theta) = \cos^2 \theta$

in contrast, at a soft interface classically all trajectories are reflected



quantum-mechanically the particles **can tunnel** from one side to the other with probability:

$$w(\theta) = e^{-\pi (k_F d) \sin^2 \theta}.$$

FIG. 1. (Color online) Angular dependence of quasiparticle transmission through the electrostatically generated n-p junction in graphene.

Klein effect Klein tunneling

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FIG. 1. (Color online) Angular dependence of quasiparticle transmission through the electrostatically generated n-p junction in graphene.

Klein effect Klein tunneling



where <T> is the mean transmission probability







Similar data published in: P. Rickhaus, R. Maurand, M.H. Liu et al. Nature Comm. 4, 2342 (2013)







P. Rickhaus, R. Maurand, M.H. Liu et al. Nature Comm. 4, 2342 (2013)

The Focusing of Electron Flow and a Veselago Lens in Graphene *p-n* Junctions

Vadim V. Cheianov, ^{1*} Vladimir Fal'ko, ¹ B. L. Altshuler^{2,3}

The focusing of electric current by a single p-n junction in graphene is theoretically predicted. Precise focusing may be achieved by fine-tuning the densities of carriers on the n- and p-sides of the junction to equal values. This finding may be useful for the engineering of electronic lenses and focused beam splitters using gate-controlled n-p-n junctions in graphene-based transistors.



Fig. 1. Graphene *p-n* junction (PNJ). Monolayer of graphite is placed over the split gate, which is used to create *n*- (**left**) and *p*-doped (**right**) regions. The energy diagram shows the position of the Fermi level with respect to the touching point of the valence and the conduction bands.



the real **Klein-tunneling** experiment



from paper Katsnelson, Novoselov, Geim, Nature. Phys. 2, 620 (2006)

$$\begin{split} \psi_1(x,y) &= \begin{cases} (\mathrm{e}^{ik_x x} + r\mathrm{e}^{-ik_x x})\mathrm{e}^{ik_y y}, & x < 0, \\ (a\mathrm{e}^{iq_x x} + b\mathrm{e}^{-iq_x x})\mathrm{e}^{ik_y y}, & 0 < x < D, \\ t\mathrm{e}^{ik_x x + ik_y y}, & x > D, \end{cases} \\ \psi_2(x,y) &= \begin{cases} s(\mathrm{e}^{ik_x x + i\phi} - r\mathrm{e}^{-ik_x x - i\phi})\mathrm{e}^{ik_y y}, & x < 0, \\ s'(a\mathrm{e}^{iq_x x + i\theta} - b\mathrm{e}^{-iq_x x - i\theta})\mathrm{e}^{ik_y y}, & 0 < x < D, \\ st\mathrm{e}^{ik_x x + ik_y y + i\phi}, & x > D, \end{cases} \end{split}$$



transmission is **always one at normal incidence** in monolayer graphene

7. Pseudodiffusion in graphene



assume all is graphene, also the contacts but contacts at high doping (very large)

problem is similar to Klein tunneling matching of wave functions

Tworzydlo et al. Phys. Rev. Lett. 96, 24680 (2006)

Tero Heikkilä's book

$$T(k_y) = \frac{2q_x^2}{2q_x^2 + k_y^2(1 - \cos(2q_xL))},$$
(10.43)

(here, x is along junction, y is transverse. For $k_y=0$, i.e. normal incidence, transmission probability is 1)





assume all is graphene, also the contacts but contacts at high doping (very large)

problem is similar to Klein tunneling matching of wave functions

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Tworzydlo et al. Phys. Rev. Lett. 96, 24680 (2006)

"pseudo-diffusion in graphene"

PRL 100, 156801 (2008)

PHYSICAL REVIEW LETTERS

week ending 18 APRIL 2008

Shot Noise in Graphene

L. DiCarlo,¹ J. R. Williams,² Yiming Zhang,¹ D. T. McClure,¹ and C. M. Marcus¹ ¹Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA ²School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA (Received 20 November 2007; published 14 April 2008)

We report measurements of current noise in single-layer and multilayer graphene devices. In four single-layer devices, including a p-n junction, the Fano factor remains constant to within $\pm 10\%$ upon varying carrier type and density, and averages between 0.35 and 0.38. The Fano factor in a multilayer device is found to decrease from a maximal value of 0.33 at the charge-neutrality point to 0.25 at high carrier density. These results are compared to theories for shot noise in ballistic and disordered graphene.





"pseudo-diffusion in graphene"

PRL 100, 196802 (2008)

PHYSICAL REVIEW LETTERS

week ending 16 MAY 2008

Shot Noise in Ballistic Graphene

R. Danneau,^{1,*} F. Wu,¹ M. F. Craciun,² S. Russo,² M. Y. Tomi,¹ J. Salmilehto,¹ A. F. Morpurgo,² and P. J. Hakonen¹

(a)

g

с

900

800

700

600

¹Low Temperature Laboratory, Helsinki University of Technology, Espoo, Finland

²Kavli Institute of Nanoscience, Delft University of Technology Delft, The Netherlands

(Received 27 November 2007; published

We have investigated shot noise in graphene field effect devices low frequency (f = 600-850 MHz). We find that for our graphene ratio W/L, the Fano factor \mathfrak{F} reaches a maximum $\mathfrak{F} \sim 1/3$ at the \mathfrak{L} with increasing charge density. For smaller W/L, the Fano factor a results are in good agreement with the theory describing that transp arises from evanescent electronic states.



FIG. 1 (color online). (a) Experimental setup for detecting shot noise at T = 4.2-30 K. (b) Schematic of the principle of our measurements in terms of the noise power reflection $|\Gamma|^2$. (c) Illustration of a typical graphene sample fabricated for our shot noise study.



⁵⁰⁰ FIG. 3 (color online). F extracted at V_{bias} = 40 mV for three different samples, all having W/L ≥ 3, as a function of δV =
 (d) V_{gate} - V_{Dirac}. For the two unintentionally highly p-doped samples (orange and green dots), the Dirac point was estimated via extrapolation of the minimum conductivity at ^{4e²}/_{πh}.



9. Outlook

Transparent electrodes

Production of a 100-m-long high-quality graphene transparent conductive film by roll-to-roll chemical vapor deposition and transfer process

Toshiyuki Kobayashi,^{a)} Masashi Bando, Nozomi Kimura, Keisuke Shimizu, Koji Kadono, Nobuhiko Umezu, Kazuhiko Miyahara, Shinji Hayazaki, Sae Nagai, Yukiko Mizuguchi, Yosuke Murakami, and Daisuke Hobara Advanced Materials Laboratories, Sony Corporation, Atsugi-Shi, Kanagawa 243-0014, Japan



100 Meter lang !

Transparent electrodes



Transparent Conductor Market by Application





Flexibility...



Mechanically strong

- Reißfestigkeit $\sigma_A = 42 \text{ N m}^{-1}$ (>> σ_A (Stahl) = 0.084 0.4 N m⁻¹ für Graphendicke)
 - => Trägt 4 kg (z.B. Katze)



• Perfekte Barriere für Gase und Flüssigkeiten

Mechanically strong



?

Stretchability of graphene

Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene

Changgu Lee,^{1,2} Xiaoding Wei,¹ Jeffrey W. Kysar,^{1,3} James Hone^{1,2,4}*

Fig. 1. Images of suspended graphene membranes. (A) Scanning electron micrograph of a large graphene flake spanning an array of circular holes 1 µm and 1.5 µm in diameter. Area I shows a hole partially covered by graphene, area II is fully covered, and area III is fractured from indentation. Scale bar, 3 µm. (B) Noncontact mode AFM image of one membrane, 1.5 µm in diameter. The solid blue line is a height profile along the dashed line. The step height at the edge of the membrane is



25% möglich gewöhnliche Materialien liegen bei 1%

dabei ca. 120 Gpa mehr als 10 x besser als Stahl !

> Anwendung Dehnsensor!

about 2.5 nm. (C) Schematic of nanoindentation on suspended graphene membrane. (D) AFM image of a fractured membrane.

SCIENCE VOL 321 18 JULY 2008

Mechanically strong

Graphene used to create more pleasurable condoms

Nobel Prize winning super-material graphene is being used to create thinner and stronger condoms that could be more pleasurable to use



Ein neues Wundermaterial für Kondome, Graphene, möchte der Microsoft-Gründer und reichste Mensch der Welt, Bill Gates, im Kampf der Bill and Melinda Gates Foundation gegen die weltweite Ausbreitung von HIV und AIDS, aber auch Armut, wissenschaftlich weiter entwickeln lassen und zwar am National Graphene Institute Manchester in Großbritannien. Bis 2015 sollen die neuen Kondome an den Start kommen.

Bill Gates will bessere Graphene Kondome statt Latex Kondome für die Welt

21.11.2013, mehr zum Thema Tests

Graphene is impermeable

Impermeable Atomic Membranes from Graphene Sheets

J. Scott Bunch, Scott S. Verbridge, Jonathan S. Alden, Arend M. van der Zande, Jeevak M. Parpia, Harold G. Craighead, and Paul L. McEuen*



NANO LETTERS 2008 Vol. 8, No. 8 2458-2462



Figure 2. Scatter plot of the gas leak rates vs thickness for all the devices measured. Helium rates are shown as solid triangles (\blacktriangle), argon rates are shown as solid squares (\blacksquare) and air rates are shown as hollow squares (\square).

Anwendungen: einstellbarer mechanischer Schwingkreis Drucksensor Gasdichtung Nanobehältnis für Medikamente

Graphene electronics



Dehnsensor aus Graphen

Graphene-based transparent strain sensor CARBON 51 (2013) 236-242



Other 2D materials

BN = Isolator





guiding



$$n' = \pm k_F = \sqrt{\pi | n}$$

 $n_1'\sin(\alpha_1) = n_2'\sin(\alpha_2)$

total internal reflection if:

 $n_1'\sin(\alpha_1) > n_2'$



two cases: **conventional optical guiding** (refractive indicies have the same sign) and **pn-guiding** *Williams, et al. Nature Nano* 6, 222–5 (2011).

