Boundary conditions in the Dirac approach to graphene devices

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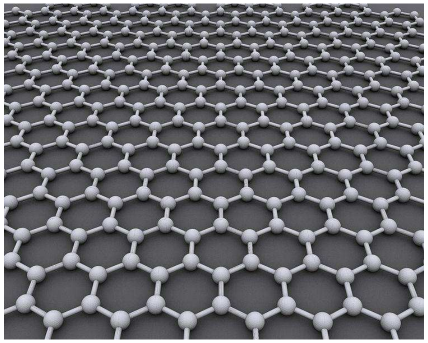
Contents

Graphene

-Truly two-dimensional material

-Honeycomb lattice

-Unique electronic properties



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).

The lattice

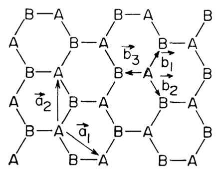
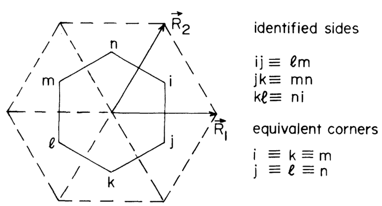


FIG. 1. The honeycomb lattice as a superposition of two triangular sublattices. The basis vectors are $\vec{a}_1 = (\sqrt{3}/2, -\frac{1}{2})a$; $\vec{a}_2 = (0,1)a$ and the sublattices are connected by $\vec{b}_1 = (1/2\sqrt{3}, \frac{1}{2})a$; $\vec{b}_2 = (1/2\sqrt{3}, -\frac{1}{2})a$; $\vec{b}_3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

A sites generated by a_1 and a_2

b_1, b_2, b_3 connect A with B sites

The reciprocal lattice



R_1 and R_2 vectors generate reciprocal lattice

Only two non-equivalent vertices

Tight binding Hamiltonian

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

In the momentum space

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

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

$\phi(k) = \alpha\left(e^{ik.b_1} + e^{ik.b_2} + e^{ik.b_3}\right) = 0$ at the six corners of the Brilloun 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 ($a \to 0$) up to first order in a

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

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

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

Dirac Hamiltonian for massless fermions in 2+1 dimensions with Fermi velocity $v_F = \frac{\alpha a \sqrt{3}}{2} \approx 10^6 \frac{m}{s}$

P.R. Wallace, Physical Review **71**, 622 (1947)

Gordon W. Semenoff, Physical Review Letters **53**, 2449 (1984)

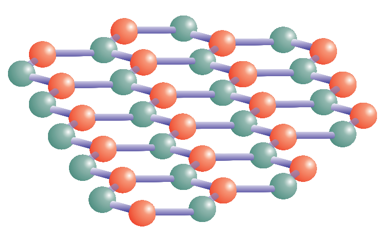
C.L. Kane and E.J. Mele, Physical Review Letters **78**, 1932 (1997)

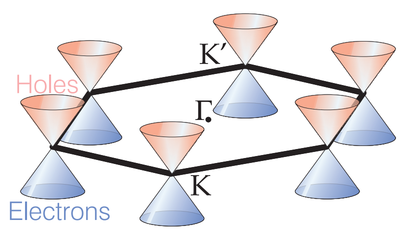
EFFECTIVE THEORY FOR CHARGE CARRIERS MASSLESS DIRAC like theory in 2+1, reducible representation and two ”flavors”

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 gapless material





Opening a gap

How useful is graphene?

GAPLESS material

To obtain grafene-based transistors a controllable gap must be opened

Samples of finite size a natural guess to open a gap

Measurements of the electronic conductivity in devices do show a gap

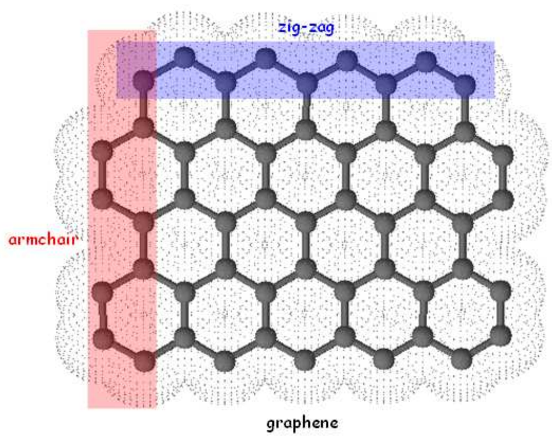
Melinda Y. Han, Barbaros Özyilmaz, Yuanbo Zhang and Philip Kim, Phys. Rev. Lett. **98**, 206805 (2007).

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

Melinda Y. Han, Juliana C. Brant and Philip Kim, Phys. Rev. Lett. **104**, 056801 (2010).

Study a finite size sample

Most theoretical approaches presuppose orientation dependence of the adequate boundary conditions



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. Are separately imposed in each valley
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

$$\boxed{(I + \sigma_1 \, e^{-i\alpha\sigma_2})\Psi_+\rfloor_{x=x_0} = (I + \sigma_1 \cos(\alpha) + \sigma_3 \sin(\alpha))\Psi_+\rfloor_{x=x_0} = 0}$$

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

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

Nanoribbons

Put a second Boundary at $x = W$

Experiments show gap, symmetric around 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 $k_y \to -k_y$
  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
- 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 show a transport gap as a function of the gate voltage.

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

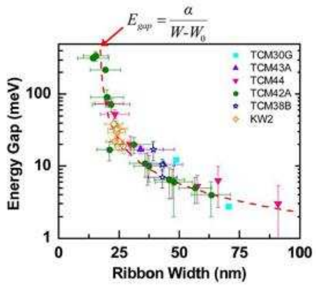
$\forall \alpha \neq \pm\frac{\pi}{2}$, recovering units, $\Delta E \leq \frac{\hbar v_F \pi}{W} = \frac{3}{2}\pi t \frac{a}{W} = 12.37eV\frac{a}{W}$ (a is the next neighbor distance). For MIT bag boundary conditions ($\alpha = 0, \pi$) the equal sign holds. The numerical value of ΔE we obtained is in agreement with values obtained by Yu-Ming Lin et al, but smaller than the energy gap obtained by Melinda Y. Han, Juliana C. Brant and Philip Kim.

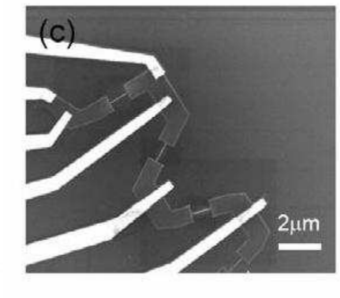
Experiment performed by Yu-Ming Lin et al. shows equally spaced plateaux in the conductivity

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

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.





Yu-Ming Lin, Vassili Perebeinos, Zhihong Chen and Phaedon Avouris, Phys. Rev. **B78**, 161409(R) (2008).

Melinda Y. Han, Juliana C. Brant and Philip Kim, Phys. Rev. Lett. **104**, 056801 (2010).

Melinda Y. Han, Barbaros Özyilmaz, Yuanbo Zhang and Philip Kim, Phys. Rev. Lett. **98**, 206805 (2007).

Quantum dots

Treat the case of a circular graphene dot of radius R

Polar coordinates

Boundary Value problem

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

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

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

$\gamma^r = \sigma_1 \cos\theta + \sigma_2 \sin\theta$ 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 present a gap

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

Spectrum for $\alpha \neq \pm\frac{\pi}{2}$

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

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

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).

Casimir energy of nanotubes and nanoribbons

Graphene nanotube

-Compactify y direction with compactification lenght L and finite lenght W in the perpendicular direction

-Impose MIT bag boundary conditions at $x = 0$ and $x = W$

To obtain nanoribbon take $\frac{L}{W} \to \infty$ limit

Casimir energy with zeta regularization

$$E_C = -\frac{g_s\, g_v}{2} \left(\sum_{E_{n,l}>0} E_{n,l}^{-s} + \sum_{E_{n,l}<0} |E_{n,l}|^{-s} \right) \Bigg|_{s=-1}$$

g_s and g_v spin and valley degenerations

Spectrum $\quad E_{n,l} = \pm \left[\left((n + \frac{1}{2}) \frac{\pi}{W} \right)^2 + \left((l + \frac{\delta}{2}) \frac{2\pi}{L} \right)^2 \right]^{\frac{1}{2}}$

$n = 0, ..., \infty \qquad l = -\infty, ..., \infty$

δ to allow arbitrary periodicity in the compact direction

$$\frac{E_C}{L} = -\frac{g_s\, g_v}{L}\sum_{l=-\infty}^{\infty}\sum_{n=0}^{\infty}\left[\left[(n+\frac{1}{2})\frac{\pi}{W}\right]^2 + \left[(l+\frac{\delta}{2})\frac{2\pi}{L}\right]^2\right]^{-\frac{s}{2}}\Bigg|_{s=-1}$$

Mellin transforming

$$\frac{E_C}{L} = -\left(\frac{2\pi}{L}\right)^{-s}\frac{g_s\, g_v}{L\Gamma\left(\frac{s}{2}\right)}\int_0^{\infty} dt\, t^{\frac{s}{2}-1}\sum_{l=-\infty}^{\infty}\sum_{n=0}^{\infty} e^{-t\left(\left[(n+\frac{1}{2})\frac{L}{2W}\right]^2+\left[l+\frac{\delta}{2}\right]^2\right)}\Bigg|_{s=-1}$$

To be able to take the $L \longrightarrow \infty$ limit, we write the l-sum in terms of a Jacobi theta function and use standard inversion formula for it.

$$\frac{E_C}{L} = -\left(\frac{2\pi}{L}\right)^{-s}\frac{g_s g_v \pi^{\frac{1}{2}}}{L\Gamma\left(\frac{s}{2}\right)}\left\{\sum_{n=0}^{\infty}\int_0^{\infty} dt\, t^{\frac{s-1}{2}-1} e^{-t\left[(n+\frac{1}{2})\frac{L}{2W}\right]^2}\right.$$

$$\left. +4\sum_{l=1}^{\infty}\sum_{n=0}^{\infty}\int_0^{\infty} dt \cos(\pi l\delta) t^{\frac{s-1}{2}-1} e^{-t\left[(n+\frac{1}{2})\frac{L}{2W}\right]^2-\frac{\pi^2 l^2}{t}}\right\}\Bigg|_{s=-1}$$

Performing the integral and writing first term as a Hurwitz zeta function

$$\frac{E_C}{L} = -\left(\frac{2\pi}{L}\right)^{-s} \frac{g_s g_v \pi^{\frac{1}{2}}}{L\Gamma\left(\frac{s}{2}\right)} \left\{ \Gamma\left(\frac{s-1}{2}\right) \left(\frac{L}{2W}\right)^{1-s} \zeta_H(s-1, \frac{1}{2}) \right.$$

$$\left. \left. + 4\sum_{l=1}^{\infty} \sum_{n=0}^{\infty} \cos(\pi l \delta) \left(\frac{\pi l}{\left(n+\frac{1}{2}\right)\frac{L}{2W}}\right)^{\frac{s-1}{2}} K_{\frac{s-1}{2}}\left(\left(n+\frac{1}{2}\right)\frac{\pi l L}{W}\right) \right\} \right|_{s=-1}$$

Relating the Hurwitz zeta function to the corresponding Riemann one, and using the reflection formula for this last

Nanotube compactification length L arbitrary periodicity (δ)

MIT bag boundary conditions at the extremes

$$\frac{E_C}{L} = \frac{2g_s\, g_v}{LW} \sum_{l=1,n=0}^{\infty} \cos\left(\pi\, l\, \delta\right) \frac{\left(n+\frac{1}{2}\right)}{l} K_1\left(\left(n+\frac{1}{2}\right)\frac{\pi\, l\, L}{W}\right) - \frac{3g_s\, g_v}{32\pi W^2}\zeta_R(3)$$

Nanoribbon limit $L \longrightarrow \infty$

$$\frac{E_C}{L} = -\frac{3}{8\pi W^2}\zeta_R(3)$$

Independent of δ

Attractive force

Same result obtained considering

$$\frac{E_C}{L} = -\frac{g_s g_v}{2\pi}\int_{-\infty}^{\infty} dk_y \sum_{n=0}^{\infty} \left[\left[\left(n+\frac{1}{2}\right)\frac{\pi}{W}\right]^2 + k_y^2\right]^{-\frac{s}{2}} \Bigg|_{s=-1}$$

Alternative expression obtained extending n-sum

$$\frac{E_C}{W} = \frac{2g_s\, g_v}{LW} \sum_{l=-\infty, n=1}^{\infty} (-1)^n \frac{|l+\frac{\delta}{2}|}{n} K_1 \left(|l + \frac{\delta}{2}| \frac{4n\pi\, W}{L} \right) + \frac{g_s\, g_v}{\pi L^2} \sum_{n=1}^{\infty} \frac{\cos\left(n\pi\, \delta\right)}{n^3} \, .$$

S. Bellucci and A.A. Saharian, Phys. Rev. **D80**, 1050003 (2009).

Allows to take $\frac{W}{L} \to \infty$ limit (long nanotube). In this case

$$\frac{E_C}{W} = \frac{g_s\, g_v}{\pi L^2} \sum_{n=1}^{\infty} \frac{\cos\left(n\pi\, \delta\right)}{n^3}$$

Final comments

MIT bag boundary conditions seem to agree reasonably well with experiments with nanoribbons

Predict the existence of a gap which does not depend on the orientation

Equally spaced energy levels

Only boundary conditions which give a symmetric spectrum around zero in the case of nanodots

We performed the calculation of the Casimir energy for nanotubes of arbitrary chirality

In the nanoribbon limit, the Casimir energy shows there is an attractive force between the edges of the robbon