Boundary conditions in the Dirac approach to graphene devices

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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

![Image](image1.png)

**FIG. 1.** The honeycomb lattice as a superposition of two triangular sublattices. The basis vectors are \( \mathbf{a}_1 = (\sqrt{3}/2, -\frac{1}{2}) \), \( \mathbf{a}_2 = (0, 1) \), \( \mathbf{b}_1 = (1/2\sqrt{3}, \frac{1}{2}) \), \( \mathbf{b}_2 = (1/2\sqrt{3}, -\frac{1}{2}) \), \( \mathbf{b}_3 = (-\sqrt{3}, 0) \).

\( A \) sites generated by \( a_1 \) and \( a_2 \)

\( b_1, b_2, b_3 \) connect \( A \) with \( B \) sites

The reciprocal lattice

![Image](image2.png)

**Identified sides**

\( i = \ell m \)

\( j = mn \)

\( k = n \)

**Equivalent corners**

\( i = k = m \)

\( j = \ell = n \)

\( R_1 \) 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

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

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

\[ \phi(k) = \alpha \left( e^{ik\cdot b_1} + e^{ik\cdot b_2} + e^{ik\cdot b_3} \right) = 0 \text{ at the six corners of the Brillouin zone.} \]

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 ($a \to 0$) up to first order in $a$

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

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

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

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 $\gamma$ matrices in 2+1

$A$ and $B$ type of sites - upper and lower components of $\Psi$ in each representation

Graphene is gapless material
Opening a gap

How useful is graphene?

GAPLESS material

To obtain graphene-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 $K_{\pm}$, when necessary, boundary conditions around $K_{\mp}$ 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

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

Note: $\alpha = 0, \pi$ MIT bag boundary conditions
$\alpha = \pm \frac{\pi}{2}$ mimic zigzag boundary.

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

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 orthogonal projectors at both boundaries

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

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

$E = \pm \sqrt{k_x^2 + k_y^2}$
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. $\Delta E = \frac{\pi}{W}$
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 $k_y \rightarrow -k_y$
  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 $\alpha$
- $\forall k_y \neq 0$, values of $k_x$ not equally spaced
- Imaginary as well as real values of $k_x$ are allowed
  Calling $\kappa = ik_x$, for $E \neq \pm k_y$
  $$\kappa \cosh (\kappa W) = k_y \sin \alpha \sinh (\kappa W), \quad \text{for } |k_y| > \frac{1}{W|\sin \alpha|}$$
- 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.

\[ \forall \alpha \neq \pm \frac{\pi}{2}, \text{recovering units, } \Delta E \leq \frac{\hbar v_F \pi}{W} = \frac{3}{2} \pi t \frac{a}{W} = 12.37 eV \frac{a}{W} \] (a is the next neighbor distance). For MIT bag boundary conditions (\( \alpha = 0, \pi \)) the equal sign holds. The numerical value of \( \Delta E \) 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 \((I + i\chi) \psi(x = 0, W) = 0\), where \(n\) is the inward normal vector.
Yu-Ming Lin, Vassili Perebeinos, Zihong 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

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

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

\[
\psi(r, \theta) = \psi(r, \theta + 2\pi),
\]

\( \gamma^r = \sigma_1 \cos \theta + \sigma_2 \sin \theta \) 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 $\alpha$ 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 length $L$ and finite length $W$ in the perpendicular direction
- Impose MIT bag boundary conditions at $x = 0$ and $x = W$

To obtain nanoribbon take $\frac{L}{W} \rightarrow \infty$ 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 \( E_{n,l} = \pm \left[ \left( (n + \frac{1}{2}) \frac{\pi}{W} \right)^2 + \left( (l + \frac{\delta}{2}) \frac{2\pi}{L} \right)^2 \right]^{\frac{1}{2}} \)

$n = 0, \ldots, \infty \quad l = -\infty, \ldots, \infty$

$\delta$ to allow arbitrary periodicity in the compact direction
\[
\frac{E_C}{L} = -\frac{gs \cdot gv}{L} \sum_{l=-\infty}^{\infty} \sum_{n=0}^{\infty} \left[ \left( n + \frac{1}{2} \right) \frac{\pi}{W} \right]^2 + \left[ \left( l + \frac{\delta}{2} \right) \frac{2\pi}{L} \right]^2 \right]^{-\frac{s}{2}} \left. \right|_{s=-1}
\]

Mellin transforming

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

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

\[
\frac{E_C}{L} = -\left( \frac{2\pi}{L} \right)^{-s} \frac{gs \cdot gv \pi^{\frac{1}{2}}}{L \Gamma(\frac{s}{2})} \left\{ \sum_{n=0}^{\infty} \int_0^{\infty} dt \, t^{\frac{s-1}{2}} e^{-t \left[ \left( n + \frac{1}{2} \right) \frac{L}{2W} \right]^2} \right\}_{s=-1}
\]

\[
+4 \sum_{l=1}^{\infty} \sum_{n=0}^{\infty} \int_0^{\infty} dt \cos(\pi l \delta) t^{\frac{s-1}{2}} e^{-t \left[ \left( n + \frac{1}{2} \right) \frac{L}{2W} \right]^2 - \frac{\pi^2 t^2}{4}} \right\}_{s=-1}
\]
Performing the integral and writing first term as a Hurwitz zeta function

\[
\frac{E_C}{L} = -\left(\frac{2\pi}{L}\right)^{-s} \frac{g_s g_v \pi^2}{L \Gamma\left(\frac{s}{2}\right)} \left\{ \Gamma\left(\frac{s-1}{2}\right) \left(\frac{L}{2W}\right)^{1-s} \zeta_H(s - 1, \frac{1}{2}) \right. \\
\left. + 4 \sum_{l=1}^{\infty} \sum_{n=0}^{\infty} \cos(\pi l\delta) \left(\frac{\pi l}{n + \frac{1}{2}}\right)^{s-1} L \frac{1}{2W} K_{s-1} \left(\frac{n + \frac{1}{2}}{2} \frac{\pi l L}{W}\right) \right\} \bigg|_{s=-1}
\]

Relating the Hurwitz zeta function to the corresponding Riemann one, and using the reflection formula for this last
Nanotube compactification length $L$ arbitrary periodicity ($\delta$)  
MIT bag boundary conditions at the extremes

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

Nanoribbon limit $L \rightarrow \infty$

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

Independent of $\delta$

Attractive force

Same result obtained considering

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

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

S. Bellucci and A.A. Saharian, Phys. Rev. \textbf{D80}, 1050003 (2009).

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

\[
\frac{E_C}{W} = \frac{g_s g_v}{\pi L^2} \sum_{n=1}^{\infty} \frac{\cos (n\pi \delta)}{n^3}
\]
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 ribbon