

Quantum Field Theory Approach to the Optical Conductivity of Strained and Deformed Graphene.

W. de Paula¹, A. Chaves², O. Oliveira³ and T. Frederico¹

1-Departamento de Física, Instituto Tecnológico de Aeronáutica,

2- Department of Physics and Center of Physics, University of Minho, P-4710-057, Braga, Portugal,

3- CFisUC, Department of Physics, University of Coimbra, P - 3004 516 Coimbra, Portugal

Abstract

The computation of the optical conductivity of strained and deformed graphene is discussed within the framework of quantum field theory in curved spaces. The analytical solutions of the Dirac equation in an arbitrary static background geometry for one dimensional periodic deformations are computed, together with the corresponding Dirac propagator. Analytical expressions are given for the optical conductivity of strained and deformed graphene associated with both intra and interband transitions. The special case of small deformations is discussed and the result compared to the prediction of the tight-binding model.

1 Introduction

Graphene is a 2D material whose low energy electronic excitations can be described by a massless Dirac equation [1, 2, 3, 4, 5, 6]. The Dirac equation can be motivated starting from the tight-binding model and assuming that graphene is a flat sheet. However, almost immediately after its discovery deviations from flatland were observed with the identification of ripples and corrugations. Further, in many experimental realisations, graphene is grown on top of a supporting material which is hardly flat. On the theoretical side, the analysis of the stability of two-dimensional crystals and membranes suggests that flat materials are not realised in nature.

The introduction of a Dirac equation to describe graphene opened the possibility of using Relativistic Field Theory to investigate its properties. In this sense, graphene provides a nice laboratory where phenomena typically associated with High Energy Physics can be observed and studied. Deviations from the perfect crystal structure can easily be accommodated within the field theoretical approach calling for new fields and/or operators. Indeed, it was proven that certain types of defects require the introduction of a scalar field and/or two dimensional gauge fields. If these fields are dynamical, phenomena like spontaneous symmetry breaking are expected to

occur in graphene. Moreover, these relativistic field theories have its proper dynamics, with e.g. soliton like solutions [7], which couple to the electrons and can induce non-trivial effects. The full picture of the coupling between the various possible fields is still to be explored.

On the other side, geometric deformations of graphene are known to change its electrical conductance and optical properties. From the point of view of the electronic properties and the field theoretical approach the natural language to describe deformed graphene is via the Dirac equation in a curved space. Once more, graphene makes a new bridge between two distinct and far apart branches of physics. Recall that, electrons are confined within a 2D surface which leaves in a 3D world. Further, as discussed in [6] the use of a Dirac equation in a 2D curved space can accommodate not only geometric deformations of the pristine material but can also be used to study strained graphene.

As described in [8], certain types of geometric deformation have associated intense pseudo magnetic fields. The interpretation of Landau levels spacing in terms of a pseudo magnetic field unveil intense fields of the order ~ 300 T. For one dimensional periodic deformations like e.g. ripples, in [6] it was studied how optical properties are changed by deforming graphene. The main goal of all such studies is, of course, to learn how to tailor the properties of such a promising material as graphene.

This paper is organised as follows. In section 2 we resume the main features of the Dirac equation in a static background geometry and discuss how strain and geometric deformations can be described within such a formalism. In section 3, we discuss in detail the case of one dimensional deformations and write out the expressions for the electronic Green function. In section 4, the report on the computation of the optical conductivity for the Dirac equation in curved space using the Kubo formula.

2 Dirac Electron in Curved Space

The Dirac equation in a curved space-time with a metric tensor $g_{\mu\nu}$ reads

$$\left\{ i \Gamma^\mu D_\mu - M \right\} \Psi = 0 \quad (1)$$

where $\Psi(x)$ is the Dirac field, $\Gamma^\mu = e_A^\mu \gamma^A$ are the Dirac matrices in curved space-time, where the ‘‘vielben’’ e_A^μ defines a local Lorentzian frame such that the space-time interval is given by $ds^2 = \eta_{AB} \theta^A \theta^B$; $\eta_{AB} = \text{diag}(-1, 1, 1)$ is the Minkowski metric and $\theta^A = e_\mu^A dx^\mu$. The covariant derivative is

$$D_\mu = \partial_\mu + \frac{1}{4} \omega_\mu^{AB} \sigma_{AB} \quad \text{with} \quad \sigma_{AB} = \frac{1}{2} (\gamma_A \gamma_B - \gamma_B \gamma_A) \quad (2)$$

and the spin connection are given by

$$\omega_{\mu}^{AB} = \frac{1}{2} e^{\nu A} \left(\partial_{\mu} e_{\nu}^B - \partial_{\nu} e_{\mu}^B \right) - \frac{1}{2} e^{\nu B} \left(\partial_{\mu} e_{\nu}^A - \partial_{\nu} e_{\mu}^A \right) - \frac{1}{2} e^{\rho A} e^{\sigma B} \left(\partial_{\rho} e_{\sigma C} - \partial_{\sigma} e_{\rho C} \right) e_{\mu}^C. \quad (3)$$

For a time independent metric one can set $\theta^0 = dt$ and choose $\Gamma^0 = \gamma^0$, where γ^0 is the usual flatland gamma matrix. Furthermore, from the definition $\theta^1 = e_1^1 dx + e_2^1 dy$, $\theta^2 = e_1^2 dx + e_2^2 dy$ and taking the symmetric solution $e_2^1 = e_1^2$, it follows, after some algebra, that and the only non-vanishing spin connections are $\omega_i^{12} = -\omega_i^{21}$ for $i = 1, 2$. The Dirac equation (1) can be written in the usual form

$$i\partial_t \Psi = H \Psi \quad (4)$$

where the Hamiltonian is

$$H = -i \sum_{i,j=1}^2 \alpha_i e_i^j \nabla_j - i \sum_{i=1}^2 \alpha_i A_i + M\beta, \quad (5)$$

with

$$\beta = \gamma^0, \quad \alpha_i = \beta \gamma^i, \quad A_i = \sum_{j,k=1}^2 \frac{\epsilon_{ij}}{2} e_j^k \omega_k^{12} \quad (6)$$

and ϵ_{ij} is the two dimensional Levi-Civita symbol. Equation (5) extends, for a generic static geometry, the Hamiltonian derived in [9, 10] for radial and small deformations; see also [11]. Following the notation of [10], the first term in H includes the usual flat Dirac term and the space-dependent Fermi velocity given by the departure from unit of the corresponding "vielben". The second term can be interpreted as a geometric gauge field. Note, however, the absence of the usual i factor appearing in the minimal U(1) coupling. The last term, is a mass term and it shows up only when chiral symmetry is explicitly broken and, therefore, one can conclude that in graphene a gap is not open by a geometric deformation.

We define the geometric deformation of the graphene sheet according to the parametric equation

$$z = h(x, y). \quad (7)$$

Strain can be viewed as a local deformation and can be parametrized by the change of variables

$$x \rightarrow x' = \mathcal{X}(x, y) = x + X_x(x, y) \quad \text{and} \quad y \rightarrow y' = \mathcal{Y}(x, y) = y + Y_y(x, y), \quad (8)$$

where in terms of (x', y') the metric is euclidean and X_x , Y_y and h are the displacement fields. The transformation (8) does not change the surface curvature, in the sense that the 2D Ricci scalar defined on the graphene

sheet is invariant under the change of variables. The distance between two neighboring points is given by

$$ds^2 = (dx')^2 + (dy')^2 + dz^2 \quad (9)$$

and the corresponding metric tensor reads $g_{ij} = \mathcal{X}_i \mathcal{X}_j + \mathcal{Y}_i \mathcal{Y}_j + h_i h_j$, where \mathcal{X}_i means partial derivative with respect to x_i , and can be written as

$$g_{ij} = \delta_{ij} + 2u_{ij} \quad (10)$$

where

$$u_{ij} = \frac{1}{2} \left(\partial_i u_j + \partial_j u_i + \sum_{k=1}^2 \partial_i u_k \partial_j u_k + (\partial_i h) (\partial_j h) \right) \quad (11)$$

is the strain tensor and $u_x = X_x$, $u_y = Y_y$. In the limit of the small deformations and to first order in the in-plane displacements and to second order in the out-of-plane displacement, the strain tensor u_{ij} reproduces exactly the strain tensor considered in [10]. The difference for a finite deformation is the second order term in the in-plane displacements X_x and Y_y .

It follows from equations (10) and (11) that strain and geometric deformations play similes roles. Indeed, as long as the stress tensor is the same, there is no basic difference between strain and deformation. Furthermore, for a particular geometric deformation there is, in principle, a set of strains such that $u_{ij} = 0$ and the combined effect is flat graphene. In the same way, strained graphene can behave as flat graphene provided it is deformed conveniently production a vanishing stress tensor. One should not forget that under sufficiently large deformations, the overlap between the various electron orbitals can change significantly and change the nature of the electronic interaction and new interactions are required in the Dirac equation. In this sense, a geometric deformation is not equivalent to straining graphene.

3 One Dimensional Deformations

Let us consider the case of one dimensional deformations defined by $z = h(x)$ and $X_x(x, y) = X_x(x)$. A deformation on the x direction induces a deformation y . The stretch along y is related to the stretch in x direction via the Poisson ratio and in this sense one can expect that $Y_y(x, y) = Y_y(x)y$. However, in order to simplify the calculations we will take $Y_y(x, y) = Y_y(x)$. The corresponding Dirac Hamiltonian reads [6]:

$$\mathcal{H} = -i \frac{\alpha_x}{\sqrt{g(x)}} \partial_x - 2i \frac{u_{xy}(x)}{\sqrt{g(x)}} \partial_y - i \alpha_y \partial_y, \quad (12)$$

where

$$\sqrt{g(x)} = \sqrt{1 + 2u_{xx} - 4u_{xy}^2} \quad (13)$$

and whose eigenvectors are given by

$$\Psi_{k_x, k_y, \lambda}(x, y) = \frac{1}{\sqrt{2\xi L}} e^{ik_y(y+Y_y(x))} e^{ik_x \int^x dx' \sqrt{g(x')}} \begin{pmatrix} 1 \\ i\lambda e^{-i\theta} \end{pmatrix}, \quad (14)$$

where $\theta = \text{atan}(k_y/k_x)$, $\lambda = \pm 1$. The energy of solution (14) is $E = \lambda \sqrt{k_x^2 + k_y^2}$.

Electrons in the conduction band are described by the solutions (14) with $\lambda = +1$, while those electrons in the valence band are described by $\lambda = -1$. In the following, we will assume that the valence band is occupied. The Dirac propagator in coordinate space reads

$$G(x, y, x', y', E) = \sum_k \frac{\Psi_{k_x, k_y, +}(x, y) \Psi_{k_x, k_y, +}^\dagger(x', y')}{E - E_k + i\varepsilon} + \frac{\Psi_{k_x, k_y, -}(x, y) \Psi_{k_x, k_y, -}^\dagger(x', y')}{E + E_k - i\varepsilon}, \quad (15)$$

where $E_k = \sqrt{k_x^2 + k_y^2}$. Assuming periodic boundary conditions in x and y direction, i.e.

$$X_x(-L/2) = X_x(L/2) \quad \text{and} \quad Y_y(-L/2) = Y_y(L/2), \quad (16)$$

then

$$\sum_{k_y} \rightarrow \frac{L}{2\pi} \int dk_y \quad \text{and} \quad \sum_{k_x} \rightarrow \frac{\xi}{2\pi} \int dk_x \quad (17)$$

where we have defined

$$\xi = \int_{-L/2}^{L/2} dx \sqrt{g(x)}, \quad (18)$$

then the Green function (15) can be rewritten as

$$G(x, y, x', y', E) = \int dk_x dk_y \frac{e^{ik_y(y+Y_y(x)-y'-Y_y(x'))} e^{ik_x \int_x^x dx'' \sqrt{g(x'')}}}{8\pi^2} \left[\frac{M_+^\theta}{E - E_k + i\varepsilon} + \frac{M_-^\theta}{E + E_k - i\varepsilon} \right] \quad (19)$$

with

$$M_\lambda^\theta = \begin{pmatrix} 1 & -i\lambda e^{i\theta} \\ i\lambda e^{-i\theta} & 1 \end{pmatrix}. \quad (20)$$

In terms of x, x' and the momentum along direction y , the later expression becomes

$$G(x, x', k_y, E) = \frac{e^{ik_y(Y_y(x)-Y_y(x'))}}{8\pi^2} \int dk_x e^{ik_x \int_x^x dx'' \sqrt{g(x'')}} \left[\frac{M_+^\theta}{E - E_k + i\varepsilon} + \frac{M_-^\theta}{E + E_k - i\varepsilon} \right]. \quad (21)$$

The integration over k_x can be performed using standard techniques and gives

$$G(x, x', k_y, E) = \frac{e^{ik_y(Y_y(x) - Y_y(x'))}}{4\pi i} \frac{E}{k_0} e^{ik_0|\zeta(x, x')|} \begin{pmatrix} 1 & -ie^{i \operatorname{sgn}[\zeta(x, x')]\theta} \\ ie^{-i \operatorname{sgn}[\zeta(x, x')]\theta} & 1 \end{pmatrix}, \quad (22)$$

where

$$\zeta(x, x') = \int_{x'}^x dx'' \sqrt{g(x'')}, \quad \text{and} \quad k_0 = \sqrt{E^2 - k_y^2}. \quad (23)$$

Note that all information on the geometric of the graphene sheet is resumed in the function $\zeta(x, x')$. Strain shows up in ζ and in the extra phase $\delta_y = k_y(Y_y(x) - Y_y(x'))$ which vanishes if the graphene is dislocated uniformly along y .

4 The Optical Conductivity

The active electrons contributing to the optical conductivity can belong to the valence band, which are described by the negative energy eigenstates of H , and to the conduction band, which are the positive energy eigenstates of the hamiltonian. One can introduce a chemical potential μ associated to the occupation of the electronic bands. A negative chemical potential means a partially occupied valence band. On the other hand, a $\mu > 0$ describes a partially filled conduction band.

In our particle independent model, the optical conductivity of deformed and strained graphene can be computed via the Kubo formula [12, 13] adapted to a two dimension problem

$$\sigma_{ij} = -i \mathcal{G} \sum_{m, n} \frac{f(E_m - \mu) - f(E_n - \mu)}{\omega - \omega_{mn} + i\epsilon} v_{mn}^i v_{nm}^j, \quad (24)$$

where $\mathcal{G} = \frac{e^2 g_s}{A \omega}$, e is the electron electric charge, $g_s = 4$ is the spin and pseudospin degenerescence, $A = \xi L$ is the effective area of the graphene sheet, Ω is the light frequency, $\Omega_{mn} = E_m - E_n$ is the transition energy, $f(\epsilon) = (1 + e^{\beta \epsilon})^{-1}$ is the Fermi-Dirac distribution function, $\beta = 1/k_B T$ and $v_{mn}^i = \langle m | v_i | n \rangle$ are the matrix elements of the velocity operator in the Hamiltonian eigenvector basis.

The velocity operators are defined as $v_i = i [H, x_i] = i \alpha_j e_i^j$, where H is the hamiltonian reported in (5). From the definition it follows that

$$v_x = \frac{\alpha_x}{\sqrt{g}} \quad \text{and} \quad v_y = \alpha_y - \frac{2 u_{xy}}{\sqrt{g}} \alpha_x \quad (25)$$

with $\vec{\alpha} = \beta \vec{\gamma}$.

The real part of the longitudinal optical conductivity σ_{ii} is associated with absorption and it reads

$$\Re \sigma_{ii} = -\mathcal{G} \pi \sum_{m,n} \left[f(E_m - \mu) - f(E_n - \mu) \right] \delta(\omega - \omega_{mn}) |v_{mn}^i|^2 \quad (26)$$

where the sum over states is constrained by energy conservation.

The computation of the longitudinal optical conductivity require the matrix elements of the velocity operator

$$\langle k'_x, k'_y, \lambda' | v_x | k_x, k_y, \lambda \rangle = -\delta_{k_y, k'_y} F(\Delta k_x) \frac{\lambda e^{-i\theta} + \lambda' e^{i\theta'}}{2}, \quad (27)$$

$$\langle k'_x, k'_y, \lambda' | v_y | k_x, k_y, \lambda \rangle = i\delta_{k_x, k'_x} \delta_{k_y, k'_y} \frac{\lambda e^{-i\theta} - \lambda' e^{i\theta'}}{2} + 2\delta_{k_y, k'_y} G(\Delta k_x) \frac{\lambda e^{-i\theta} + \lambda' e^{i\theta'}}{2}, \quad (28)$$

where

$$F(p_x) = \frac{1}{\xi} \int_{-L/2}^{L/2} dx \exp \left[i p_x \int^x dx' \sqrt{g(x')} \right], \quad (29)$$

$$G(p_x) = \frac{1}{\xi} \int_{-L/2}^{L/2} dx u_{xy} \exp \left[i p_x \int^x dx' \sqrt{g(x')} \right], \quad (30)$$

The electronic transitions where matrix elements have the same λ in the initial and final state are called intraband transitions. On the other hand, those transitions where λ changes sign are called interband transitions.

Introducing the following notation for the difference of Fermi-Dirac functions

$$\Delta_{k_x, k'_x, k_y}^{\lambda\lambda'}(\mu) = n_F \left(\lambda \sqrt{k_x^2 + k_y^2} - \mu \right) - n_F \left(\lambda' \sqrt{k'_x{}^2 + k_y^2} - \mu \right), \quad (31)$$

then the conductivity is given by

$$\frac{\mathcal{R}\sigma_{xx}^{\text{inter}}}{\sigma_0} = -\frac{2\xi}{\pi^2\omega} \int dk_x \int dk'_x \int dk_y \Delta_{k_x, k'_x, k_y}^{+-}(\mu) \delta(\omega - \omega_{mn}) |F(\Delta k_x)|^2 \sin^2 \left(\frac{\theta + \theta'}{2} \right), \quad (32)$$

$$\frac{\mathcal{R}\sigma_{xx}^{\text{intra}}}{\sigma_0} = -\frac{2\xi}{\pi^2\omega} \sum_{\lambda} \int dk_x \int dk'_x \int dk_y \Delta_{k_x, k'_x, k_y}^{\lambda\lambda}(\mu) \delta(\omega - \omega_{mn}) |F(\Delta k_x)|^2 \cos^2 \left(\frac{\theta + \theta'}{2} \right), \quad (33)$$

$$\begin{aligned} \frac{\mathcal{R}\sigma_{yy}^{\text{inter}}}{\sigma_0} = & -\frac{2\xi}{\pi^2\omega} \int dk_x \int dk'_x \int dk_y \Delta_{k_x, k'_x, k_y}^{+-}(\mu) \delta(\omega - \omega_{mn}) \left[\delta_{k_x, k'_x} \cos^2 \left(\frac{\theta + \theta'}{2} \right) + \right. \\ & \left. + 4 |G(\Delta k_x)|^2 \sin^2 \left(\frac{\theta + \theta'}{2} \right) - \delta_{k_x, k'_x} \mathcal{R}\{G(\Delta k_x)\} \sin(\theta + \theta') \right], \end{aligned} \quad (34)$$

$$\frac{\mathcal{R}\sigma_{yy}^{\text{intra}}}{\sigma_0} = -\frac{2\xi}{\pi^2\omega} \sum_{\lambda} \int dk_x \int dk'_x \int dk_y \Delta_{k_x, k'_x, k_y}^{\lambda\lambda}(\mu) \delta(\omega - \omega_{mn}) 4 |G(\Delta k_x)|^2 \cos^2\left(\frac{\theta + \theta'}{2}\right), \quad (35)$$

where

$$\sigma_0 = \frac{e^2}{4}, \quad (36)$$

is the optical conductivity of flat graphene [2]. The Dirac delta function express the conservation of energy and can be used to integrate over k_y giving

$$\frac{\mathcal{R}\sigma_{xx}^{\text{inter}}}{\sigma_0} = \frac{\xi}{\pi^2\omega} \int dk_x \int dk'_x \Delta_{k_x, k'_x}^{+-}(\mu) |F(\Delta k_x)|^2 \Omega(\omega, k_x k'_x), \quad (37)$$

$$\frac{\mathcal{R}\sigma_{xx}^{\text{intra}}}{\sigma_0} = -\frac{2\xi}{\pi^2\omega} \sum_{\lambda} \int dk_x \int dk'_x \Delta_{k_x, k'_x}^{\lambda\lambda}(\mu) |F(\Delta k_x)|^2 [1 - \Omega(\omega, k_x k'_x)], \quad (38)$$

$$\frac{\mathcal{R}\sigma_{yy}^{\text{inter}}}{\sigma_0} = \Delta_{\frac{\xi}{2}, \frac{\xi}{2}}^{+,-}(\mu) - \frac{8\xi}{\pi^2\omega} \int dk_x \int dk'_x \Delta_{k_x, k'_x}^{+-}(\mu) |G(\Delta k_x)|^2 \Omega(\omega, k_x k'_x), \quad (39)$$

$$\frac{\mathcal{R}\sigma_{yy}^{\text{intra}}}{\sigma_0} = -\frac{8\xi}{\pi^2\omega} \sum_{\lambda} \int dk_x \int dk'_x \Delta_{k_x, k'_x, k_y}^{\lambda\lambda}(\mu) |G(\Delta k_x)|^2 [1 - \Omega(\omega, k_x k'_x)]. \quad (40)$$

where

$$\Omega(\omega, k_x k'_x) = \sqrt{\frac{\omega^2 - (k_x + k'_x)^2}{\omega^2 - (k_x - k'_x)^2}}. \quad (41)$$

4.1 Special case - half-filling and zero temperature and the limit of small deformations

For half-filling, i.e. for $\mu = 0$, and at zero temperature the Fermi-Dirac are such that the above expressions can be further simplified. The function Δ^{+-} showing in the interband case become 1. In what concerns the intraband transitions, the $\Delta^{\lambda\lambda}$ vanish. Therefore, for this very special case only $\mathcal{R}\sigma_{xx}^{\text{inter}}$ and $\mathcal{R}\sigma_{yy}^{\text{inter}}$ survive. In center of mass coordinates $k_m = (k_x + k'_x)/2$ and $q = k_x - k'_x$ and after integratong over k_m we arrive at

$$\frac{\mathcal{R}\sigma_{xx}^{\text{inter}}}{\sigma_0} = \frac{\xi\omega}{4\pi} \int_{-\omega}^{\omega} dq \frac{|F(q)|^2}{\sqrt{\omega^2 - q^2}}, \quad \frac{\mathcal{R}\sigma_{yy}^{\text{inter}}}{\sigma_0} = 1 - \frac{2\xi\omega}{\pi} \int_{-\omega}^{\omega} dq \frac{|G(q)|^2}{\sqrt{\omega^2 - q^2}}. \quad (42)$$

The same expression hold if in Eqs. (37)-(40) the limit $\omega \rightarrow \infty$ is taken.

For small deformations, the expressions for the optical condutivity Eqs. (37)-(40) can be simplified. Considering only the first order term in the stress tensor, the optical conductivity reads

$$\frac{\mathcal{R}\sigma_{xx}^{\text{inter}}}{\sigma_0} = 1 - \bar{u}, \quad \frac{\mathcal{R}\sigma_{yy}^{\text{inter}}}{\sigma_0} = 1, \quad (43)$$

where \bar{u} is the mean value of the strain tensor u_{xx} :

$$\bar{u}_{xx} = \lim_{L \rightarrow \infty} \frac{1}{L} \int_{L/2}^{L/2} dx u_{xx}(x); \quad (44)$$

note that the dependence on u_{xy} is of second order and so it is neglected.

Our prediction for the optical conductivity in the limit of small deformations (43) can be compared to the tight-binding model result [15]

$$\frac{\mathcal{R}\sigma_{xx}^{\text{inter}}}{\sigma_0} = 1 - 4\epsilon, \quad \frac{\mathcal{R}\sigma_{yy}^{\text{inter}}}{\sigma_0} = 1 + 4\epsilon, \quad (45)$$

where ϵ is the uniaxial strain, which in the small deformation limit, determines the full strain tensor; see [15] for details. If the tight-binding results predicts deviations from the flat graphene conductivity, (43) reports a deviation from σ_0 only for the longitudinal component $\mathcal{R}\sigma_{xx}^{\text{inter}}$. The difference in the results probably comes from ignoring the y dependence in the dislocation $Y_y(x, y)$ in calculation reported here.

5 Summary

The present reports on the use of the geometric language to investigate electrons in strained and deformed graphene and discuss the computation the optical conductivity in this framework. The case of a general one dimensional periodic deformation is studied and the exact solutions of the Dirac equation in an arbitrary static background geometric are computed. This allows us to compute exactly the corresponding Dirac propagator. Furthermore, from the Kubo formula one access the optical conductivity of graphene for an arbitrary static geometry of the graphene sheet.

We call the reader attention that experimental realisation of deformations along one direction were already achieved by e.g. bending graphene nanoribbons [14]. Within the formalism of the Dirac equation in a curved background geometry one can also describe strained graphene. Of course, the goal is to understand and control the geometry of graphene wafers in a way that hopefully, in the future, it is possible to engineer its properties based on pure geometric deformations and/or by applying appropriate strain fields.

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