Optical conductivity of curved graphene

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Abstract

We compute the optical conductivity for an out-of-plane deformation in graphene using an approach based on solutions of the Dirac equation in curved space. Different examples of periodic deformations along one direction translates into an enhancement of the optical conductivity peaks in the region of the far- and mid-infrared frequencies for periodicities \(\sim 100\, \text{nm}\). The width and position of the peaks can be changed by dialling the parameters of the deformation profiles. The enhancement of the optical conductivity is due to intraband transitions and the translational invariance breaking in the geometrically deformed background. Furthermore, we derive an analytical solution of the Dirac equation in a curved space for a general deformation along one spatial direction. For this class of geometries, it is shown that curvature induces an extra phase in the electron wave function, which can also be explored to produce interference devices of the Aharonov–Bohm type.

Keywords: graphene, optical conductivity, Dirac equation, curved graphene

1. Introduction and motivation

The dynamics of electrons in graphene can be described by tight-binding models or, equivalently, by a two-dimensional Dirac equation \([1–7]\). Graphene is a two-dimensional material embedded in three dimensions and is assumed to define a 2D flat surface. However, from the general description of stability analysis for 2D materials and membranes, see e.g. \([2]\) and references therein, one expects deviations from flatland. Ripples, with a size distribution of 50–100 Å, were observed in suspended graphene \([8]\). Furthermore, atomistic simulations using many-body interatomic potentials \([9]\) show that ripples appear spontaneously owing to thermal fluctuations. The predicted size distributions of the ripples were in good agreement with the experimental observations as shown in \([8]\). Also, structural corrugation has been observed in graphene \([10, 11]\).

The deviations of the bulk graphene from a flat surface can also be used to model topological defects \([12, 13]\). In this approach, curvature and torsion are associated with disclinations and dislocations of the medium (see e.g. \([2]\)). The connection between the geometrical approach, elasticity theory and tight-binding models was investigated, for example, in \([14]\). A geometric framework considering curvature \([15]\) has also been applied to model the electronic properties of the ‘buckyball’ \(C_{60}\). This work provides an example of how a geometrical approach can be used to address electronic properties.

Curvature in a geometrical approach can be translated into a pseudo magnetic field or, more generally, into pseudo gauge fields which can lead to observable phenomena; see e.g. the references \([2, 16–18]\).

In \([16]\) the authors suggested an experiment to measure zero-field quantum Hall effect in strained graphene, the strain being at the origin of a strong pseudo magnetic field. Furthermore, they are able to connect strain with the possibility of opening energy gaps in the graphene electronic spectrum.

Experimental evidence of strain-induced large pseudo magnetic fields were reported in \([17]\), where the Landau levels were measured by scanning tunelling microscopy. The authors claim the presence of pseudo magnetic field in graphene with intensities greater than 300 tesla.

Another example of possible effects due to the pseudo magnetic fields associated with local deformations of the
graphene is given in [18], where the authors propose a device to measure Aharonov–Bohm interferences at the nanometre scale. The interplay between the pseudo-magnetic field and an external real one has been addressed in [19], where it was shown that, due to an inherent competition between the two fields, the electric current exhibited spatial inhomogeneity not present when the real magnetic field is zero. For flat graphene, a nonlinear magnetization appears in the absence of a gap or when it is much smaller than the separation between two Landau levels, as has been shown in [20], which one could in principle combine with geometric deformations and study the competition between the pseudo- and real magnetic fields in the magnetization.

The fabrication of wrinkled graphene sheets and the measurement of the single layer topological features by atomic force microscopy was achieved in [21]. Graphene sheets can be reversibly folded and unfolded multiple times, as reported in a following work [22]. Although reference [22] was focused on the structural properties related to defects in graphene, the electronic and transport properties of the folded graphene do not reproduce those of the ‘flat’ graphene. A periodic deformation in suspended graphene was achieved in [23], where the amplitude and the periodicity of the deformation can be controlled by the boundary conditions and temperature. Another approach to engineering periodic deformations in graphene was studied in [24], where graphene was deposited on stretchable elastomeric substrates. In [25] the electrical properties of graphene were investigated by scanning tunnelling microscopy. The authors identified wrinkles in the graphene sheet, with the local curvature of the wrinkle being responsible for the breaking of the lattice symmetry, and showed that the wrinkles have a lower electrical conductance and have mid gap states. It is appropriate to recall that structural deformations can induce zero-field quantum Hall effects in strained graphene [2].

In the literature one can find several theoretical works, see e.g. [26–31], where the geometrical deformations of the graphene sheet change the electronic and optical properties of the pristine material. The optical conductivity for strained graphene (in-plane displacements) was calculated in [28, 29] using a tight-binding approach. In the present work, we rely on a quantum field theoretical approach with curvature to compute the effect of out-of-plane deformations on the graphene’s optical conductivity. To the best knowledge of the authors, this is the first time that the connection between out-of-plane deformation and graphene optical conductivity has been investigated and computed.

In the recent experiment in [32] a single graphene nanoribbon was bent and its voltage-dependent conductance measured. Further, the experiment accounted for the conductance dependence on the precise atomic structure and bending of the molecule in the junction. This type of bending is a geometric deformation in one direction.

All the reported works raise the question of how curvature can be used to tailor the electronic and optical properties of graphene and nanoribbons. In this sense, it is interesting to explore different geometries of the graphene sheet. A possible application that can explore the geometric deformations of graphene is, for example, flexible electronics. The main goal of the current work, is the theoretical investigation of one-dimensional deformations and how they can change the electronic and optical properties of graphene materials. Experimental examples of such types of deformation are given by ripples [8] or bending [32].

Our starting point is the Dirac equation in curved space in 2D+1 dimensions. For a given geometry, we study how stretching and out-of-plane displacements can be included in a geometrical framework. We provide general expressions that can be used to investigate any geometry. Furthermore, we investigate how the electronic dispersion relation, the electronic wave function and optical conductivity depend on the geometry of the graphene. Several one dimensional out-of-plane periodic deformations are worked in detail. We also calculate the expression of the operator velocity for an electron in a static metric.

We found an analytical solution of the Dirac equation in a general curved surface for deformations along a single space direction. The effects of the curvature appear as an extra phase in the electron wave function, besides its normalization, but keep the usual linear dispersion relation $E = \pm |\mathbf{k}|$. This result adds to the work of [18] the possibility of engineering Aharonov–Bohm interference type devices with one-dimensional geometric deformations of the graphene sheet. For the particular case of periodic deformations the phase structure implies the quantization of the electron energy, mimicking Bloch waves in a crystal.

The extra phase and the normalization due to the geometry of the graphene sheet, change the optical conductivity in a non-trivial way. Our analytical solutions simplify considerably the computation of the optical conductivity via the Kubo formula adapted to the two-dimensional case. It also makes easier the optimization of the geometry to tune the optical properties.

For one-dimensional out-of-plane deformations, the Dirac equation can be mapped into a Sturm–Liouville type of equation, i.e. a Schrödinger-like equation with a non-trivial potential bearing a complex functional form. In this way, the solution of the Schödinger eigenvalue equation with a non-trivial potential is mapped into a solvable geometrical problem. We detail such mapping for a particular out-of-plane geometric deformation of the graphene sheet.

The paper is organized as follows. In section 2, we review the properties of the Dirac formalism in curved space. The Hamiltonian of the system and the pseudo-gauge fields are defined. In section 2.1 we discuss how strain and out-of-plane displacements can be accommodated in a geometrical framework. In section 3, the solution of the Dirac equation for in-plane displacements are discussed. In section 4 the analytical solution of the Dirac equation for out-of-plane displacements is derived for a general one dimensional deformation. Moreover, the geometric phase is defined and its relation to a generalized Aharonov–Bohm interference device is presented for an idealized situation. In 5, the one dimensional periodic ripple is investigated in detail and the quantization condition is resolved. The Sturm–Liouville type of equation is derived and the corresponding small and large deformation limits studied. In section 6, the optical conductivity is computed for our
analytical solution of the Dirac equation via the Kubo formula. The large frequency limit will be discussed and, for this limit, we derive analytically forms for the optical conductivity which take into account the geometric of the graphene sheet. In addition, the optical conductivity is calculated for three geometric out-of-plane deformations. Finally, in section 7 we summarize and conclude. In Appendix A, expressions to handle the general case of out-of-plane deformations are provided.

2. Dirac electron in curved space

The action for a relativistic electron in a 2D+1 curved space is given by

\[ S = \int d^3x \sqrt{g} \Psi(x) \left\{ i\Gamma^\mu D_\mu - M \right\} \Psi(x), \]  

(1)

where \( \Psi(x) \) is the Dirac field and \( g = \det(g_{\mu\nu}) \), with \( g_{\mu\nu} \) being the metric tensor. The Dirac matrices in curved space-time read

\[ \Gamma^\nu = e_\mu^\nu A^\mu, \]  

(2)

where the 'vielbein' \( e_\mu^\nu \) define a local Lorentzian frame such that the space-time interval can be written as

\[ ds^2 = \eta_{\alpha\beta} \theta^\alpha \theta^\beta, \]  

(3)

with \( \eta_{\alpha\beta} = \text{diag}(1, -1, -1) \) being the Minkowski metric and \( \theta^\alpha = \epsilon^\alpha_\mu dx^\mu \). The covariant derivative is

\[ D_\mu = \partial_\mu + \frac{1}{4} \omega_{\nu\sigma}^\mu \sigma_{\alpha\beta}, \]  

(4)

with

\[ \sigma_{\alpha\beta} = \frac{1}{2} (\gamma_\alpha \gamma_\beta - \gamma_\beta \gamma_\alpha), \]  

(5)

and the spin connection

\[ \omega_{\nu\sigma}^\mu = \frac{1}{2} \epsilon^\nu_{\alpha\sigma}(\partial_\mu \epsilon^\beta_{\alpha} - \partial_\alpha \epsilon^\beta_{\mu}) - \frac{1}{2} \epsilon^\nu_{\mu\sigma}(\partial_\alpha \epsilon^\beta_{\nu} - \partial_\beta \epsilon^\alpha_{\nu}) - \frac{1}{2} \epsilon^\nu_{\alpha\beta}(\partial_\mu \epsilon^\sigma_{\alpha} - \partial_\alpha \epsilon^\sigma_{\mu}) \epsilon^\beta_{\sigma}. \]  

(6)

The Dirac equation in a curved space-time is

\[ \left\{ i\Gamma^\mu D_\mu - M \right\} \Psi = 0 \]  

(7)

and the Dirac Hamiltonian for a time independent metric reads

\[ H = \int d^3x \sqrt{g} \left\{ -i\Gamma^\mu D_\mu + M \right\} \Psi. \]  

(8)

In this particular case one can choose \( \theta^0 = dx \) and \( \Gamma^0 = \gamma^0 \), where \( \gamma^0 \) is the usual flatland gamma matrix. Furthermore, from the definition

\[ \theta^1 = e_1 dx + e_2 dy, \]  

\[ \theta^2 = e_2 dx + e_1 dy, \]  

(9)

and taking the symmetric solution \( e_1^2 = e_2^2 \), it follows, after some algebra, that the only non-vanishing spin connections are \( \omega^{12} = -\omega^{21} \) for \( i = 1, 2 \).

The Hamiltonian (8) can then be rewritten as

\[ H = H_1 + H_2 + H_3, \]  

(10)

where

\[ H_1 = \int d^3x \Psi^\dagger \left\{ -i\sqrt{g} \sum_{i,j=1}^2 \alpha_i e_i^\dagger \nabla_j \right\} \Psi, \]  

(11)

\[ H_2 = \int d^3x \Psi^\dagger \left\{ -i\sqrt{g} \sum_{i=1}^2 \alpha_i A_i \right\} \Psi, \]  

(12)

\[ H_3 = \int d^3x \Psi^\dagger \left\{ \sqrt{g} M \beta \right\} \Psi, \]  

(13)

the Dirac matrices are

\[ \beta = \gamma^0, \]  

\[ \alpha_i = \beta \gamma^i, \]  

(14)

and the pseudo-gauge fields \( A_i \) are defined, in terms of the vielben and spin connections, as

\[ A_i = \sum_{j,k=1}^2 e_{ij} \epsilon_{jk} \alpha_1^2, \]  

(15)

where \( \epsilon_{ij} \) is the two dimensional Levi-Civita symbol.

The physical interpretation of the \( H_1, H_2 \) and \( H_3 \) can be found in [1, 13, 14, 33]. In particular, the liaison between the continuum approach and a generalized tight-binding Hamiltonian without breaking the symmetries of graphene crystal structure can be found in [33]. The term \( H_1 \), which reproduces the usual Dirac Hamiltonian for a flat geometric, gives rise to a position-dependent Fermi velocity. Possible experimental implications rooted in the minimal U(1) coupling. It induces a Dirac cone shift in momentum space—see [33]. The term \( H_3 \) is a mass term multiplied by the determinant of the metric tensor. In the language of field theory, \( M \sqrt{g} \) can be viewed as a scalar field.

The properties of graphene can be traced to the hybridization of one \( s \) orbital and two in-plane \( p \) orbitals leading to the formation of \( \sigma \) bands, and the remaining \( p_z \) orbital builds \( \pi \) bands. The latter determines the electronic properties of flat graphene. A deformation of the graphene sheet changes the overlap of the various orbitals and, therefore, changes the electronic dynamics. Strain, or in-plane deformations, keeps the relative orientation of the various orbitals and its main effect is essentially a rescaling of the various parameters characterizing the intensity of the interactions. On the other hand, out-of-plane deformations change the relative orientation of the \( p_z \) orbital, modifying the overlap between the various atomic orbitals, and, in principle, can lead to new types of interaction. For example, as summarized in [1] out-of-plane deformations can lead to the introduction (in the continuum field theoretical approach) of a new vector-like field. These new interactions, connected with the out-of-plane deformation, are associated with second order derivatives of the deformation (see e.g. [1, 33]).
while the in-plane deformation is associated with first order derivatives. Therefore, one expects these new interactions, coming from bending \( p_z \) orbitals, to give subleading contributions to the properties of graphene. In the present work we will consider only the interactions coming from the geometric deformation of the flat Hamiltonian and will ignore any possible new interaction.

In the current work, we focus on time independent metrics and, for this class of metrics, it can be shown that the Hamiltonian (10) is Hermitian [34]. In this way, one ensures that the \( H \) eigenvalues are real numbers.

2.1. Strain and out-of-plane displacements

Let us consider that a flat graphene surface lies on the \( xOy \) plane. If graphene is not flat, it defines the surface

\[
z = h(x, y).
\]

The function \( h(x, y) \) parametrizes the out-of-plane displacements and induces curvature.

Strain in graphene can be viewed as a local deformation which can be parametrized by the change of variables

\[
x \rightarrow x' = \mathcal{X}(x, y) \quad \text{and} \quad y \rightarrow y' = \mathcal{Y}(x, y),
\]

where in terms of \((x', y')\) the metric is euclidean. The transformation defined by (17) 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 spatial distance between two neighboring points is given by

\[
dx^2 = (dx')^2 + (dy')^2 + dz^2.
\]

The corresponding metric tensor reads

\[
g_{ij} = \mathcal{X}_i \mathcal{X}_j + 3 \mathcal{Y}_i \mathcal{Y}_j + h h_{ij},
\]

where \( \mathcal{X}_i \) means partial derivative with respect to \( x_i \).

Let us consider deformations described by

\[
x' = x + u_x(x, y),
\]

\[
y' = y + u_y(x, y),
\]

\[
z = h(x, y),
\]

where \( u_x, u_y \) and \( h \) are the displacement fields. The corresponding metric tensor is given by

\[
g_{ij} = \delta_{ij} + 2u_{ij},
\]

where the strain tensor is given by

\[
u_{ij} = \frac{1}{2} \left( \partial_i u_j + \partial_j u_i + \sum_{k=1}^2 \partial_i \partial_j u_k + \partial_i h \partial_j h \right).
\]

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 reproduces exactly the strain tensor considered in [14]. The difference for a finite deformation is the second order term in the in-plane displacements \( u_{ij} \).

3. In-plane displacements

Let us consider the case of in-plane deformations where \( z = h(x, y) = 0 \). Recall that, in this case the transformation (17) does not introduce curvature on graphene and, therefore, the solution of the Dirac equation can be found in the \((x', y')\) reference frame where the electron behaves as a free particle. The solution in the \((x, y)\) reference is obtained from the one in \((x', y')\) via a generalized boost as described in [41].

For in-plane displacements one can write the general solution for the Dirac equation (7) in terms of the vector \( \vec{k} = k_x \hat{e}_x + k_y \hat{e}_y \), as

\[
\Psi = \left\{ i \Gamma^p \partial_p + M \right\} \chi(t) e^{i\sqrt{\mathcal{Z}} (\vec{x} + \vec{u}(x, y))}
\]

where

\[
\chi(t) = \chi e^{iEt}
\]

and

\[
E = \sqrt{\vec{k} \vec{k} + M^2}
\]

In two dimensional representation, \( \chi \) is a Pauli spinor. We call to the reader's attention, that our solution is defined up to a normalization factor.

4. Out-of-plane displacements

The Dirac equation for a general out-of-plane deformation of the graphene sheet described by equation \( z = h(x, y) \) is computed in Appendix A, and reads

\[
\left\{ i \gamma^0 \partial_0 + i \gamma^i \partial_i + \frac{1}{2} \alpha^{ij} \gamma_{ij} \right\} \Psi = 0,
\]

where

\[
\Gamma^i = \frac{1}{(V h)^2} \left\{ \gamma^a h^b (\epsilon^{mnp} h_{a} + \frac{h^i}{\sqrt{1 + (V h)^2}} \right\}
\]

where \( h_a = \partial h / \partial x^a, \nabla h = h \partial_e + h \partial_i, \) and \( \partial_i \) the unit vector along direction \( i \).

The nonvanishing spinconnection components are

\[
\alpha^{ij} = \alpha^{ji} = (-h h_{ik} + h h_{ki}) \tilde{\Omega}(x, y)
\]

where

\[
\tilde{\Omega}(x, y) = \frac{1 + \sqrt{1 + 2 h^2}}{1 + h^2 + h^2}.\]

The Dirac equation (28) can be rewritten introducing the pseudo gauge field \( A_i \) defined in (15). However, to keep track of the out-of-plane deformation, parameterized in terms of the function \( h(x, y) \), and see how the deformation impacts on the electronic and optical properties of graphene we will not use such types of formalism.

In this section we are interested in a general deformation along one direction where \( z = h(x) \). For the particular case under discussion, the Dirac equation simplifies into
The wave function is determined up to a global normalization factor. In the sense, can be considered a 'pure-gauge' configuration. We would like to call the reader's attention to the fact that

\[ C \text{ is not the pseudo-gauge field } \tilde{A} \text{ defined in equation (15) but can be introduced to remove the new electron wave function phase. For example, while } \tilde{A} \text{ can give rise to pseudo-magnetic fields [26, 27, 30], the pure-gauge field } C \text{ does not.} \]

4.1 Aharonov–Bohm phases

The effect of the out-of-plane deformation along one direction translates into a new phase,

\[ \delta(x) = k \int dx' \sqrt{1 + h'^2(x')} , \tag{41} \]

The electron wave function, which can be explored to produce interference devices based on Aharonov–Bohm type effects. The new phase \( \delta(x) \) is a measure of the local curvature. If in the electron path there are regions of different out-of-plane deformations, being either different lengths or different metrics, they mimic a double slit Young experiment and the difference of phase between the two paths is realized in practice.

In figure 1 we illustrate an idealized Aharonov–Bohm one-dimensional interference device of a double slit Young type experiment. Classically, the electron can follow either path 1 or 2. If, on the left hand side, the electron is described by the wave function \( \Psi_1 \), on the right side of the apparatus the electron is described by a superposition of the wave functions, say \( \Psi_1 \) associated with path 1, and \( \Psi_2 \) associated with path 2. The phase \( \delta \) given by equation (41). By a convenient choice of the curvature or the length of path 2 one can tune \( \delta \) in order to produce interference effects. A conventional Aharonov–Bohm phase, due to the presence of a solenoid type electromagnetic field, can be added to the geometric phase \( \delta \) and explored to build up or destroy the presence of curvature.

An example of a device relying on the Aharonov–Bohm effect, in association with a rotational symmetric deformation of the geometry, was proposed in [18]. Recently, in [32] the authors were able to bend a nanoribbon, which could be associated with a metric of the type discussed here, i.e. \( z = h(x) \). Their technique envisages that, in the future, it may be possible to build an electron multipath arrangement, using coherently several of their experimental apparatuses.

5. One dimensional periodic out-of-plane deformations

Let us now consider the out-of-plane displacements corresponding to a periodically corrugated graphene parametrized as (see figure 2)

\[ E_0 = \sqrt{1 + h^2(x)} \]

Fractals, they mimic a double slit Young experiment and the difference of phase between the two paths is realized in practice.
This type of geometry simulates ripples along the $x$ direction and defines a 1D crystal. For periodic solutions which require $\delta(2\pi) = \delta(0) + 2\pi r$, where $r$ is an integer number, $k_s$ and, therefore, the energy are quantized. The quantization condition gives

$$\frac{k_s}{\omega} = 2\pi r. \quad (43)$$

where $\xi$ is the arc length in units of $1/\omega$ and is given by

$$\xi = \int_0^{2\pi} d\nu \sqrt{1 + h^2(v)}, \quad (44)$$

computed with the dimensionless argument $v = \omega x$.

For example, for $h(x) = A \cos(\omega x)$ the quantization condition (44) gives the spectra, as a function of $\eta = A \omega$, shown in figure 3. For small deformations, i.e. for $\eta \ll 1$, equation (43) reads

$$\frac{k_s}{\omega} = r \left(1 - \frac{\eta^2}{4} + \cdots \right). \quad (45)$$

The quadratic behavior in $\eta$ is clearly visible in figure 3.

5.1. On the Sturm–Liouville equation

For the geometry given by $h(x) = A \cos(\omega x)$, the Dirac equations (35) and (36) can be reduced to a second order differential equation in $\varphi_+$. Indeed, for a wave function of the form

$$\varphi_+(x, y) = e^{ik_s y} \left(1 + A^2 \omega^2 \sin^2(\omega x) \right)^{1/4} \psi,$$

the second order differential equation in $\varphi_+$ can be cast in a Sturm–Liouville form

$$\left\{ - \frac{d^2}{dy^2} + V(y) \right\} \psi(y) = \xi \epsilon(y) \phi(y), \quad (47)$$

where $v = \omega x$, $\xi = (E^2 - M^2 - k_s^2)/\omega^2$, $\epsilon(y)$ and $\phi(y)$ are functions of $y$.

6. Optical conductivity

In our description of geometrically deformed (out-of-plane) graphene, the active electrons belong to two bands distinguished by the sign of the corresponding single particle energy eigenstates of the hamiltonian (10); see (A.12) in the first quantized form. The electron valence levels are the negative energy eigenstates of $H$, while the conduction band is associated with the positive energy eigenstates of the hamiltonian.

The chemical potential $\mu$ outlines 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 graphene can be computed via the Kubo formula [44] adapted to a two dimension problem as

$$\sigma(\omega) = \frac{2ie}{h} \int_0^\infty \frac{dE}{E} \left( \tilde{n}(E) - \tilde{f}(E) \right) \frac{d\epsilon}{dE} \frac{d\phi}{dE},$$

where $\tilde{n}(E)$ is the occupation probability of the electronic states above $E$ and $\tilde{f}(E)$ is the Fermi function.
\[ \sigma_{ij} = -i \mathcal{G} \sum_{m,n} \frac{f(E_m - \mu) - f(E_n - \mu)}{\Omega - \Omega_{mn} + i\epsilon} v_{nm} v_{im}, \]  

(49)

where

\[ \mathcal{G} = \frac{\epsilon^2 g_e}{3\Omega}, \]  

(50)

\( e \) is the electron electric charge, \( g_e = 4 \) is the spin and pseudospin degenerescence, \( \Omega \) is the area of the graphene sheet, \( \Omega = \epsilon \Omega_{mn} = E_m - E_n \) is the transition energy, \( f(x) = (1 + e^{-x})^{-1} \) is the Fermi-Dirac distribution function, \( \beta = 1/k_BT \) and \( v_{nm} = \{m|v|n\} \) are the matrix elements of the velocity operator in the Hamiltonian eigenvector basis \((37)\).

The velocity operators are defined as \( v_i = i [H, x_i] \), where \( H \) is the hamiltonian. For a general surface geometry \( H \) is given in \((A.12)\) and it follows that

\[ v_i = \alpha_i e_i = \frac{1}{h_i^2 + h_j^2} \left\{ \frac{h_j^2}{\sqrt{1 + h_i^2 + h_j^2}} \alpha_i - h_j \left( 1 - \frac{1}{\sqrt{1 + h_i^2 + h_j^2}} \right) \alpha_j \right\}, \]  

(51)

where \( \alpha = \beta \vec{r} \), \( h_1 \equiv h_x \) and \( h_2 \equiv h_y \). The first term in \((51)\) reproduces the usual operator form for Dirac electrons in flat geometries, i.e. \( v_i = \alpha_i \), up to a geometrical factor which includes the surface deformation, through derivatives of the profile function \( h(x, y) \). The second term add the contribution of a transverse velocity operator to the chosen direction and vanishes in the limit where \( h_i \to 0 \), i.e. a flat surface.

The real part of the longitudinal optical conductivity \( \sigma_{ii} \) is associated with the following

\[ \Re \sigma_{ii} = -\mathcal{G} \sum_{m,n} [f(E_m - \mu) - f(E_n - \mu)] \times \delta(\Omega - \Omega_{mn}) |v_{im}|^2, \]  

(52)

where the sum over states is constrained by energy conservation. It can be shown that the transverse part \( \sigma_{ij} \) is proportional to the mass term \( M \) or the graphene half-gap. Typical values for \( M \) are of the order of meV or less and, therefore, one can safely disregard the transverse component of the optical conductivity. For example, for a gapless flat graphene the transverse conductivity vanishes, unless the magnetic field is active \([46]\).

The electronic transitions associated with optical absorption can occur between levels with different energy signs, named interband transitions and represented by \( \sigma_{\text{inter}}^{\text{int}} \), or between levels with the same energy sign, i.e. intraband transitions described by \( \sigma_{\text{intr}}^{\text{int}} \). For temperatures \( T \sim 300 \) K and finite chemical potential \( \mu \sim 100 \) meV, the intraband transitions have to be taken into account \([45]\). Indeed, as discussed below, the largest values for the optical conductivity are associated with the intraband transitions.

### 6.1. Periodic deformations along a single direction

For a deformation along a single direction where \( z = h(x) \), the velocity operators can be read from \((51)\) and are given by

\[ v_x = \frac{\alpha_x}{\sqrt{1 + h_x^2}}, \quad \text{and} \quad v_y = \frac{\alpha_y}{\sqrt{1 + h_y^2}}. \]  

(53)

The operator \( v_x \) acquires the factor \( 1/\sqrt{1 + h_x^2} \), which can be interpreted as the projection of the unitary vector \( \hat{e}_x \) into the deformed graphene surface. For a general two-dimensional deformation, such a simple geometric interpretation is not possible.

The calculation of the real part of the longitudinal optical conductivity \( \Re \sigma_{ii} \) requires the matrix elements (m.e.’s) of the velocity operator, \( \langle \vec{k}' \cdot s | v_i | \vec{k} \cdot s \rangle \), between eigenstates of the hamiltonian with positive \((s = +)\) and negative \((s = -)\) eigenvalues; see equation \((37)\) for definition of the spinors. For a periodic deformation, the quantization condition \((43)\) determines

\[ k_x \equiv k_r = \frac{2\pi n a}{\xi} \quad \text{and} \quad \vec{k} = k_x \hat{e}_x + k_y \hat{e}_y. \]  

(54)

Translation invariance along the \( y \) direction implies that the m.e.’s are diagonal in \( k_y \), but mix different values of \( r \) and \( r' \). The energy conservation condition \( \Omega_{mn} = \Omega \) in \((52)\) gives us

\[ k_r^2 = \frac{\Omega^2}{4} - \frac{1}{2} (k_r^2 + k_s^2) + \frac{(k_r^2 - k_s^2)^2}{4\Omega^2} - M^2. \]  

(55)

For interband transitions, the solution of the energy conservation constraint

\[ \sqrt{k_r^2 + k_s^2 + M^2} + \sqrt{k_r^2 + k_s^2 + M^2} = \Omega, \]  

(56)

requires \( \Omega^2 > |k_r^2 - k_s^2| \) and its solution is given by \((55)\). On the other hand, for intraband transitions, energy conservation reads

\[ \sqrt{k_r^2 + k_s^2 + M^2} - \sqrt{k_r^2 + k_s^2 + M^2} = \Omega, \]  

(57)

and, therefore, \( \Omega^2 < k_r^2 - k_s^2 \) with \( k_r \) given by \((55)\).

In the following, we will show results for the following geometric deformations

\[ h_1(x) = \frac{A}{\omega} \cos u \quad A = 3.13, \]  

\[ h_2(x) = \frac{A}{\omega} \left( \int_{-\pi/2}^u \frac{dv}{\sqrt{(v - \pi/2)^2 + b}} \right)^2 \quad A = 0.05, \quad b = 0.05, \]  

\[ h_3(x) = \frac{A}{\omega} \exp \left\{ -\frac{(u - \pi/2)^2}{2b} \right\} \quad A = 4.9, \quad b = 0.1 \]  

(58)

where \( u = \omega x \), \( 2\pi a/\omega \) is the spatial periodicity of the deformation. Note that for the geometries defined by \( h_2(x) \) and \( h_3(x) \) the first derivative has a discontinuity at \( x = 0, \pm 2\pi a/\omega, \pm 4\pi a/\omega, \ldots \) but the square of its second derivative, which enters in the definition of \( \xi \), is always a continuous function of \( x \). The geometric profiles associated with \( h_1(x) \), \( h_2(x) \) and \( h_3(x) \) can be seen in figure 4.

The examples provide by the profiles \( h_1(x) \), \( h_2(x) \) and \( h_3(x) \) show that optical conductivity is sensitive to the deformation induced in the graphene surface. Of course, this raises the question of optimizing the geometry to either tune the value of the conductivity or maximize/minimize \( \sigma_{ii} \). Although these
are important questions from the practical point of view, they
will not be discussed here. However all the necessary expres-
sions are provided and the interested reader can use them to
tune, maximize or minimize the optical conductivity.

6.1.1. Interband transitions. For interband transitions, the
matrix elements of the velocity operator depend only on the
discrete labels \( r \) and \( r' \); see equations (54) and (55) for defi-
1
nitions. Let us introduce the shorthand notation for the m.e.’s
\( v_{rr} \) and an analogous form for the m.e.’s of \( v_{rr} \). It follows that

\[
\begin{align*}
v_{rr, \text{inter}} &= -\frac{G^{0,0}}{2k_f} \left( \frac{i (k_y - k_{y'})}{E_k + M} - \frac{i (k_x + k_{x'})}{E_k - M} \right), \\
v_{rr, \text{inter}} &= \delta_{rr} \frac{M k_y + i k_x E_k}{E_k} \left( \frac{1}{E_k^2 - M^2} \right),
\end{align*}
\]

where

\[
G^{0,0} = F(r-r') \left( 1 + \frac{M}{E_k} \right) \left( 1 + \frac{M}{E_{k'}} \right).
\]

The information on the geometry of the graphene sheet is
summarized in the function

\[
F(t) = \int_0^{2\pi} d u \, e^{i \phi(t,u)},
\]

through the phase-factor

\[
\phi(t,u) = 2\pi \frac{t}{\xi} \int_0^u d \nu \sqrt{1 + h_1^2(\nu)}.
\]

In the absence of deformation, i.e. for \( h = 0 \), the function
\( F(t) \) reduces to \( 2\pi \delta_{t,0} \) as expected from the transla-
tional invariance along \( x \) modulo the periodic boundary condi-
tion. The function \( F(t) \) encodes the information on the
geometry of the graphene sheet and shapes the contribu-
tion of both inter- and intra-band transitions to the optical con-
ductivity.

The function \( |F(t)| \) is plotted on figure 5 for the periodic
geometric deformations given in (58). The profiles on figure 5
have the same arc length \( \xi/2 \pi = 2.29 \).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{The \( |F(r-r')/2\pi| \) function for the profiles defined in (58).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Optical conductivity for intraband transitions for the geometries (58), a chemical potential \( \mu = 250 \text{ meV} \), \( 2\pi/\omega = 100 \text{ nm} \) and the same arc length \( \xi \).}
\end{figure}

The real part of the optical conductivity along the deforma-
tion profile is given by:

\[
\Re \frac{\sigma_{\text{inter}}}{\sigma_0} = -\frac{8\omega}{\Omega^2} \sum_{r,r'} \Delta_{rr'} \left( \frac{1}{E_r^2 - E_{r'}^2} \right)^2,
\]

where \( \sigma_0 = e^2/4 \) is the bulk value,

\[
D_{rr'} = \sqrt{1 - 2 \left( E_{r'}^2 + E_r^2 + 2M^2 \right) + \left( E_{r'}^2 - E_r^2 \right)^2},
\]

with the dimensionless quantities \( k_r = k_r/M, M = M/\Omega \) and \( \xi \) is defined in (44). \( k_r \) is given by (55) and it satisfies the
energy conservation condition (56). The difference between
the Fermi-Dirac functions is defined as

\[
\Delta_{rr'} = f(\lambda E_r - \mu) - f(\lambda E_{r'} - \mu).
\]

The real part of the optical conductivity along the \( y \) direc-
tion reads

\[
\Re \frac{\sigma_{\text{intra}}}{\sigma_0} = -\frac{\omega}{\Omega^2} \sum_{r} \Delta_{rr} \left[ \frac{1}{E_r^2 - E_{r}^2} + \frac{1}{E_r^2 - E_{r}^2} \right],
\]

From its definition it follows that the dimensionless optical
conductivity is a function of the dimensionless quantities \( \beta = \omega/\Omega \), \( \omega/\Omega \), \( \mu/\Omega \) and \( M/\Omega \), i.e.

\[
\Re \frac{\sigma_{\text{intra}}}{\sigma_0} = \mathcal{S}_{\beta} \left( \beta, \frac{\omega}{\Omega}, \frac{\mu}{\Omega}, \frac{M}{\Omega} \right).
\]

This type of behavior is not seen in \( \Re \sigma_{\text{inter}}/\sigma_0 \) as it encodes
the information on the geometry of the graphene surface via
the function \( F(t) \). The scaling properties of \( \Re \sigma_{\text{inter}}/\sigma_0 \) summarized in equation (68) simplify considerably the analysis of the numerics.

The optical conductivities given by (64) and (67) have
singularities, the Van Hove singularities, associated with the
zeros of denominator of \( D_{rr'} \). For zero electron mass, the Van
Hove singularities do not contribute to \( \Re \sigma_{\text{inter}}/\sigma_0 \) as they are
cancelled by the vanishing of the m.e.’s of the velocity. This is
no longer valid in the case of \( M \neq 0 \). The cancellation does not
occur in $\Re \sigma_v / \sigma_0$ and, therefore, the discrete spectrum of $k_x$, due to the periodic boundary conditions, gives a nonvanishing contribution to the conductivity. However, $\Re \sigma_v / \sigma_0 \to 1$ as one approaches the bulk graphene limit, i.e. when $\omega \to 0$.

For real graphene, the Van Hove singularities are washed out by disorder and imperfections in the graphene and in the periodic deformation. In what concerns the optical conductivity, this can be simulated by performing an average in the parameters of the model, see e.g. [45]. The results reported below for $\sigma_{\text{int}}^\text{intra}$ and $\sigma_{\text{int}}^\text{inter}$ are an average over $\omega$, assuming a gaussian distribution of frequencies with standard deviation of $\surd 10$. For $\sigma_{\text{int}}^\text{intra}$ such effects are tiny and there is no need to average the results.

### 6.12. Intraband transitions

For intraband transitions the m.e.'s of $v_\gamma$ are diagonal in the momentum states $k$ and, therefore, $\sigma_{\gamma\gamma}^\text{intra} = \sigma_{\gamma\gamma}^\text{inter} = 0$.

The conductivity $\Re \sigma_{\gamma\gamma}^\text{intra}$ is given by (64) after replacing the m.e.'s of $v_\gamma$ by

$$ v_{\gamma,\text{intra}} = \frac{iG_{rr}}{2\bar{\xi}} \left( -ik_x + k_y - ik_x - k_y \right), $$

and $\Delta_{rr}^\pm \rightarrow \Delta_{rr}^\pm$, with $\lambda = \pm 1$. It follows that

$$ \frac{\Re \sigma_{\gamma\gamma}^\text{intra}}{\sigma_0} = -\frac{8\omega}{\Omega \bar{\xi}} \sum_{r',r,\lambda} \Delta_{rr}^\pm D_{r'r}^\pm |v_{r',\text{intra}}|^2. $$

For flat graphene $r' = r$ and the Pauli Principle forbids a transition to the same state, therefore, the intraband optical conductivity vanishes. On the other hand, if the graphene sheet is deformed, $r' \neq r$ transitions are allowed and $\Re \sigma_{\gamma\gamma}^\text{intra} \neq 0$.

In what concerns the dependence with the chemical potential, an increase in $\mu$ means a larger phase space for intraband transitions and, therefore, an increase in the intraband optical conductivity. In addition, given that the number of possible electronic interband transitions is determined mainly by the chemical potential, $\mu$ also determines the contribution of the Van Hove singularities to $\Re \sigma_v / \sigma_0$.

### 6.2. Numerical results

In this section, we report on the numerical results for the optical conductivity for inter, see equations (64) and (70), and intraband transitions, see equation (67), considering the geometric profiles defined in (58). In what follows, the Dirac electron is supposed to be massless, the spatial periodicity $2\pi / \omega$ is varied between 30 and 200 nm and the chemical potential is varied in the range 40–450 meV for a temperature $T = 300$ K.

As described below, we have observed quite different behaviors for the conductivities associated with the inter and intraband transitions. The intraband transitions give much larger contributions to the optical conductivity in the far-infrared region, where it dominates for $\Omega \sim \omega$ and for a finite chemical potential. On the other hand, as $\Omega$ increases the contributions to the conductivity approach its asymptotic values and the larger values are now associated with the interband transitions.

Let us start looking to the contribution of the intraband transitions to the optical conductivity. Figure 6 shows the intraband optical conductivity for the geometries defined in (58) computed for a chemical potential $\mu = 250$ meV, a spatial periodicity $2\pi / \omega = 100$ nm and the same arc length $\xi$. The behavior of $\Re \sigma_{\gamma\gamma}^\text{intra}$ is determined mainly by the Van Hove singularities and is modelled by the geometry of the graphene sheet. In the limit of $\omega \to \infty$ and $\xi \to 0$ the first peak of figure 6 narrows and moves towards $\Omega = 0$, becoming the Drude peak, that is expected for an infinite and disorder-free system [45].

---

**Figure 7.** Optical conductivity associated with intraband transitions for the Gaussian geometry defined in (58) with a $2\pi / \omega = 100$ nm and for different chemical potentials $\mu$. Note that the widths become larger as $\mu$ increases from 50 meV to 450 meV.

**Figure 8.** Band structure for the Gaussian profile defined in (58). For a given chemical potential $\mu$ (dashed line), the possible intraband transitions can only occur from the shaded area to states above the dashed line. The dominant contribution to $\Re \sigma_{\gamma\gamma}^\text{intra}$ is represented by the arrow.

From its definition, it follows that

$$ \frac{\Re \sigma_{\gamma\gamma}}{\sigma_0} = \mathcal{S}_{\gamma\gamma}(\beta \omega, \Omega / \omega, \frac{\omega \mu}{\Omega}, \frac{M}{\omega}, \omega h(\alpha \omega)). $$

This relation applies both to the contribution of the intra and interband transitions to the optical conductivity.
The Van Hove singularities in $\Re \sigma_{\text{xx}}$ are defined by the zeros of the denominator in equation (65)

$$D_{rr}^\Omega = \left| 1 - \frac{(k_x^2 - k_y^2)^2}{k_y} \right|,$$

which occur for $|k_x| = |k_y| = 1$, see equation (57), and $r \neq r'$. Given that the m.e.’s of $v_i$ and the denominator of $D_{rr}^\Omega$ do not vanish simultaneously, the positions of the Van Hove peaks happen for $\Omega = 2\pi \omega s / \xi$, where $s = |r - r'| = 1, 2, 3 \ldots$

Figure 6 shows a peak structure at $\Omega = 17$ s meV. The peaks are associated with the Van Hove singularities and each Van Hove peak is modulated by the corresponding $|F(\pm s)|^2$ function. As can be seen in figure 5, $|F(\pm s)|^2$ decreases fast with $s$ and, therefore, the higher peak intensity occurs for smaller $s$. Indeed, the first peak corresponds to $s = 1$, and subsequent ones to $s = 2, 3, \ldots$. For the profile function $h_1(x) = A \cos \omega x$, the function $F(\pm s)$ vanishes at odd $s$ and, for this particular geometry, there are no peaks for odd $s$.

The maxima of the various peaks are proportional to $|F(\pm s)|^2$ and, therefore, its relative value is a signature of the function $|F(\pm s)|^2$. This can also be read comparing figures 5 and 6.

The behavior of $F(\pm s)$ at large $s$ also explains why the contribution of the intraband transitions to the optical conductivity vanishes in the limit of $\Omega \gg \omega$. Indeed, for sufficiently large $\Omega$ or small $\omega$, equation (57) implies that $k_x \gg k_y$ and, therefore, $F(r - r')$ is essentially zero as $r - r'$ becomes large.

The widths of various peaks in the optical conductivity associated with the intraband transitions depend on the chemical potential $\mu$. For example, for the Gaussian profile, see (58), the quantization condition (43) provides the band structure of figure 8. For a given chemical potential $\mu$ (dashed line), the intraband transitions that can contribute to the optical conductivity can only occur from and to the shaded area. The dominant contribution to $\Re \sigma_{\text{xx}}^{\text{intr}}$ is represented by the arrow in figure 8; see [45] for a discussion.

The phase space for the intraband transitions increases with $\mu$ and, therefore, the corresponding widths also increase with the chemical potential.

Figure 9. Contribution of the interband transitions to the optical conductivity for different geometries with $\mu = 40$ meV and a fixed spatial periodicity of $2\pi \omega = 100$ nm. From bottom to top one sees $\Re \sigma_{\text{xx}}^{\text{inter}} / \sigma_0$ computed with $h_1(x)$ (gray), $h_2(x)$ (blue), and $h_3(x)$ (red) defined in (58).

Figure 10. Contribution of the interband transitions to the optical conductivity for the geometric profile $A \cos \omega x$ for different amplitudes. From top to bottom $\Re \sigma_{\text{xx}}^{\text{inter}} / \sigma_0$ follows the sequence $A \omega = (1, 2, 4)$ and $\xi = (7.64, 10.54, 17.63)$. The periodicity is given by $2\pi \omega = 100$ nm and the chemical potential is fixed at 40 meV.

Figure 7 illustrates the effect of changing the chemical potential for the Gaussian profile with $2\pi \omega = 100$ nm. As shown, the positions of the peaks are found at $\Omega = s 17$ meV and their width increases with $\mu$. Similar curves can be drawn for the other profiles in (58).

Let us turn our attention to the optical conductivity associated with interband transitions. Recall that the matrix elements of $v_i$ vanish for the interband transitions at the pole frequency, see equation (65), and, in this way, the Van Hove singularities do not contribute to $\Re \sigma_{\text{xx}}^{\text{inter}}$. Indeed, as can be seen in figures 9–11, $\Re \sigma_{\text{xx}}^{\text{inter}}$ has no peak structure.

The maxima of the peaks associated with the Van Hove singularities, i.e. the pole contribution to the optical conductivity in $\Re \sigma_{\text{xx}}^{\text{intr}}$ look rather different than the corresponding contribution for $\Re \sigma_{\text{xx}}^{\text{inter}}$. If for the former quantity, see equation (70), there is a double sum in $r$ and $r'$ and the frequency $\Omega$ contributes to the conductivity whenever $\Omega = 2 \pi s \omega / \xi$ for $s = 1, 2, 3 \ldots$. For the latter one, see equation (67), it involves a single sum over $r$ and only the frequency $\Omega = 4 \pi \omega r / \xi$ contributes to the conductivity. Then, for a given $\Omega$ associated with a pole on the optical conductivity, $\Re \sigma_{\text{xx}}^{\text{intr}}$ adds the contribution of an infinite number of poles, while $\Re \sigma_{\text{xx}}^{\text{inter}}$ sees only a single pole and one expects higher peak values for $\Re \sigma_{\text{xx}}^{\text{intr}}$ when compared with $\Re \sigma_{\text{xx}}^{\text{inter}}$. Note that the number of frequencies associated with the Van Hove singularities is determined by the chemical potential. Furthermore, the widths of the peaks associated with interband and intraband transitions is expected to be distinct, with Van Hove peak intraband transitions showing a larger width. The diverse widths of the Van Hove peaks for the intra and interband transitions was already discussed in [45] for graphene nanoribbons.

The optical conductivity $\Re \sigma_{\text{xx}}^{\text{inter}}$ associated with the interband transitions for different geometries, a chemical potential $\mu = 40$ meV, a fixed spatial periodicity $2\pi \omega = 100$ nm and for profiles having the same arc length $\xi$ is shown in figure 9. As expected no Van Hove singularities are observed and the conductivity approaches a plateaux whose value depends on the particular geometry. Note, however, that the values for $\Re \sigma_{\text{xx}}^{\text{intr}}$
are not that sensitive to the graphene profiles and are significantly smaller than the corresponding optical conductivity for the intraband transitions—see figures 7 and 6.

The effect on the interband conductivity of changing the arc length $\xi$ for the profile $h(s) = A \cos \omega s$ can be seen in figure 10. The curves are for $2\pi \omega = 100$ nm, a chemical potential of 40 meV and $(A, \omega, \xi) = (1, 7.64), (2, 10.54), (4, 17.63)$. As figure 10 shows, a larger $\xi$ means a smaller $\mathbf{R} \sigma_{xx}^{\text{inter}}$. This behavior with $\xi$ can be understood as the matrix elements in $\mathbf{R} \sigma_{xx}^{\text{inter}}$. The behavior with $\xi$ can be understood as the matrix elements in $\mathbf{R} \sigma_{xx}^{\text{inter}}$.

In figure 11 the contribution of the various transitions to the optical conductivity are illustrated for the case of a Gaussian profile with spatial periodicity $2\pi \omega = 100$ nm and chemical potential $\mu = 250$ meV. The highest conductivity occurs for $\mathbf{R} \sigma_{xx}^{\text{inter}}$, detailed in figure 7, and occurs for low frequency, i.e. in the far-infrared region of the spectra.

The conductivity associated with interband transitions show a plateaux as $\Omega$ increases. As $\Omega \to \infty$, the effects due to $T$, $\mu$ and the periodic boundary condition can be disregarded and, as clearly seen in the figure, the bulk value is approached for $\mathbf{R} \sigma_{xx}^{\text{inter}} / \sigma_0 \to 1$. In what concerns the high frequency limit for $\mathbf{R} \sigma_{xx}^{\text{inter}}$, its plateau value correlates with the geometry of the graphene sheet and it can be shown that

$$\frac{\mathbf{R} \sigma_{xx}^{\text{inter}}}{\sigma_0} \to \left(\frac{2\pi}{\xi}\right)^2 + \frac{2}{\xi^2} \sum_{t=1}^{n} |F(t)|^2$$

as $\Omega \to \infty$.

7. Summary

The present work makes use of a geometric framework to investigate electrons in graphene. In particular, we look at in-plane and out-of-plane displacements as deformations and the corresponding Dirac equation in curved 2D space is derived. We focus on a static metric that ensures an hermitian Hamiltonian [34].

A general deformation along a single spatial direction is investigated and we are able to provide an analytical solution of the corresponding Dirac equation in a curved space. The solution shows that, for this class of geometries, curvature induces an extra phase in the electron wave function. This opens the possibility of engineering Aharonov–Bohm interference type devices with geometric deformations of the graphene sheet in one direction.

An experimental realization of deformations along one direction has already been achieved by bending graphene nanoribbons [32]. This allows us to hope that, in the future, it may be possible to tailor the geometry of graphene wafers to create controlled devices with tuned conductance properties. Along these lines, we have considered an idealized apparatus to explore Aharonov–Bohm interferences based on geometrical deformations in one spatial direction.

For periodic deformations a quantization rule for the energy is found from the phase structure. This suggests the presence of electron Bloch waves in the background of a ‘crystal structure’ created by the periodicity of the deformation, which is illustrated for a periodic out of plane ripple.

The Sturm–Liouville type of equation associated with the Dirac equation in curved space was obtained for the ripple, illustrating the possibility of mapping complex potentials into solvable geometric problems.

The induced deformations of the graphene/nanoribbon surface has the potential to modify the charge carriers properties, namely the associated electronic states and optical properties. For periodic out-of-plane deformations, the quantisation rule for the energy eigenvalues, the phase structure of the eigenstates of the Dirac Hamiltonian on the surface of the curved graphene, change in a sensible form the optical conductivity. Different examples of periodic deformations along the arbitrary $x$-direction shows an enhancement of the optical conductivity in the far and mid-infrared frequency range for periodicities $\sim 100$ nm. The enhancement of the optical conductivity comes mainly from the interband transitions and is associated with the Van Hove singularities modulated by the geometry of the graphene sheet. The difference of the contributions of the Van Hove singularities to the interband and intraband optical conductivities explains the observed scales for $\sigma_{xx}$. Furthermore, we have shown that the manipulation of the profile functions can alter both the width and position of the peaks. This opens up the problem of finding the geometric profile to maximize the optical conductivity or to tune the geometric profile and produce a given value for the conductivity. We have not explored these questions here, but all the expressions derived allow investigation of such important problems.

As reported in section 6.2, the optical conductivity of a curved graphene sheet depends on the polarization of the photon relative to the direction along which the graphene is deformed. This anisotropy in the optical conductivity can be explored to create a dichroism effect. For a linearly polarized incident photon with momenta perpendicular to the graphene sheet and polarization angle $\theta$, measured relative to the $x$-axis, the rotation of the polarization angle in the graphene sheet is given by...
\[
\tan \theta' = \frac{2 + Z\sigma_{xx}\tan \theta}{2 + Z\sigma_{yy}} \tag{73}
\]

where \(Z\) is the medium impedance and \(\theta'\) is the polarization angle of the refractive electromagnetic wave. In the above expression we have neglected the contributions from \(\sigma_{xy}\). For a graphene sheet in vacuum, \(Z_0 = 0.013 \ll 1\), where \(Z_0 = \sqrt{\mu_0/\varepsilon_0} \approx 377\Omega\) is the vacuum impedance, and \(\theta' = \theta\). Further, if \(\sigma_{xx} = \sigma_{yy}\) the polarization angle remains essentially unchanged and \(\theta' = \theta\). For photon frequencies of the order of \(\omega\), the large values of \(Z_{xx}\) and \(Z_{yy}\) correspondingly suppress, relative to \(Z_{xy}\), the optical conductivity is dominated by the interband transitions. For photon frequencies \(\omega \ll \omega_0 \approx 0.013\), for such frequencies, the optical response \(\sigma_{xx}^{\text{magn}}\) is suppressed, relative to \(\sigma_{xy}\), the vacuum impedance, and \(\theta' = \theta\). For photon frequencies \(\omega \gg \omega_0\), or placing the graphene sheet on medium with a large impedance, see equation (73), like e.g. a magnetic medium, with \(\mu \gg \mu_0\), or placing it inside a waveguide—see [45] for discussions.

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**Appendix A. Out-of-plane displacements: the general case**

In order to fix our notation and conventions, here we give details of the Dirac equation on a curved 2D space. An analogous formalism was also presented in [31].

Let us consider a two-dimensional out-of-plane displacement parametrized as

\[ z = h(x, y). \]

The associated metric reads

\[
(g_{\mu \nu}) = \begin{pmatrix}
1 & 0 & 0 \\
0 & -h_{x}^2 - 1 & -h_{x}h_{y} \\
0 & -h_{x}h_{y} & -h_{y}^2 - 1
\end{pmatrix} \tag{A.1}
\]

where \(h_{x}\) and \(h_{y}\) stands for the partial derivative with respect to \(x\) and \(y\). Defining the local Lorentzian frame by \(ds^2 = \eta_{\alpha \beta} \partial^{\alpha} \partial^{\beta}\), where \(\partial^{\alpha} = e^{\alpha}_{\mu} \partial^{\mu}\), one can write

\[
\partial^{\alpha} = dt, \quad \partial^0 = Adx + Bdy, \tag{A.2}
\]

\[
\partial^2 = Cdx + Ddy.
\]

Rewriting \(ds^2\) in terms of \(A, B, C\) and \(D\) we get

\[
A^2 + C^2 = 1 + h_{x}^2, \quad B^2 + D^2 = 1 + h_{y}^2, \quad AB + CD = h_{x}h_{y}. \tag{A.3}
\]

This system has many solutions but we will consider those which are \(x\) and \(y\) symmetric and assume \(B = C\). This is not sufficient to define a unique solution. Indeed, the system has four different possible solutions but, in the following, we will take

\[
A = \frac{h_{x}^2 + h_{y}^2}{h_{x}^2 + h_{y}^2}, \quad B = \frac{-h_{x}h_{y}}{h_{x}^2 + h_{y}^2}, \quad D = \frac{h_{x}^2}{h_{x}^2 + h_{y}^2} \tag{A.4}
\]

The nonvanishing matrix elements of the ‘vielbein’

\[
(e^{\mu}_{\alpha}) = \begin{pmatrix}
e^{0}_{0} & e^{0}_{1} & e^{0}_{2} \\
e^{1}_{0} & e^{1}_{1} & e^{1}_{2} \\
e^{2}_{0} & e^{2}_{1} & e^{2}_{2}
\end{pmatrix}
\]

are

\[
e^{0}_{0} = 1, \quad e^{1}_{0} = h_{x}^2 + h_{y}^2, \quad e^{2}_{0} = h_{y}, \quad e^{0}_{1} = -h_{x}, e^{1}_{1} = h_{x}^2 + h_{y}^2, \quad e^{2}_{1} = e^{2}_{2} = h_{x}. \tag{A.5}
\]

The nonvanishing spin connection components are

\[
a^{\alpha}_{\beta} = -a^{\alpha}_{\beta} = \left( -h_{x}h_{y} + h_{x}h_{y} \right) \tilde{\Omega}(x, y) \tag{A.6}
\]

where

\[
\tilde{\Omega}(x, y) = \frac{-1 + \sqrt{1 + h_{x}^2 + h_{y}^2}}{\left( h_{x}^2 + h_{y}^2 \right)^{\frac{1}{2}}}. \tag{A.7}
\]

Finally, the Dirac equation reads

\[
\left\{ i\gamma^{0} \partial_{0} + i\gamma^{1} \left( \partial_{1} + \frac{1}{2} a^{1}_{0} \right) \right\} \Psi = 0 \tag{A.8}
\]

\[
+ i\gamma^{2} \left( \partial_{2} + \frac{1}{2} a^{2}_{0} \right) \Psi = 0. \tag{A.9}
\]
with
\[
\Gamma^4 = \frac{1}{h_2^2 + h_2^2} \left\{ \frac{h_2^2 + \gamma_5^2}{\sqrt{1 + h_2^2 + h_2^2}} \right\} y^1 - h_2^2 \left\{ \frac{1 - \gamma_5^2}{\gamma_5^2} \right\} y^2 \tag{A.10}
\]
and \( \Gamma^2 \) being obtained from \( \Gamma^4 \) after interchanging \( x \leftrightarrow y \) and \( y^1 \leftrightarrow y^2 \). The Dirac equation (A.9) can be rewritten in the Hamiltonian form
\[
i \delta_0 \psi = H \psi \tag{A.11}
\]
where
\[
H = -i \hbar \Gamma^4 \left\{ \partial_x + \frac{1}{2} \omega \gamma^5 \right\} - i \hbar \Gamma^2 \left\{ \partial_x + \frac{1}{2} \omega \gamma^5 \right\} + \beta m
\tag{A.12}
\]
and \( \beta = \gamma^0 \).

**Appendix B. Sturm–Liouville equation: small and large curvature limits**

Let us discuss the small and large curvature limits where the Sturm–Liouville equation reduces to a well-know differential equation.

In the small curvature limit, i.e. for \( \eta = A \omega \ll 1 \), the second order differential equation (47) reduces to the Mathieu equation \[42\]
\[
d^2\psi \over dr^2 + (a - 2q \cos(2v)) \psi = 0
\tag{B.1}
\]
where
\[
a = \xi \left(1 + \eta^2 \right) \quad \text{and} \quad q = \frac{\eta^2}{4} (\xi - 1). \tag{B.2}
\]

Note that with such definitions \( q \) can take, in principle, any value. Using a different approach, the limit of the small curvature for a corrugated graphene sheet was also considered \[37\], where the authors reduced the problem to the solution of a Mathieu equation\[4\]. The small deformation limit was studied using a geometrical language in \[31\], where the authors built the corresponding Dirac equation but did not consider its general solution, as provided in our work.

The solutions of the Mathieu equation can be classified according to their parity. Using the notation of \[42\], the parity even corresponds to \( c_0(v, q) \) for \( r = 1, 2 \), and with \( a = a_0(q) \), while the parity odd are associated with \( s_0(v, q) \) for \( r = 1, 2 \), and with \( a = b_0(q) \). The relations \( a = a_0(q) \) and \( a = b_0(q) \) define the relation \( \xi = \xi(q) \) which can be rewritten in terms of the energy. The solutions \( c_0(v, q) \) and \( s_0(v, q) \) have period \( \pi \) for \( r \) even and \( 2\pi \) for \( r \) odd.

For small \( q \), it follows that the even parity solutions have a \( \xi \) spectrum given by
\[
\xi^{(\pm)} = 0 + O(\eta^2),
\]
\[
\xi^{(\pm)} = r^2 \left(1 - \frac{\eta^2}{2}\right) + O(\eta^4) \quad \text{for} \quad r \geq 1. \tag{B.3}
\]

On the other hand, the \( \xi \) spectrum for the odd parity solutions reads
\[
\xi^{(-)} = r^2 \left(1 - \frac{\eta^2}{2}\right) + O(\eta^4) \quad \text{for} \quad r \geq 1. \tag{B.4}
\]

Note that the spectra of the periodic solutions of the Mathieu equation reproduce exactly the results found in \[45\], where \( K/\omega \) takes the role of \( \sqrt{\xi} \).

For large deformations given by \( \eta = A \omega \gg 1 \), equation (47) reduces to a different Mathieu equation
\[
\frac{d^2\psi}{dr^2} + (a - 2q \cos(2v)) \psi = 0
\tag{B.5}
\]
where
\[
a = 2q = \frac{\xi^2}{2}. \tag{B.6}
\]

A similar analysis as for the small curvature limit but relying on the asymptotic series for \( a(q) \) give
\[
\xi \sim 1/\eta^2 \tag{B.7}
\]
for \( r \neq 0 \) with \( \xi \) vanishing if \( r = 0 \). As can be seen in figure 3, replacing \( K/\omega \) by \( \sqrt{\xi} \), the large \( \eta \) behavior is compatible with the prediction of (B.7).

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