Boundary conditions in the Dirac approach to graphene devices

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We study a family of local boundary conditions for the Dirac problem corresponding to the continuum limit of graphene, both for nanoribbons and nanodots. We show that, among the members of such family, MIT bag boundary conditions are the ones which give the best agreement with experiment.

It would be redundant to start this paper with a detailed description of the wonderful properties of graphene. In this respect, the interested reader is referred to[1]. As predicted theoretically[2,3] twenty years before its production in a laboratory[4], electron transport in graphene is described by a massless Dirac equation, which leads to distinctive electronic properties[5,6]. Indeed, many such properties where studied experimentally, starting with the determination of the quantum Hall effect[7], and found to agree with the predictions of a "relativistic" and massless Dirac field theory[8].

The aforementioned properties allow to envisage many possible applications. However, a crucial point in achieving such goals as the construction of graphene-based transistors is the opening of a controllable band gap in an otherwise gapless material. The use of samples of finite size is a natural guess when trying to do so[6]. In fact, several measurements of the electric conductivity in graphene devices do show the existence of a gap (see, for instance,[9–12]).

Unlike the case of usual semiconductors, the confinement of charge carriers to a finite region cannot be modeled, in the continuous Dirac theory, by the condition that the fields vanish at the boundaries. Most theoretical approaches to this problem presuppose an orientation dependence of the adequate boundary conditions[13,14], which is in contradiction with the experimental results[9]. A nice general study of possible boundary conditions in the Dirac problem and of their symmetries in the case of nanotubes was presented in[15]. It is the aim of this paper to study one possible family of boundary conditions and compare the predictions arising from taking different members of such family with experimental results.

We will choose the orientation of the lattice as in reference[2], so that, by taking the two nonequivalent Dirac points as $K_\pm = (0, \pm\frac{4\pi}{3a})$, we get the total Hamiltonian as a direct sum of

$$H_\pm = \hbar v_F(-i\sigma_2\partial_x \pm i\sigma_1\partial_y)\,, \tag{1}$$

where $v_F = \frac{3at}{2\hbar}$ is the Fermi velocity of graphene, with $a = 0.14nm$ the distance between nearest neighbors and $t = 2.7eV$ the nearest neighbor hopping energy.

Such Hamiltonian corresponds to a free Dirac equation in $2+1$ dimensions, where the gamma matrices are given, in each valley, by $\gamma^0_\pm = i\sigma_3$, $\gamma^1_\pm = \sigma_1$, $\gamma^2 \pm = \pm\sigma_2$. We will study the corresponding eigenvalue problems $H_\pm\Psi_\pm(x,y) = E_\pm\Psi_\pm(x,y)$, when the domain of the differential operator is 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[14],
3. Are defined through a self-adjoint projector[14,15].

From now on, we will study the problem around K_+, leaving the discussion on how to combine boundary conditions in both valleys for later on. We will consider the boundary to be placed at a given $x = x_0$ value. Throughout our calculations, we will take $v_F = \hbar = 1$, and recover the right units when comparing our predictions with experimental results.

The condition 2. is a close to confinement as one can get in a Dirac theory and it leads to a self-adjoint Hamiltonian (thus, to real energies). It is easy to check that the current perpendicular to the boundary is proportional to $\Psi^\dagger_+\sigma_2\Psi_+$, while the current along the boundary is proportional to $\Psi^\dagger_+\sigma_1\Psi_+$. So, the most general local boundary conditions satisfying conditions 1. to 3. above are given by $(I + \sigma_1\, e^{-i\alpha\sigma_2})\Psi_+\rfloor_{x=x_0} = 0$, which is a one-parameter family. Note that $\alpha = 0, \pi$ correspond to the so-called MIT bag boundary conditions[16], while $\alpha = \pm\frac{\pi}{2}$ are the conditions used to mimic a zigzag boundary[13]. Each member of this family imposes a different condition on the density of tangential current at the boundary. In fact, one has $\Psi^\dagger_+\sigma_1\Psi_+\rfloor_{x=x_0} = -\cos(\alpha)\Psi^\dagger_+\Psi_+\rfloor_{x=x_0}$. In particular, zigzag boundary conditions enforce the vanishment of the tangential current at the boundary, while MIT ones equate it to the density of charge.

In view of the translational invariance along the y direction we will propose, for each k_y, $\Psi_+(x,y) = e^{ik_y\, y}\psi_+(x)$.

We start with the case of the half plane, with its boundary at $x = 0$, in order to analyze the existence of edge states (or the lack thereof). In order to do so, it is convenient to perform a unitary transformation of the eigenfunctions, $\tilde\psi(x) = e^{-i\frac{\alpha}{2}\sigma_2}\psi_+(x)$. This leads us to the eigenvalue problem,

$$\begin{aligned}&[-i\sigma_2\partial_x - \sigma_1 k_y\cos\alpha + \sigma_3 k_y\sin\alpha]\,\tilde\psi(x) = E\tilde\psi(x)\\ &(I+\sigma_1)\,\tilde\psi(x=0) = 0\,,\end{aligned} \tag{2}$$

together with the normalizability condition when $x \to \infty$.

It is a simple exercise to show that, for all $\alpha \neq 0, \pi$ (i.e., all boundary conditions different from the MIT bag ones) there are, apart from bulk sates, some edge states, corresponding to $E = k_y \cos\alpha$, with $k_y \sin\alpha > 0$, which are eigenfunctions decreasing exponentially with x, thus concentrated at the boundary.

The existence of these states is well known for zigzag boundary conditions ($\alpha = \pm\frac{\pi}{2}$), in which case they are zero energy modes[5]. This shows that, in a compact region with a single smooth boundary, the boundary problem will not satisfy the Lopatinsky-Shapiro condition (equivalently, they would not define a Fredholm operator)[17]. In the remaining cases, these modes correspond to real, nonzero, energies. We will comment on this point when treating circular quantum dots.

For a comparison with experiments, we will first discuss the case of a graphene nanoribbon, which requires the imposition of a boundary condition at a second boundary, placed at $x = W$.

Experiments concerning nanoribbons[9,10,12] show a gap which, moreover, is symmetric around the Dirac point. There are two ways of obtaining a symmetric spectrum, i.e., choosing exactly the same projector to define the boundary condition at $x = W$ or choosing, instead, the orthogonal one. It is easily shown that the first alternative allows for the existence of zero modes, no matter the value of α. They appear for all values of k_y when $\alpha = \pm\frac{\pi}{2}$ and for $k_y = 0$ in the remaining cases. So, we will limit our discussion to the second alternative, which is also consistent with the fact that the sign of the inward normal is opposite at both boundaries.

Our boundary value problem will now be,

$$\begin{aligned} &[-i\sigma_2\partial_x - \sigma_1 k_y \cos\alpha + \sigma_3 k_y \sin\alpha]\,\tilde{\psi}(x) = E\tilde{\psi}(x) \\ &(I + \sigma_1)\,\tilde{\psi}(x = 0) = 0 \\ &(I - \sigma_1)\,\tilde{\psi}(x = W) = 0\,. \end{aligned} \tag{3}$$

In all cases one has $E = \pm\sqrt{k_x^2 + k_y^2}$. However, MIT bag boundary conditions are unique in that the spectrum is determined by the equation $\cos(k_x W) = 0$, which doesn't depend on k_y, and they allow only real values of k_x. Thus we have, in these two cases ($\alpha = 0, \pi$),

$$E_n = \pm\sqrt{\left(\frac{(n+\frac{1}{2})\pi}{W}\right)^2 + k_y^2}\,. \tag{4}$$

This leads to an energy gap $\Delta_E = \frac{\pi}{W}$.

The remaining values of α, instead, lead to a spectrum determined by

$$k_x \cos(k_x W) = k_y \sin\alpha \sin(k_x W) \quad \text{for } E \neq \pm k_y\,, \tag{5}$$

and

$$k_y = \frac{1}{W \sin\alpha}, \quad \text{for } E = \pm k_y\,. \tag{6}$$

Note that both equations break the invariance under $k_y \to -k_y$. It is difficult to imagine why this invariance would be broken in a ribbon, which extends to $-\infty < y < \infty$, in the absence of electromagnetic fields. Such invariance could only be recovered by imposing exactly the same boundary conditions on the eigenfunctions around the other valley.

Moreover, for $k_y = 0$ one has $k_x = \frac{(n+\frac{1}{2})\pi}{W}$, no matter the value of α. For all the remaining values of k_y, at variance with the situation in the MIT case, the admissible values of k_x are not equally spaced.

But, more important, equation (5) allows for imaginary as well as real values of k_x. Calling $\kappa = i\,k_x$ one has, for $E \neq \pm k_y$,

$$\kappa\cosh(\kappa W) = k_y \sin\alpha \sinh(\kappa W), \text{ for } |k_y| > \frac{1}{W|\sin\alpha|}\,. \tag{7}$$

When $|\sin\alpha| = 1$, i.e., zigzag boundary conditions, this equation allows for energies arbitrarily close to zero when $\kappa \to \infty$. As a consequence, no gap exists in this case, which is a well known fact[5]. For the remaining values of α, the eigenenergies coming from equation (5) never tend to zero. The analysis of the minimal value of $|E|$ can be performed analytically. From such analysis one concludes that, for all α, the energy gap satisfies $\Delta E \leq \frac{\pi}{W}$.

The experiments on nanoribbons[9,10,12] show a transport gap as a function of the gate voltage, when performed at low temperature and bias voltage. This eliminates zigzag boundary conditions as candidates to describe the physical situation. For the remaining values of α we have, recovering units, $\Delta E \leq \frac{\hbar v_F \pi}{W} = \frac{3}{2}\pi t\frac{a}{W}$. For MIT bag boundary conditions ($\alpha = 0, \pi$) the equal sign holds. Moreover, reference[10] shows equally spaced plateaux in the conductivity, which suggests that MIT bag boundary conditions are the ones to be imposed in the continuous model.

As for the numerical value of the gap, reference[12] presents a study of several graphene nanoribbons, of different widths, all of which show a gap in the gate voltage corresponding to a one-particle energy gap fitted to $\Delta_m = 36eV\frac{a}{W}$. This is roughly three times our result for MIT boundary conditions, i.e., $\Delta E = 12.7eV\frac{a}{W}$. Reference[10] finds, for a sample of width $W = 30nm$, a value of the energy gap $\Delta E = 46meV$, in very good agreement with our result for such case, i.e., $\Delta E = 57meV$ (note, that, in this case, our prediction is higher than the measured gap). Obviously, both experiments disagree. The origin of such discrepancy is not clear to us, since both use similar values of the capacitance for comparable samples.

Finally, as shown clearly by reference[9], and at odds with most theoretical models[13,14] (which would impose different boundary conditions depending on the orientation of the boundary) the measured gap in the gate voltage doesn't depend on the orientation of the boundary. This will certainly be the case in our continuous model if MIT bag boundary conditions are written as $(I + \not{n})\,\psi(x = 0, W) = 0$, where n is the inward pointing normal vector corresponding to each boundary. More-

over, consistently imposing MIT boundary conditions around K_- leads to the same gap in both valleys.

In order to further compare the predictions of different members of our family of boundary conditions with the experiment, we will now treat the case of a circular graphene dot of radius R. To this end, we adopt polar coordinates. Taking the gamma matrices for the theory around K_+ as before, we are led to the boundary value problem (with $v_F = \hbar = 1$),

$$\begin{aligned} &\left[-i\gamma^\theta\partial_r + i\frac{\gamma^r}{r}\partial_\theta\right]\psi(r,\theta) = E\psi(r,\theta) \\ &\left(I - \gamma^r e^{-i\alpha\gamma^\theta}\right)\psi(r=R,\theta) = 0 \\ &\psi(r,\theta) = \psi(r,\theta+2\pi)\,, \end{aligned} \tag{8}$$

where $\gamma^r = \sigma_1\cos\theta + \sigma_2\sin\theta$ and $\gamma^\theta = \sigma_2\cos\theta - \sigma_1\sin\theta$.

Solving this boundary value problem is a simple exercise (see, for instance[18]). The first outcome is that zigzag boundary conditions ($\alpha = \pm\frac{\pi}{2}$) allow for an infinite amount of zero modes, as expected from the facts that they don't satisfy the Lopatinski-Shapiro condition and that we are now treating a compact region with a smooth boundary. As for the remaining conditions in the family, none of them allows for zero modes. Since experiments on quantum dots also present a gap, we will concentrate on the remaining cases ($\cos\alpha \neq 0$), which give a spectrum determined by

$$\begin{aligned} &(1-\sin\alpha)J_n(|E|R) + s\cos\alpha)J_{n+1}(|E|R) = 0,\ n = 0, ..., \infty \\ &(1-\sin\alpha)J_{n+1}(|E|R) - s\cos\alpha)J_n(|E|R) = 0,\ n = 0, ..., \infty \end{aligned} \tag{9}$$

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

Now, the experiment[11] 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.

Note that reference[18] had already suggested that this could be the case. Indeed, this is the first guess a particle physicist would make when asked for confinement in a Dirac theory. The comparison with experimental results presented in this paper shows this to be, most probably, the case.

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