Space Dependent Fermi Velocity in Strained Graphene

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We investigate some apparent discrepancies between two different models for curved graphene: the one based on tight-binding and elasticity theory, and the covariant approach based on quantum field theory in curved space. We demonstrate that strained or corrugated samples will have a space-dependent Fermi velocity in either approach that can affect the interpretation of local probe experiments in graphene. We also generalize the tight-binding approach to general inhomogeneous strain and find a gauge field proportional to the derivative of the strain tensor that has the same form as the one obtained in the covariant approach.

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As is well known, the low-energy electronic excitations in graphene are modeled by a massless Dirac Hamiltonian that is able to describe many spectroscopic and transport experiments with surprising accuracy [1]. The Fermi velocity is the only free parameter in the model and, as such, all the observable quantities critically depend on it. It plays the same role as the effective mass in the usual Fermi liquid theory. Recent experiments [2–4] have been able to measure the renormalization of the Fermi velocity predicted in Ref. [5], which means that the Fermi velocity is not a constant but increases as the energy is decreased near the Dirac point. In this Letter, we will show that the corrugations and strain present in most of the samples give rise to a space-dependent Fermi velocity, a fact that can change the interpretation of some experiments.

The presence of ripples in all the graphene samples and the influence of the lattice distortions on the electronic properties of the material are two of the most interesting aspects of graphene that still remain as open problems in the field. To study the issue, the most popular model proposed in the literature is based on a combination of tight-binding and elasticity theory [6,7] that induces ''elastic'' vector fields coupled to the electronic density (for an extensive review on the subject see Ref. [8] and the references therein). This approach has given rise to the proposal of ''strain engineering'' [9,10]. An important highlight in the field has been the observation of a reorganization of the spectrum resembling Landau levels in strained graphene due to the effective magnetic field [11] whose existence was theoretically predicted [10,12].

An alternative model to explore the influence of corrugations on the electronic properties of graphene is based on the formulation of quantum field theory (QFT) in curved space that is well known in cosmology and gravitation [13,14]. This possibility, suggested for modeling spherical fullerenes [15,16], was fully explored for general geometries [17–20]. The QFT approach is rooted on the spinorial nature of the low-energy electronic excitations of graphene and on the robustness of the Fermi points under deformations of the lattice [21], and hence it should work well in the low-energy scale.

Since both models are natural and predictive, one should expect that they will provide the same results when applied to curved graphene samples with given shapes. Nevertheless, there are a few discrepancies that are immediately apparent without entering into much detail. One is the prediction of the QFT approach of a space-dependent Fermi velocity [19]. The origin of it lies on the vector indices of the Pauli matrices that made them space dependent when going to curved geometries. There is also a homogeneous contribution coming from volume effects. Another obvious discrepancy is related to in-plane distortions. These give rise in the elasticity approach to the coupling of the spinor to vector fields (named ''fictitious magnetic fields'' in the literature), which in turn have observational consequences. Since in-plane distortions do not induce intrinsic curvature to the sample, the analogue of the fictitious vector fields in the QFT approach, the spin connection, is zero. A third apparent discrepancy comes from the different symmetry of the vector fields associated to intrinsically curved samples where the two approaches can be used. The best example is provided by the Gaussian bump [19] whose associated vector field is axially symmetric in the QFT scheme and has trigonal symmetry in the TB-elasticity models [22].

Although the tight-binding derivation of the low-energy effective Dirac Hamiltonian is the most popular, probably for historical reasons [23], it has been known since 1958 that the Dirac structure is more general and follows from the lattice symmetry and a low-energy expansion [24]. New directions studying the effective low-energy Hamiltonians for distorted lattices on symmetry grounds [25–29] paved the way to a better understanding of the correspondence between the lattice formulations and the QFT covariant approach. In this Letter, we partially follow this path and explore the correspondence between lattice

and continuum formulations with special emphasis on the spacial dependence of the effective Fermi velocity. We will show that a space-dependent Fermi velocity arises from the tight-binding elasticity approach when going beyond the linear approximation and that the two formalisms can be compared if a metric coming from elasticity is chosen in the QFT approach.

The QFT geometric description of curved graphene and the elasticity theory.—The QFT geometric description of curved graphene has been discussed in detail in Ref. [30]. It is based on the stability of the Fermi points of the hexagonal lattice under moderate lattice distortions [21], and on the subsequent description of the low-energy excitations around the Fermi points as massless Dirac fermions. Hence, a natural way to incorporate the effect of the observed corrugations at low energies is to couple the Dirac equation to the given curved background.

To make the connection between the two approaches explicit, we will work out the QFT Hamiltonian in a curved space arising from a metric related to the strain tensor by $g_{ij} = \eta_{ij} + 2u_{ij}$ [31,32], where η_{ij} is the flat metric (the identity matrix), and the strain tensor is defined as $u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i + \partial_i h \partial_j h)$, where u_i and h are in and out of plane displacements, respectively. Since the metric g is already phenomenological, we could include in its definition a material dependent parameter β similar to the one obtained from the TB approach. We choose to leave its value at 1 for the time being.

The Dirac Hamiltonian in a curved space described by a metric g_{ij} is given by

$$H = i \int d^2x \sqrt{g} \bar{\psi} \gamma^a e_a^i (\partial_i + \Omega_i) \psi, \tag{1}$$

where $\bar{\psi} = \psi^\dagger \gamma^0$, $\gamma^0 \gamma^i = \sigma^i$ are the Pauli matrices, and a sum is implicit in repeated indices. The effect of the metric is encoded in the tetrads e_a^i, the metric determinant $\sqrt{g}$, and the spin connection Ω_i. Expanding these objects to first order in u_{ij} (see Part A of the Supplemental Material [33]), we obtain the Hamiltonian

$$H = i \int d^2x \psi^\dagger (\sigma_a \partial_a + u_{ii} \sigma_a \partial_a - \sigma_a u_{ab} \partial_b + \frac{1}{2} \sigma_a (\partial_a u_{ii} - \partial_i u_{ia})) \psi. \tag{2}$$

The first term in Eq. (2) is the usual Dirac term. The next two terms are the space-dependent Fermi velocity, and the last two are the corresponding geometric gauge field, as interpreted in Ref. [19]. Note that the terms of the type $i(u_{ij}\partial_k + 1/2 \partial_k u_{ij})$ are Hermitian by partial integration: for every term in the Fermi velocity there must be a corresponding geometric gauge field that guarantees Hermiticity. Also, note the extra factor of i as compared to the minimal coupling of a U(1) gauge field, $\partial_i + ieA_i$, which is Hermitian by itself. The effective Hamiltonian around the other Fermi point will have the same Fermi velocity but a minus sign in the gauge field couplings.

Space-dependent Fermi velocity from tight binding.—We now proceed to compute the effective Hamiltonian in the presence of strain directly from the tight-binding model. The general tight-binding Hamiltonian is

$$H = -\sum_{\vec{x},n} t_{\vec{x},n} a_{\vec{x}}^\dagger b_{\vec{x}+\vec{\delta}_n} + \text{c.c.}, \tag{3}$$

where $\vec{x}$ runs over the position of all unit cells and the three nearest neighbor vectors are defined as

$$\vec{\delta}_1 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \qquad \vec{\delta}_2 = a\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \qquad \vec{\delta}_3 = a(0, -1), \tag{4}$$

with a the equilibrium nearest neighbor distance.

In order to make an easier contact with previous works in the literature and to illustrate the method, we will first consider the case of homogeneous strain $t_{\vec{x},n} = t_n$ and then generalize it to arbitrary inhomogeneous strain. In the tight-binding approximation, the only effect of strain is to modify the hopping integrals as the distance between the atoms changes. Even if the strain does not depend on position, the three nearest neighbor hoppings t_n may vary independently. To first order in the distance change Δu_n, we may write

$$t_n = t_0(1 - \beta \Delta u_n), \tag{5}$$

where $\beta = |\partial \log t / \partial \log a|$ and t_0 the equilibrium hopping. The relative distance change to first order in strain is

$$\Delta u_n = \frac{\delta_n^i \delta_n^j}{a^2} u_{ij}. \tag{6}$$

Notice that when considering inhomogeneous strain as in Part C of the Supplemental Material [33], this equation has to be completed with terms proportional to the derivative of the strain tensor. The lowest order in this case is

$$\Delta u_n = \frac{\delta_n^i \delta_n^j}{a^2} u_{ij} + \frac{\delta_n^i \delta_n^j \delta_n^k}{2a^2} \partial_i u_{jk}. \tag{7}$$

We now expand in Bloch waves

$$a_{\vec{x}} = \sum_{\vec{k} \in BZ} e^{i\vec{k}\vec{x}} a_{\vec{k}}, \qquad b_{\vec{x}} = \sum_{\vec{k} \in BZ} e^{i\vec{k}\vec{x}} b_{\vec{k}}, \tag{8}$$

and consider momenta close to the Dirac points $\vec{k} = \vec{K} + \vec{q}$, with $\vec{K} = (4\pi/(a3\sqrt{3}), 0)$ (the result for the other Dirac point can be obtained by changing $\vec{K} \to -\vec{K}$ throughout). The Hamiltonian in momentum space is

$$H = -\sum_{n=1}^{3} t_n \begin{pmatrix} 0 & e^{-i(\vec{K}+\vec{q})\cdot\vec{\delta}_n} \\ e^{i(\vec{K}+\vec{q})\cdot\vec{\delta}_n} & 0 \end{pmatrix}. \tag{9}$$

Expanding to first order in q we obtain

$$H \approx -\sum_{n=1}^{3} t_n \begin{pmatrix} 0 & e^{-i\vec{K}\vec{\delta}_n} \\ e^{i\vec{K}\vec{\delta}_n} & 0 \end{pmatrix} (1 + i\sigma_3 \vec{q}\cdot\vec{\delta}_n). \quad (10)$$

We now use the following identity:

$$\begin{pmatrix} 0 & e^{-i\vec{K}\cdot\vec{\delta}_n} \\ e^{i\vec{K}\cdot\vec{\delta}_n} & 0 \end{pmatrix} = i\frac{\vec{\sigma}\cdot\vec{\delta}_n}{a}\sigma_3, \quad (11)$$

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ are the two Pauli matrices. Using Eqs. (5) and (6) for t_n, the Hamiltonian is

$$H \approx -\sum_{n=1}^{3} t_0 \left(1 + \frac{\beta}{a^2}\vec{\delta}_n u \vec{\delta}_n\right)\left(\frac{i}{a}\sigma_3\vec{\sigma}\cdot\vec{\delta}_n\right)(1 + i\sigma_3\vec{q}\cdot\vec{\delta}_n). \quad (12)$$

We can now collect the different terms of this expression with the use of the identities given in Part B of the Supplemental Material [33]. Labeling the various terms by their order in the expansion in q, u we get

$$H = H_q + H_u + H_{q,u}, \quad (13)$$

with

$$H_q = v_0\sigma_i q_i, \quad (14)$$

$$H_u = \frac{v_0}{2a}\beta\sigma_i K_{ijk}\epsilon_{kl}u_{jl}, \quad (15)$$

$$H_{u,q} = \frac{v_0}{4}\beta[2\sigma^i q_j u_{ij} + \sigma^i q_i u_{jj}], \quad (16)$$

where we have defined $v_0 = 3t_0 a/2$ and K_{ijk} as the invariant C_3 tensor given in Eq. (16) of the Supplemental Material [33], and Ref. [8]. It is easy to see that, if needed, the expansion of the low-energy Hamiltonian in powers of q_i and u_{ij} can be done to any order. The first two contributions are well known: H_q is the usual Dirac Hamiltonian, and H_u is the standard strain-induced gauge coupling [8]: $H_u = v_0\sigma_i A_i$ with components

$$A_x = \frac{\beta}{2a}(u_{xx} - u_{yy}), \qquad A_y = \frac{\beta}{2a}(-2u_{xy}). \quad (17)$$

The new contribution $H_{u,q}$ is the main result of this Letter. This result is consistent with the one obtained from the symmetry analysis in Refs. [28,29], and fixes the coefficients of the symmetry-allowed terms in terms of a microscopic model. We will see its full significance in what follows.

Inhomogeneous strain.—Treating inhomogeneous strain is a delicate issue due to the lack of translation invariance of the system. The usual procedure [29] consists of taking the homogeneous Hamiltonian in k space and going to real space by the replacement rule

$$u_{ij}q_k \to i\left(u_{ij}\partial_k + \frac{1}{2}\partial_k u_{ij}\right), \quad (18)$$

which guarantees Hermiticity. Using this rule, the term (16) becomes

$$H_{u,q} = i\frac{v_0}{4}\sigma_i\left(2u_{ij}\partial_j + u_{jj}\partial_i + \partial_j u_{ij} + \frac{1}{2}\partial_i u_{jj}\right), \quad (19)$$

which allows us to write the Hamiltonian as

$$H = iv_{ij}(r)\sigma_i\partial_j + iv_0\sigma_i\Gamma_i + v_0\sigma_i A_i. \quad (20)$$

The field A_i is the one obtained in the standard approach (17). We also get the tensorial and space-dependent Fermi velocity

$$v_{ij} = v_0\left[\eta_{ij} + \frac{\beta}{4}(2u_{ij} + \eta_{ij}u_{kk})\right], \quad (21)$$

obtained in (16). The new term is a "geometric" gauge field given by

$$\Gamma_i = \frac{\beta}{4}\left(\partial_j u_{ij} + \frac{1}{2}\partial_i u_{jj}\right), \quad (22)$$

which was obtained in the covariant approach (2). Being proportional to the derivative of the strain tensor, it only appears in the case of inhomogeneous strain. All these terms are also found in the symmetry analysis [28,29].

As discussed in Ref. [34], the former procedure can miss some terms. We have checked that this is the complete result to this order in derivatives by directly performing the Fourier transform of the real-space Hamiltonian in the first stage of the tight binding for the general case of inhomogeneous strain. The details can be found in Part C of the Supplemental Material [33].

Discussion and future.—The purpose of this Letter was to discuss the equivalence of the tight-binding and the QFT approaches in the description of curved or strained graphene with special emphasis on the space-dependent Fermi velocity. The main result is that the two approaches give rise to the same type of terms for the space-dependent Fermi velocity although with different numerical values of the coefficients. The symmetry approach gives rise to the same type of terms with independent—and undetermined—coefficients whose value has to be fixed by the model. We have also derived the "geometric" gauge field in the tight-binding approach for the case of inhomogeneous strain.

Referring to the QFT approach, we have seen that the definition of the metric of the curved space in terms of the strain tensor allows us to get physical effects from the covariant formalism even in the case of having only in-plane distortions.

An interesting related issue concerns whether new terms can appear in the effective tight-binding Hamiltonian independently of the change of the hoppings that are produced just by changes in the relative positions of the atoms. If one assumes $\beta = 0$, the discrete TB Hamiltonian in that case is just

$$H = -\sum_{<ij>} t_0 a_i^\dagger b_j + \text{c.c.}, \quad (23)$$

with i, j running through nearest neighbor atoms. It is easy to see that moving the atoms from their positions does not change the Hamiltonian at all. i, j are just labels numbering the atoms and need not refer to physical position in any sense. Hence, the energies and eigenfunctions of the system are not modified by this strain, even if inhomogeneous (for $\beta = 0$). However, this does not imply that there will not be observable consequences. The fact that the atoms are in different positions does change the way in which external position-dependent probes see the system. In short, when the atoms are displaced, the discrete label i maps to a physical position in the strained frame. If we describe the physics in the lab frame so as to be able to couple an external field, then vectors in the strained frame have to be rotated to the lab frame. This gives rise to a β-independent contribution of the type obtained recently in Ref. [35] and will be discussed in detail elsewhere.

Although the space-dependent Fermi velocity is obtained at higher order in a tight-binding expansion, its presence has important physical consequences and it cannot be obviated. The important issue in this discussion is the influence of the various factors entering the effective Hamiltonian on the observable physical quantities. In particular, in Ref. [19] it was shown that in the QFT approach the local density of states is not affected by the vector fields to first order in perturbation theory. The oscillations in the local density of states obtained in that work came from the combination of variable Fermi velocity and volume effects. Similarly, it has been shown in Ref. [36] that long-range correlated vector fields do not alter the minimal conductivity of graphene that is in turn severely changed by long-range correlated disorder in the form of a random distribution of Fermi velocity [37]. We also note that while this Letter was completed, we learned in an experiment that points to the observation of a 5–10% spatial fluctuation of the Fermi velocity in samples on SiO_2 [2].

As we have seen, the standard QFT approach is rooted in considering the spinor describing the low-energy electronic excitations of graphene as a covariant spinor under a geometric point of view. Since the time coordinate remains "flat," the Lorentz symmetry is reduced to translation and rotations. This approach has been pushed forward in Ref. [38] considering graphene as a QFT in curved spacetime what gives rise to very interesting consequences as the possibility to observe a Hawking-Unruh temperature in the curved graphene samples.

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