Planar QED description of graphene: from the quantum Hall effect to nanodevices

E.M. Santangelo

Departamento de Física - Universidad Nacional de La Plata

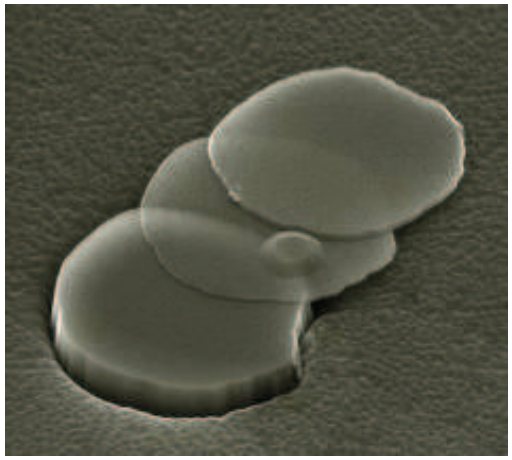
Argentina

What is Quantum Field Theory? (Manolo's Fest)

Benasque, September 2011

Work done in colaboration with C.G. Beneventano

real cake

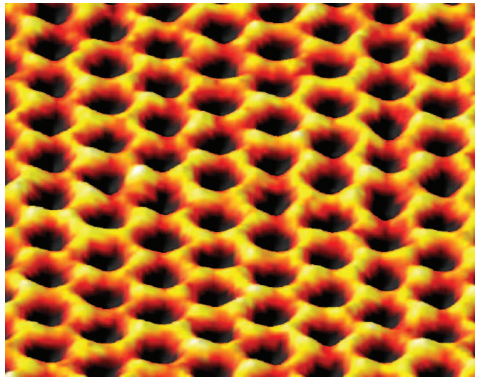


real graphene

Contents

Graphene: Electrons in “Flatland”

Truly bidimensional array of carbon atoms. Unique properties



Proposed in 1984:

- G.W. Semenoff, Phys. Rev. Lett. **53**, 2499 (1984).

ALMOST obtained in 2004:

- K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Science **306**, 666 (2004).

Effective model for charge carriers

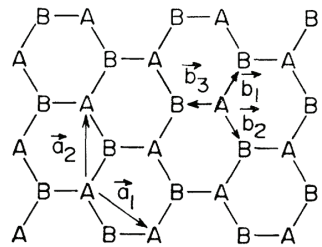


FIG. 1. The honeycomb lattice as a superposition of two triangular sublattices. The basis vectors are $\vec{a}_1 = (\sqrt{3}/2, -\frac{1}{2})a$; $\vec{a}_2 = (0, 1)a$ and the sublattices are connected by $\vec{b}_1 = (1/2\sqrt{3}, \frac{1}{2})a$; $\vec{b}_2 = (1/2\sqrt{3}, -\frac{1}{2})a$; $\vec{b}_3 = (-1/\sqrt{3}, 0)a$.

A sites generated by a_1 and a_2

b_1, b_2, b_3 connect A to B sites

Tight binding Hamiltonian

$$H = t \sum_{A,i} \left(U^\dagger(A) V(A + b_i) + V^\dagger(A + b_i) U(A) \right) .$$

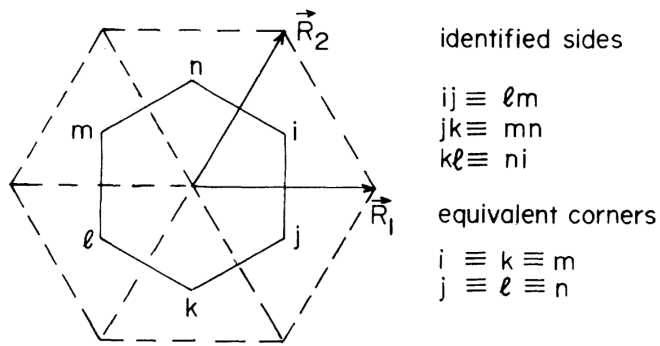
In momentum space

$$H = \int_{\Omega_B} \frac{d^2q}{(2\pi)^2} \left(U^\dagger(k), V^\dagger(k)\right) H(k) \begin{pmatrix} U(k) \\ V(k) \end{pmatrix} ,$$

$$H(k) = \begin{pmatrix} 0 & \phi(k) \\ \phi(k)^* & 0 \end{pmatrix}$$

$$\phi(k) = t \left(e^{ik.b_1} + e^{ik.b_2} + e^{ik.b_3}\right) ,$$

$\phi(k) = 0$ at the six corners of the Brillouin zone.



Take $K_\pm = \pm\frac{4\pi}{\sqrt{3}a}\left(0, \frac{1}{\sqrt{3}}\right)$ as the two non-equivalent ones. Conduction and valence bands touch at $K_\pm$.

Expand around $K_\pm$ ($k = K_\pm + p$). In the continuum limit ($a \to 0$, with $t\,a$ constant), to first order

$$\phi(p + K_\pm) \approx \frac{ta\sqrt{3}}{2}(-ip_x \mp p_y)$$

Calling $\Psi_\pm = \begin{pmatrix} U(p + K_\pm) \\ V(p + K_\pm) \end{pmatrix}$

We obtain

$$\boxed{H_\pm = v_F \begin{pmatrix} 0 & -ip_x \mp p_y \\ ip_x \mp p_y & 0 \end{pmatrix}}$$

Dirac Hamiltonian for massless fermions in 2+1 dimensions with

Fermi velocity $v_F = \frac{ta\sqrt{3}}{2} \approx 10^6 \frac{m}{s}$

P.R. Wallace, Phys. Rev. **71**, 622 (1947)

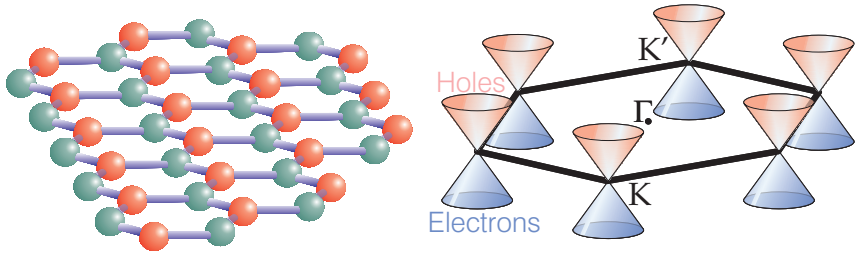
Gordon W. Semenoff, Phys. Rev. Lett. **53**, 2449 (1984)

Effective theory graphene - Dirac like theory in a reducible representation

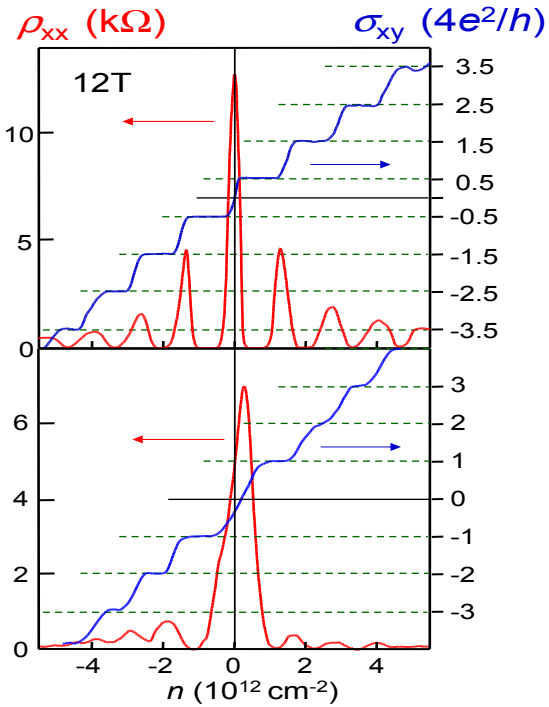
Valleys $K_\pm$ - the two irreducible representations of γ matrices in 2+1

A and B type of sites - upper and lower components of Ψ in each representation

Graphene is a gapless material



Hall conductivity for mono and bi-layer graphene



Note that the behavior around the origin is ”unexpected”

Our approach to the Hall conductivity through planar QED

- Study of Dirac fields in 3-dimensional Euclidean space, with chemical potential in the presence of a constant magnetic field perpendicular to the $x - y$ plane.
- Evaluate the partition function and density of fermion number (or charge) at finite temperature, via zeta regularization.
- Lorentz boost to include electric field and determination of Hall's current.
- Analysis of different selections of the phase of the determinant at each valley, and of the effect on Hall's conductivity.

C.G.Beneventano and E.M.S., Jour. Phys. A 39, 7457 (2006).

C.G.Beneventano, P. Giacconi, E.M.S. and R. Soldati, Jour. Phys. A: Math. Theor. **40**, F435 (2007).

C.G.Beneventano and E.M.S., Jour. Phys. A: Math. Theor. **41**, 164035 (2008).

Partition function at finite temperature and density

Study a massless Dirac Field in 3-dimensional Euclidean space, at finite temperature

Uniform magnetic field B perpendicular to the sample + chemical potential μ

Choose Landau gauge: $A = (i\frac{\mu}{e}, -By, 0)$ and $0 < \tau < \beta = \frac{1}{kT}$

Evaluate the Euclidean effective action

$$\log \mathcal{Z} = \log \; det(i\partial\!\!\!/ + eA\!\!\!/)_{AP}$$

Antiperiodic boundary conditions to insure Fermi statistics

Use zeta regularization

$$\log \mathcal{Z} = -\frac{d}{ds}\Big]_{s=0} \zeta(s, \frac{(i\partial\!\!\!/ + eA\!\!\!/)_{AP}}{\alpha}) = -\frac{d}{ds}\Big]_{s=0} \sum \omega_n^{-s}$$

To apply zeta regularization: solve eigenvalue problem for the Dirac operator, with L^2 integrability condition, and (to satisfy antiperiodicity)

$$\Psi_{k,l}(\tau, x, y) = \frac{e^{i\lambda_l \tau} e^{ikx}}{\sqrt{2\pi\beta}} \begin{pmatrix} \varphi_{k,l}(y) \\ \chi_{k,l}(y) \end{pmatrix} \qquad \boxed{\lambda_l = (2l+1)\frac{\pi}{\beta}}$$

The spectrum has two pieces: $\tilde{\lambda}_l = (2l+1)\frac{\pi}{\beta} - i\mu$

1) Asymmetric piece (associated to a zero mode of the Hamiltonian)

$$\boxed{\omega_l = \tilde{\lambda}_l \quad \text{with} \quad l = -\infty, ..., \infty}$$

2) Symmetric piece

$$\boxed{\omega_{l,n} = \pm\sqrt{\tilde{\lambda}_l^2 + 2neB} \quad \text{with} \quad n = 1, ..., \infty \quad l = -\infty, ..., \infty}$$

Degeneracy (per unit area) in all cases:

$$\boxed{\Delta_L = \frac{eB}{2\pi}}$$

In the other irreducible representation of γ matrices (around the valley K_-), the asymmetric piece of the spectrum changes the sign

Analytic extension of $\zeta(s, \frac{(i\not{\partial}+e\not{A})_{AP}}{\alpha})$

Two contributions:

$$\zeta_1(s,\mu) = \Delta_L \sum_{l=-\infty}^{\infty} \left[(2l+1)\frac{\pi}{\alpha\beta} - i\frac{\mu}{\alpha}\right]^{-s}$$

$$\zeta_2(s,\mu,eB) = (1+(-1)^{-s})\,\Delta_L \sum_{\substack{n=1\\ l=-\infty}}^{\infty} \left[\frac{2neB}{\alpha^2} + \left((2l+1)\frac{\pi}{\alpha\beta} - i\frac{\mu}{\alpha}\right)^2\right]^{-\frac{s}{2}}$$

The extension of $\zeta_2(s,\mu)$ is standard. One uses the Mellin transform

$$z^{-s} = \frac{1}{\Gamma(s)}\int_0^\infty dt\, t^{s-1} e^{-tz} \qquad \Re(z) > 0$$

and the definition of the Jacobi theta function $\Theta_3(z,x) = \sum_{l=-\infty}^{\infty} e^{-\pi x l^2} e^{2\pi z l}$, together with its well known inversion formula: $\Theta_3(z,x) = \frac{1}{\sqrt{x}} e^{(\frac{\pi z^2}{x})} \Theta_3\left(\frac{z}{ix}, \frac{1}{x}\right)$

The analytic extension of $\zeta_1(s,\mu)$ introduces the "PHASE"

$$\zeta_1(s,\mu) = \Delta_L \sum_{l=-\infty}^{\infty} \left[(2l+1)\frac{\pi}{\alpha\beta} - i\frac{\mu}{\alpha}\right]^{-s}$$

$$\zeta_1(s,\mu) = \Delta_L \left(\frac{2\pi}{\alpha\beta}\right)^{-s} \left[\sum_{l=0}^{\infty} \left[(l+\frac{1}{2}) - i\frac{\mu\beta}{2\pi}\right]^{-s} + \right.$$

$$\left. \sum_{l=0}^{\infty} \left[-(l+\frac{1}{2}) - i\frac{\mu\beta}{2\pi}\right]^{-s}\right]$$

$$= \Delta_L \left(\frac{2\pi}{\alpha\beta}\right)^{-s} \left[\zeta_H\left(s, \frac{1}{2} - \frac{i\mu\beta}{2\pi}\right) + \right.$$

$$\left. + \sum_{l=0}^{\infty} e^{-is\theta} \left((2l+1)\frac{\pi}{\beta} - i\mu\, e^{-i\theta}\right)^{-s}\right]$$

Usual choice (don't go through zeros): $(-1)^{-s} = e^{i\pi sign(\mu)s}$ $\kappa = -1$

Opposite choice (go through infinite zeros): $(-1)^{-s} = e^{-i\pi sign(\mu)s}$ $\kappa = 1$

$$\zeta_1(s,\mu) = \Delta_L \left(\frac{2\pi}{\beta\alpha}\right)^{-s} \left[\zeta_H\left(s, \frac{1}{2} - \frac{i\mu\beta}{2\pi}\right) + \right.$$

$$\left. e^{-i\kappa\pi sign(\mu)s}\zeta_H\left(s, \frac{1}{2} + \frac{i\mu\beta}{2\pi}\right)\right]$$

Contribution to the effective action:

$$\log Z_1(\kappa) = \Delta_L \left\{\log\left[2\cosh(\frac{\mu\beta}{2})\right] + \kappa\frac{|\mu|\beta}{2}\right\}$$

Total effective action per unit area and one irreducible representation

$$\log Z(\kappa) = \Delta_L \left\{\log\left[2\cosh(\frac{\mu\beta}{2})\right] + \kappa\frac{|\mu|\beta}{2} + \beta\sqrt{2eB}\zeta_R\left(-\frac{1}{2}\right)\right.$$

$$\left. + \sum_{n=1}^{\infty} \log\left[\left(1 + e^{-(\sqrt{2neB}-\mu)\beta}\right)\left(1 + e^{-(\sqrt{2neB}+\mu)\beta}\right)\right]\right\}$$

Same in the other representation (valley) if the phase is chosen with the same criterium. No fundamental reason for doing so. So, around the other valley $\kappa \to \kappa'$ (± 1).

Hall current in the presence of electric field

Fermion number (per unit area) in one i.r. $N = \frac{1}{\beta}\frac{d}{d\mu}\log\mathcal{Z}$

$$N(\kappa) = \Delta_L \left\{ \frac{1}{2}\left[\tanh\left(\frac{\mu\beta}{2}\right) + \kappa sign(\mu)\right] \right.$$

$$\left. + \sum_{n=1}^{\infty}\left[\frac{e^{-(\sqrt{2neB}-\mu)\beta}}{1+e^{-(\sqrt{2neB}-\mu)\beta}} - \frac{e^{-(\sqrt{2neB}+\mu)\beta}}{1+e^{-(\sqrt{2neB}+\mu)\beta}}\right]\right\}$$

Charge density: $j^0 = -eN$

Zero temperature limit ($\beta \to \infty$) of charge density (recovering physical units)

Without electric field:

$$j^0(2ec^2\hbar Bn < \mu^2 < 2eBc^2\hbar(n+1)) =$$

$$\frac{-(n+\frac{1+\kappa}{2})ce^2B}{h}\, sign(\mu)$$

To include electric field E'_y

Perform a Lorentz boost with velocity $v_x = -\frac{E'_y c}{B'_z}$ $(E'_y < eB'_z)$ gives as a result

$$j'^0 = \frac{-(n + \frac{1+\kappa}{2})ce^2 B'_z}{h} \, sign(\mu)$$

$$j'^x = \frac{-(n + \frac{1+\kappa}{2})e^2 E'_y}{h} \, sign(\mu) \, , \quad j'^y = 0$$

Hall conductivity, one irreducible representation and two ”flavors” (spins of the electron)

$$\boxed{\sigma_{xy} = \frac{-2(n + \frac{1+\kappa}{2})e^2}{h} \, sign(\mu)}$$

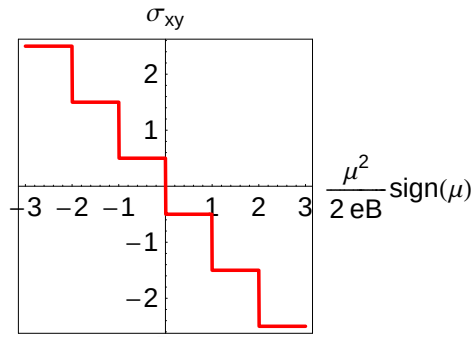
How to combine the phases in both representations?

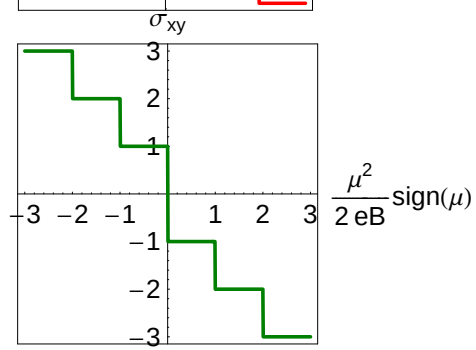
Our results in graphics

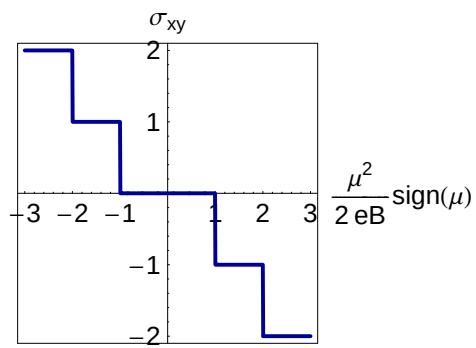
Opposite phases (monolayer)

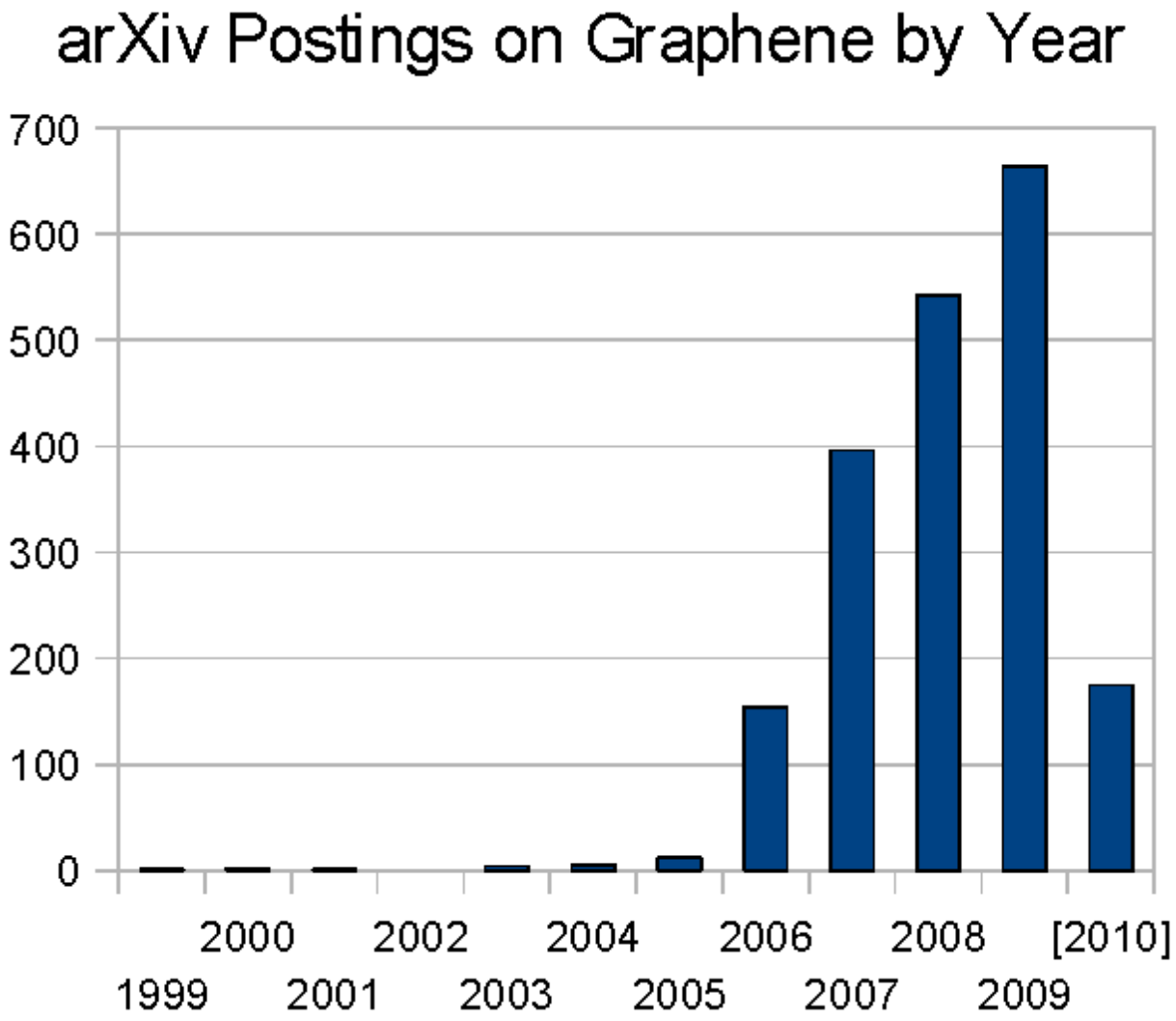
Both $\kappa = +1$ (bilayer)

Both $\kappa = -1$ (?)








arXiv Postings on Graphene by Year
700
600
500
400
300
200
100
0
2000
2002
2004
2006
2008
[2010]
1999
2001
2003
2005
2007
2009

Applications of graphene and boundary conditions in the continuum model

Many applications foreseen:

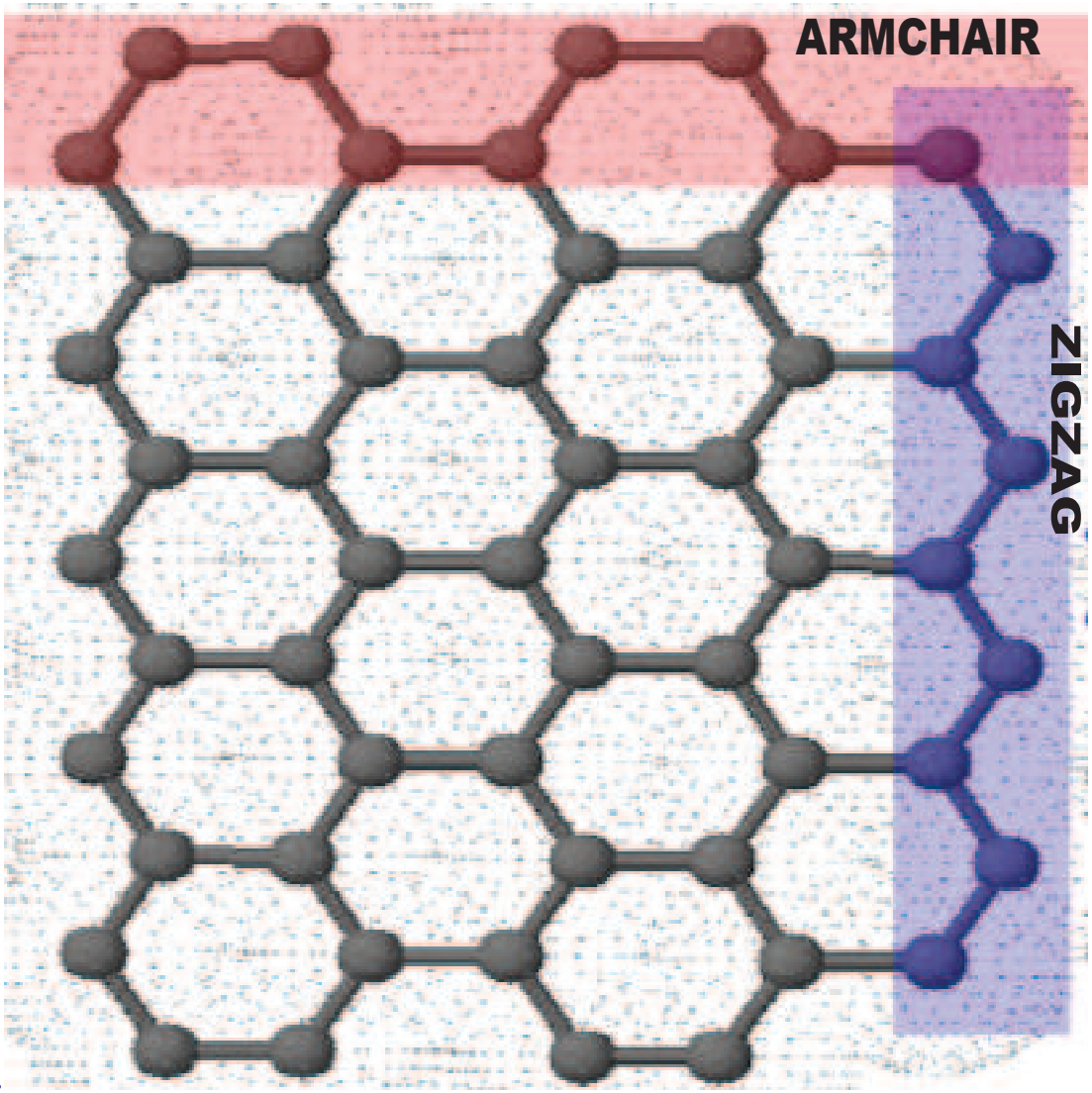
- Graphene touchscreens, microdisplays and monitors,
- Graphene solar cells,
- Graphene biosensors,...

Major dream is to construct graphene-based ultra fast computers

NEED TO OPEN A GAP

To this end, nothing like...

BOUNDARIES



Our work on boundary conditions

Study a family of local boundary conditions (b.c.) for massless Dirac fields for nanoribbons and nanodots

Show that MIT bag b.c. give the best agreement with experiments

C.G.B and E.M. Santangelo, arXiv:1011.2772

Study the eigenvalue problems $H_\pm \Psi_\pm(x,y) = E_\pm \Psi_\pm(x,y)$,
with $H_\pm = -i\sigma_2\partial_x \pm \sigma_1\partial_y$

Domain of the differential operator defined by a family of local boundary conditions which:

1. Don't mix valleys
2. Give a vanishing flux of current perpendicular to the boundary
3. Are defined through a self-adjoint projector

Study the problem around K_+. When necessary, boundary conditions around K_- will be discussed.

Put a boundary at x_0

$\Psi_+^\dagger \sigma_2 \Psi_+$ proportional to perpendicular current

$\Psi_+^\dagger \sigma_1 \Psi_+$ proportional to current along boundary

The most general one-parameter family of b.c. satisfying 1 to 3

$$\boxed{(I + \sigma_1\, e^{-i\alpha\sigma_2})\Psi_+\rfloor_{x=x_0} = 0}$$

Note: $\alpha = 0, \pi$ MIT bag boundary conditions

$\alpha = \pm\frac{\pi}{2}$ mimic zigzag boundary.

$$\Psi_+^\dagger \sigma_1 \Psi_+\rfloor_{x=x_0} = -\cos(\alpha)\Psi_+^\dagger \Psi_+\rfloor_{x=x_0}$$

Zigzag b.c. $\Rightarrow$ tangential current at the boundary vanishes

MIT $\Rightarrow$ current along the boundary proportional to density of charge

Propose, for each k_y, $\Psi_+(x,y) = e^{ik_y\, y}\psi_+(x)$

Half Plane

Take the boundary at $x = 0$

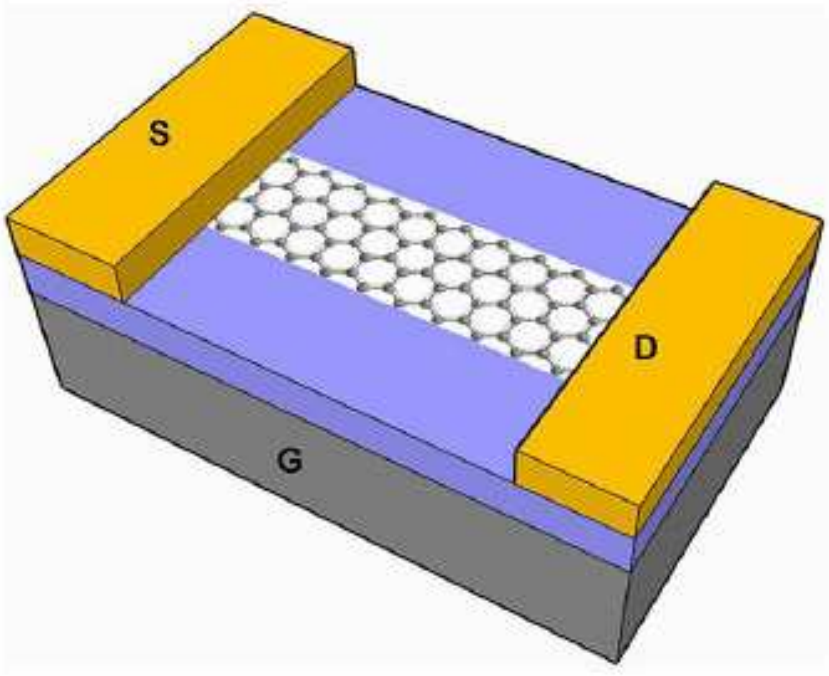
Solve the eigenvalue problem with the normalizability condition when $x \to \infty$

For all $\alpha \neq 0, \pi$, there are apart from bulk states, edge states, corresponding to $E = k_y \cos\alpha$, with $k_y \sin\alpha > 0$, eigenfunctions decreasing exponentially with x.

Correspond to $E = 0$ in the zigzag case $\Rightarrow$

Note: This shows zigzag b.c. do not define, in a compact region with smooth boundary, a Lopatinski-Shapiro (elliptic) boundary problem.

Graphene nanoribbon transistor



Nanoribbons and boundary conditions in QED

Put a second Boundary at $x = W$

Experiments show a gap, which is symmetric around the Dirac Point

Two ways of obtaining a symmetric spectrum:

1. Same projector at both boundaries-ZERO MODES $\forall\alpha$ (Appear for all values of k_y for $\alpha = \pm\frac{\pi}{2}$, and for $k_y = 0$ for $\alpha \neq \pm\frac{\pi}{2}$.
2. Orthogonal projectors at both boundaries

We take ortogonal projectors at both boundaries

$$H_+\Psi_+(x,y) = E_+\Psi_+(x,y)\,,$$

$$(I + \sigma_1\, e^{-i\alpha\sigma_2})\Psi_+\rfloor_{x=0} = 0\,, \quad (I - \sigma_1\, e^{-i\alpha\sigma_2})\Psi_+\rfloor_{x=W} = 0$$

$$E = \pm\sqrt{k_x^2 + k_y^2}$$

Spectrum for MIT ($\alpha = 0, \pi$)

$$\cos(k_x W) = 0 \Rightarrow E_n = \pm\sqrt{\left(\frac{(n+\frac{1}{2})\pi}{W}\right)^2 + k_y^2}$$

- equally spaced spectrum in k_x
- energy gap for MIT bag b.c. $\boxed{\Delta E = \frac{\pi}{W}}$

Spectrum for all $\alpha \neq 0, \pi$

$$k_x \cos(k_x W) = k_y \sin\alpha \sin(k_x W), \quad \text{for } E \neq \pm k_y \,,$$

$$k_y = \frac{1}{W \sin\alpha}, \quad \text{for } E = \pm k_y \,.$$

- Both equations break the invariance under $k_y \to -k_y$
  Only recovered by imposing exactly the same boundary conditions on the eigenfunctions around the other valley
- For $k_y = 0$, $k_x = \frac{(n+\frac{1}{2})\pi}{W}$, no matter the value of α

- $\forall k_y \neq 0$, values of k_x not equally spaced, but continuous
- Imaginary as well as real values of k_x are allowed
  Calling $\kappa = i\, k_x$, for $E \neq \pm k_y$

$$\kappa \cosh(\kappa W) = k_y \sin\alpha \sinh(\kappa W), \text{ for } |k_y| > \frac{1}{W|\sin\alpha|}$$

- For $\alpha = \pm\frac{\pi}{2}$ (zigzag b.c.) **energies arbitrarily close to zero** $\Rightarrow$ NO GAP
- $\forall \alpha \neq \pm\frac{\pi}{2}$ $\Delta E \leq \frac{\pi}{W}$

Comparison with the experiments

Experiments DO show a transport gap as the gate voltage grows, when performed at low temperature and bias voltage.

Zigzag boundary conditions are then eliminated as candidates to describe this physical situation.

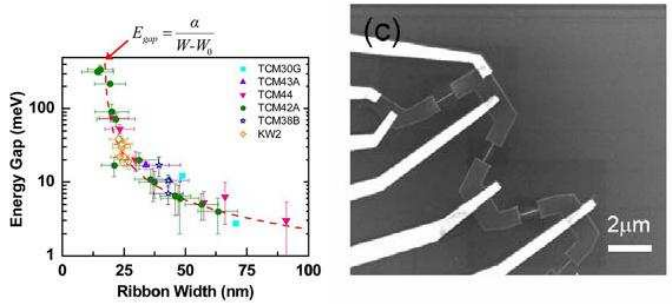
$\forall \alpha \neq \pm\frac{\pi}{2}$, recovering units, $\Delta E \leq \frac{\hbar v_F \pi}{W} = \frac{3}{2}\pi t \frac{a}{W} = 12.37 eV \frac{a}{W}$ (a is the nearest neighbor distance).

For MIT bag boundary conditions ($\alpha = 0, \pi$) the equal sign holds.

Experiment performed by Yu-Ming Lin et al. shows equally spaced plateaux in the conductivity

This suggests that MIT bag boundary conditions are the ones to be imposed in the continuous model.

We obtained, for MIT bag b.c. $\Delta E = 12.7 eV \frac{a}{W}$. For a sample of width $W = 30nm$, $\Delta E = 46 meV$ in good agreement with values obtained by Yu-Ming Lin et al. In general, a bit smaller than the energy gap obtained by Melinda Y. Han, Juliana C. Brant and Philip Kim.



Experiment performed by Melinda Y. Han, Barbaros Özyilmaz, Yuanbo Zhang and Philip Kim shows the measured gap in the gate voltage doesn't depend on the orientation of the boundary.

This is the case if MIT bag boundary conditions are written as $(I + \not{n})\,\psi(x = 0, W) = 0$, where n is the inward normal vector.

Quantum dots

Treat the case of a circular graphene dot of radius R

Polar coordinates

Boundary Value problem

$$\left[-i\gamma^\theta \partial_r + i\frac{\gamma^r}{r}\partial_\theta\right]\psi(r,\theta) = E\psi(r,\theta)$$

$$\left(I - \gamma^r e^{-i\alpha\gamma^\theta}\right)\psi(r=R,\theta) = 0$$

$$\psi(r,\theta) = \psi(r,\theta+2\pi)\,,$$

$$\gamma^r = \sigma_1\cos\theta + \sigma_2\sin\theta \text{ and } \gamma^\theta = \sigma_2\cos\theta - \sigma_1\sin\theta.$$

Zigzag boundary conditions ($\alpha = \pm\frac{\pi}{2}$) allow for an infinite amount of zero modes

This was expected from the facts that they don't satisfy the Lopatinski-Shapiro condition and the region is compact with a smooth boundary.

Experiments on quantum dots also DO present a gap

Treat cases $\alpha \neq \pm\frac{\pi}{2}$

Spectrum

$$(1-\sin\alpha)J_n(|E|R)+s\cos\alpha)J_{n+1}(|E|R) = 0,\ n = 0, ..., \infty$$

$$(1-\sin\alpha)J_{n+1}(|E|R)-s\cos\alpha)J_n(|E|R) = 0,\ n = 0, ..., \infty$$

J_n is the Bessel function of order n, and s is the sign of the energy.

The experiment performed by S.Schnez et al shows clearly that the gap in a quantum dot is symmetric around the Dirac point.

This, again, points to the MIT boundary conditions as the right conditions to impose on the continuum model in order to reproduce the experimental results, since all the remaining values of α produce a spectral asymmetry.

S.Schnez, F. Molitor, C. Stampfer, J. Güttinger, I. Shorubalko, T. Ihn and K. Ensslin, Appl. Phys. Lett. **B94**, 012107 (2009).

Conclusions

The relativistic model of graphene can nicely describe the most salient properties of graphene, mainly the Hall conductivity.

Elliptic boundary conditions are the conditions to choose if one wants to define a quantum theory and, in particular, a quantum charge.

In this sense, MIT bag boundary conditions are the best candidate. They also show the best agreement with experiment, but...

not all the Condensed Matter physicists love relativistic theories; not many of them care about such things as ellipticity.

OUR TOAST TO MANOLO'S HAPPINESS

Thanks and...