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Bending and flexural phonon scattering: Generalized Dirac equation for an electron moving in curved graphene

Q1 Richard Kerner [a,*], Gerardo G. Naumis [b], Wilfrido A. Gómez-Arias [b]

[a] LPTMC, Université Pierre et Marie Curie – CNRS UMR 7600, Tour 23, 5-ème étage, Boite 121, 4 Place Jussieu, 75005 Paris, France
[b] Depto. de Física-Química, Instituto de Física, Universidad Nacional Autónoma de México (UNAM). Apdo. Postal 20-364, 01000 México D.F., Mexico

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ABSTRACT

A generalized Dirac equation is derived in order to describe charge carriers moving in curved graphene, which is the case for temperatures above 10 K due to the presence of flexural phonons, or in bent graphene. Such interaction is taken into account by considering an induced metric, in the same spirit as the general relativity approach for the description of fermionic particle moving in a curved space-time. The resulting equation allows to include in a natural way the presence of other phonon branches as well as an external electromagnetic field. For a monochromatic sinusoidal bending of the graphene, the problem can be recasted as a Mathieu equation with a complex driven parameter, indicating the possibility of a resonance pattern.

1. Introduction

Graphene is a new material that has been attracting a lot of attention since its experimental discovery [1]. This carbon allotrope has unique transport properties [2,3], like a high electronic mobility [4] and thermal conductivity [5], which are believed to be important for future applications in nano-devices [6,7]. However, there are certain discrepancies in the values of the electronic mobilities depending on whether the samples are suspended or in a substrate [8,9]. At low temperatures, impurity scattering can be responsible for this effect, which eventually leads to a metal–insulator transition since the mobility edge appears near the Fermi energy [10], as has been confirmed in graphene doped with H [11]. However, above $T > 10$ K such discrepancies are believed to be a consequence of the crucial role of the graphene's surface vibrations (known as flexural phonons [12]) in the electron scattering, as has been shown very recently by applying tension to graphene sheets [9]. From a microscopic point of view, the scattering results from changes in the distances between atoms, leading to fluctuations of π-orbitals electron wavefunctions overlaps [13]. Furthermore, since graphene can be curved by applying strain and stress, it has been proposed to do "strain engineering" in order to tailor the electronic properties [14]. Long-wavelength strains in graphene induce a pseudomagnetic gauge field which can modify electron propagation [15].

On the other hand, the behavior of charge carriers in graphene can be adequately described by the two-dimensional Dirac equation, as has been firmly established by Hall effect measurements [4,16,12]. It enables to evaluate the interaction between charge carriers and phonons via minimal coupling with a pseudopotential [12]. However, as long as the description of the graphene sheet remains strictly two-dimensional, the so-called *flexural modes* and *strain*, resulting from the transversal deformations, cannot be taken into account in a natural geometrical manner. This is why we propose to use the known formalism of covariant calculus in order to adapt the Dirac equation to the curved surface.

Our argument is as follows:

Since charge carriers in flat graphene are described by massless Dirac fermions [4,16], it is natural to ask if it is possible to modify the Dirac equation taking into account the flexural mode interaction. Two paths can be followed in order to answer this question. One is to start from the usual tight-binding approach and use Taylor expansion of the overlap integral on the displacement field [12,13,17]. Here we present an alternative point of view, in which the interaction is included by making the observation that a graphene membrane can be considered as a curved space. The effective equation must be covariant due to simple and general physical arguments. The desired equation can be considered as the Dirac equation in curved space-time, as in general

Q2 * Corresponding author.
E-mail address: richard.kerner@upmc.jussieu.fr (R. Kerner).

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relativity. Also, since the planar vibrational modes are described by a vectorial potential [12,13,17], our approach allows to describe all phonon branches and the electromagnetic potential in a single equation. Notice that in fact, the problem of the two-dimensional Dirac equation including a vectorial potential has been solved recently [18,19]. As we shall show in the conclusion, the present approach has certain advantages over the Taylor expansion of the tight-binding parameters.

To finish this introduction, let us briefly sketch the ideas behind the present approach. For graphene at low temperatures, its surface can be considered as flat. The corresponding unperturbed Hamiltonian operator used to describe charges evolving on the graphene sheet can be written as an effective Dirac equation [4,16]:

$$i\hbar\frac{\partial}{\partial t}\Psi=\hat{H}\Psi \quad \text{with } \hat{H}=-i\hbar v_F[\gamma^x\nabla_x+\gamma^y\nabla_y], \tag{1}$$

where v_F is the *Fermi velocity*, with

$$\gamma^x=\sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \gamma^y=\sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}. \tag{2}$$

Note that at this stage there is no difference between covariant and contravariant indices, because we have

$$\gamma^i\gamma^j+\gamma^j\gamma^i=\sigma_i\sigma_j+\sigma_j\sigma_i=2g_{ij}\mathbf{1},\quad (i,j=x,y) \tag{3}$$

with $g_{ij}=\delta_{ij}$, so that obviously the contravariant metric raising the indices is also $g^{ij}=\delta^{ij}$. But this is no more true when the underlying two-dimensional space is not flat, but corrugated, with a non-trivially deformed metric, as the case is for graphene at $T\gg 10$ K. This is why the Dirac equation in two dimensions should be now generalized in order to incorporate the fact that the metric on the surface of constraint is no more flat, but curved. Luckily enough, the problem of covariant formulation of Dirac's equation in a curved space has been quite deeply investigated since a long time ago [20,21], so that we can follow the same steps in this particular case: introduce the non-Euclidean two-dimensional metric on the graphene sheet, then adapt the Clifford algebra and find the Christoffel connection, and finally assemble all these in the covariant version of Dirac's equation:

$$\hat{\tilde{H}}\Psi\sim[\tilde{\gamma}^x\tilde{\nabla}_x+\tilde{\gamma}^y\tilde{\nabla}_y]\Psi. \tag{4}$$

Here not only the contravariant metric is deformed, but also the γ-matrices should be modified in order to satisfy new anti-commutation relations with the induced metric instead of the flat one as before; finally, $\tilde{\nabla}_j$ contains not only the electromagnetic and on plane phonon interaction visualized by the vector potential included in the usual gauge-invariant way, but also the Christoffel symbols of the metric $\tilde{g}_{ij}$:

$$\tilde{\nabla}_j\Psi=(\partial_j-eA_j)\Psi+\tilde{\Gamma}^m_{jk}\tilde{g}^{ki}\tilde{\Sigma}_{mi}\Psi, \tag{5}$$

where the Christoffel symbols $\tilde{\Gamma}^m_{jk}$ are defined as usual, by means of the modified metric:

$$\tilde{\Gamma}^i_{jk}=\tfrac{1}{2}\tilde{g}^{im}[\partial_j\tilde{g}_{mk}+\partial_k\tilde{g}_{jm}-\partial_m\tilde{g}_{jk}] \tag{6}$$

and $\tilde{\Sigma}_{mk}$ is the matrix-valued anti-symmetric tensor defined by means of the modified gamma-matrices:

$$\tilde{\Sigma}_{mk}=\tfrac{1}{8}[\tilde{\gamma}_m\tilde{\gamma}_k-\tilde{\gamma}_k\tilde{\gamma}_m]. \tag{7}$$

This term is often called "spinorial connection" [20,21]. The result of the calculations, up to the second-order terms in powers of deformation $\partial_i f$, is as follows:

$$\begin{aligned}\hat{\tilde{H}}\sim{}&\hat{H}_0+\sigma_z(\overrightarrow{\text{grad}}\, f)\cdot(\vec{\nabla})-(\overrightarrow{\text{grad}}\, f\cdot\vec{\sigma})(\overrightarrow{\text{grad}}\, f\cdot\vec{\nabla})\\ &+\tfrac{1}{8}\vec{\sigma}\cdot\overrightarrow{\text{grad}}[(\partial_x f)^2+(\partial_y f)^2]-\tfrac{1}{4}[\vec{\sigma}\cdot\overrightarrow{\text{grad}}\, f]\Delta f.\end{aligned} \tag{8}$$

The full derivation of this equation is given in the Appendix; here we can start to investigate the solutions describing a charged carrier's behavior on the deformed graphene sheet, interacting with flexural phonons.

A similar approach has been proposed in Ref. [22], where a non-holonomous fielbein was used in order to take into account the non-Euclidean metric of the deformed graphene sheet. The problem addressed in their paper is static, and the curved-space effect is computed in a particular case of a symmetric Gaussian bump. The use of the non-holonomous local frame leads to extra terms in the connection coefficients akin to torsion which are absent in our case because we use holonomous frame based on local coordinate system. The covariant form of Dirac's operator we give is more general because it is valid in any local coordinates and enables us to describe the curvature effects of time-dependent deformations propagating on the graphene sheet.

Except for this difference, both forms of the covariant generalization of Dirac's equation are based on the same universal formulae defining the spin connection which can be found in standard monographs, in particular in Ref. [20].

2. The generalized Dirac equation on corrugated graphene

To show how Eq. (74) is used, we consider that the displacement field can be written using a simple set of basis functions provided by standing waves [23],

$$\begin{aligned}\vec{u}=\frac{2}{\sqrt{N}}\sum_{\mu,\mathbf{q}>0}\vec{e}_{\,\mu}(\vec{q})[Q^{(c)}_{\mu,\vec{q}}\cos(\vec{q}\cdot\vec{R}-\omega_\mu(\vec{q})t)\\ +Q^{(s)}_{\mu,\vec{q}}\sin(\vec{q}\cdot\vec{R}-\omega_\mu(\vec{q})t)],\end{aligned} \tag{9}$$

where $\mathbf{e}_\mu(\mathbf{q})$ is the polarization vector for a wave-vector $\vec{q}$, μ is the phononic branch, $\omega_\mu(\vec{q})$ the dispersion relationship and $\vec{R}=(x,y)$ is the position. Notice that the notation $\mathbf{q}>0$ indicates that $q_x>0$ and $q_y>0$. $Q^{(c)}_{\mu,\vec{q}}$ and $Q^{(s)}_{\mu,\vec{q}}$ are operators given in terms of the creation (annihilation) phonon operators [23] $a_{\mu,\vec{q}}$ ($a^\dagger_{\mu,\vec{q}}$),

$$Q^{(\alpha)}_{\mu,\vec{q}}=\frac{1}{\sqrt{2M\omega_\mu(\vec{q})}}\left(a^{(\alpha)}_{\mu,\vec{q}}+a^{(\alpha)\dagger}_{\mu,\vec{q}}\right), \tag{10}$$

where α runs over c and s and M is the carbon atom's mass.

Thus, for flexural phonons the function $f(x,y,t)$ is given by

$$f(x,y,t)=\frac{2}{\sqrt{N}}\sum_{\mathbf{q}>0}\left[Q^{(c)}_{F,\vec{q}}\cos\phi_{\mathbf{q}}+Q^{(s)}_{F,\vec{q}}\sin\phi_{\mathbf{q}}\right], \tag{11}$$

where $\mu=F$ means that we are dealing with flexural phonons, and the phase $\phi_{\mathbf{q}}$ is defined as $\phi_{\mathbf{q}}=\vec{q}\cdot\vec{R}-\omega_\mu(\vec{q})t$. For the flexural branch, $\omega_F(\vec{q})=\alpha_F\|\vec{q}\|^2$ where $\alpha_F\approx 4.6\times 10^{-7}$ m^2/s. Notice that $Q^{(c)}_{F,\vec{q}}$ and $Q^{(s)}_{F,\vec{q}}$ have length units, so $f(x,y,t)$ has the same units, while $\partial_x f$ and $\partial_y f$ are dimensionless.

The generalized Dirac equation only needs as input the partial derivatives of $f(x,y,t)$,

$$\partial_x f=\frac{2}{\sqrt{N}}\sum_{\mathbf{q}>0}q_x\left[Q^{(c)}_{F,\vec{q}}\cos\phi_{\mathbf{q}}+Q^{(s)}_{F,\vec{q}}\sin\phi_{\mathbf{q}}\right], \tag{12}$$

$$\partial_y f=\frac{2}{\sqrt{N}}\sum_{\mathbf{q}>0}q_y\left[Q^{(c)}_{F,\vec{q}}\cos\phi_{\mathbf{q}}+Q^{(s)}_{F,\vec{q}}\sin\phi_{\mathbf{q}}\right]. \tag{13}$$

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For example, if we keep only the linear correction in Eq. (74), the Hamiltonian reads as follows:

$$\tilde{\hat{H}} = v_F \begin{pmatrix} 0 & \hat{\pi}_x - i\hat{\pi}_y \\ \hat{\pi}_x + i\hat{\pi}_y & 0 \end{pmatrix} + \frac{2v_F}{\sqrt{N}} \sum_{\mathbf{q}>0} \left[Q^{(c)}_{F,\vec{q}} \cos\phi_{\mathbf{q}} + Q^{(s)}_{F,\vec{q}} \sin\phi_{\mathbf{q}} \right] \times \begin{pmatrix} q_x\hat{\pi}_x + q_y\hat{\pi}_y & 0 \\ 0 & -q_x\hat{\pi}_x - q_y\hat{\pi}_y \end{pmatrix}. \quad (14)$$

Using the fact that the Fermi velocity is much higher than the flexural modes' speeds, we can drop the time dependence and apply perturbation theory to solve the equation. To understand the nature of the solutions, in the following section we will consider the case of a pure monochromatic wave which is equivalent to a sinusoidal bend of the surface.

3. Approximate solutions

Choosing the deformation function representing simple monochromatic plane wave proportional to

$$f(x,y) = a\cos(\mathbf{q}\cdot\mathbf{r})$$

with a representing the amplitude of the flexural wave or bending, and inserting it in the first order version of the covariant two-dimensional curved Dirac equation, we get the following differential system:

$$(\pi_x - i\pi_y)\psi_B + a\cos\Phi_{\mathbf{q}}(q_x\pi_x + q_y\pi_y)\psi_A = (i\hbar/v_F)\partial_t\psi_A,$$

$$(\pi_x + i\pi_y)\psi_A + a\cos\Phi_{\mathbf{q}}(-q_x\pi_x - q_y\pi_y)\psi_B = (i\hbar/v_F)\partial_t\psi_B. \quad (15)$$

In the particular case of no time dependence in $f(x,y,t)$, the spatial and temporal evolution can be separated. The temporal part of the wave function has the form $\exp(-i\omega t)$, where ω is a frequency. Then, being left with the spatial part of the deformation function only, $a\cos(\mathbf{q}\cdot\mathbf{r})$, and choosing $\mathbf{q} = [q,0]$, we get, after dividing by $-i\hbar$:

$$(\partial_x - i\partial_y)\psi_B + a\cos(qx)q\partial_x\psi_A = E\psi_A,$$

$$(\partial_x + i\partial_y)\psi_A - a\cos(qx)q\partial_x\psi_B = E\psi_B, \quad (16)$$

where the parameter E is defined as $E \equiv i\hbar\omega/\hbar v_F \equiv i\epsilon/(\hbar v_F)$ where ϵ is the energy, and now ψ_A and ψ_B denote only the spatial part of the wavefunction. In order to separate the variables, let us suppose that the stationary solution is of the form

$$\psi_A(x,y) = \mathcal{F}(y)\Phi_A(x), \quad \psi_B(x,y) = \mathcal{F}(y)\Phi_B(x).$$

Then Eqs. (16) take on the form:

$$\mathcal{F}(y)\Phi_B{}'(x) - i\mathcal{F}'(y)\Phi_B(x) + aq\mathcal{F}(y)\cos(qx)\Phi_A{}' = E\mathcal{F}(y)\Phi_A$$

and similarly for Φ_A,

$$\mathcal{F}(y)\Phi_A{}'(x) + i\mathcal{F}'(y)\Phi_A(x) - aq\mathcal{F}(y)\cos(qx)\Phi_B{}' = E\mathcal{F}(y)\Phi_B.$$

After dividing by $\mathcal{F}(y)$, we see that the variables will separate easily if we set

$$\frac{\mathcal{F}'}{\mathcal{F}} = \text{Const.},$$

which means that $\mathcal{F}(y)$ is an exponential function with real or pure imaginary exponent, depending on the sign of the constant. We choose the negative sign in order to ensure the bounded character of the function $\mathcal{F}(y)$ and to recover the case of flat graphene in the appropriate limit; this leads to the following ansatz:

$$\psi_A(x,y) = e^{iK_y y}\Phi_A(x), \quad \psi_B^{\pm} = e^{\pm iK_y y}\Phi_B^{\pm}(x). \quad (17)$$

The function $\psi_B^{\pm}$ has two signs because in principle, ψ_A and ψ_B are the components of a spinor, and we need to build two solutions, one with energy E and the other $-E$. For the case of flat graphene, it is known that one can pass from one solution to the other by changing the sign of one component. These two solutions are necessary to represent electrons and holes. Here we will concentrate in electrons, although the solution for holes can be found in a similar way. For that reason, in what follows we will search the solution for ψ_B^+, dropping the sign for simplicity. Inserting the ansatz (17) into Eq. (16) we get

$$[\partial_x - i(iK_y)]\Phi_B(x) + qa\cos(qx)\partial_x\Phi_A(x) = E\Phi_A(x),$$

$$[\partial_x + i(iK_y)]\Phi_A(x) - qa\cos(qx)\partial_x\Phi_B(x) = E\Phi_B(x),$$

which amounts to

$$[\partial_x + K_y]\Phi_B(x) + qa\cos(qx)\partial_x\Phi_A(x) = E\Phi_A(x),$$

$$[\partial_x - K_y]\Phi_A(x) - qa\cos(qx)\partial_x\Phi_B(x) = E\Phi_B(x).$$

This system of equations being linear, we can compose the general solution summing over partial solutions with given K_y, i.e. using the Fourier development. In order to have an elementary insight in solutions' properties, let us consider first the zero mode corresponding to an incident current in the x direction, letting $K_y = 0$. For other modes (with $K_y \neq 0$) the diagonalization is not straightforward and can be achieved only by successive approximations. In this paper we only consider the case $K_y = 0$, which is the most relevant concerning a typical conductivity experiment. But with the basic zero mode the diagonalization of the system (16) is particularly easy, because it takes on the simplified form:

$$\partial_x\Phi_B(x) + qa\cos(qx)\partial_x\Phi_A(x) = E\Phi_A(x),$$

$$\partial_x\Phi_A(x) - qa\cos(qx)\partial_x\Phi_B(x) = E\Phi_B(x). \quad (18)$$

This system is diagonalized by derivation of one of its parts with respect to x and subsequent substitution of the first derivative from the second equation. The resulting ordinary second-order differential equation is common for both components Φ_A and Φ_B:

$$(1 + a^2q^2\cos^2(qx))\frac{d^2\Phi_A}{dx^2} - 2a^2q^3\sin(qx)\cos(qx)\frac{d\Phi_A}{dx} = E(E - aq^2\sin(qx))\Phi_A \quad (19)$$

or, in a more standard form,

$$\frac{d^2\Phi_A}{dx^2} - \frac{a^2q^3\sin(2qx)}{(1 + a^2q^2\cos^2(qx))}\frac{d\Phi_A}{dx} - \frac{E(E - aq^2\sin(qx))}{(1 + a^2q^2\cos^2(qx))}\Phi_A = 0 \quad (20)$$

and the same equation for Φ_B, but with $+$ sign before the second term. Let us introduce a new parameter

$$\eta = aq^2,$$

which will turn out to be useful while considering various physical energy limits. We can rewrite the two equations now:

$$\frac{d^2\Phi_A}{dx^2} - \frac{qa\eta\sin(2qx)}{(1 + a\eta\cos^2(qx))}\frac{d\Phi_A}{dx} - \frac{E(E - \eta\sin(qx))}{(1 + a\eta\cos^2(qx))}\Phi_A = 0, \quad (21)$$

$$\frac{d^2\Phi_B}{dx^2} - \frac{qa\eta\sin(2qx)}{(1 + a\eta\cos^2(qx))}\frac{d\Phi_B}{dx} - \frac{E(E + \eta\sin(qx))}{(1 + a\eta\cos^2(qx))}\Phi_B = 0. \quad (22)$$

Now we remind that in our notation, the parameter E has become purely imaginary:

$$E = i\frac{\hbar\omega}{\hbar v_F} \equiv i\frac{\epsilon}{\hbar v_F}, \quad (23)$$

where ϵ is the energy deviation from the Dirac cone energy (ϵ_D), i.e. the total electron energy is $\epsilon_{Total} = \epsilon_D + \epsilon$. These observations are important to keep in mind in order to understand the nature of solutions in what follows.

Eq. (20) is of the standard form

$$y'' + P(x)y' + Q(x)y = 0. \quad (24)$$

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The well-known ansatz

$$y(x) = Z(x)e^{-1/2\int P(x)\,dx}$$

reduces the equation for $Z(x)$ to the even simpler form:

$$Z'' + C(x)Z = 0, \tag{25}$$

where

$$C(x) = Q(x) - \tfrac{1}{2}P'(x) - \tfrac{1}{4}P^2(x). \tag{26}$$

In order to have an insight concerning the properties of solutions, let us treat first the case of weak amplitudes, when the bending of the graphene sheet is small enough so that we can neglect its powers higher than two; we assume therefore that

$$a\eta \ll 1.$$

Assuming that the energy E is of the same order as $a\eta$ (since near the Dirac cone $\epsilon \ll 1$), we get the simplified linearized version of our equations:

$$\frac{d^2\Phi_A}{dx^2} - qa\eta\,\sin(2qx)\frac{d\Phi_A}{dx} - E(E - \eta\,\sin(qx))\Phi_A = 0. \tag{27}$$

Now we have

$$P(x) = -qa\eta\,\sin(2qx), \quad Q(x) = -E(E - \eta\,\sin(qx))$$

and

$$\int P(x)\,dx = -qa\eta \int \sin(2qx)\,dx = \frac{a\eta}{2}\cos(2qx) \tag{28}$$

so that

$$\Phi_A(x) = Z(x)e^{-a\eta/4\,\cos(2qx)}. \tag{29}$$

The function $Z(x)$ satisfies the following ordinary linear differential equation:

$$Z'' + \left[E\eta\,\sin(qx) - E^2 - \eta^2\,\cos(2qx) - \frac{a\eta^3}{4}\,\sin(2qx)\right]Z = 0 \tag{30}$$

and inserting the expression (23), we get

$$Z'' + \left[\left(\frac{\epsilon}{\hbar v_F}\right)^2 + \frac{i\epsilon}{\hbar v_F}\eta\,\sin(qx) - \eta^2\,\cos(2qx) - \frac{a\eta^3}{4}\,\sin(2qx)\right]Z = 0. \tag{31}$$

One easily checks that in the limit of planar geometry, when there is no deformation, i.e. $f=0$ because $a=0$ and consequently, the parameter $\eta = 0$ vanishes, too, one gets the harmonic oscillator equation for Z:

$$Z'' + \left(\frac{\epsilon}{\hbar v_F}\right)^2 Z = 0$$

and the carrier's space wave function represents a monochromatic wave propagating in the x-direction,

$$\Phi_A = e^{i(\omega t - (\epsilon/\hbar v_F)x)} = e^{i(\omega t - K_x x)},$$

where we have put

$$K_x = \frac{\epsilon}{\hbar v_F},$$

which has the right physical dimension, cm^{-1}. We can write now, neglecting the cubic term containing η^3, the following approximate equation for $Z(x)$:

$$Z'' + [K_x^2 + iK_x\eta\,\sin(qx) - \eta^2\,\cos(2qx)]Z = 0. \tag{32}$$

Two limits that are of particular interest can be treated separately and lead to well-known equations:

(a) When $K_x \ll \eta$, corresponding to electrons between the Dirac energy and effective energy $a\eta$ (it is worthwhile to remember that near the Dirac point, K_x is nearly zero since it measures the deviation from the momentum $\mathbf{K}_D$ at each Dirac cone [12], thus the complete momentum is $\hbar\,\mathbf{K}_{Total} \equiv \hbar(\mathbf{K}_D + \mathbf{K})$). Then Eq. (32) reduces to

$$Z'' - \eta^2\,\cos(2qx)Z = 0, \tag{33}$$

which is unstable by nature, because there is no constant term looking like fundamental frequency in a Mathieu's equation; here the oscillating term changes sign and the solution for Z cannot be kept bounded. This means that the electrons whose energy is too low ($K_x < \eta$) are unable to propagate in the graphene sheet. Notice that the inclusion of the linear term on η leads basically to the same kind of unbounded solution.

(b) When $K_x \gg \eta$, corresponding to high energies (over the Fermi energy, $K_x \gg K_F$, the equation for Z becomes

$$Z'' + K_x^2\left[1 + i\left(\frac{\eta}{K_x}\right)\sin(qx)\right]Z = 0. \tag{34}$$

This equation has the form of a Mathieu equation with a complex driven parameter, which appears for example in the eddy currents problem in an elliptic solenoid [24]. Defining a new variable $\tilde{x}$ such that

$$qx = 2\tilde{x} + (\pi/2). \tag{35}$$

Eq. (34) can be rewritten as

$$Z'' + [A + i2s\,\cos(2\tilde{x})]Z = 0, \tag{36}$$

where the parameters A and s are

$$A = \frac{4K_x^2}{q^2}, \quad s = \frac{2K_x\eta}{q^2}, \tag{37}$$

i.e. there is a supplementary condition in the Mathieu equation since $A(s) = (q/\eta)^2 s^2$. They are given by the complex Mathieu functions [24] $cer(\tilde{x}, -is)$, $cei(\tilde{x}, -is)$ and $ser(\tilde{x}, -is)$, $sei(\tilde{x}, -is)$. The solution can be written as a superposition of solutions with coefficients C_j and D_j,

$$Z(\tilde{x}) = \sum_j [C_j ce_j(\tilde{x}, -is) + D_j se_j(\tilde{x}, -is)],$$

where for example [24],

$$ce_{2n}(\tilde{x}, -is) = cer_{2n}(\tilde{x}, -is) + icei_{2n}(\tilde{x}, -is) = \sum_{r=0}^{\infty} A_{2r}^{(2n)}\cos(2r\tilde{x}, -is) \tag{38}$$

and $A_{2r}^{(2n)}$ is a complex coefficient, with a recurrence relation defined using an auxiliary variable V_{2r},

$$V_{2r} = \frac{A_{2r+2}^{(2n)}}{A_{2r}^{(2n)}} \tag{39}$$

such that

$$(4r^2 - A_0)V_{2r-2} + s(V_{2r}V_{2r-2} + 1) = 0. \tag{40}$$

The functions $ce_{2n+1}(x)$ have a similar nature. A second set of solutions are obtained in the form [24]

$$se_{2n}(\tilde{x}, -is) = \sum_{r=0}^{\infty} B_{2r}^{(2n)}\,\sin(2r\tilde{x}, -is). \tag{41}$$

As an example, the function $ce_2(\tilde{x}, -is)$ for $s = 0.16$ is given by [24].

$$ce_2(\tilde{x}, -0.16i) = 1 + 25i\,\cos(2\tilde{x}) - 0.328\,\cos(4\tilde{x}) - 0.00164i\,\cos(6\tilde{x}) + \cdots \tag{42}$$

or for $s=4.8$, the solution is,

$$ce_2(\tilde{x},-4.8i) = 1-(1.367-0.588i)\cos(2\tilde{x})+(0.013-0.468i)\cos(4\tilde{x}) +(0.065+0.015i)\cos(6\tilde{x})+\cdots$$

The resulting solutions display the phenomenon of parametric resonance. The pattern of resonance is the same as in the case of graphene under electromagnetic radiation [19], which has been obtained using the Whittaker method with a modification of the Strang recurrence relations, to take into account that the driven parameter in the Mathieu equation is complex [19].

4. Conclusions

We have employed the generalized Dirac equation to describe the interaction of charge carriers moving in curved graphene with its flexural phonons, or in bent graphene. To produce the equation, an appropriate metric was found and the principle of covariance has been applied. The resulting equation contains a linear correction plus several non-linear terms. Some of these non-linear terms correspond to the Taylor expansion of the overlap integral approach [12], while others, including the linear correction, are new. Such terms may lead to interesting effects, like resonances between various phonon modes, or between flexural phonons and the oscillating external electromagnetic field. We expect these non-linear terms to become important at higher temperatures. Also, we obtained a threshold for electron propagation. For those electrons above this threshold, the corresponding equations are just a set of coupled Mathieu equations, which indicates the possibility of parametric resonances.

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Appendix A. Covariant Dirac equation in curved space

At any finite temperature, phonons produce a displacement field ($\vec{u}$). We start in this section by finding the resulting metrics and its Christoffel connection on corrugated graphene. Let the surface materialized by the graphene sheet be described by

$$z=f(x,y,t), \tag{43}$$

where x,y are the coordinates in the graphene sheet, and z is the out of plane displacement. Notice that here we only consider the flexural phonon branch, since the planar phonons can be described by inclusion in a vectorial potential [12], whose solution is basically known [18,19].

As now the differential dz becomes a linear combination of dx and dy, we have

$$dz=\frac{\partial f}{\partial x}\,dx+\frac{\partial f}{\partial y}\,dy \tag{44}$$

and the induced metric on the sheet is given by the following formula:

$$ds^2=g_{ij}\,dx^i\,dx^j,\quad (i,j=x,y,z), \tag{45}$$

where g_{ij} is the metric tensor. Or, in a more explicit form,

$$ds^2=dx^2+dy^2+dz^2=dx^2+dy^2+\left(\frac{\partial f}{\partial x}\,dx+\frac{\partial f}{\partial y}\,dy\right)^2 \tag{46}$$

and it is obviously a metric in a two-dimensional (but curved) space parametrized by two space variables (x,y). After opening the last expression we get the explicit form of the induced metric, which is

$$\tilde{g}_{jk}=\begin{pmatrix} 1+(\frac{\partial f}{\partial x})^2 & \frac{\partial f}{\partial x}\frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial x}\frac{\partial f}{\partial y} & 1+(\frac{\partial f}{\partial y})^2 \end{pmatrix}. \tag{47}$$

This can be written as

$$\tilde{g}_{jk}=g_{jk}+h_{jk}\quad \text{with } j,k=x,y, \tag{48}$$

where $g_{ij}=\mathrm{diag}(1,1)$ is the flat metric in two-dimensional space, and h_{ij} is the perturbation (supposed small as compared with 1) provoked by the corrugation of the sheet. The matrix (47) is symmetric and real, therefore it can be diagonalized by an appropriate linear transformation.

Also the inverse (contravariant) metric can be easily found. The determinant of the matrix corresponding to the covariant metric tensor (47) is easily found to be

$$\det\begin{pmatrix} 1+(\frac{\partial f}{\partial x})^2 & \frac{\partial f}{\partial x}\frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial x}\frac{\partial f}{\partial y} & 1+(\frac{\partial f}{\partial y})^2 \end{pmatrix}=(1+(\partial_x f)^2+(\partial_y f)^2) \tag{49}$$

and the inverse matrix, corresponding to the contravariant metric g^{jk} is

$$g^{jk}=\frac{1}{Q}\begin{pmatrix} 1+(\frac{\partial f}{\partial y})^2 & -\frac{\partial f}{\partial x}\frac{\partial f}{\partial y} \\ -\frac{\partial f}{\partial x}\frac{\partial f}{\partial y} & 1+(\frac{\partial f}{\partial x})^2 \end{pmatrix}, \tag{50}$$

where we used the abbreviate notation for the determinant, $Q=1+(\partial_x f)^2+(\partial_y f)^2$.

The deformation h_{jk} is entirely composed of quadratic terms containing products of *spatial* partial derivatives of the deformation function $f(x,y,t)$,

$$h_{jk}\simeq \partial_j f\partial_k f \tag{51}$$

and it is easy to check that the corresponding Christoffel symbols reduce to

$$\tilde{\Gamma}^i_{jk}=\tfrac{1}{2}\tilde{g}^{im}(\partial_j\tilde{g}_{mk}+\partial_k\tilde{g}_{jm}-\partial_m\tilde{g}_{jk})=\tilde{g}^{im}\partial_m f\partial^2_{jk}f. \tag{52}$$

Both quantities disappear when $f=0$, and the metric becomes flat again.

The Dirac equation in two dimensions should be now generalized in order to incorporate the fact that the metric on the surface of constraint is no more flat, but curved. Now we will obtain the covariant generalization of the Dirac equation.

The equation we want to produce can be written as the new deformed quantum-mechanical Hamiltonian acting on a two-component spinor Ψ as follows:

$$\hat{H}\,\Psi\sim[\tilde{\gamma}^x\tilde{\nabla}_x+\tilde{\gamma}^y\tilde{\nabla}_y]\Psi. \tag{53}$$

Here not only the contravariant metric is deformed, but also the γ-matrices should be modified in order to satisfy new anti-commutation relations with the induced metric instead of the flat one as before; finally, $\tilde{\nabla}_j$ contains not only the electromagnetic and on plane phonon interaction visualized by the vector potential included in the usual gauge-invariant way, but also the Christoffel symbols of the metric $\tilde{g}_{ij}$:

$$\tilde{\nabla}_j\Psi=(\partial_j-eA_j)\Psi+\tilde{\Gamma}^m_{jk}\tilde{g}^{ki}\tilde{\Sigma}_{mi}\Psi, \tag{54}$$

where the Christoffel symbols $\tilde{\Gamma}^m_{jk}$ are defined as usual, by means of the modified metric:

$$\tilde{\Gamma}^i_{jk}=\tfrac{1}{2}\tilde{g}^{im}[\partial_j\tilde{g}_{mk}+\partial_k\tilde{g}_{jm}-\partial_m\tilde{g}_{jk}] \tag{55}$$

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and $\tilde{\Sigma}_{mk}$ is the matrix-valued anti-symmetric tensor defined by means of the modified gamma-matrices:

$$\tilde{\Sigma}_{mk} = \tfrac{1}{8}[\tilde{\gamma}_m\tilde{\gamma}_k - \tilde{\gamma}_k\tilde{\gamma}_m]. \tag{56}$$

This term is often called "spinorial connection" [20,21].

We are looking for two "deformed" generators of the Clifford algebra $\tilde{\gamma}_x$ and $\tilde{\gamma}_y$ that would satisfy

$$\tilde{\gamma}_x\tilde{\gamma}_x = \left(1+\left(\frac{\partial f}{\partial x}\right)^2\right)\mathbf{1}, \quad \tilde{\gamma}_x\tilde{\gamma}_y+\tilde{\gamma}_y\tilde{\gamma}_x = 2\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\mathbf{1},$$
$$\tilde{\gamma}_y\tilde{\gamma}_y = \left(1+\left(\frac{\partial f}{\partial y}\right)^2\right)\mathbf{1}. \tag{57}$$

In order to do this, we must introduce the third Pauli matrix, because the deformation of the sheet pushes it out of the strict two-dimensional plane (x,y).

The undeformed Clifford algebra satisfying anti-commutation relations in a three-dimensional *flat* space is defined as follows:

$$\gamma_j\gamma_k+\gamma_k\gamma_j = 2g_{jk}\mathbf{1} \quad \text{with } g_{jk}=\mathrm{diag}(1,1,1),\ j,k=1,2,3, \tag{58}$$

which can be generated by three Pauli matrices as follows:

$$\gamma_1=\sigma_x, \quad \gamma_2=\sigma_y, \quad \gamma_3=\sigma_z \tag{59}$$

with

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix}, \quad \sigma_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix}, \quad \sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix} \tag{60}$$

we have indeed

$$(\gamma_x)^2=\mathbf{1}, \quad (\gamma_y)^2=\mathbf{1}, \quad (\gamma_z)^2=\mathbf{1}$$

and the three matrices anticommuting with each other.

The ansatz for the two deformed space-like γ-matrices is simple: if we set

$$\tilde{\gamma}_x=\sigma_x+a\sigma_z, \quad \tilde{\gamma}_y=\sigma_y+b\sigma_z \tag{61}$$

then the coefficients a and b should be, as it was easy to check,

$$a=\frac{\partial f}{\partial x}, \quad b=\frac{\partial f}{\partial y} \tag{62}$$

so that

$$\tilde{\gamma}_x=\sigma_x+\frac{\partial f}{\partial x}\sigma_z, \quad \tilde{\gamma}_y=\sigma_y+\frac{\partial f}{\partial y}\sigma_z. \tag{63}$$

Now we have to produce their *contravariant* counterparts that appear in the Dirac equation [21]. We have

$$\tilde{\gamma}^x=\tilde{g}^{xx}\tilde{\gamma}_x+\tilde{g}^{xy}\tilde{\gamma}_y, \quad \tilde{\gamma}^y=\tilde{g}^{yx}\tilde{\gamma}_x+\tilde{g}^{yy}\tilde{\gamma}_y, \tag{64}$$

which gives explicitly

$$\tilde{\gamma}^x=\frac{1}{Q}\left[(1+(\partial_y f)^2)\sigma_x+(\partial_x f)\sigma_z-(\partial_x f)(\partial_y f)\sigma_y,\right],$$

$$\tilde{\gamma}^y=\frac{1}{Q}\left[(1+(\partial_x f)^2)\sigma_y+(\partial_y f)\sigma_z-(\partial_x f)(\partial_y f)\sigma_x\right]. \tag{65}$$

Recalling that $Q=1+(\partial_x f)^2+(\partial_y f)^2$, we can add and subtract in the numerators of the above formula respectively the following terms: $(\partial_x f)^2\sigma_x$ in the first one, and $(\partial_y f)^2\sigma_y$ in the second one; this will enable us to separate the undeformed matrices σ_x and σ_y and the genuine deformation terms containing spatial derivatives of f. This gives the following result:

$$\tilde{\hat{H}} \sim \sigma^x\tilde{\nabla}_x+\sigma^y\tilde{\nabla}_y+\frac{\sigma_z}{Q}(\overrightarrow{\mathrm{grad}}\, f\cdot\vec{\tilde{\nabla}})-\frac{1}{Q}(\overrightarrow{\mathrm{grad}}\, f\cdot\vec{\sigma})(\overrightarrow{\mathrm{grad}}\, f\cdot\vec{\tilde{\nabla}}), \tag{66}$$

where the vectors and their scalar products are two-dimensional, i.e. we mean

$$\overrightarrow{\mathrm{grad}}\, f=[\partial_x f,\partial_y f], \quad \vec{\sigma}=[\sigma_x,\sigma_y], \quad \vec{\tilde{\nabla}}=[\tilde{\nabla}_x,\tilde{\nabla}_y]$$

so that

$$(\overrightarrow{\mathrm{grad}} f)\cdot(\vec{\sigma})=\partial_x f\sigma_x+\partial_y f\sigma_y, \text{etc.}$$

We see that already in the numerators we have not only linear, but also quadratic terms, notwithstanding the presence of quadratic terms in the denominator (contained in the normalizing factor Q). If we decided to keep *linear terms only*, then the modified Hamiltonian would contain only one extra term proportional to the matrix σ_z:

$$\tilde{\hat{H}}_{lin} \sim \hat{H}_0+\delta\hat{H}=\sigma^x\nabla_x+\sigma^y\nabla_y+\sigma_z(\overrightarrow{\mathrm{grad}}\, f\cdot\vec{\nabla}). \tag{67}$$

Note that also the differential operator ∇ is taken in its primary form, because the connection coefficients contain only quadratic expressions in derivatives of f. Observe that this equation is akin to the one obtained using a Taylor expansion of the overlap integral in a tight-binding approach.

However, if we choose to keep all terms up to quadratic ones, then we must take into account also the Christoffel coefficients in $\tilde{\nabla}$. It is easy to check the following explicit form of our Christoffel symbols; keeping only the second order expressions means that we can use the simplified formula in which $\tilde{g}^{ij}$ is replaced by $g^{ij}=\delta^{ij}$. We have then

$$\Gamma^x_{xx}=\partial_x f\partial^2_{xx}f, \quad \Gamma^x_{xy}=\Gamma^x_{yx}=\partial_x f\partial^2_{xy}f, \quad \Gamma^x_{yy}=\partial_x f\partial^2_{yy}f,$$

$$\Gamma^y_{xx}=\partial_y f\partial^2_{xx}f, \quad \Gamma^y_{xy}=\Gamma^y_{yx}=\partial_y f\partial^2_{xy}f, \quad \Gamma^y_{yy}=\partial_y f\partial^2_{yy}f. \tag{68}$$

In covariant derivatives, these coefficients are contracted with g^{jk} and the *anti-symmetric* matrices Σ_{km},

$$\Gamma^i_{jk}g^{km}\Sigma_{im}.$$

We are using the undeformed matrices Σ_{jk} and not the deformed ones, $\tilde{\Sigma}_{jk}$, because we shall keep the expressions up to the second power of derivatives of f, which are already contained in the Christoffel symbols. This, taking into account that only diagonal terms in g^{ik} do not vanish and are equal to one, leads to the following result when explicited: for $j=x$ we have

$$\Gamma^x_{xx}g^{xx}\Sigma_{xx}+\Gamma^x_{xy}g^{yy}\Sigma_{xy}+\Gamma^y_{xx}g^{xx}\Sigma_{yx}+\Gamma^y_{xy}g^{yy}\Sigma_{yy}$$

and for $j=y$ we get a similar expression:

$$\Gamma^x_{yx}g^{xx}\Sigma_{xx}+\Gamma^x_{yy}g^{yy}\Sigma_{xy}+\Gamma^y_{yx}g^{xx}\Sigma_{yx}+\Gamma^y_{yy}g^{yy}\Sigma_{yy}.$$

The non-vanishing metric tensor components are equal to one, whereas the Σ-matrices are anti-symmetric in their two lower indices, so what is left is only

$$\Gamma^x_{xy}\Sigma_{xy}+\Gamma^y_{xx}\Sigma_{yx}=(\partial_x f\partial^2_{xy}f-\partial_y f\partial^2_{xx}f)\Sigma_{xy},$$

$$\Gamma^x_{yy}\Sigma_{xy}+\Gamma^y_{yx}\Sigma_{yx}=(\partial_y f\partial^2_{yx}f-\partial_x f\partial^2_{yy}f)\Sigma_{yx}. \tag{69}$$

These are the only terms remaining to be included in the covariant derivatives as follows:

$$\tilde{\nabla}_x=(\partial_x-eA_x)+(\partial_x f\partial^2_{xy}f-\partial_y f\partial^2_{xx}f)\Sigma_{xy},$$

$$\tilde{\nabla}_y=(\partial_y-eA_y)+(\partial_y f\partial^2_{yx}f-(\partial_x f\partial^2_{yy}f)\Sigma_{yx}.$$

In the Hamiltonian, they appear multiplied from the left by the corresponding $\tilde{\gamma}$-matrices, but here, evaluating the terms coming from the Christoffel connection coefficients, already quadratic in deformation f, we may keep only their undeformed version, which our case are just the two Pauli matrices σ^x and σ^y, so that the part of the deformed Hamiltonian keeping track of the Christoffel connection is

$$\sigma^x\tilde{\nabla}_x+\sigma^y\tilde{\nabla}_y=\sigma^x(\partial_x-eA_x)+\sigma^x[(\partial_x f)(\partial^2_{xy}f)-(\partial_y f)(\partial^2_{xx}f)]\Sigma_{xy}$$
$$+\sigma^y(\partial_y-eA_y)+\sigma^y[(\partial_y f)(\partial^2_{yx}f)-(\partial_x f)(\partial^2_{yy}f))]\Sigma_{yx}. \tag{70}$$

Taking into account the fact that

$$(\sigma_x)^2=\mathbf{1},\quad (\sigma_y)^2=\mathbf{1},\quad \sigma_x\sigma_y=-\sigma_y\sigma_x,\quad \text{and}\quad \sigma^x\Sigma_{xy}=\tfrac{1}{4}\sigma_y$$

and adding and subtracting terms like $(\partial_y f)(\partial^2_{yy}f)$ to the first expression and $(\partial_x f)(\partial^2_{xx}f)$ to the second, we get the following invariant form of the extra terms induced by the Christoffel connection:

$$\tfrac{1}{4}\sigma^y[(\partial_x f)(\partial^2_{xy}f)+(\partial_y f)(\partial^2_{yy}f)-(\partial_y f)(\partial^2_{yy}f)-(\partial_y f)(\partial^2_{xx}f)] +\tfrac{1}{4}\sigma^x[(\partial_y f)(\partial^2_{xy}f)+(\partial_x f)(\partial^2_{xx}f)-(\partial_x f)(\partial^2_{xx}f)-(\partial_x f)(\partial^2_{yy}f)] \quad (71)$$

This in turn can be written in a more compact (and elegant !) way as follows:

$$\tfrac{1}{8}\vec{\sigma}\cdot\overrightarrow{\text{grad}}[(\partial_x f)^2+(\partial_y f)^2]-\tfrac{1}{4}[\vec{\sigma}\cdot\overrightarrow{\text{grad}}\, f]\Delta f \quad (72)$$

with

$$\Delta f=\partial^2_{xx}f+\partial^2_{yy}f.$$

It is worthwhile to note that the expression (72) vanishes when f is a pure monochromatic wave, $f=A\cos(\omega t-K_x x-K_y y)$, but is different from zero as soon as there is a superposition of such expressions, e.g. for a standing wave. Now we are able to write down the full Hamiltonian for an electron on a sheet, taking into account that sheet's proper motions described by the deformation from horizontal plane given by $z=f(x,y,t)$, up to the second order (quadratic terms in derivatives of f):

$$\hat{\hat{H}}\sim\hat{H}_0+\frac{1}{Q}\sigma_z(\overrightarrow{\text{grad}}\, f)\cdot(\vec{\nabla})-\frac{1}{Q}(\overrightarrow{\text{grad}}\, f\cdot\vec{\sigma})(\overrightarrow{\text{grad}}\, f\cdot\vec{\nabla}) +\frac{1}{8}\vec{\sigma}\cdot\overrightarrow{\text{grad}}[(\partial_x f)^2+(\partial_y f)^2]-\frac{1}{4}[\vec{\sigma}\cdot\overrightarrow{\text{grad}}\, f]\Delta f. \quad (73)$$

The normalizing factor $1/Q$ in front of two first contributions can be set to 1, because it contains the squares of derivatives of f, and if developed, will create terms of order 3 and 4 when multiplied by the terms behind.

The quantum-mechanical Hamiltonian is obtained from this expression by multiplying it by $-i\hbar$ and v_F. Let us define the operator of generalized momentum,

$$\hat{\vec{\pi}}=\hat{\vec{p}}-e\vec{A}=-i\hbar\overrightarrow{\text{grad}}-e\vec{A},$$

where $\vec{A}$ is a vector potential that describes an electromagnetic field [18,19] or in plane longitudinal and transversal phonons [17]. Then we can write:

$$\hat{\tilde{H}}=v_F\begin{pmatrix}0 & \hat{\pi}_x-i\hat{\pi}_y\\ \hat{\pi}_x+i\hat{\pi}_y & 0\end{pmatrix} +v_F\begin{pmatrix}(\partial_x f)\hat{\pi}_x+(\partial_y f)\hat{\pi}_y & 0\\ 0 & -(\partial_x f)\hat{\pi}_x-(\partial_y f)\hat{\pi}_y\end{pmatrix}$$

$$-v_F(\overrightarrow{\text{grad}}\, f\cdot\vec{\sigma})(\overrightarrow{\text{grad}}\, f\cdot\hat{\pi}) -i\hbar v_F\left[\frac{1}{8}\vec{\sigma}\cdot\overrightarrow{\text{grad}}[(\partial_x f)^2+(\partial_y f)^2\right]-\frac{1}{4}[\vec{\sigma}\cdot\overrightarrow{\text{grad}}\, f]\Delta f]. \quad (74)$$

This last equation is the generalized Dirac equation. It is interesting to observe that in the Hamiltonian derived here, the first order correction and the term $\vec{\sigma}\cdot\overrightarrow{\text{grad}}[(\partial_x f)^2+(\partial_y f)^2]/8-[\vec{\sigma}\cdot\overrightarrow{\text{grad}}\, f]\Delta f/4$ are akin to the ones obtained from a vectorial potential approach [12]. However, Eq. (74) contains more terms.

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