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Anisotropic AC conductivity of strained graphene

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Abstract

The density of states and the AC conductivity of graphene under uniform strain are calculated using a new Dirac Hamiltonian that takes into account the main three ingredients that change the electronic properties of strained graphene: the real displacement of the Fermi energy, the reciprocal lattice strain and the changes in the overlap of atomic orbitals. Our simple analytical expressions for the density of states and the AC conductivity generalize previous expressions for uniaxial strain. The results suggest a way to measure the Grüneisen parameter β that appears in any calculation of strained graphene, as well as the emergence of a sort of Hall effect due to shear strain.

Keywords: strained graphene, density of states, AC conductivity

(Some figures may appear in colour only in the online journal)

1. Introduction

Graphene [1], a two-dimensional form of carbon, has attracted an enormous amount of attention from both experimental and theoretical studies to understand and take advantage of its remarkable properties [2, 3]. Among its most exotic properties, one can cite a linear band dispersion of charge carriers at the so-called Dirac points; hence in graphene the charge carriers behave as massless Dirac fermions [4]. This has suggested the possibility of studying phenomena originally predicted for relativistic particle physics in such a unique condensed-matter system.

The mechanical properties, strength and flexibility, of graphene are also unique. Graphene is the strongest material ever measured, with an effective Young's modulus of $\sim$1 TPa, and can reversibly withstand elastic deformations up to 25% [5]. This unusual interval of elastic response results in a peculiar interplay between its electronic and morphological properties, which has opened a new opportunity to explore the strain modifications of the electronic properties of graphene: strain engineering [6–8]. This concept has a successful history in strained silicon technology.

In the literature, the most popular approach to study the electronic implications of graphene lattice deformations is based on a combination of a tight-binding (TB) model of the electrons and linear elasticity theory [9–18].

Among the most investigated strain-induced implications, one of the most relevant is the opening of a gap at the Fermi level, due to its importance for the functionality of graphene-based logic devices. For uniaxial strain, which is the case usually considered, it has been shown that the strain-induced opening of a band gap depends critically on the direction of strain and requires values as large as 23% [9]. Nevertheless, it has been shown that a combination of shear and uniaxial strain can be used to open a gap for more easily accessible reversible deformations [10]. Needless to say, another strain implication is the anisotropy in the electron dynamics, which has been theoretical and experimentally established [15–19].

Unfortunately, it has been found that the usual approach to treat strain contains problems. The most important one is that the Fermi energy falls far from the unstrained Dirac point [16]. A new Dirac Hamiltonian has been proposed to solve this and other problems by taking into account the main three ingredients that change the electronic properties of strained graphene: the real displacement of the Fermi energy, the reciprocal lattice strain and the changes in the overlap of

atomic orbitals [16]. In several previous studies of the subject, the first ingredient was missing, while the second one has only very recently been found. It was called lattice corrections [12, 15], but later on it was explained as the image of strain in the reciprocal space [16]. As a result, many theoretical computations concerning experimental strain situations need to be revised. Here we provide the first application of this new Hamiltonian which enables us to generalize the alternating-current (AC) conductivity expression for strained graphene and, thereby, to propose possible applications.

In fact, numerous theoretical works and several experiments have been devoted to investigating the optical conductivity properties of graphene [20–35]. Gusynin *et al* [20] presented analytical expressions for the AC conductivity in unstrained graphene. Pellegrino *et al* [25] reported the uniaxial strain effects on the AC conductivity within the tight-binding approximation. Pereira *et al* [26] also studied the uniaxial strain effects on the AC conductivity, but within the Dirac-cone approximation. However, in the graphene literature an AC conductivity expression under uniform strain which can straightforwardly be used for comparison with experimental data is not available.

This work has several purposes. The first is to provide an accurate and general description of the AC conductivity using the new Dirac Hamiltonian [16]. Then we provide simple analytical expressions for the density of states and the AC conductivity which generalize some previous expressions for uniaxial strain [26].

As an example, we provide an experimental proposal to measure the Grüneisen parameter β, which is a vital quantity to perform calculations in strained graphene, as well as a kind of Hall effect due to strain.

The layout of this paper is as follows. In section 2 we present the Dirac-like model used for uniformly strained graphene. In section 3 we study the density of states of strained graphene, which is required in section 4 to study the conductivity using the Kubo formula. Finally, in section 4 the conclusions are given.

2. Strained graphene model

From a combination of a tight-binding description and linear elasticity theory, recently it has been reported that the low-energy Dirac Hamiltonian for electrons in graphene under uniform strain is given by [16]

$$H \simeq \hbar v_0 \boldsymbol{\sigma}\cdot(\bar{\boldsymbol{I}} - \beta\bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}})\cdot\boldsymbol{q}, \tag{1}$$

where v_0 is the Fermi velocity for the undeformed lattice, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the two Pauli matrices, $\bar{\boldsymbol{I}}$ is the 2×2 identity matrix, $\bar{\boldsymbol{\epsilon}}$ is the strain tensor, β is the Grüneisen parameter and $\boldsymbol{q}$ is the momentum measured relative to the $\boldsymbol{K}_{\rm D}$ Dirac point [9, 16, 19], which does not coincide with the $\boldsymbol{K}$ high-symmetry points of the strained Brillouin zone, as detailed in figure 1. To first order in strain the shift of the $\boldsymbol{K}_{\rm D}$ Dirac point can be written as [16]

$$\boldsymbol{K}_{\rm D} \simeq \boldsymbol{K} + \boldsymbol{A} \simeq (\bar{\boldsymbol{I}} + \bar{\boldsymbol{\epsilon}})^{-1}\cdot\boldsymbol{K}_0 + \boldsymbol{A}, \tag{2}$$

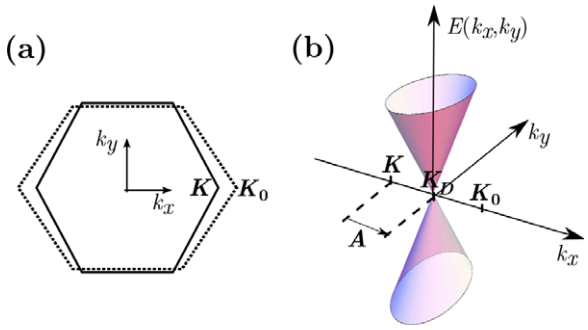

Figure 1. (a) $\boldsymbol{K}_0$ ($\boldsymbol{K}$) is a high-symmetry point of the first Brillouin zone, denoted by the dashed (solid) line, for unstrained (strained) graphene. The strained Brillouin zone corresponds to graphene stretched in the x direction. (b) Sketch of the strain-induced shift of the $\boldsymbol{K}_{\rm D}$ Dirac point and the distorted Dirac cone. The displacement of $\boldsymbol{K}_{\rm D}$ from $\boldsymbol{K}$ is given by the vector $\boldsymbol{A}$.

where $\boldsymbol{K}_0$ is a high-symmetry point of the unstrained Brillouin zone and $\boldsymbol{A}$ is related to the strain tensor $\bar{\boldsymbol{\epsilon}}$ by

$$A_x = \frac{\beta}{2a_0}(\bar{\epsilon}_{xx} - \bar{\epsilon}_{yy}), \qquad A_y = -\frac{\beta}{2a_0}(2\bar{\epsilon}_{xy}), \tag{3}$$

where a_0 is the unstrained carbon–carbon distance. Note that here the vector $\boldsymbol{A}$ is related to the Dirac-cone shift, whereas in the theory of the strain-induced pseudomagnetic field it is interpreted as a pseudovector potential [4]. The relevance of the strain-induced shift of the Dirac points, to obtain an effective Dirac-like Hamiltonian for strained graphene, has been noted earlier [9, 19]. In [19], one can find a detailed discussion about this shift and a closed expression of $\boldsymbol{K}_{\rm D}(t_n)$ as a function of the three nearest-neighbour hopping parameters $t_{1,2,3}$. However, the advantage of (2) lies in that $\boldsymbol{K}_{\rm D}$ is an explicit function of the strain tensor and thus enables us to obtain the Hamiltonian (1). The novelty of our model resides in its explicit dependence on the strain tensor, which is essential in order to achieve functionality for performing strain engineering.

Let us emphasize the three contributions appearing in (1): $\hbar v_0\boldsymbol{\sigma}\cdot\boldsymbol{q}$ is the low-energy Dirac Hamiltonian for unstrained graphene; the β-dependent term $-\hbar v_0\beta\boldsymbol{\sigma}\cdot\bar{\boldsymbol{\epsilon}}\cdot\boldsymbol{q}$ is associated with the strain-induced changes in hopping parameters; and the β-independent term $\hbar v_0\boldsymbol{\sigma}\cdot\bar{\boldsymbol{\epsilon}}\cdot\boldsymbol{q}$ is only a consequence of the reciprocal space distortion due to lattice deformation.

From (1) one can recognize a direction-dependent Fermi velocity, which can be written in tensorial notation as

$$\bar{\boldsymbol{v}} = v_0(\bar{\boldsymbol{I}} - \beta\bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}}). \tag{4}$$

To test (4), let us consider the seemingly trivial case of an isotropic strain $\bar{\boldsymbol{\epsilon}}_i = \epsilon\bar{\boldsymbol{I}}$. Under $\bar{\boldsymbol{\epsilon}}_i$, the new carbon–carbon distance is $a = a_0(1+\epsilon)$. On the other hand, the new hopping parameter to first order in strain is $t = t_0(1-\beta\epsilon)$. Therefore, the new Fermi velocity is

$$v = \frac{3ta}{2\hbar} \simeq \frac{3t_0a_0}{2\hbar}(1-\beta\epsilon+\epsilon) \simeq v_0(1-\beta\epsilon+\epsilon),$$

and in tensorial notation $\bar{\boldsymbol{v}} = v_0(\bar{\boldsymbol{I}} - \beta\bar{\boldsymbol{\epsilon}}_i + \bar{\boldsymbol{\epsilon}}_i)$, which can be directly obtained from the generalized expression (4).

Since the Fermi velocity, the most important parameter in graphene physics, is changed by the strain, one would expect changes in the conductivity.

3. Density of states

Another ingredient that influences the conductivity is the density of states (DOS). Furthermore, the DOS is accessible through scanning tunnelling microscopy experiments and thus can serve to test the new Dirac Hamiltonian (1).

In general, the DOS can be computed from the Green's function defined as

$$G^{\pm}(E) = \lim_{\eta\to 0} \frac{1}{E \pm i\eta - H} \tag{5}$$

by taking the imaginary part of its trace,

$$D(E) = \mp\frac{1}{\pi}\mathrm{Im}\{\mathrm{Tr}G^{\pm}(E)\}. \tag{6}$$

However, using the previous formula and a representation of $G^{\pm}(E)$ in momentum space, the local density of states (LDOS) can be calculated as

$$\rho(E) = \iint \mathrm{Tr}[E - H(q_x, q_y)]^{-1}\mathrm{d}q_x\mathrm{d}q_y, \tag{7}$$

where $H(q_x, q_y)$ is the Hamiltonian (1). The DOS and the LDOS are related by $D(E) = A\rho(E)$, where A is the area of the strained sample. The computation of (7) is straightforward if one proposes the change of integration variables

$$\boldsymbol{q} = (\bar{\boldsymbol{I}} - \beta\bar{\boldsymbol{\epsilon}} + \bar{\boldsymbol{\epsilon}})^{-1} \cdot \boldsymbol{q}^*. \tag{8}$$

This transformation yields

$$\rho(E) = \iint J\mathrm{Tr}[E - H_0(q_x^*, q_y^*)]^{-1}\mathrm{d}q_x^*\mathrm{d}q_y^*, \tag{9}$$

where J is the Jacobian determinant of (8) and $H_0(q_x^*, q_y^*) = \hbar v_0 \boldsymbol{\sigma}\cdot\boldsymbol{q}^*$ is the unstrained Hamiltonian. It can be proved that the Jacobian determinant is given as $J = 1/\det(\bar{\boldsymbol{v}}/v_0)$. Then, for the LDOS it immediately follows that

$$\rho(E) = \rho_0(E)/\det(\bar{\boldsymbol{v}}/v_0), \tag{10}$$

where $\rho_0(E)$ is the LDOS for unstrained graphene and reads $\rho_0(E) = 2|E|/(\pi\hbar^2 v_0^2)$. Finally, up to first order in strain, the LDOS gives

$$\rho(E) \simeq \rho_0(E)(1 + \beta\mathrm{Tr}\bar{\boldsymbol{\epsilon}} - \mathrm{Tr}\bar{\boldsymbol{\epsilon}}), \tag{11}$$

which is a generalized expression available for any uniform strain, and not only for uniaxial strain, as in previous works [26]. Note that A can be written as $A \simeq A_0(1 + \mathrm{Tr}\bar{\boldsymbol{\epsilon}})$, A_0 being the area of the unstrained sample. Therefore, the DOS is given by

$$D(E) = A\rho(E) \simeq D_0(E)(1 + \beta\mathrm{Tr}\bar{\boldsymbol{\epsilon}}), \tag{12}$$

where $D_0(E) = A_0\rho_0(E)$ is the DOS of the unstrained sample of graphene.

Since $\beta - 1 > 0$, the strain effect in the LDOS (DOS) depends on the sign of $\mathrm{Tr}\bar{\boldsymbol{\epsilon}}$, which can be written as $\mathrm{Tr}\bar{\boldsymbol{\epsilon}} = A/A_0 - 1$. Thus, for an expanded sample $(A/A_0 > 1)$ the strain effect in the LDOS (DOS) is a slope enhancement, whereas for $(A/A_0 < 1)$ the effect is a decrease of slope. It is also worth mentioning that for the case of shear strain, i.e. $\bar{\epsilon}_{xx} = \bar{\epsilon}_{yy} = 0$ and $\bar{\epsilon}_{xy} = \bar{\epsilon}_{yx} = \epsilon$, the LDOS (DOS) does not change.

4. AC conductivity of strained graphene

Let us now obtain the AC conductivity $\bar{\boldsymbol{\sigma}}(w)$ of graphene under uniform strain by combining (1) and the Kubo formula, assuming a linear response to an external electric field with frequency w. Following the representation used in [22, 23], the frequency-dependent conductivity tensor $\bar{\boldsymbol{\sigma}}(w)$ can be written as a double integral with respect to two energies E, E',

$$\bar{\sigma}_{ij}(w) = \frac{i}{\hbar}\iint \mathrm{Tr}\{j_i\delta(H - E')j_j\delta(H - E)\} \times \frac{1}{E - E' + w - i\alpha}\frac{f(E) - f(E')}{E - E'}\mathrm{d}E\mathrm{d}E', \tag{13}$$

where $f(E) = (1 + \exp[E/(k_B T)])^{-1}$ is the Fermi function at temperature T and $j_l = -ie[H, r_l]$ is the velocity operator in the l-direction, with $l = x, y$.

To calculate (13) it is convenient once again to use the change of integration variables (8). In the new variables (q_x^*, q_y^*), the Hamiltonian transforms as $H = H_0(q_x^*, q_y^*)$ and the velocity operator components are obtained using the chain rule,

$$\begin{aligned} j_x &= -ie[H, r_x] = e\frac{\partial H}{\partial q_x}, \\ &= e\left(\frac{\partial H}{\partial q_x^*}\frac{\partial q_x^*}{\partial q_x} + \frac{\partial H}{\partial q_y^*}\frac{\partial q_y^*}{\partial q_x}\right), \\ &= (1 - \tilde{\beta}\epsilon_{xx})j_x^* - \tilde{\beta}\epsilon_{xy}j_y^*, \end{aligned} \tag{14}$$

and

$$j_y = (1 - \tilde{\beta}\epsilon_{yy})j_y^* - \tilde{\beta}\epsilon_{xy}j_x^*, \tag{15}$$

where $j_x^* = e(\partial H/\partial q_x^*)$ and $j_y^* = e(\partial H/\partial q_y^*)$ are the current operator components for unstrained graphene and $\tilde{\beta} = \beta - 1$. Plugging these expressions into (13) and calculating up to first order in strain, we obtain

$$\bar{\sigma}_{xx}(w) \simeq (1 - 2\tilde{\beta}\bar{\epsilon}_{xx})\sigma_0(w), \tag{16}$$

$$\bar{\sigma}_{yy}(w) \simeq (1 - 2\tilde{\beta}\bar{\epsilon}_{yy})\sigma_0(w), \tag{17}$$

$$\bar{\sigma}_{xy}(w) = \bar{\sigma}_{yx}(w) \simeq -2\tilde{\beta}\bar{\epsilon}_{xy}\sigma_0(w), \tag{18}$$

with

$$\sigma_0(w) = \frac{i}{\hbar}\iint \mathrm{Tr}\{j_i^*\delta(H_0 - E')j_i^*\delta(H_0 - E)\} \times \frac{1}{E - E' + w - i\alpha}\frac{f(E) - f(E')}{E - E'}\mathrm{d}E\mathrm{d}E'. \tag{19}$$

Note that the frequency-dependent conductivity tensor of unstrained graphene $\bar{\boldsymbol{\sigma}}_0(w)$ is given by $\bar{\boldsymbol{\sigma}}_0(w) = \sigma_0(w)\bar{\boldsymbol{I}}$, as has been calculated in [20–23]. Finally, from (16)–(19) it follows that the frequency-dependent conductivity tensor of graphene under uniform strain can be written as

$$\bar{\boldsymbol{\sigma}}(w) \simeq \sigma_0(w)(\bar{\boldsymbol{I}} - 2\beta\bar{\boldsymbol{\epsilon}} + 2\bar{\boldsymbol{\epsilon}}). \tag{20}$$

Our expression (20) generalizes the reported AC conductivity in [26] for the case of a uniaxial strain and allows us to make a quick evaluation of the AC conductivity of graphene under any uniform strain configuration. However, due to the approximations considered one may wonder how dependable

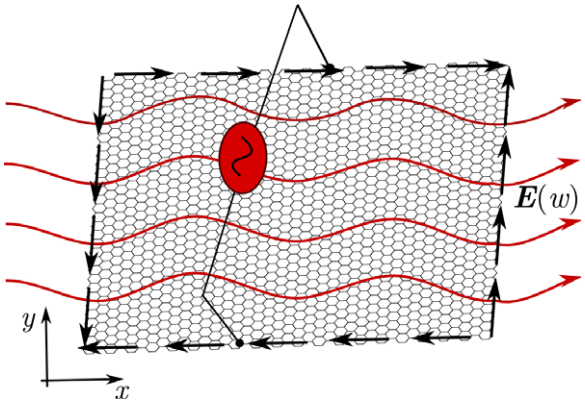

Figure 2. Sketch of the observation of Hall voltage in a rectangular graphene sample under shear strain and an oscillating electric field $\boldsymbol{E}(w)$ in the x direction (curved red lines). The black arrows at the sample boundaries represent the force field that leads to the shear deformation. The Hall voltage is measured in the y direction.

our linear corrections in (20) are. Pereira *et al* [26] showed from *ab initio* calculation for uniaxially strained graphene that $\bar{\boldsymbol{\sigma}}(w)$ linearly depends on strain up to at least 10%, which is a broad range of stretching where the linear corrections are quite dependable. Very recently, the transmittance of graphene under uniaxial strain has been measured [36]. The observed modulation of the transmittance with respect to the polarization direction of the incoming light was quantitatively explained using expressions for the anisotropic AC conductivity of strained graphene obtained in [26]. Thus, as (20) reproduces the results of [26], these experiments confirm the validity of the predictions from our equation (20).

Unlike the DOS, the AC conductivity is modified for shear strain. From (20), a sort of Hall effect is predicted due to shear strain, as sketched in figure 2, since a component $\sigma_{xy}(w)$ appears whenever $\epsilon_{xy} \neq 0$. This result is novel because a strain-induced Hall effect in graphene has been only discussed in nonuniform strain configurations.

Moreover, a possible application follows from (20). If the conductivity can be measured with precision for different strain configurations one can obtain by means of (20) an experimental value of the Grüneisen parameter β. For example, if the conductivity σ_{xx} of a graphene sample is measured for uniaxial strains in the x direction of 1%, 2%, 3%,..., the scope of the lineal graph of σ_{xx} versus strain is $-2(\beta - 1)$. Knowledge of β is vital for the characterization of the strain-induced effects on the electronic band structure.

5. Conclusions

In conclusion, using the Kubo formula and a new Dirac Hamiltonian that takes into account the real strain-induced displacement of the Fermi energy, we have derived the AC conductivity for graphene under uniform strain. As an example, the corresponding expression gives a way to measure the Grüneisen parameter β that appears in any calculation of strained graphene. Also, we have reported a generalized expression for the density of states, which does not change for shear strain. However, under shear strain we have reported a sort of Hall effect which had not been discussed for uniform strain.

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