Graphene: massless electrons in flatland.

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What is graphene

One atom thick layer of carbon atoms arranged in a hexagonal/honeycomb structure. More precisely it can be seen as a triangular Bravais lattice with a basis.

The fact that the Bravais lattice has a basis is a key element to explain many of the properties of graphene.
Graphene as an unrolled nanotube
A brief history

• 1564: “Lead pencil” based on graphite was invented

• 1946 P. R Wallace writes paper on band structure of graphene

• 2004 K.S. Novoselov et al. realize and identify graphene experimentally

• 2005 Y.B. Zhang et al. observe quantum Hall effect and Berry's phase in graphene
Is it interesting?

Realization of graphene
Why is graphene interesting: band structure

Each carbon atom as 4 bonds, 1 pz and 3 sp2 orbitals. The sp2 (s hybridized with p) leads to trigonal planar structure with formation of a σ-bond between carbon atoms. The pz orbitals bind covalently with neighbors forming a half filled π-band.

- **Graphene is truly 2D!**

  Tight binding model, P. R. Wallace (1947)

- **Graphene has 2D Dirac cones**
Dirac cones in graphene

From tight binding model we have that at the corners of the BZ the low energy Hamiltonian is:

\[ H = \hbar v_F \sigma \cdot p \]

Chiral Massless Dirac Fermions

Electrons obey laws of 2D QED!

The Fermi velocity \( v_F \) is \( \sim 1/300 \) the speed of light \( c \). We have slow ultrarelativistic electrons.

QED with a pencil and some scotch!
Chirality

The sublattice symmetry implies that we have a conserved quantity: 

**chirality**

defined by the operator:

\[ \hat{h} \equiv \frac{1}{2} \sigma \cdot \frac{p}{|p|} \]

The Dirac point is protected by the conservation of chirality.

Transport implication:

Back-scattering is suppressed.

*Courtesy of M. Fuhrer, University of Maryland*
Klein paradox

If we solve the Dirac equation in presence of a potential barrier:

We find that for particular directions the transmission probability, $T$, is equal to 1, in particular $T=1$ for forward scattering:

The never before observed Klein paradox has been observed for the first time in graphene.
Screening of charge impurities in graphene

\[ V(r) = -\frac{Ze}{r} \]

\[ \frac{H}{\hbar \nu_f} = \sigma \cdot p + Z \alpha \frac{1}{r} \]

Gershtein, Popov, Zeldovich, Perolomov, Greiner, et al. 
Electronic Structure Of Superheavy Atoms 
Undercritical and supercritical screening

Difficult to test in QED, we need $Z > 137$.

But in graphene $\alpha \sim 1$; we only need $Z \sim 1$. 

Shytov et al. (2007)
Problem: transport at the Dirac point

\[ \sigma \propto D(E) \tau \]

Experimentally: \( \sigma \) is a sample dependent constant!
Effect of disorder

At the Dirac point disorder induces electron-hole puddles

Suggested theoretically:

Observed experimentally:
J. Martin et al., Nature Physics, 4, 144 (2008)
System

Linear scaling region well explained by presence of random charged impurities

\[ V_g = e\langle n\rangle / C \]

Graphene

Average distance of impurities from the graphene layer

Impurities

SiO\textsubscript{2}

Substrate

Si

Back-gate
**Thomas-Fermi-Dirac theory**

Start from the energy functional $E[n]$ and then minimize it with respect to the electron density $n$. In presence of disorder for the total energy we have:

\[ E[n] = E_{\text{kin}}[n(r)] + E_H[n(r)] + E_{\text{exch}}[n(r)] - \int_A V_D n(r) d^2r - \mu \int_A n(r) d^2r \]

and then:

\[ \frac{\delta E}{\delta n} = 0 \]

\[ \hbar v_F \text{sign}(n) \sqrt{\pi n} + \frac{e^2}{2\epsilon_0} \int d^2 r' \frac{n(r')}{|r - r'|} + \Sigma(n) - V_D - \mu = 0 \]

Where $\Sigma$ is the exchange self energy:

\[ \Sigma \approx r_s \sqrt{|n| \ln |n|} \]

The correlation energy contribution is quite smaller and scales as the self energy:

\[ \frac{\delta E_c}{\delta n} \approx F[r_s] \sqrt{|n| \ln |n|} \]

\[ F[r_s] < r_s \]

and of opposite sign
Construction of disorder potential

- We assume charge distribution with zero average. A nonzero average it simply translates in a voltage gate off-set.

\[ \langle C(r) \rangle = 0 \]

- We assume the charge positions to be uncorrelated.

\[ \langle C(r_1)C(r_2) \rangle = n_{\text{imp}} \delta(r_2 - r_1) \]

\[ \langle C(q) \rangle = 0 \]

\[ \langle C^2(q) \rangle = n_{\text{imp}} \]

- We then calculate \( C(q) \) using random number with Gaussian distribution and variance equal to impurity density.

- Assuming the impurities to be in a layer at distance \( d \) we finally calculate \( V_D \)

\[ V_D(q) = 2\pi e^{-qd} \]

\[ q \]

\[ C(q) \]
Dirac point: single disorder realization

We can see that many-body effects, exchange, tend to suppress the density fluctuations as it can be seen from the “histogram” plot of the density distribution.
Density rms and correlation length, as function of impurity density

$A_0$: area fraction over which $|n(r) - \langle n \rangle| < n_{rms}/10$

$\delta Q \equiv n_{rms} \pi \xi^2$

Small region of size $\xi$, $\sim 10$ nm, fixed by non-linear screening, and high density. $\delta Q \sim 2e$. Result in agreement with recent STM experiment [V. Brar et al. unpublished]

Wide regions of size $\sim L$ (sample size) and low density. $\delta Q \sim 10e$. 

Carrier density properties
Inhomogeneous conductivity

The inhomogeneous character of the $n$ will be reflected in inhomogeneous transport properties such as the conductivity, $\sigma$, and the mean free path, $l$. Because in presence of disorder the density is strongly inhomogeneous, and different from zero almost everywhere, we assume the RPA-Boltzmann expression [Ando J. Phys. Soc. (2006); Nomura & MacDonald, PRL (2006); Hwang, Adam, Das Sarma, PRL (2007); Cheianov & Falko, PRL (2006), Adam et al. PNAS (2007)] to be valid locally also at the Dirac point:

$$\sigma(r) = F(r_s) \frac{2e^2 |n(r)|}{\hbar} \frac{n_{imp}}{n_s}$$

For $r_S = 0.8$ is $F(r_S) = 10$. 

![Graph showing conductivity and density distributions](image)
Effective medium theory

We use the Landauer-Bruggeman [Bruggeman Ann. Phys (1935), Landauer J. Appl. Phys. (1952)] Effective Medium Theory. In this approach an effective medium conductivity, $\sigma_{\text{eff}}$, is calculated requiring that the spatial average of the electric field fluctuations induced by the inhomogeneity of $\sigma$ is equal to zero. In 2D this requirement translates into the equation:

$$\int d^2 r \frac{\sigma(r) - \sigma_{\text{eff}}}{\sigma(r) + \sigma_{\text{eff}}} = 0$$

For graphene this equation, after disorder averaging, takes the form:

$$\left\langle \int d^2 r \frac{\sigma(r) - \sigma_{\text{eff}}}{\sigma(r) + \sigma_{\text{eff}}} \right\rangle = 0 \iff \int dn \frac{\sigma_0 \frac{|n|}{n_{\text{imp}}}}{\sigma_0 \frac{|n|}{n_{\text{imp}}} + \sigma_{\text{eff}}} P(n) = 0$$

$$\sigma(r) = F(r_s) \frac{2e^2}{h} \frac{|n(r)|}{n_{\text{imp}}}$$

We know $P(n)$: obtained using the Thomas-Fermi-Dirac approach.

ER, S. Adam, S. Das Sarma, arxiv:0809.1425
Effective medium theory: regime of validity

The Effective Medium Theory is valid when:

\[ l \ll \left[ \frac{\nabla \sigma}{\sigma} \right]^{-1} \quad l \ll \left[ \frac{\nabla n}{n} \right]^{-1} \]

From Boltzmann-RPA result

In general we have seen that \( \xi \) is \( \sim 10 \) nm, smaller than the typical \( l \). However:

- \( \xi \) characterizes small regions that are quite sparse and, in first approximation, we can assume their contribution to the conductivity to be small;

- Close to the Dirac point most of the sample is characterized by wide regions with small density. Because is \( l(r) = \sigma(r)/\sqrt{\pi n(r)} \); in this regions \( l \) is quite smaller than the length scale over which \( n \) varies.

b) Resistive contribution due to boundaries between e-h puddles is small., [Cheianov & Falko, PRB (2006); Cheianov et al, PRL (2007); Fogler et al. PRB (2008)].

This contribution becomes less important with the size of the e-h puddles.
Results away from the Dirac point.

Up to high carrier densities densities fluctuations dominate.

The density probability distribution has bimodal character.

Dirac-point physics dominates over finite range of gate voltages.
EMT: conductivity vs. gate voltage

- Finite value of the conductivity at Dirac point;
- Recovers linear behavior at high gate voltages;
- Describes crossover;
- Shows importance of exchange-correlation at low voltages.

S. Adam et al. PNAS (2007)
EMT: minimum conductivity vs. impurity density

Dependence of conductivity on impurity density in qualitative and quantitative agreement with experiments.

S. Adam et al. PNAS (2007)
Tuning $r_s$

C. Jang et al. PRL (2008)

$$r_s = \frac{\epsilon^2}{\hbar v_F \bar{\epsilon}}$$

$$\bar{\epsilon} = \frac{\epsilon_T + \epsilon_S}{2}$$

Vacuum

$$\epsilon_T = 1$$

$$r_s = 0.81$$

Graphene

$$\epsilon_S = 3.9$$

Ice

$$\epsilon_T = 3.2$$

$$r_s = 0.56$$
How $r_s$ enters the theory

- $r_s$ affects the ground-state carrier distribution:

\[
\frac{1}{\hbar v_F} \frac{\delta E}{\delta n} = \text{sign}(n) \sqrt{\pi n} + r_s \int d^2r' \frac{n(r')}{|r - r'|} + r_s \hat{\Sigma}(n) - r_s \hat{V}_D - \mu
\]

- $r_s$ controls the scattering time:

\[
\frac{1}{\tau} = \frac{\sqrt{\pi v_F n_{imp}}}{\hbar \sqrt{n}} F(r_s)
\]


and therefore the local value of the conductivity

\[
\sigma = 2 \frac{e^2}{h} E_F \tau = 2 \frac{e^2}{h} \frac{n}{n_{imp}} \frac{1}{F(r_s)}
\]
EMT: $r_s$ dependence of the minimum conductivity

Conclusions

• Graphene is interesting.

• Close to the Dirac-point, disorder induced density inhomogeneities are extremely important to understand graphene properties, especially transport.

• We understand transport in current samples close to Dirac point;

• Interactions not strong enough to cause long-range order but essential to understand transport close to the Dirac point;

• Many things not covered and still largely unexplored: bilayers; graphene nanostructures, ...