

# Transport properties of graphene across strain-induced nonuniform velocity profiles

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We consider the effect of uniaxial strain on ballistic transport in graphene, across single and multiple tunneling barriers. Specifically, we show that applied strain not only shifts the position of the Dirac points in reciprocal space, but also induces a deformation of the Dirac cones, and that both effects are of the same order on the applied strain intensity. We therefore study the deviations thereby induced on the angular dependence of the tunneling transmission across a single barrier, as well as on the conductivity and Fano factor across a single barrier and a superstructure of several, periodically repeated, such sharp barriers. Our model is generalized to the case of nonuniform barriers, where either the strain or the gate potential profiles may depend continuously on position. This should afford a more accurate description of realistic “origami” nanodevices based on graphene, where “foldings” are expected to involve several lattice spacings.

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## I. INTRODUCTION

Graphene is an atomically thin, two-dimensional layer of carbon atoms arranged according to a honeycomb lattice. After having been speculated since long ago as the ideal building block of graphite and other  $sp^2$  carbon compounds, it has been recently obtained in the laboratory,<sup>1</sup> thereby kindling an extraordinary outburst of experimental as well as theoretical research activity.<sup>2,3</sup> Reduced dimensionality and its peculiar structure conspire toward the formation of low-energy quasiparticles, which can be described as massless Dirac fermions with a cone dispersion relation in reciprocal space around the so-called Dirac points  $\mathbf{K}$ ,  $\mathbf{K}'$ , and a linearly vanishing density of states (DOS) at the Fermi level. This is reflected in several electronic properties already in the noninteracting limit, e.g., Klein tunneling,<sup>4–8</sup> the reflectivity,<sup>9</sup> the optical conductivity,<sup>10–14</sup> and the plasmon dispersion relation.<sup>15–18</sup>

Graphene is also remarkable for its exceptional mechanical properties, as is generic for most carbon compounds. For instance, notwithstanding its reduced dimensionality, graphene is characterized by a relatively large tensile strength and stiffness,<sup>19</sup> with graphene sheets being capable to sustain elastic deformations as large as  $\approx 20\%$ .<sup>20–24</sup> Larger strains would then induce a semimetal-to-semiconductor transition, with the opening of an energy gap,<sup>25–28</sup> and it has been demonstrated that such an effect critically depends on the direction of applied strain.<sup>14,29</sup> The effect of uniaxial strain on the linear-response electronic properties of graphene has been studied on quite general grounds.<sup>30</sup>

Recently, it has been suggested that graphene-based electronic devices might be designed by suitably tailoring the electronic structure of a graphene sheet under applied strain.<sup>31</sup> Indeed, a considerable amount of work has been devoted to the study of the transport properties in graphene across strain-induced single and multiple barriers.<sup>32,33</sup> There, the main effect of strain has usually been considered to be that of shifting the position of the Dirac points in reciprocal space. However, it has been demonstrated that a nonuniform space

variation of the underlying gate potential would result in a modulation of the Fermi velocity.<sup>32,34,35</sup>

Here, we show that both effects are of the same order on the applied strain intensity, and should therefore be considered on the same ground, when studying the transport properties of strained graphene. We shall therefore explicitly consider not only the strain-induced displacement of the Dirac points in reciprocal space, but also a strain-induced deformation of the Dirac cones, resulting in a strain-dependent anisotropic Fermi velocity. Specifically, we will consider tunneling through a single strain-induced sharp barrier, possibly subjected to a gate potential, and through a superstructure made of several such barriers, periodically repeated. More interestingly, we will generalize our results to the problem of transport through a tunneling structure, characterized by a *nonuniform* variation of both the Fermi velocity and of the gate potential, as can, e.g., be brought about by a continuous deformation or applied uniaxial strain.

The paper is organized as follows. After introducing our model in Sec. II, we discuss the effect of a strain-induced modulation of the Fermi velocity on the angular dependence of the transmission across a single sharp barrier, as well as on the conductivity and Fano factor for ballistic transport (Sec. III). We then consider the case of several such barriers, arranged in a periodic fashion (Sec. IV). In Sec. V, we generalize our results to the case of *nonuniform* strain across a smooth barrier. Finally, in Sec. VI we summarize and give directions for future investigation.

## II. MODEL

In unstrained graphene, low-energy quasiparticles can be described by the linear Hamiltonian in momentum space,

$$H^{(0)} = \hbar v_F \mathbb{I} \boldsymbol{\sigma} \cdot \mathbf{p}, \quad (1)$$

where  $v_F$  is the Fermi velocity,  $\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$ , with  $\sigma_i$  and  $\tau_i$  ( $i = 1, 2, 3$ ) Pauli matrices and  $\mathbb{I}$  the identity matrix associated with the two-dimensional spaces of the sublattices ( $A$  and  $B$ ,

say), and of the two valleys around the Dirac points ( $\mathbf{K}$  and  $\mathbf{K}'$ ), respectively. Equation (1) acts on the four-component spinors,<sup>36,37</sup>

$$\Psi_{\mathbf{p}} = (\Psi_{A,\mathbf{K}}(\mathbf{p}), \Psi_{B,\mathbf{K}}(\mathbf{p}), \Psi_{B,\mathbf{K}'}(\mathbf{p}), -\Psi_{A,\mathbf{K}'}(\mathbf{p}))^{\top}, \quad (2)$$

where  $\mathbf{p}$  is measured from the Dirac point one is referring to. Here and below, a superscript zero denotes absence of strain. The effect of uniaxial strain in real space is that of modifying the lattice vectors as  $\delta_{\ell} = (\mathbb{I} + \boldsymbol{\varepsilon}) \cdot \delta_{\ell}^{(0)}$  ( $\ell = 1, 2, 3$ ), where  $\delta_1^{(0)} = a(\sqrt{3}, 1)/2$ ,  $\delta_2^{(0)} = a(-\sqrt{3}, 1)/2$ ,  $\delta_3^{(0)} = a(0, -1)$  are the relaxed (unstrained) vectors connecting two nearest-neighbor (NN) carbon sites, with  $a = 1.42 \text{ \AA}$ , the equilibrium C-C distance in a graphene sheet,<sup>2</sup> and  $\boldsymbol{\varepsilon}$  is the strain tensor,<sup>26</sup>

$$\boldsymbol{\varepsilon} = \frac{1}{2}\varepsilon[(1 - \nu)\mathbb{I} + (1 + \nu)A(\theta)], \quad (3)$$

where

$$A(\theta) = \cos(2\theta)\sigma_z + \sin(2\theta)\sigma_x, \quad (4)$$

where the Pauli matrices now are understood to act on vectors of the two-dimensional direct or reciprocal lattice. In Eq. (3),  $\theta$  denotes the angle along which the strain is applied, with respect to the  $x$  axis in the lattice coordinate system,  $\varepsilon$  is the strain

modulus, and  $\nu$  is Poisson's ratio. While in the hydrostatic limit  $\nu = -1$  and  $\boldsymbol{\varepsilon} = \varepsilon\mathbb{I}$ , in the case of graphene one has  $\nu = 0.14$ , as determined from *ab initio* calculations,<sup>38</sup> to be compared with the known experimental value  $\nu = 0.165$  for graphite.<sup>39</sup> The special values  $\theta = 0$  and  $\theta = \pi/2$  refer to strain along the zigzag and armchair directions, respectively.

The possibility of describing the effects of strain through Eq. (3), i.e., elastically, implies that applied strain does not induce any irreversible process or mechanical failure of the graphene sheet, such as dislocations, grain boundaries, or cracks. In fact, such dramatic effects are not expected for strain below  $\sim 20\%$ , as is predicted by calculations within density-functional theory,<sup>21,40</sup> and confirmed experimentally by means of atomic force microscopy (AFM).<sup>41</sup>

In momentum space, the effect of uniaxial strain on the Hamiltonian Eq. (1) is likewise accounted for by the strain tensor, Eq. (3). This is usually described as a shift in momentum space of the location of the Dirac points. However, starting from the more general, tight-binding Hamiltonian,<sup>2</sup> expanding to first order in the strain modulus, and to second order in the impulses, one may show that applied strain also induces a deformation of the Dirac cones, at the same (first) order in  $\varepsilon$ . Explicitly, one finds

$$\begin{aligned} H = & \hbar v_F \sigma_1 \left\{ \left[ 1 + \left( \frac{1}{2} - \kappa_0 \right) \varepsilon (1 - \nu) + \left( \frac{1}{2} - \frac{1}{2} \kappa_0 \right) \varepsilon (1 + \nu) \cos(2\theta) \right] p_x + \left( \frac{1}{2} - \frac{1}{2} \kappa_0 \right) \varepsilon (1 + \nu) \sin(2\theta) p_y \right\} \\ & + \hbar v_F \sigma_2 \left\{ \left[ 1 + \left( \frac{1}{2} - \kappa_0 \right) \varepsilon (1 - \nu) - \left( \frac{1}{2} - \frac{1}{2} \kappa_0 \right) \varepsilon (1 + \nu) \cos(2\theta) \right] p_y + \left( \frac{1}{2} - \frac{1}{2} \kappa_0 \right) \varepsilon (1 + \nu) \sin(2\theta) p_x \right\} \\ & - \frac{1}{4} \hbar v_F \tau_3 \left[ \sigma_1 (p_x^2 - p_y^2) - 2\sigma_2 p_x p_y \right] - \hbar v_F \tau_3 \sigma_1 \varepsilon (1 + \nu) \cos(2\theta) + \hbar v_F \tau_3 \sigma_2 \varepsilon (1 + \nu) \sin(2\theta), \end{aligned} \quad (5)$$

where  $\kappa_0 = (a/2t)|\partial t/\partial a| \approx 1.6$  is related to the logarithmic derivative of the nearest-neighbor hopping  $t$  at  $\varepsilon = 0$ .

Our model is based on the tight-binding approximation for the band structure, including only nearest-neighbor hopping. To this level of approximation, one does not observe any strain-induced modification of the work function  $\Phi$ . In order to include also such effects, one needs to consider also next-nearest-neighbor hopping.<sup>2</sup> Making use of the expression for the hopping function between two neighboring carbon  $p$  orbitals involved in a  $\pi$  bond, as a function of the bond length  $\ell$ ,  $V_{pp\pi}(\ell) = t_0 e^{-3.37(\ell/a-1)}$ , with  $t_0 = -2.7 \text{ eV}$ ,<sup>26</sup> one finds

$$\Phi = \frac{3}{2}(1 - \nu)\sqrt{3}a \left. \frac{dV_{pp\pi}(\ell)}{d\ell} \right|_{\ell=\sqrt{3}a} \quad \varepsilon \approx 1.7 \text{ eV} \times \varepsilon, \quad (6)$$

viz. a scalar term, going linear with the strain modulus  $\varepsilon$ , whose order of magnitude agrees with the *ab initio* results of Ref. 23. At any rate, the work function, Eq. (6), can be absorbed in an effective scalar potential  $U$ , which we conventionally refer to as a gate potential below.

Another effect that is not explicitly considered in our model is the deformation of the  $\pi$  orbitals due to off-plane bending, as would be, e.g., generated by an AFM tip. However, a change in the hopping parameters due to the bending of the graphene sheet can be described as an effective in-plane strain.<sup>42</sup> Specifically, one may expect that strain induced by an AFM tip would be characterized by cylindrical symmetry, which is beyond the scope of the present work, where

only linear barriers are considered. We note in passing that other efficient ways to realize controllable strain consists in depositing graphene on top of deformable substrates.<sup>43,44</sup>

The spectrum of the strained Hamiltonian, Eq. (5), is still linear, but now around the shifted Dirac points  $\mathbf{q}_D \mathbf{a} = \pm(\kappa_0 \varepsilon (1 + \nu) \cos(2\theta), -\kappa_0 \varepsilon (1 + \nu) \sin(2\theta))^{\top}$ . To first order in the wave-vector displacement  $\mathbf{q} = \mathbf{p} \mp \mathbf{q}_D$  from such shifted Dirac points, one finds

$$H = \hbar v_F \boldsymbol{\sigma} \cdot \mathbf{q}', \quad (7)$$

where

$$\mathbf{q}' = \{[1 - \kappa \varepsilon (1 - \nu)]\mathbb{I} - \kappa \varepsilon (1 + \nu)A(\theta)\}\mathbf{q}, \quad (8)$$

and  $\kappa = \kappa_0 - \frac{1}{2}$ . However, it is convenient to work in the reference frame with the  $x$  axis along the direction of applied strain. This is accomplished by a rotation in the sublattice  $AB$  space, described by the unitary matrix

$$U(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\theta} \end{pmatrix}, \quad (9)$$

so that

$$H = \hbar v_F U^{\dagger}(\theta) [\sigma_1 (1 - \lambda_x \varepsilon) q_x + \sigma_2 (1 - \lambda_y \varepsilon) q_y] U(\theta), \quad (10)$$

where  $\lambda_x = 2\kappa$ ,  $\lambda_y = -2\kappa\nu$ . After the rotation, Eq. (9), the location of the Dirac points is given by

$$\mathbf{q}_D \mathbf{a} = \pm(\kappa_0\varepsilon(1+\nu)\cos(3\theta), -\kappa_0\varepsilon(1+\nu)\sin(3\theta))^\top. \quad (11)$$

The density operator can be expressed as

$$\rho(\mathbf{r}) = \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}), \quad (12)$$

where  $\Psi(\mathbf{r}) = (2\pi)^{-2} \int d^2\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{r}} \Psi(\mathbf{k})$ . Correspondingly, the current density operator can be derived as<sup>45</sup>  $\mathbf{J} = -\frac{ie}{\hbar}[H, \mathbf{r}]$ , yielding

$$J_i(\mathbf{r}) = -ev_F\Psi^\dagger(\mathbf{r})(1-\lambda_x\varepsilon)U^\dagger(\theta)\sigma_i U(\theta)\Psi(\mathbf{r}). \quad (13)$$

In the following, for the sake of definitiveness, we shall restrict to the valley  $\mathbf{K}$  only, thus having  $\mathbf{q} = \mathbf{p} - \mathbf{q}_D$ .

### III. TUNNELING ACROSS A SINGLE BARRIER

Potential barriers for single quasiparticle tunneling in graphene are conventionally designed by suitably changing the underlying gate voltage. Recently, it has been suggested that an equivalent effect may be induced by local uniaxial strain.<sup>31,42</sup> Therefore we start by considering a strain-induced one-dimensional steplike barrier, characterized by uniaxial strain applied along the direction  $\theta$ , with respect to the  $x$  axis, Eq. (3), with strain modulus  $\varepsilon$  for  $0 \leq x \leq D$ , and zero otherwise. Correspondingly, the Hamiltonian and current density vector are given by Eqs. (10) and (13), respectively. In addition, for the sake of generality, we may also consider a nonzero gate potential  $V_g$  within the barrier (Fig. 1).

Since we are interested in stationary solutions and the strain barrier is uniform along the  $y$  direction, the energy  $E$  and the component  $k_y$  of the wave vector of an incoming wave are conserved. We look therefore for solutions of the stationary Dirac equation of the form

$$\psi(x, y) = \begin{cases} U^\dagger(\theta)\psi_I(x)e^{ik_y y}, & x < 0, \\ U^\dagger(\theta)\psi_{II}(x)e^{ik_y y}, & 0 \leq x \leq D, \\ U^\dagger(\theta)\psi_{III}(x)e^{ik_y y}, & x > D, \end{cases} \quad (14)$$

where

$$\psi_I(x) = \left[ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ s e^{i\varphi} \end{pmatrix} e^{ik_x x} + \frac{r}{\sqrt{2}} \begin{pmatrix} 1 \\ -s e^{-i\varphi} \end{pmatrix} e^{-ik_x x} \right], \quad (15a)$$

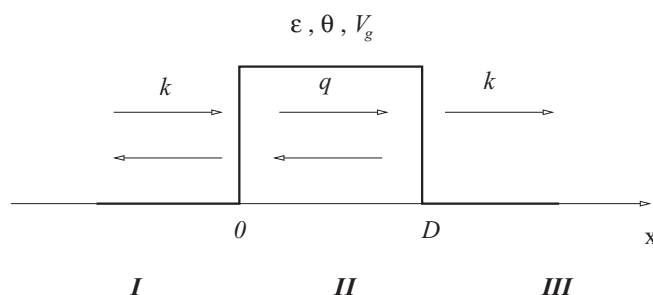


FIG. 1. One-dimensional single tunneling barrier along the  $x$  direction. Region II ( $0 \leq x \leq D$ ) is characterized by applied strain  $\varepsilon$  along the  $\theta$  direction, as well as by a gate voltage  $V_g$ .

$$\psi_{II}(x) = \left[ \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ s' e^{i\alpha} \end{pmatrix} e^{i(q_x + q_D)x} + \frac{b}{\sqrt{2}} \begin{pmatrix} 1 \\ -s' e^{-i\alpha} \end{pmatrix} e^{-i(q_x - q_D)x} \right], \quad (15b)$$

$$\psi_{III}(x) = t \begin{pmatrix} 1 \\ s e^{i\varphi} \end{pmatrix} e^{ik_x x}. \quad (15c)$$

In Eqs. (15),  $\varphi$  denotes the angle of incidence with respect to the barrier,  $k_x = (|E|/\hbar v_F) \cos \varphi$ ,  $k_y = (|E|/\hbar v_F) \sin \varphi$ ,  $(E - U_g)^2 = \hbar^2 v_F^2 [(1 - \lambda_x \varepsilon)^2 q_x^2 + (1 - \lambda_y \varepsilon)^2 (k_y - q_{Dy})^2]$ ,  $s' = \text{sgn}(E - U_g)$ , with  $U_g = -eV_g$ . Propagating waves correspond to real values of  $q_x$ , while evanescent waves correspond to having  $q_x$  purely imaginary.

Given the stationary character of the solution, the continuity equation implies that  $\nabla \cdot \mathbf{J} = 0$  everywhere. In particular,  $\langle \mathbf{J} \rangle \equiv \langle \psi | \mathbf{J} | \psi \rangle$  may only depend on  $x$ , therefore  $\langle J_x \rangle$  is constant. The latter condition implies, at the barrier boundaries,

$$\psi_I(0^-) = (1 - \lambda_x \varepsilon)^{-1/2} \psi_{II}(0^+), \quad (16a)$$

$$(1 - \lambda_x \varepsilon)^{-1/2} \psi_{II}(D^-) = \psi_{III}(D^+). \quad (16b)$$

Enforcing the above conditions in Eqs. (15), one eventually finds for the tunneling transmission,  $T = |t|^2$ ,

$$T = \frac{C^2 \cos^2 \varphi}{C^2 \cos^2 \varphi \cos^2(q_x D) + (1 - s s' S \sin \varphi)^2 \sin^2(q_x D)}, \quad (17)$$

where  $q_y = k_y - q_{Dy}$ ,  $q_x = (1 - \lambda_x \varepsilon)^{-1} |(E - U_g)^2 / \hbar^2 v_F^2 - (1 - \lambda_y \varepsilon)^2 q_y^2|^{1/2}$ ,  $C = (1 - \lambda_x \varepsilon) \hbar v_F q_x / |E - U_g|$ ,  $S = (1 - \lambda_y \varepsilon) \hbar v_F q_y / |E - U_g|$ .

#### A. Angular dependence

In order to discuss the dependence of the tunneling transmission on the incidence angle  $\varphi$ , we preliminarily observe that propagation within the barrier is allowed whenever

$$\hbar^2 v_F^2 (1 - \lambda_y \varepsilon)^2 (k_y - q_{Dy})^2 \leq (E - U_g)^2, \quad (18)$$

where  $k_y = (E/\hbar v_F) \sin \varphi$ . Within such a range, one has moreover total transmission ( $T = 1$ ) whenever

$$q_x D = n\pi, \quad (19)$$

$n$  being an integer. Equation (18) differs from the usual condition for propagation across strain-induced barriers<sup>31</sup> in that we are not only considering a shift of the Dirac point  $\mathbf{q}_D$ , but also a strain-induced deformation of the Dirac cone, here exemplified by the substitution  $v_F \mapsto v_F(1 - \lambda_y \varepsilon)$ .

Figures 2 and 3 show our results for the tunneling transmission  $T = T(\varphi)$ , Eq. (17), as a function of the incidence angle  $\varphi$ , for  $E = 80$  meV,  $D = 100$  nm (Fig. 2) and  $E = 150$  meV,  $D = 100$  nm (Fig. 3). In both figures, the left (respectively, right) panel refers to uniaxial strain applied along the zigzag ( $\theta = 0$ ; respectively, armchair,  $\theta = \pi/2$ ) direction.

In the case of strain applied along the zigzag direction ( $\theta = 0$ , Figs. 2 and 3, left panels), curves (b) neglect a strain-induced deformation of the Dirac cone. Comparison with curves (c), where such a deformation is fully included, shows that the effect of a strain-induced anisotropy of the Fermi velocity

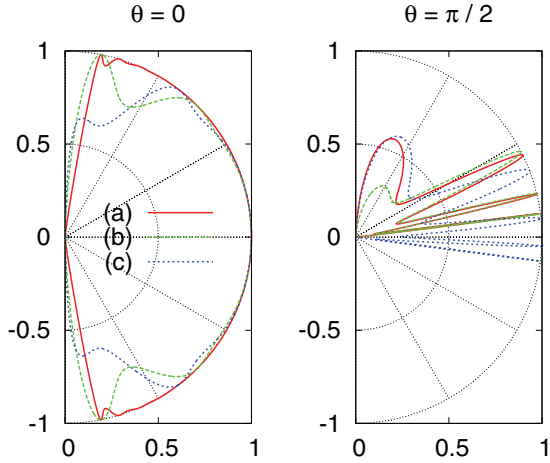


FIG. 2. (Color online) Dependence on the incidence angle  $\varphi$  of the tunneling transmission  $T$ , Eq. (17). Left panel refers to strain applied along the zigzag direction ( $\theta = 0$ ), and (a)  $\varepsilon = 0.03$ ,  $U_g = 0$  meV; (b)  $\varepsilon = 0.03$ ,  $U_g = -20$  meV (the strain-induced deformation of the Dirac cone is neglected); (c)  $\varepsilon = 0.03$ ,  $U_g = -20$  meV. Right panel refers to strain applied along the armchair direction ( $\theta = \pi/2$ ), and (a)  $\varepsilon = 0.01$ ,  $U_g = 0$  meV; (b)  $\varepsilon = 0.01$ ,  $U_g = 0$  meV (the strain-induced deformation of the Dirac cone is neglected); (c)  $\varepsilon = 0.01$ ,  $U_g = -20$  meV.

is that of shifting the angular location of the maxima [ $T = 1$ , Eq. (19)] of the tunneling transmission. Such an effect becomes more important with increasing energy (from Fig. 2 to Fig. 3), while the number of peaks increases, Eq. (19), and the angular range in which the propagating regime is allowed widens. The effect of a strain-induced deformation of the Dirac cone is even more dramatic in the absence of a gate potential [ $U_g = 0$  meV, curve (a)]. Indeed, in such a case, neglecting the Fermi velocity anisotropy for strain applied along the zigzag direction would yield a uniform tunneling transmission  $T = 1$ , for all incidence angles  $\varphi$ , whereas we find that transmission via propagating waves is allowed only for  $|\varphi| \leq \arcsin[(1 - \lambda_y \varepsilon)^{-1}]$ , with small oscillations below  $T = 1$  within, and evanescent waves beyond that range. A similar analysis applies to the case of strain applied along the armchair direction ( $\theta = \pi/2$ , Figs. 2

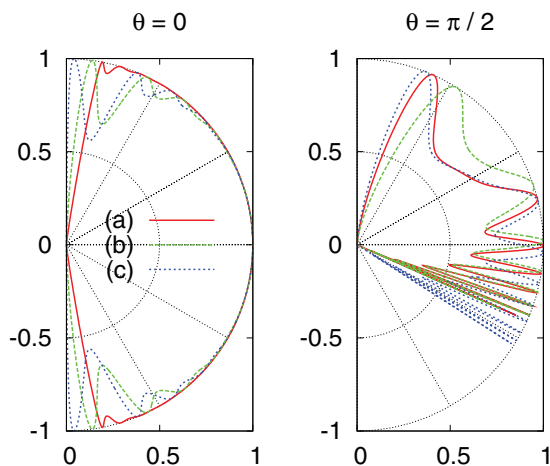


FIG. 3. (Color online) Same as Fig. 2, but for  $E = 150$  meV and  $D = 100$  nm.

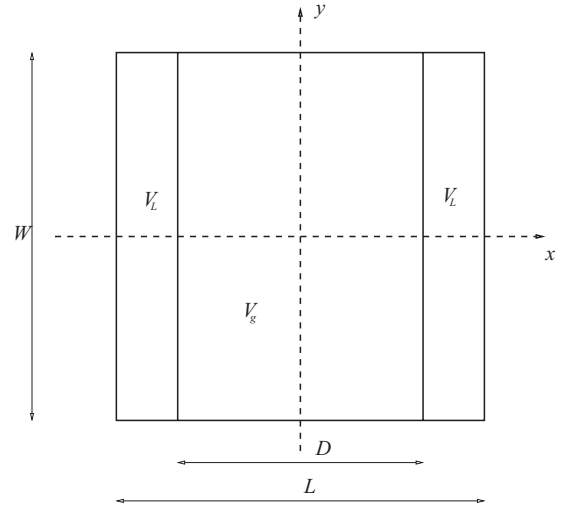


FIG. 4. Schematic top view of a graphene layer contacted by metallic leads, as considered in Sec. III B.

and 3, right panels), which is characterized by an asymmetric transmission  $T = T(\varphi)$ , with pronounced oscillations for  $\varphi > 0$  close to the propagating edge.

The origin of such an asymmetry of the  $\varphi$  dependence of the transmission can be traced back to the particular Dirac cone vertex  $\mathbf{q}_D$ , whose shift is here considered. Global symmetry would be restored upon inclusion of the other Dirac cone. In that case, one would obtain the same picture, but with  $\varphi \mapsto -\varphi$ . It should be emphasized that the stationarity condition, Eq. (19), characterizes the occurrence of peaks in the transmission  $T(\varphi)$  in any case. In addition, for a potential barrier, in the absence of strain, one also recovers complete transmission ( $T = 1$ ) at  $\varphi = 0$  (Klein tunneling).

Summarizing, at variance with previous studies,<sup>31</sup> from Eq. (17) one obtains that the overall effect of a strain-induced deformation of the Dirac cones is that of shifting the transmission peaks, and of reducing the range in  $\varphi$  at which transmission takes place.

## B. Ballistic transport

We now consider a more realistic device, viz. a graphene strip of length  $L$  and width  $W$ , subjected to two leads at a distance  $D$  (Fig. 4).<sup>33,34,46,47</sup> Following Ref. 46, we assume that  $W/L \gg 1$ , and that the gate potential within the strip is much less than the potential of the leads,  $|V_g| \ll |V_L|$ . Moreover, we assume the graphene strip to be characterized by uniaxial strain, with modulus  $\varepsilon$  and strain direction  $\theta$ , and explicitly consider the deformation of the Dirac cones induced by the applied strain. The energy levels of Ref. 46 are therefore modified into

$$E = U_L + s\hbar v_F \sqrt{k_x^2 + k_y^2}, \quad x < 0, \quad x > D, \quad (20a)$$

$$= U_g + s'\hbar v_F \sqrt{(1 - \lambda_x \varepsilon)^2 q_x^2 + (1 - \lambda_y \varepsilon)^2 q_y^2}, \quad 0 < x < D, \quad (20b)$$

where again  $q_y = k_y - q_{Dy}$ , and  $U_L = -eV_L$  and  $U_g = -eV_g$ . The limit  $|V_L| \rightarrow \infty$  is equivalent to the limit  $\varphi \rightarrow 0$ , and the transmission, Eq. (17), reduces to

$$T_\alpha^{\text{prop}}(k_y) = \frac{1}{\cos^2(q_x D) + \eta(k_y) \sin^2(q_x D)}, \quad (21)$$

for propagating waves in the valley  $\alpha = \mathbf{K}$ , where

$$\eta(k_y) = \frac{(E - U_g)^2}{(E - U_g)^2 - \hbar^2 v_F^2 (1 - \lambda_y \varepsilon)^2 (k_y \pm q_{Dy})^2}, \quad (22)$$

and the minus (respectively, plus) sign applies to the valley  $\alpha = \mathbf{K}$  (respectively,  $\alpha = \mathbf{K}'$ ). Analogous expressions hold for the transmission  $T_\alpha^{\text{evan}}(k_y)$  in the evanescent case, with  $\eta(k_y) \mapsto -\eta(k_y)$ ,  $\cos(q_x D) \mapsto \cosh(q_x D)$ , and  $\sin(q_x D) \mapsto \sinh(q_x D)$ . The transmission for a general (propagating or evanescent) wave therefore reads

$$T_\alpha(k_y) = \Theta[\eta(k_y)] T_\alpha^{\text{prop}}(k_y) + \{1 - \Theta[\eta(k_y)]\} T_\alpha^{\text{evan}}(k_y), \quad (23)$$

where  $\Theta(t)$  is the Heaviside (step) function. Integrating over  $k_y$  and summing over both valleys, one obtains the conductance across the barrier (Landauer formula),<sup>48,49</sup>

$$G = \frac{2e^2}{h} W \sum_\alpha \int_{-\infty}^{\infty} \frac{dk_y}{2\pi} T_\alpha(k_y), \quad (24)$$

where the factor of 2 takes into account for the spin degeneracy, the conductivity

$$\sigma = \frac{D}{W} G, \quad (25)$$

and the Fano factor<sup>50,51</sup>

$$F = 1 - \frac{\sum_\alpha \int_{-\infty}^{\infty} \frac{dk_y}{2\pi} T_\alpha^2(k_y)}{\sum_\alpha \int_{-\infty}^{\infty} \frac{dk_y}{2\pi} T_\alpha(k_y)}. \quad (26)$$

In Eq. (25) for the conductivity, the summation over the valleys contributes with an additional factor of 2, whereas this factor cancels in the definition of the Fano factor, Eq. (26).

Before discussing our results, let us observe that the inclusion of a strain-induced deformation of the Dirac cone in the expressions of the conductivity, Eq. (25), and of the Fano factor, Eq. (26), amounts to the replacements

$$D \mapsto D_{\text{eff}} \equiv \xi D, \quad (27a)$$

$$E \mapsto E_{\text{eff}} \equiv \zeta E, \quad (27b)$$

for the strip width and incident energy, respectively, in the corresponding expressions,  $\sigma^{(0)}$  and  $F^{(0)}$ , say, without cone deformation, with

$$\xi = \frac{1 - \lambda_y \varepsilon}{1 - \lambda_x \varepsilon}, \quad (28a)$$

$$\zeta = \frac{1}{1 - \lambda_y \varepsilon}. \quad (28b)$$

In particular, one explicitly finds

$$\sigma(D, E) = \xi^{-1} \sigma^{(0)}(D_{\text{eff}}, E_{\text{eff}}). \quad (29)$$

As a consequence, while  $\lim_{E \rightarrow 0} \sigma^{(0)}(D, E) = 4e^2/\pi h$ , a universal constant,<sup>52</sup> in the presence of applied uniaxial strain one finds

$$\lim_{E \rightarrow 0} \sigma(D, E) = \frac{1}{\xi} \frac{4e^2}{\pi h}. \quad (30)$$

Only in the case of hydrostatic strain ( $\nu = -1$ ,  $\lambda_x = \lambda_y$ ,  $\xi = 1$ ) does one recover the universal limit, regardless of the strain modulus.<sup>34</sup> On the other hand, one finds  $\lim_{E \rightarrow 0} F(D, E) = \frac{1}{3}$ , corresponding to strongly sub-Poissonian noise,<sup>46</sup> regardless of applied strain.

In the opposite limit, the conductivity across a single barrier in the absence of strain is linear in energy,  $\sigma^{(0)} \approx (e^2/h) D |E| / \hbar v_F$  for  $E \rightarrow \infty$ , with damped oscillations characterized by a pseudoperiod  $\Delta E$  such that<sup>47</sup>  $D \Delta E / \hbar v_F = \pi$ . In the presence of strain, such results are modified by Eqs. (28), so that  $\sigma(E) \approx \sigma_\infty(E)$  for  $E \rightarrow \infty$ , with

$$\sigma_\infty(E) = \frac{4e^2}{h} \frac{D |E|}{4} \zeta, \quad (31)$$

with damped oscillations characterized by a pseudoperiod given by

$$\xi \zeta D \frac{\Delta E}{\hbar v_F} = \pi. \quad (32)$$

In view of the fact that  $|\lambda_x| > |\lambda_y|$ , one may conclude that applied strain induces a slight change in the slope of  $\sigma$  vs  $|E|$ , while it modifies the pseudoperiod of the oscillations more substantially.

Figure 5 shows our results for the scaled conductivity in the presence of uniaxial strain ( $\varepsilon = 0.03 - 0.15$ ) applied along the armchair direction ( $\theta = \pi/2$ ). When the conductivity  $\sigma(E)$  is normalized with respect to its asymptotic limit, Eq. (31), and plotted against energy  $E$  scaled with the strain-dependent pseudoperiod  $\Delta E$ , Eq. (32), results corresponding to different values of the strain modulus collapse into a single curve, displaying damped oscillations, as prescribed by Eq. (32). Similarly, Fig. 6 reports our results for the Fano factor as a function of scaled energy. Again, the results for all the strain moduli here considered ( $\varepsilon = 0.03 - 0.15$ ) collapse into

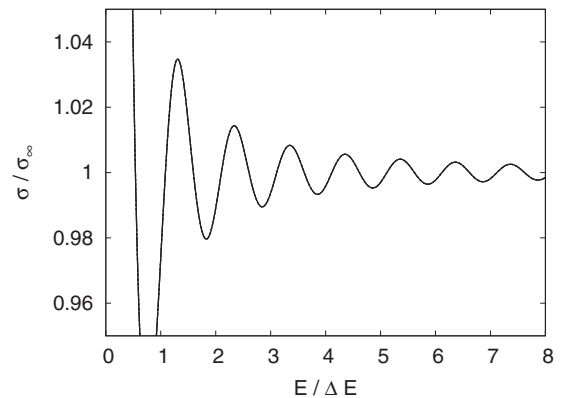


FIG. 5. Conductivity across a graphene strip ( $D = 100$  nm) normalized to asymptotic large-energy behavior, Eq. (31), vs energy scaled to the pseudoperiod, Eq. (32). Actually shown are four curves, all collapsing into a single one, corresponding to strain applied along the armchair direction ( $\theta = \pi/2$ ), with  $\varepsilon = 0.03, 0.05, 0.10, 0.15$ .

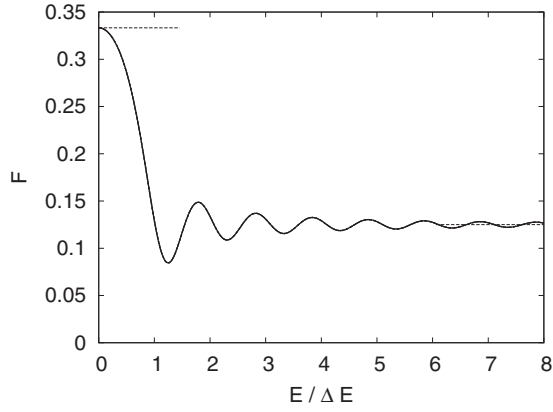


FIG. 6. Fano factor for ballistic transport across a graphene strip. All parameters are as in Fig. 5. Dashed lines represent the universal low- and large-energy asymptotic values,  $F(0) = \frac{1}{3}$  and  $F_\infty = \frac{1}{8}$ , respectively.

a single, oscillating curve. Note that the universal limits  $F(E=0) = \frac{1}{3}$  and  $F_\infty \equiv \lim_{E \rightarrow \infty} F(E) = \frac{1}{8}$  are recovered in all cases, regardless of applied strain. Such results do not depend on the direction  $\theta$  of applied strain.

#### IV. TRANSMISSION ACROSS MULTIPLE BARRIERS

We next consider quasiparticle tunneling across  $N$  identical barriers, each of width  $\ell$ , two nearest-neighbor (NN) barriers being separated by the distance  $\ell$ , such that  $2N\ell = D$  (Fig. 7). We assume a position-dependent strain modulus  $\varepsilon(x)$  and gate potential energy  $U(x)$ , with

$$\varepsilon(x) = \varepsilon_-, \quad (m-1)\ell \leq x \leq m\ell, \quad (33a)$$

$$= \varepsilon_+, \quad m\ell \leq x \leq (m+1)\ell, \quad (33b)$$

and

$$U(x) = U_-, \quad (m-1)\ell \leq x \leq m\ell, \quad (34a)$$

$$= U_+, \quad m\ell \leq x \leq (m+1)\ell, \quad (34b)$$

with  $m = 1, \dots, 2N-1$ . We further consider the possibility of contacting the two extrema of the chain of barriers with leads at the potential  $V_L$ . Equations (16) then suggest to look for a solution of the Dirac equation in the form

$$\psi(x, y) = U^\dagger(\theta) \frac{\phi(x)}{\sqrt{1 - \lambda_x \varepsilon(x)}} e^{ik_y y} \quad (35)$$

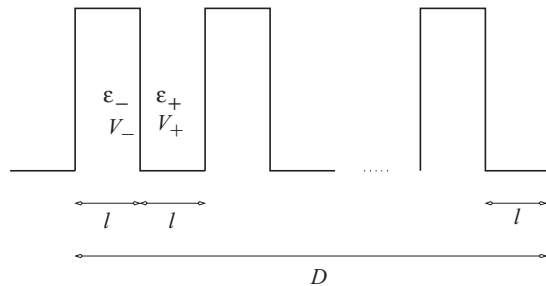


FIG. 7. Schematic plot of the multiple barrier, as considered in Sec. IV.

so that  $\phi(x)$  is a continuous function at the barriers' edges. The stationary Dirac equation for  $\phi(x)$  can then be casted in the form of an evolution equation,<sup>47</sup> so that  $\phi(x) = \mathbb{T}^{(N)}(x, x_0)\phi(x_0)$ , where the evolution matrix  $\mathbb{T}^{(N)}(x, x_0)$  in turn obeys the equation

$$\begin{aligned} \frac{d}{dx} \mathbb{T}^{(N)}(x, x_0) = & \left[ i q_{D_x}^{(0)} \varepsilon(x) \tau_z \mathbb{I} + \frac{i}{\hbar v_F} \frac{E - U(x)}{1 - \lambda_x \varepsilon(x)} \sigma_x \right. \\ & \left. + \frac{1 - \lambda_y \varepsilon(x)}{1 - \lambda_x \varepsilon(x)} (k_y - q_{D_y}^{(0)} \varepsilon(x) \tau_z) \sigma_z \right] \\ & \times \mathbb{T}^{(N)}(x, x_0), \end{aligned} \quad (36)$$

with  $\mathbb{T}^{(N)}(x_0, x_0) = \mathbb{I}$ . For a single barrier, the evolution matrix is related to the transfer matrix by<sup>52</sup>

$$\mathbb{M}^{(1)}(x, x_0) = Q_s^{-1}(\varphi) \mathbb{T}^{(1)}(x, x_0) Q_s(\varphi), \quad (37)$$

where

$$Q_s(\varphi) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ s e^{i\varphi} & -s e^{-i\varphi} \end{pmatrix} \quad (38)$$

includes the incidence angle  $\varphi$  of the incoming spinor, Eq. (15a), and  $s = \text{sgn}(E)$ . In the limit of metallic leads ( $|V_L| \rightarrow \infty$ ), one has  $\varphi \rightarrow 0$ , with  $Q_+(0) = \frac{1}{\sqrt{2}}(\sigma_z + \sigma_x)$ ,  $Q_+^{-1}(0) = Q_+(0)$ , and  $Q_-(0) = Q_+(0)\sigma_x$ ,  $Q_-^{-1}(0) = \sigma_x Q_+(0)$ . The elements of the transfer matrix can be further related to the elements of the scattering matrix across the barrier,

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}, \quad (39)$$

where  $r$ ,  $t$  (respectively,  $r'$ ,  $t'$ ) are the amplitudes of the reflected and transmitted waves in region I (respectively, III), cf. Fig. 1. Indeed, one explicitly finds<sup>52,53</sup>

$$\mathbb{M}^{(1)} = \begin{pmatrix} (t^\dagger)^{-1} & r'(t')^{-1} \\ -(t')^{-1}r & (t')^{-1} \end{pmatrix}. \quad (40)$$

Therefore, for the conductance across a single barrier, one finds

$$G = \frac{2e^2}{h} \text{Tr}(t^\dagger t) = \frac{2e^2}{h} \text{Tr}((\mathbb{M}_{11}^{(1)\dagger} \mathbb{M}_{11}^{(1)})^{-1}), \quad (41)$$

where  $\text{Tr} \equiv W \sum_\alpha \int_{-\infty}^{\infty} dk_y / 2\pi$ . Correspondingly, the transmission for an incoming quasiparticle with energy  $E$  and transverse wave vector  $k_y$  in valley  $\alpha$  is  $T_\alpha(k_y) = (\mathbb{M}_{11}^{(1)\dagger} \mathbb{M}_{11}^{(1)})^{-1}$ , and the expressions for the conductivity, Eq. (25), and Fano factor, Eq. (26), follow straightforwardly.

The solution of Eq. (36) for the transfer matrix is derived analytically in the Appendix, both for a single and for a multiple barrier, in the presence of strain-induced deformation of the Dirac cone. Making use of Eqs. (A10) for the transmission  $T_\alpha(k_y)$  in Landauer's formula for the conductivity, Eq. (25), and in the definition for the Fano factor, Eq. (26), one again finds that the conductivity in strained graphene and strained graphene where the strain-induced velocity anisotropy has

been neglected are related by means of Eqs. (28) and (29), but now with  $D = 2N\ell$ , and

$$\xi = \frac{1}{2}(\xi_+ + \xi_-), \quad (42a)$$

$$\zeta = \frac{1}{2}(\zeta_+ + \zeta_-), \quad (42b)$$

$$\xi_{\pm} = \frac{1 - \lambda_y \varepsilon_{\pm}}{1 - \lambda_x \varepsilon_{\pm}}, \quad (42c)$$

$$\zeta_{\pm} = \frac{1}{1 - \lambda_y \varepsilon_{\pm}}. \quad (42d)$$

Equation (30) in the limit  $E \rightarrow 0$  then follows straightforwardly, with  $\xi$  given now by Eq. (42a). Moreover, the conductivity at large energies is characterized by an overall linear behavior, interrupted by dips with decreasing depth, which result from the coherent superposition of the damped oscillations produced by scattering off the edges of the single barriers. The energies  $E_n$  at which such dips occur are asymptotically given by (cf. the Appendix)

$$\frac{E_n}{\hbar v_F} \frac{D}{N} \frac{1}{2} (\xi_+ \zeta_+ + \xi_- \zeta_-) = n\pi, \quad (43)$$

with  $n$  an integer.

Figure 8 shows our numerical results for the conductivity in strained graphene, with strain applied nonuniformly along the armchair direction, across a superlattice of  $N = 10$  barriers. At variance with Fig. 5, we have not scaled  $\sigma$  with its asymptotic behavior at large energies, Eq. (31). As expected, the overall linear behavior of  $\sigma(E)$  is interrupted by dips, whose approximate energy location is given by Eq. (43). While such dips get damped as energy increases, they are nonetheless enhanced with respect to the case in which the strain-induced deformation of the Dirac cones is neglected,<sup>33</sup> especially those corresponding to even integer values of  $n$  in Eq. (43). Correspondingly, the Fano factor (Fig. 9) is

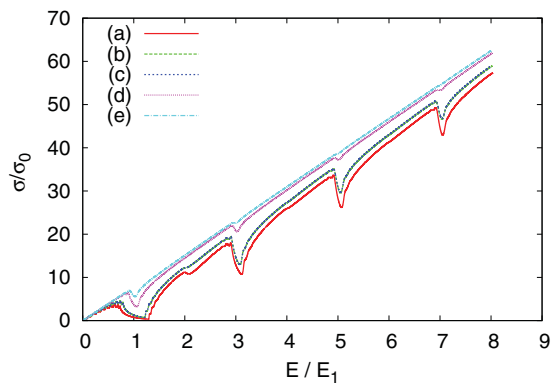


FIG. 8. (Color online) Conductivity  $\sigma(E)$  in units of  $\sigma_0 = 4e^2/h$ , vs energy  $E$ , scaled with respect to the approximate location of the first dip,  $E_1$ , as given by Eq. (43). Subsequent dips then occur close to integer values of the ratio  $E/E_1$ . Uniaxial strain is applied along the armchair direction ( $\theta = \pi/2$ ) in the case of a multibarrier superlattice, with  $N = 10$  barriers,  $\ell = 25$  nm ( $D = 500$  nm). Different curves refer to nonuniform strain moduli within and outside NN barriers (cf. Fig. 7), with (a)  $\varepsilon_+ = 0.004$ ,  $\varepsilon_- = 0$ ; (b)  $\varepsilon_+ = 0.003$ ,  $\varepsilon_- = 0$ ; (c)  $\varepsilon_+ = 0.002$ ,  $\varepsilon_- = -0.001$ ; (d)  $\varepsilon_+ = 0.002$ ,  $\varepsilon_- = 0.001$ ; (e)  $\varepsilon_+ = 0.0005$ ,  $\varepsilon_- = 0$ . In all cases, we set  $U_{\pm} = 0$ , for the sake of simplicity.

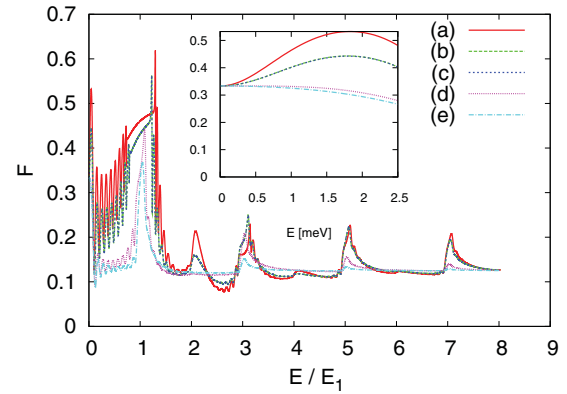


FIG. 9. (Color online) Fano factor  $F$  vs scaled energy  $E/E_1$ , for transport across a multibarrier superlattice, with nonuniform uniaxial strain applied along the armchair direction ( $\theta = \pi/2$ ). All parameters are as in Fig. 8. Inset shows the universal low-energy asymptotic behavior in the various cases. In the limit  $E \rightarrow 0$ , the universal asymptotic value,  $F(0) = \frac{1}{3}$ , is recovered.

characterized by essentially analogous features, with bumps occurring at approximately  $E_n$ , Eq. (43). In particular, the universal limit at low energy,  $F(0) = \frac{1}{3}$ , is recovered as in the single-barrier case, regardless of applied strain.

Figure 10 shows our numerical results for the conductivity in strained graphene, but now for nonuniform strain applied along the zigzag direction. At variance with the armchair case (Fig. 8), for strain applied along the zigzag direction the conductivity seems not to be characterized by prominent dips as a function of energy. This may be explained by a reduced coherent superposition of the effects due to each single barrier. However, if the trailing linear dependence on energy is divided out (Fig. 10, inset), one may again recognize “oscillations,” with extrema approximately occurring at  $E_n$ , as given by

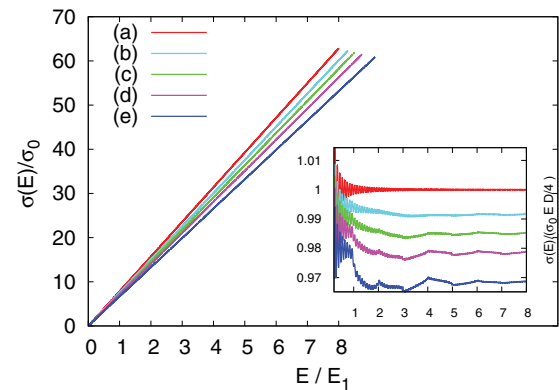


FIG. 10. (Color online) Conductivity  $\sigma(E)$  in units of  $\sigma_0 = 4e^2/h$ , vs energy  $E$ , scaled with respect to  $E_1$ , as given by Eq. (43). Uniaxial strain is applied along the zigzag direction ( $\theta = 0$ ) in the case of a multibarrier superlattice, with  $N = 10$  barriers,  $\ell = 25$  nm ( $D = 500$  nm). Different curves refer to nonuniform strain moduli within and outside NN barriers (cf. Fig. 7), with (a)  $\varepsilon_+ = 0$ ,  $\varepsilon_- = 0$ ; (b)  $\varepsilon_+ = 0.03$ ,  $\varepsilon_- = 0$ ; (c)  $\varepsilon_+ = 0.05$ ,  $\varepsilon_- = 0$ ; (d)  $\varepsilon_+ = 0.07$ ,  $\varepsilon_- = 0$ ; (e)  $\varepsilon_+ = 0.10$ ,  $\varepsilon_- = 0$ . In all cases, we set  $U_{\pm} = 0$ , for the sake of simplicity. Inset shows the conductivity scaled with respect to its large-energy asymptotic limit,  $\sigma/\sigma_{\infty}$ , as a function of scaled energy,  $E/E_1$ .

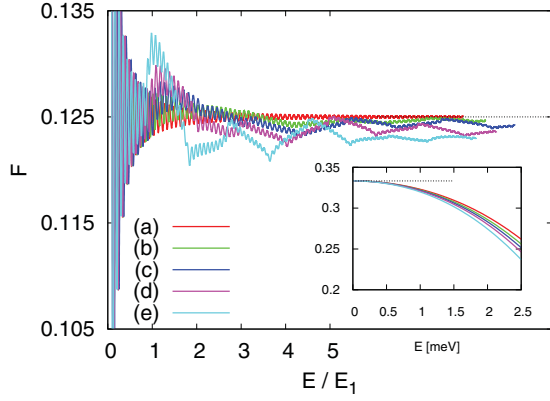


FIG. 11. (Color online) Fano factor  $F$  vs scaled energy  $E/E_1$ , for transport across a multibarrier superlattice, with nonuniform uniaxial strain applied along the zigzag direction ( $\theta = 0$ ). All parameters are as in Fig. 10. Note the deviations from the large-energy asymptotic limit for the unstrained case,  $F_\infty = \frac{1}{8}$  (dashed line). The low-energy universal limit,  $F(0) = \frac{1}{3}$  (inset, dashed line), is recovered, regardless of strain.

Eq. (43). At variance with the armchair case, the Fano factor exhibits a strain-dependent asymptotic limit, for large energies (Fig. 11), with increasing deviations from the unstrained behavior  $F_\infty = \frac{1}{8}$ , with increasing strain modulus  $\varepsilon$  (at least within the strain range that has been numerically investigated). On the other hand, both the oscillations as a function of scaled energy  $E/E_1$  and the low-energy limit  $F(0) = \frac{1}{3}$  (Fig. 11, inset) are recovered.

## V. TRANSMISSION ACROSS A SMOOTH BARRIER: EFFECT OF CONTINUOUS STRAIN

Although considerable insight is afforded by analytical solutions to the problem of tunneling across single or multiple *sharp* barriers, there is sufficient evidence, both experimental<sup>54</sup> and theoretical,<sup>32</sup> that barrier edge effects are also important to determine the transport properties across corrugated graphene. Here, we therefore consider the case in which uniaxial strain is applied in a nonuniform but continuous fashion to a graphene sheet, which can be modeled by a single barrier with *smooth* strain and gate potential profiles,  $\varepsilon = \varepsilon(x)$  and  $U = U(x)$ , respectively. Such a description includes and generalizes, in particular, a continuous Fermi wave-vector profile, as considered in Ref. 32.

On quite general grounds, one may expect that a smooth potential profile (whether induced by strain or by gating) introduces a new length scale,  $a$  say [as in Eq. (48) below], which is the linear size over which the potential strain varies appreciably. Such a new length scale has then to be compared with the atomic scale, measured by the lattice step  $a$ , on one hand, and with the Fermi wavelength  $\lambda_F = \hbar v_F / (2\pi E)$  corresponding to the incident energy  $E$ , on the other. The approximation of a sharp barrier (no smoothing) then holds whenever  $a \ll \lambda_F$ , i.e., at sufficiently large incident energies. On the other hand, the detailed structure of the barrier needs to be considered when  $a \sim \lambda_F$ . In both cases, we are interested to the more general and realistic cases where  $a \ll \lambda_F$ , where one may additionally neglect the occurrence of  $\mathbf{K}-\mathbf{K}'$

coupling. Indeed, truly sharp electrostatic barriers on the order of the electron wavelength are quite difficult to be realized, as is, e.g., demonstrated by the occurrence of Fabry-Pérot oscillations of the conductance in graphene heterostructures as narrow as  $\sim 20$  nm, where a resonant cavity is formed between two electrostatically created bipolar junctions.<sup>55</sup> Such oscillations are more accurately described when the smooth structure of these potential barriers is taken into account, whereas intervalley scattering can be safely neglected (see Supplementary Information in Ref. 55). Another instance of nonuniform barrier, where smoothing effects are important, is the strain-induced ripples superlattice experimentally realized in Ref. 43, in which smoothing is essential on a length scale of  $\sim 100$  nm, whereas intervalley processes are negligible.

The kinetic part of the Hamiltonian for graphene subjected to uniform strain  $\varepsilon$  along the direction  $\theta$  is

$$H = U^\dagger(\theta) \sigma_i \hbar v_i \left( \frac{1}{i} \nabla_i - q_{D_i} \right) U(\theta), \quad (44)$$

where  $v_i = v_F(1 - \lambda_i \varepsilon)$ , and summation over the repeated index  $i = 1, 2$  is understood. In order to generalize Eq. (44) to the case of a nonuniform, but continuous strain profile  $\varepsilon = \varepsilon(x)$ , one may be tempted to perform the replacements  $v_i \mapsto v_i(\mathbf{r}) \equiv v_F[1 - \lambda_i \varepsilon(x)]$  and  $\mathbf{q}_D \mapsto \mathbf{q}_D(\mathbf{r})$ , Eq. (11), with  $\varepsilon = \varepsilon(x)$ . However, the resulting Hamiltonian must be symmetrized, in order to preserve hermiticity, thus leading to the model Hamiltonian for a nonuniform strain profile:

$$H = U^\dagger(\theta) \sigma_i \frac{1}{2} \left[ \hbar v_i(\mathbf{r}) \left( \frac{1}{i} \nabla_i - q_{D_i}(\mathbf{r}) \right) + \left( \frac{1}{i} \nabla_i - q_{D_i}(\mathbf{r}) \right) \hbar v_i(\mathbf{r}) \right] U(\theta). \quad (45)$$

Equation (45) includes the effect of nonuniform, continuous strain both as a shift in the position of the Dirac points, and as a deformation of the Dirac cones (nonuniform and anisotropic Fermi velocity), at variance e.g., with Ref. 35, where a nonuniform velocity is considered, but an isotropic profile is assumed. As in the case of a single, sharp barrier (Sec. III), continuity of the current density, Eqs. (16), suggests to seek for a solution of the stationary Dirac equation in a form analogous to Eq. (35), viz.

$$\psi(x, y) = U^\dagger(\theta) \frac{\phi(x)}{\sqrt{v_x(x)}} e^{ik_y y}. \quad (46)$$

One explicitly finds [cf. Eq. (36)]

$$\frac{d\phi(x)}{dx} = \left[ \frac{1 - \lambda_y \varepsilon(x)}{1 - \lambda_x \varepsilon(x)} (k_y - q_{D_y}^{(0)} \varepsilon(x)) \sigma_z + i \frac{E - U(x)}{[1 - \lambda_x \varepsilon(x)] \hbar v_F} \sigma_x + i q_{D_x}^{(0)} \varepsilon(x) \mathbb{I} \right] \phi(x). \quad (47)$$

We have solved Eq. (47) numerically, for the nonuniform, smooth strain profile

$$\varepsilon(x) = \frac{\varepsilon_0}{\tanh(D/4a)} \left( \frac{1}{1 + e^{-x/a}} - \frac{1}{1 + e^{-(x-D)/a}} \right), \quad (48)$$

as shown in Fig. 12. Such a strain profile is essentially flat for  $|x - D/2| \ll a$ , where  $\varepsilon(x) \approx \varepsilon_0$ , and for  $|x - D/2| \gg a$ , where  $\varepsilon(x) \approx 0$ . In the limit  $a/D \rightarrow 0$ , Eq. (48) tends to the sharp barrier considered in Sec. III. Therefore asymptotically



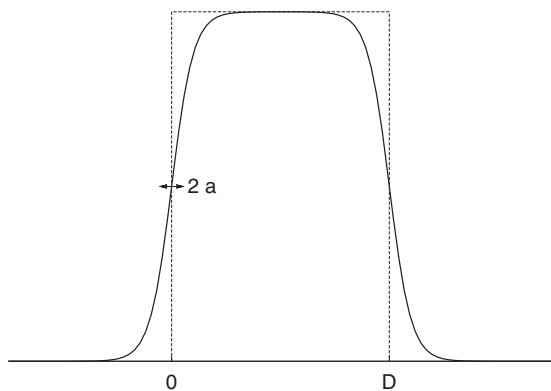


FIG. 12. Schematic single tunneling barrier, with smooth strain profile, Eq. (48). Dashed line depicts a sharp barrier, corresponding to the limit  $a \rightarrow 0$ .

for  $|x| \rightarrow \infty$ , the solutions of Eq. (47) must merge into Eqs. (15), in regions I and III. We have therefore taken an initial value  $\phi(x = x_0)$  in the form of Eq. (15c), for  $x_0 = 5D$ , and integrated Eq. (47) backward for  $x \ll 0$ . Comparing the numerical solution with Eq. (15a), one may extract the reflection coefficient  $r$ , relative to an incident wave with unit amplitude incoming from  $x > 0$ , as the Fourier weight with respect to its negative frequency component, whence the transmission  $T(\phi)$  follows straightforwardly. As a cross check of our procedure, we have also verified that the continuity equation, Eq. (16), holds true, within the numerical error.

Figures 13 and 14 show our numerical results for the tunneling transmission  $T(\varphi)$  across the smooth strain barrier, Eq. (48), with  $D = 100$  nm and different values of the smoothing parameter,  $a/D$ . Figure 13 refers to an incidence energy  $E = 80$  meV, corresponding to an incident wavelength  $\lambda_F = \hbar v_F / (2\pi E) \approx 1.3$  nm. One finds that transmission of

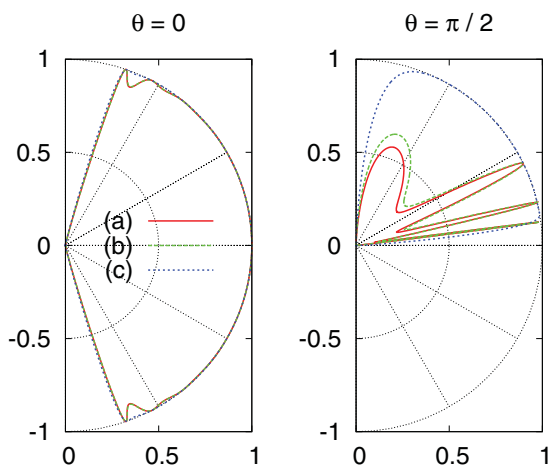


FIG. 13. (Color online) Tunneling transmission vs incidence angle  $\varphi$  across a smooth strain barrier, Eq. (48), with  $D = 100$  nm, and incidence energy  $E = 80$  meV ( $\lambda_F = \hbar v_F / (2\pi E) \approx 1.3$  nm). Left panel refers to strain applied along the zigzag direction ( $\theta = 0$ ), with  $\varepsilon_0 = 0.1$ . Right panel refers to strain applied along the armchair direction ( $\theta = \pi/2$ ), with  $\varepsilon_0 = 0.01$ . In both cases, the different lines correspond to different values of the smoothing parameter, viz. (a)  $a = 0$  (sharp barrier); (b)  $a = 10^{-2}D = 1$  nm; (c)  $a = 10^{-1}D = 10$  nm. In all cases,  $U(x) = 0$ , for the sake of simplicity.

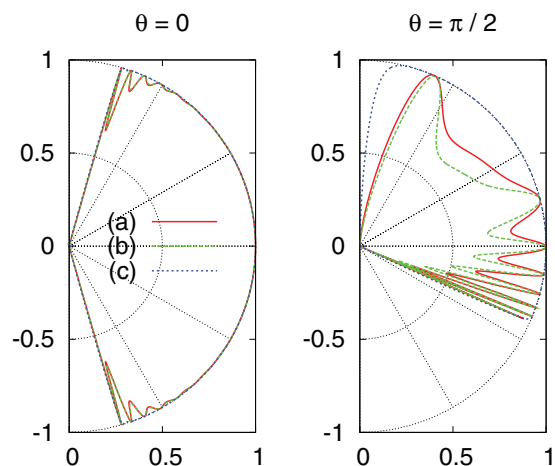


FIG. 14. (Color online) Same as Fig. 13, but with  $E = 150$  meV ( $\lambda_F \approx 0.7$  nm).

propagating waves is allowed for incidence angles  $\varphi$  such that  $\varphi_{cr-} \leq \varphi \leq \varphi_{cr+}$ , with

$$\varphi_{cr\pm} = \pm \arcsin\left(\frac{1}{1 - \lambda_y \varepsilon_0}\right), \quad (49)$$

in the zigzag case ( $\theta = 0$ ), and  $\varphi > \varphi_{cr}$ , with

$$\arcsin\left(-\frac{1}{1 - \lambda_y \varepsilon_0} + \frac{\hbar v_F}{|E|} \varepsilon_0 \kappa (1 - \nu)\right), \quad (50)$$

in the armchair case ( $\theta = \pi/2$ ), independent of the smoothing parameter  $a/D$ . Outside that window, transmission takes place via evanescent waves only, and  $T(\varphi) \approx 0$ . For strain applied along the zigzag direction ( $\theta = 0$ , Fig. 13, left panel), Eq. (49) predicts the existence of critical angles  $|\varphi_{cr\pm}| < \pi/2$ . This is a direct consequence of the strain-induced deformation of the Dirac cones [ $\lambda_y \neq 0$  in Eq. (49)]. Both in case of strain applied along the zigzag and armchair directions, increasing the smoothness parameter  $a/D$  away from the limit of a sharp barrier ( $a/D = 0$ ) suppresses the oscillations in  $T(\varphi)$  within the propagating window, until  $a > \lambda_F$ , in which case transmission is almost undisturbed by the presence of the barrier. These results are confirmed by Fig. 14, where we consider quasiparticles with larger incident energy  $E = 150$  meV, corresponding to a smaller Fermi wavelength  $\lambda_F \approx 0.7$  nm. While the transmission window widens and the number of oscillations increases, smoothing the strain profile immediately washes out the deviations of the tunneling transmission from unity. In ending this section, we note that the procedure applied to extracting the tunneling transmission from the numerical solution of Eq. (47) can be generalized, in principle, to the case of an arbitrary nonuniform strain potential, such as a superlattice of several smooth barriers, such as Eq. (48).

## VI. CONCLUSIONS

We have studied the effect of a strain-induced modulation of the Fermi velocity on several transport properties of graphene, such as the angular dependence of the tunneling transmission, the conductivity, and the Fano factor. After considering the cases of a single sharp tunneling barrier, and of a superstructure of several, periodically repeated, such sharp barriers, we have

specifically studied the case in which both the modulus of applied uniaxial strain, and possibly an applied gate potential, depend continuously on position. This is expected to afford a more accurate description of real “origami” device,<sup>31</sup> in which “foldings” of a graphene sheet would conceivably involve several lattice spacings. In the case of sharp tunneling barriers, we have demonstrated that the effect of a strain-induced deformation of the Dirac cone is of the same order of the strain-induced shift of the Dirac points, and should therefore be taken into account on the same basis. In particular, we have found that strain modifies the quasiperiod in energy that regulates the occurrence of dips in the conductivity across a superstructure of several sharp barriers, due to coherent scattering off their edges. Such effect is, however, less dramatic in the energy dependence of the Fano factor. Finally, we have generalized our results to embrace the case of a generic *nonuniform* strain, and possibly a gate potential, profile. Besides allowing a more accurate analysis of tunneling transmission across smooth barriers, especially at low incident energies, which are expected to be more sensitive to local deviations from uniformity, such an approach can be applied to describe arbitrary strain superstructures, albeit numerically.

Among the already available experimental results, which could be described in terms of a strain-induced deformation of the Dirac cones, we mention Raman spectroscopy<sup>56</sup> and the strain dependence of both the longitudinal and the recently predicted transverse plasmon mode.<sup>30,57</sup> Moreover, transmittance measurements with polarized light between the near-infrared and the ultraviolet on uniaxially strained graphene may provide information on the Dirac cone deformation.<sup>9,30</sup>

*Note added in proof.* Recently, we became aware of Ref. 59, where the effect of anisotropic mechanical strain on some transport properties of graphene is studied.

### ACKNOWLEDGMENTS

F. M. D. P. acknowledges D. M. Basko for discussions and correspondence over the general area embraced by the present work.

### APPENDIX: TRANSFER MATRIX ACROSS A MULTIPLE BARRIER

In the case of a single barrier [( $N = 1$ ,  $2\ell = D$ ), Fig. 7], Eq. (36) for the transfer matrix admits the analytical solution

$$\begin{aligned} \mathbb{M}^{(1)}(D,0) &= \exp(iq_{Dx}^{(0)}\varepsilon D) \exp\left(\frac{i}{\hbar v_F} \frac{(E - U_g)D}{1 - \lambda_x \varepsilon} \sigma_z\right. \\ &\quad \left. + \frac{1 - \lambda_y \varepsilon}{1 - \lambda_x \varepsilon} (k_y - q_{Dy}^{(0)})D \sigma_x\right), \end{aligned} \quad (\text{A1})$$

corresponding to the initial condition  $\mathbb{M}^{(1)}(0,0) = \mathbb{I}$ , and to a uniform strain  $\varepsilon$  and to a gate potential energy  $U_g$  across the barrier. The second matrix exponential in Eq. (A1) can be made more explicit, by making use of the following identity for a linear combination of the Pauli matrices,

$$\exp(\mathbf{a} \cdot \boldsymbol{\sigma}) = \frac{\sinh a}{a} \mathbf{a} \cdot \boldsymbol{\sigma} + \mathbb{I} \cosh a, \quad (\text{A2})$$

where  $a = (\sum_i a_i^2)^{1/2}$ , and  $a_i \in \mathbb{C}$  ( $i = 1, 2, 3$ ).

We next consider a single barrier, but now with nonuniform strain modulus and gate potential energy, i.e.,  $\varepsilon(x) = \varepsilon_-$  and  $U(x) = U_-$  within the barrier ( $0 < x < \ell$ ), and  $\varepsilon(x) = \varepsilon_+$  and  $U(x) = U_+$  beyond the barrier’s second edge ( $\ell < x < 2\ell$ ; cf. Fig. 7). In this case, one finds  $\mathbb{M}^{(1)}(2\ell, 0) = \mathbb{M}_+( \ell) \mathbb{M}_-( \ell)$ , where  $\mathbb{M}_\pm(\ell)$  are given by Eq. (A1), with  $D \mapsto \ell$ ,  $\varepsilon \mapsto \varepsilon_\pm$ , and  $U \mapsto U_\pm$ . One finds

$$\mathbb{M}^{(1)}(2\ell, 0) = e^{iq_{Dx}^{(0)}(\varepsilon_+ + \varepsilon_-)\ell} \tilde{\mathbb{M}}_1, \quad (\text{A3})$$

where  $\tilde{\mathbb{M}}_1$  is a unimodular matrix,  $\det \tilde{\mathbb{M}}_1 = 1$ . Specifically, one finds

$$(\tilde{\mathbb{M}}_1)_{11} = \lambda + i\eta, \quad (\text{A4})$$

where

$$\begin{aligned} \lambda &= \frac{\sinh(q_- \ell) \sinh(q_+ \ell)}{q_- q_+} (\kappa_- \kappa_+ - u_- u_+) \\ &\quad + \cosh(q_- \ell) \cosh(q_+ \ell), \end{aligned} \quad (\text{A5a})$$

$$\begin{aligned} \eta &= \frac{u_-}{q_-} \sinh(q_- \ell) \cosh(q_+ \ell) \\ &\quad + \frac{u_+}{q_+} \sinh(q_+ \ell) \cosh(q_- \ell), \end{aligned} \quad (\text{A5b})$$

with

$$\kappa_\pm = \frac{1 - \lambda_y \varepsilon_\pm}{1 - \lambda_x \varepsilon_\pm} (k_y - q_{Dy}^{(0)} \varepsilon_\pm), \quad (\text{A6a})$$

$$u_\pm = \frac{E - U_\pm}{\hbar v_F (1 - \lambda_x \varepsilon_\pm)}, \quad (\text{A6b})$$

$$q_\pm = \sqrt{\kappa_\pm^2 - u_\pm^2}, \quad (\text{A6c})$$

whence Eq. (41) follows straightforwardly.

Finally, in the case of  $N$  barriers ( $D = 2N\ell$ , Fig. 7), iterating Eq. (A3)  $N$  times, one has

$$\mathbb{M}^{(N)}(D, 0) = e^{iq_{Dx}^{(0)}(\varepsilon_+ + \varepsilon_-)N\ell} \tilde{\mathbb{M}}_1^N, \quad (\text{A7})$$

where for the  $N$ th power of the unimodular matrix  $\tilde{\mathbb{M}}_1$  one may use an identity due to Chebyshev,<sup>58</sup> and specifically obtain

$$(\tilde{\mathbb{M}}_1^N)_{11} = \frac{\sinh(Nz)}{\sinh z} (\tilde{\mathbb{M}}_1)_{11} - \frac{\sinh[(N-1)z]}{\sinh z}. \quad (\text{A8})$$

Here, we have denoted the eigenvalues of  $\tilde{\mathbb{M}}_1$  by  $e^{\pm z}$ , with  $z \in \mathbb{C}$ . Finally, one finds for the transmission

$$\begin{aligned} T(k_y) &= [(\mathbb{M}^{(N)}(D, 0))_{11}^* (\mathbb{M}^{(N)}(D, 0))_{11}]^{-1} \\ &= \left[ \cosh^2(Nz) + \frac{\eta^2}{\lambda^2 - 1} \sinh^2(Nz) \right]^{-1}. \end{aligned} \quad (\text{A9})$$

Since  $\lambda = \frac{1}{2} \text{Tr} \tilde{\mathbb{M}}_1 = \cosh z$ , one finds explicitly

$$\begin{aligned} T_\alpha(k_y) &\equiv T_\alpha^{\text{prop}}(k_y) \\ &= \left[ \cos^2(Ny) + \frac{\eta^2}{\lambda^2 - 1} \sin^2(Ny) \right]^{-1}, \end{aligned} \quad (\text{A10a})$$

with  $y = \arccos \lambda$ , if  $|\lambda| < 1$ ,

$$\begin{aligned} &\equiv T_\alpha^{\text{evan}}(k_y) \\ &= \left[ \cosh^2(Nx) + \frac{\eta^2}{\lambda^2 - 1} \sinh^2(Nx) \right]^{-1}, \end{aligned} \quad (\text{A10b})$$

with  $x = \ln|\lambda + \sqrt{\lambda^2 - 1}|$ , if  $|\lambda| > 1$ ,

$$= [1 + \eta^2 N^2]^{-1}, \quad (\text{A10c})$$

if  $|\lambda| = 1$ . In particular, one finds  $\lambda \sim \cos(u_+ \ell + u_- \ell)$ , for  $E \rightarrow \infty$ , whence Eq. (43) follows.

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