

Gauge fields from strain in graphene

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We revise the tight-binding approach to strained or curved graphene in the presence of external probes such as photoemission or scanning tunneling microscopy experiments. We show that extra terms arise in the continuum limit of the tight-binding Hamiltonian which cannot be accounted for by changes in the hopping parameters due to lattice deformations, encoded in the parameter β . These material-independent extra couplings are of the same order of magnitude as the standard ones and have a geometric origin. They include corrections to the position-dependent Fermi velocity and to a new vector field. We show that the new vector field does not couple to electrons like a standard gauge field and that no β -independent pseudomagnetic fields exist in strained graphene.

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I. INTRODUCTION

One of the most interesting aspects of graphene is the tight relation between its morphological and electronic properties. Although this issue has been explored at length in the theoretical literature^{1,2} and there is a fair number of related experiments,^{3–9} recent results^{10–12} have given an extra push to the subject that will be explored in this work.

In the continuum limit of the standard tight-binding (TB) approach, lattice deformations couple to the electronic excitations in the form of effective gauge fields and scalar potentials.^{2,13} In particular, the so-called pseudomagnetic fields have acquired a physical reality after the observation of Landau levels from strain in graphene samples¹⁴ predicted theoretically in Refs. 15 and 16. These deformation gauge fields are at the basis of the proposed strain modifications of the electronic properties (strain engineering) of graphene^{15,17–21} and have been used in the design and modeling of recent experiments exploring the physics of lattice systems either with cold atoms^{22,23} or with artificial lattices made with CO molecules in a Cu surface.¹¹ Hence it is very important to establish the accuracy and completeness of the TB description, to ascertain whether there are modifications to the model and, if so, how they will affect the experiments.

In the standard approach the parameter that links the TB electronics with the continuum elasticity theory, β , is related to the electron-phonon coupling and appears in the definition of the strain-induced effective magnetic fields. β reflects the changes in the hopping parameter t of the TB model with the changes of the relative distances between atomic nearest neighbors due to the lattice deformations. In a recent work²⁴ it was claimed that extra β -independent pseudomagnetic fields arise in the standard TB description coming from the displacements of the atomic positions of the lattice. Following this work there have been attempts to correct the previous calculations leading to “strain Landau levels.”²⁵ Moreover, inspired by a geometric approach to

curved graphene,^{26–30} the continuum TB Hamiltonian was supplemented in Ref. 31 with additional β -dependent terms arising from a higher order derivative expansion, which can be interpreted as a position-dependent Fermi velocity and a new vector field.

In what follows we will show that no β -independent pseudomagnetic fields exist in strained graphene: The only pseudogauge fields are the well-known β -dependent fields in Eq. (2). We will indeed identify all the new terms arising from “frame effects” (i.e., due to the actual atomic positions) needed to complete the TB description whenever the system is coupled to external probes. But we will see that they only modify the coefficients of the position-dependent Fermi velocity and the new vector field obtained in Ref. 31. We will further clarify the nature of the new vector field and show that it does not act as a pseudogauge field, although it may have interesting physical effects, such as pseudospin precession. We will also show that the extra gauge fields suggested in Ref. 24 can be completely eliminated by a gauge transformation and have no physical consequences. Finally we will discuss the experimental context in which the newly derived terms might lead to observable effects.

II. FRAME EFFECTS

We will assume for simplicity that there are no short-range interactions or disorder connecting the two Fermi points of graphene, so that the low-energy description around each point remains valid. As is well known in the TB-elasticity approach,^{2,32} elastic deformations of the lattice give rise, in the continuum limit, to vector potentials that mimic the coupling of real magnetic fields to the electronic current. The standard TB Hamiltonian in the continuum limit is

$$H_{TB} = -iv_0 \int d^2x \psi^\dagger \sigma_j (\partial_j + iA_j) \psi, \quad (1)$$

where $v_0 = 3ta/2$ is the Fermi velocity for the perfect lattice, with t the hopping parameter for nearest neighbors and a the lattice constant; $j = 1, 2$ (summation over a repeated index is understood over the article), and σ_j are the Pauli matrices. The potential A_j is related to the strain tensor by

$$A_1 = \frac{\beta}{2a}(u_{xx} - u_{yy}), \quad A_2 = \frac{\beta}{2a}(-2u_{xy}), \quad (2)$$

where $\beta = |\partial \ln t / \partial \ln a|$. 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. Note that one usually assumes that crystal deformations are small and (1) is valid only up to $O(u_{ij}^2)$ corrections. We will follow this practice for the rest of the paper.

As shown in Ref. 31, if one uses the TB approach to go one order higher in the derivative expansion, the Hamiltonian (1) becomes

$$H_{TB} = -i \int d^2x \psi^\dagger [v_{ij}(x) \sigma_i \partial_j + v_0 \sigma_i \Gamma_i + i v_0 \sigma_i A_i] \psi, \quad (3)$$

where the field A_i is the one given in (2), v_{ij} is the tensorial and space dependent Fermi velocity, $v_{ij} = v_0[\eta_{ij} - \frac{\beta}{4}(2u_{ij} + \eta_{ij} u_{kk})]$, and Γ_i is a new vector field given by

$$\Gamma_i = \frac{1}{2v_0} \partial_j v_{ij} = -\frac{\beta}{4} \left(\partial_j u_{ij} + \frac{1}{2} \partial_i u_{jj} \right). \quad (4)$$

The key observation of the present work is that TB Hamiltonians describing strained graphene,^{2,32} and (3) in particular, are commonly derived in a specific reference system, the ‘‘crystal frame.’’ The reason is that the Bloch waves $a_k = \sum_x e^{-i\vec{k}\cdot\vec{x}} a_x$ used to diagonalize the TB Hamiltonian are written using the atomic *equilibrium* positions $\{x\}$, which are regularly spaced and independent of the crystal deformation. On the other hand, in the presence of strain the positions measured in the ‘‘laboratory frame’’ are the actual positions of the atoms y_i . The two sets of coordinates are related by $y_i = x_i + u_i(x)$, where u_i is the in-plane horizontal displacement vector. Note that the vertical displacements h are identical in both systems. In the classical theory of elasticity, crystal (laboratory) frame coordinates are usually referred to as Lagrangian (Eulerian) coordinates.³³

Thus, the TB Hamiltonian (3) is actually the crystal frame Hamiltonian $H_c(x)$. In order to describe the interaction of electrons with external probes or fields, we must use the laboratory frame Hamiltonian $H_{\text{Lab}}(y)$; i.e., the TB Hamiltonian has to be rewritten in laboratory frame coordinates. The TB Hamiltonian is the sum of the Dirac Hamiltonian H_0 plus the terms induced by the lattice deformations. As these are already $O(u_{ij})$, we have to compute change-of-frame corrections only for the u_{ij} -independent piece $(H_0)_c$ of the crystal Hamiltonian. The computation is simplified by using the symmetric convention for the derivatives of the fermion fields

$$(H_0)_c = -i v_0 \int d^2x \psi_c^\dagger(x) \sigma_i \overleftrightarrow{\partial}_i \psi_c(x), \quad (5)$$

where $\psi^\dagger \overleftrightarrow{\partial}_i \psi \equiv 1/2[\psi^\dagger \partial_i \psi - (\partial_i \psi^\dagger) \psi]$ and the subscript in ψ_c indicates that this is the fermion field operator in the crystal

frame. The derivatives transform according to

$$\frac{\partial}{\partial x_i} = \frac{\partial y_k}{\partial x_i} \frac{\partial}{\partial y_k} = (\delta_{ik} + \partial_i u_k) \partial_k = (\delta_{ik} + \tilde{u}_{ik} + \omega \varepsilon_{ik}) \partial_k, \quad (6)$$

where $\tilde{u}_{ik} = (\partial_i u_k + \partial_k u_i)/2$ is the linear piece of the strain tensor and $\omega \varepsilon_{ik} = (\partial_i u_k - \partial_k u_i)/2$. We also have to transform the integration measure

$$d^2x = \left| \det \left(\frac{\partial x_k}{\partial y_i} \right) \right| d^2y = |\det(\delta_{ik} - \tilde{u}_{ik} - \omega \varepsilon_{ik})| d^2y \simeq (1 - \tilde{u}_{ii}) d^2y. \quad (7)$$

On the other hand, $\psi_c^\dagger \psi_c$ is the particle density operator in the crystal frame. As the number of fermions in any region should be frame independent, we must impose $\psi_c^\dagger \psi_c d^2x = \psi^\dagger \psi d^2y$, where $\psi(y)$ is the laboratory frame field operator. This implies

$$\psi_c(x) = \left| \det \left(\frac{\partial x_k}{\partial y_i} \right) \right|^{-1/2} \psi(y), \quad (8)$$

which exactly cancels the Jacobian in (7). The net result is

$$\begin{aligned} & -i v_0 \int d^2x \psi_c^\dagger(x) \sigma_i \overleftrightarrow{\partial}_i \psi_c(x) \\ & \simeq -i v_0 \int d^2y [\psi^\dagger(y) \sigma_i \overleftrightarrow{\partial}_i \psi(y) + (\tilde{u}_{kl} + \omega \varepsilon_{kl}) (\psi^\dagger \sigma_k \overleftrightarrow{\partial}_l \psi)], \end{aligned} \quad (9)$$

where the derivatives in the last term act only on the fermion fields. Finally, the dependence on the antisymmetric piece $\omega \varepsilon_{ij}$ may be eliminated by a local rotation of the spinors

$$\psi(y) \rightarrow e^{-(i/2)\omega \sigma_3} \psi(y) \simeq \psi(y) - \frac{i}{2} \omega \sigma_3 \psi(y). \quad (10)$$

Indeed, the identity $i \sigma_k \sigma_3 = \varepsilon_{kl} \sigma_l$ shows that this rotation cancels the term proportional to ω in (9). A contribution proportional to $\partial_k \omega$ vanishes as well due to the anticommutation relation $\{\sigma_3, \sigma_k\} = 0$ for $k = 1, 2$. This yields

$$H_{\text{Lab}} = H_{TB} + H_{\text{Geom}}, \quad (11)$$

where H_{TB} is given by (3) and

$$\begin{aligned} H_{\text{Geom}} &= -i v_0 \int d^2x \tilde{u}_{kl} (\psi^\dagger \sigma_k \overleftrightarrow{\partial}_l \psi) \\ &= -i v_0 \int d^2x \psi^\dagger \left[\tilde{u}_{kl} \sigma_k \partial_l + \frac{1}{2} (\partial_l \tilde{u}_{kl}) \sigma_k \right] \psi. \end{aligned} \quad (12)$$

In the last line we have used integration by parts to revert to the asymmetric derivative convention. Note that, to first order in the strain, β -dependent terms are the same in both frames. Equations (11) and (12) are the main results in this paper.

As $\beta \simeq 2$, the new β -independent terms in H_{Geom} are of the same order of magnitude as those in the standard TB Hamiltonian (3). In particular, the space-dependent Fermi velocity derived in the TB formalism in Ref. 31 will become

$$v_{ij} = v_0 \left[\delta_{ij} - \frac{\beta}{4} (2u_{ij} + \delta_{ij} u_{kk}) + \tilde{u}_{ij} \right] \quad (13)$$

with the corresponding correction for the vector field

$$\Gamma_i = \frac{1}{2v_0} \partial_j v_{ij} = -\frac{\beta}{4} \left(\partial_j u_{ij} + \frac{1}{2} \partial_i u_{jj} \right) + \frac{1}{2} \partial_j \tilde{u}_{ij}. \quad (14)$$

The Hamiltonian H_{Lab} can also be obtained by performing the TB calculation directly in the laboratory frame. This derivation is explicitly given in the Appendix, where we also show that the additional pseudogauge field found in Ref. 24 has zero curl everywhere and can be eliminated by a gauge transformation of the electronic wave function. As Γ_i is the only “new” vector field in strained or curved graphene, in what follows we will comment briefly on its physical significance and compare it with the well-known pseudogauge field A_i in Eq. (2). First of all, note that, unlike A_i , Γ_i is not a functionally independent field. The reason is that the Hamiltonian (3) is Hermitian only for $\Gamma_i = \frac{1}{2v_0} \partial_j v_{ij}$. Thus, a position-dependent Fermi velocity requires the existence of the new vector field Γ_i .

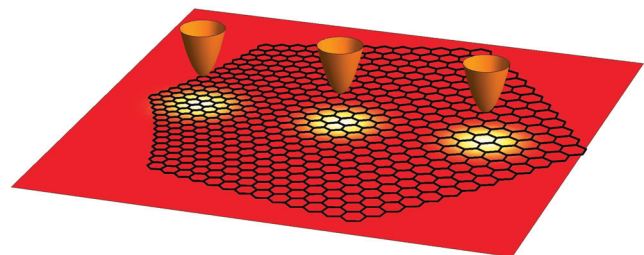
A look at (3) might suggest that Γ_i is some sort of purely imaginary³⁴ counterpart to A_i . However, this is obviously wrong, as gauge potentials have to be real (Hermitian). The true nature of Γ_i is made apparent if we use the identity $i\sigma_k\sigma_3 = \varepsilon_{kl}\sigma_l$ to rewrite the relevant term as $-iv_0\sigma_i\Gamma_i = v_0\sigma_i\tilde{\Gamma}_i$, with

$$\tilde{\Gamma}_1 = \Gamma_2\sigma_3, \quad \tilde{\Gamma}_2 = -\Gamma_1\sigma_3. \quad (15)$$

Note that $\tilde{\Gamma}_i$ is matrix-valued and Hermitian. This shows that the vector field Γ_i plays the role a Hermitian connection for the SO(2) group of local pseudospin rotations (10) generated by σ_3 . As a consequence, a position-dependent Fermi velocity will be accompanied by pseudospin rotation (“pseudospin precession”), i.e., by electronic transitions between the two sublattices. In more physical terms, whereas electrons propagating in a (pseudo)gauge field acquire a path-dependent complex phase, the new vector field induces pseudospin rotation, very much like an optically active medium turns the polarization plane of light. Thus Γ_i is not a gauge field and cannot give rise to the characteristic Landau levels of real or pseudomagnetic fields: The only pseudogauge field in strained graphene is the well-known A_i given by (2). Note also that, in general, observable effects will not be associated with the field $\tilde{\Gamma}_i$ itself but with its curl, which by (15) is proportional to the divergence of Γ_i . This is even more obvious in the covariant model,³¹ where Γ_i appears as the spin connection associated with fermions propagating in a curved background and its divergence is proportional to the scalar curvature R .

III. SOME PHYSICAL EXAMPLES

To see the physical implications of this work for actual measurements we now work out some practical examples. Consider first a density of states measurement. The frame effects discussed are rather trivial in this case but enough to exemplify the issue. The effect of the coordinate change will affect scanning tunneling microscopy (STM) measurements when the tip resolution is large in units of the lattice constant (no atomic resolution). The local density of states (LDOS) in the laboratory frame can be computed approximately in the local limit, for a sufficiently smooth u_{ij} . To do this, $\rho(E, u_{ij})$ is computed assuming u_{ij} is constant, and then its dependence on the position is restored in the final expression $\rho(E, x) \equiv \rho(E, u_{ij}(x))$. The LDOS can be computed in momentum



$$\vec{u} = (x^2 - y^2, 2xy)$$

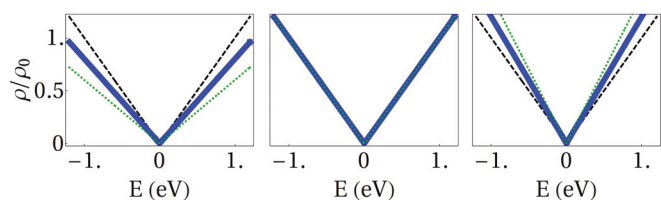


FIG. 1. (Color online) Pictorial view of the strain field discussed in the text and the changes it produces in the density of states. The dotted (green) line represents the contribution from β -dependent terms alone, while the thick (blue) line represents the total correction including frame effects. The black, dashed line represents the density of states of the perfect lattice. The three plots correspond to $x = -L, 0, L$ for the displacement discussed in the text with $u_{\text{max}} = 0.2$.

space

$$\rho(E) = \int dq_x dq_y \text{tr}[E - H(q_x, q_y)]^{-1} \quad (16)$$

with the Hamiltonian (11) by diagonalizing v_{ij} , which amounts to a change of integration variables

$$\rho(E) = \int \frac{dq_+ dq_-}{v_+ v_-} \text{tr}(E - H_0)^{-1}, \quad (17)$$

with H_0 the unperturbed Hamiltonian and v_{\pm} the velocity eigenvalues. This yields

$$\rho(E) = \frac{4}{2\pi} \frac{E}{v_+ v_-} = \rho_0(E) \frac{v_0^2}{v_+ v_-} \quad (18)$$

(the factor of 4 is due spin and valley degeneracy) which to first order in strain can be computed to give

$$\rho(E, x) = \rho_0(E)(1 + \beta \text{tr} u - \text{tr} \tilde{u}). \quad (19)$$

A simple but interesting example is provided by in-plane strains that are quadratic in the position, such as those associated to the triangular bumps that led to the observation of pseudo-Landau levels in STM¹⁰ and that have been explicitly produced in artificial graphene.¹¹ Remember that the TB gauge field associated with a strain tensor u_{ij} is $\vec{A} \propto (u_{xx} - u_{yy}, -2u_{xy})$. Consider first a deformation vector given by $\vec{u} = (x^2 - y^2, 2xy)u_{\text{max}}/4L$ shown in the upper part of Fig. 1. It is easy to see that the associated pseudomagnetic field will be zero in this case. The trace of the strain tensor is $\text{tr} u = u_{\text{max}}x/L$, hence

a line scan along the y direction will give a perfect constant V shape [$\rho(E, x) \sim |E|$], while along the x direction there will be a dilatation effect such that $\rho(E, x) \sim [1 + u_{\max}(\beta - 1)x/L]|E|$, as depicted in the lower part of Fig. 1 for different values of x . Due to the frame effects discussed in this work there is an additional, material-independent change in the magnitude of the LDOS that adds on top of the β -dependent contributions. This is important to consider if one wants to measure the space-dependent Fermi velocity from a local probe with resolution larger than the lattice constant.

An interesting thing happens if we now consider the same deformation vector but exchange u_x and u_y , i.e., $\vec{u} \propto (2xy, x^2 - y^2)$. In this case there will be no volume effect ($\text{tr} u = 0$) and the strain will give rise to a constant pseudomagnetic field whose associated density of states will show similar Landau level oscillations along any scan line. A 90° rotation of the strain deformation will give the same V shape with a Fermi velocity increasing this time along $x = \text{constant}$. Finally, for the strain $\vec{u} \propto (x^2 - y^2, -2xy)$ both the trace and the pseudomagnetic field will be zero and there will be no effect altogether. It can be shown that the geometric vector field coming from the frame change does not affect the DOS at the linear order in u_{ij} considered in this work.

On the other hand, these examples are a simple illustration of the fact that the honeycomb lattice is very anisotropic and, of course, does not have full rotational symmetry;³⁵ hence similar looking deformations give rise to very different effects in the STM images. The important point is that, in the case of general strain, the frame effects discussed in this work will be responsible for additional spatial modulation of the intensity of the LDOS while preserving its energy dependence.

Frame effects will also be important when the absolute orientation of the lattice changes locally. An example of this effect can be observed in the polarization dependence of the ARPES signal.³⁶ The usual ARPES pictures of Dirac cones see only one half of the cones, due to the form of the matrix element of the lattice electron at the K point with the free electron that comes out. This effect sees the absolute orientation of the lattice: If the lattice is rotated with respect to the polarization of light, the part of the Dirac cone that is observed also rotates. As before, in order to describe the physics in the laboratory frame, vectors in the crystal frame have to be rotated to the laboratory frame. This is again a β -independent contribution. Note, however, that the suppression of part of the observed Dirac cones in ARPES is due to the interference between photoelectrons emitted from the two sublattices and, as such, goes beyond the continuum limit considered in this paper. Effects of local lattice rotations in ARPES have been reported recently in Ref. 37. The frame effects associated with lattice rotations could also be observed in optical experiments like those described in Ref. 38.

IV. CONCLUSIONS

As a summary, we have shown that the TB description of general crystal systems on distorted lattices must be supplemented with geometric terms originating in the change of coordinates needed to describe interactions with external probes. These are of course always present in the experiments. The correct Hamiltonian to use when trying to fit

experiments is $H_{lab} = H_{TB} + H_{Geom}$. The new terms are material independent and different from the usual gauge fields arising from deformation-induced changes in the hopping parameter. We have worked out in detail the case of strained graphene and tried to clarify some confusions in the literature. We have seen that the extra terms are of the same form as those already present in the complete TB Hamiltonian (3), but come with β -independent coefficients. Moreover, aside from the well-known pseudogauge fields in Eq. (2), the only vector field in strained graphene is the connection Γ_i (also present in the geometric formalism³¹), which is compatible with the symmetry analysis³⁹⁻⁴² and required by the Hermiticity of the Hamiltonian whenever we have a position-dependent Fermi velocity. We have clarified that Γ_i is not a gauge field and will not give rise to the standard Landau levels in the density of states, although it may have other physical effects, such as pseudospin precession. We have also shown that the extra gauge fields claimed in Ref. 24 can be gauged away and do not lead to physical consequences. The frame effects described in this work will be relevant to local experiments with resolution $\lambda \gg a$, for which a continuum limit is appropriate.

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APPENDIX: THE TIGHT-BINDING DERIVATION IN THE LABORATORY FRAME

The extra terms to be added to the standard TB calculation due to frame effects can also be obtained by redoing the TB calculation directly in the laboratory frame. That is, we consider the TB Hamiltonian $H = -\sum_{\langle ij \rangle} t_{ij} a_i^\dagger b_j + \text{H.c.}$, but now we map the labels to positions in the laboratory frame

$$H = -t \sum_{\vec{y}, n} a_{\vec{y}}^\dagger b_{\vec{y}+\vec{\delta}_n} + \text{H.c.}, \quad (\text{A1})$$

where $\vec{y} = \vec{x} + \vec{u}(x)$ with $\vec{x} = m_1 \vec{a}_1 + m_2 \vec{a}_2$, and $\vec{\delta}_n$ are the three nearest-neighbor vectors (we follow Ref. 31 for their definition and other conventions). As our interest here is in the β -independent terms generated by the change of frames, we have assumed that the hopping parameters t_{ij} take their equilibrium value t . The real meaning of the relabeling in (A1) is that nonequilibrium atomic positions are used in the Fourier expansions

$$\begin{aligned} a_{\vec{y}}^\dagger &= \sum_k e^{-i\vec{k} \cdot [\vec{x} + \vec{u}(x)]} a_k^\dagger, \\ b_{\vec{y}+\vec{\delta}_n} &= \sum_k e^{i\vec{k} \cdot [\vec{x} + \vec{\delta}_n + \vec{u}(x+\delta_n)]} b_k. \end{aligned} \quad (\text{A2})$$

Note that, due to the fact that crystal momentum \vec{k} is purely two-dimensional, only the in-plane components \vec{u} of a three-dimensional displacement ($\vec{u}(x), h(x)$) will appear in the Fourier expansions in (A2). As a consequence, only the linear piece \tilde{u}_{ij} of the strain tensor can give rise to frame effects, while the out-of-plane contribution $\partial_i h \partial_j h$ does not play any role in this regard. The same conclusion was reached in the main text by noting that only \vec{u} enters the coordinate transformation that relates crystal and laboratory frames.

To see how this will change the effective theory at the K point, it is instructive to analyze a_y further before computing the Hamiltonian. If we restrict the states to $\vec{k} = \vec{K} + \vec{\delta k}$ with $\delta k < \Lambda$, we get

$$a_y = e^{i\vec{K}\cdot\vec{x}} e^{i\vec{K}\cdot\vec{u}(x)} \sum_{\delta k}^{\Lambda} e^{i\vec{\delta k}\cdot\vec{x}} e^{i\vec{\delta k}\cdot\vec{u}(x)} a_k \quad (\text{A3})$$

and, comparing with the corresponding expression $a_x = e^{i(\vec{K}+\vec{\delta k})\cdot\vec{x}} a_k$ in the crystal frame, we observe two new contributions. The first one is $e^{i\vec{K}\cdot\vec{u}(x)}$, which we can factor outside the integral. This is a trivial phase factor that can be reabsorbed into a_y by a gauge transformation and has no effect on the physics. As shown below, if we do not reabsorb this phase, it will show up in the effective theory as a new gauge field $A_i = \partial_i(K_j u_j) = (\tilde{u}_{ij} + \omega\epsilon_{ij})K_j$. But this gauge field has zero curl by construction and produces no pseudomagnetic fields, even for position-dependent strains. The second term $e^{i\vec{\delta k}\cdot\vec{u}(x)}$ cannot be eliminated by a gauge transformation in this way, and will induce extra terms in the Hamiltonian which precisely correspond to those in Eq. (9) after the field rescaling (8) is performed.

Back to the actual computation, plugging (A2) into (A1) gives

$$H = -t \sum_{x,n} \sum_{k,k'} e^{-i\vec{k}\cdot[\vec{x}+\vec{u}(x)]} e^{i\vec{k}'\cdot[\vec{x}+\vec{\delta}_n+\vec{u}(x+\delta_n)]} a_k^\dagger b_{k'} + \text{H.c.} \quad (\text{A4})$$

It is convenient to use a symmetric parametrization for the momenta: $k \rightarrow k + q/2, k' \rightarrow k - q/2$, which corresponds to the symmetric derivative convention in (5). Expanding to linear

order in u yields

$$H = -t \sum_{x,n} \sum_{k,q} e^{-i\vec{q}\cdot\vec{x}} e^{i(\vec{k}-\vec{q}/2)\cdot\vec{\delta}_n} a_{k+q/2}^\dagger b_{k-q/2} \times \left[1 + -\frac{i}{2} \vec{q} \cdot [\vec{u}(x) + \vec{u}(x + \delta_n)] - i\vec{k} \cdot [\vec{u}(x) - \vec{u}(x + \delta_n)] \right] + \text{H.c.}, \quad (\text{A5})$$

which, in terms of the Fourier coefficients of the displacement $u(x) = \sum_q e^{i\vec{q}\cdot\vec{x}} u(q)$, can be rewritten as

$$H = -t \sum_{n,k,q} e^{i(\vec{k}-\vec{q}/2)\cdot\vec{\delta}_n} a_{k+q/2}^\dagger b_{k-q/2} \times \left[\delta(\vec{q}) - \frac{i}{2} \vec{u}(q) \cdot (\vec{q} (1 + e^{i\vec{q}\cdot\vec{\delta}_n}) + 2\vec{k} (1 - e^{i\vec{q}\cdot\vec{\delta}_n})) \right] + \text{H.c.} \quad (\text{A6})$$

Expanding around the K point and performing the sums over n as usual yields the matrix element

$$H_{k,q} = \frac{3ta}{2} [\delta(q)\sigma_i k_i + i q_i u_j(q)\sigma_i (K_j + k_j) - i q_i u_i(q)\sigma_j k_j], \quad (\text{A7})$$

where we have redefined $\delta k \rightarrow k$. Replacing $i q_i u_j(q) = \tilde{u}_{ij}(q) + \omega(q)\epsilon_{ij}$ we finally obtain

$$H_{k,q} = v_0 [\delta(q)\sigma_i k_i + (\tilde{u}_{ij} + \omega\epsilon_{ij})\sigma_i K_j + (\tilde{u}_{ij} + \omega\epsilon_{ij})\sigma_i k_j - \tilde{u}_{ii}\sigma_j k_j]. \quad (\text{A8})$$

The last two terms are precisely those obtained from the direct coordinate transformation (6) and (7) of the continuum Dirac equation before the field rescaling (8), which eliminates the term proportional to \tilde{u}_{ii} . As anticipated, there is also a seemingly new gauge field

$$A_i = (\tilde{u}_{ij} + \omega\epsilon_{ij})K_j = \partial_i(u_j K_j) \quad (\text{A9})$$

which is a total derivative and has zero associated magnetic field.⁴³ It can be completely eliminated by the gauge transformation $\psi \rightarrow e^{-i\vec{K}\cdot\vec{u}(x)}\psi$.

¹A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *Rev. Mod. Phys.* **81**, 109 (2009).

²M. A. H. Vozmediano, M. I. Katsnelson, and F. Guinea, *Phys. Rep.* **496** (2010).

³W. Bao, F. Miao, Z. Chen, H. Zhang, W. Jang, C. Dames, and C. N. Lau, *Nat. Nanotechnol.* **4**, 562 (2009).

⁴M. Teague, A. Lai, J. Velasco, C. Hughes, A. Beyer, M. Bockrath, C. Lau, and N. Yeh, *Nano Lett.* **9**, 2542 (2009).

⁵F. Ding, H. Ji, Y. Chen, A. Herklotz, K. Dorr, Y. Mei, A. Rastelli, and O. G. Schmidt, *Nano Lett.* **10**, 3453 (2010).

⁶M. Huang, H. Yan, T. F. Heinz, and J. Hone, *Nano Lett.* **10**, 4074 (2010).

⁷N. Yeh, M. Teague, S. Yeom, B. L. Standley, R. T.-P. Wu, D. A. Boyd, and M. W. Bockrath, *Surf. Sci.* **605**, 1649 (2010).

⁸H. Tomori, A. Kanda, H. Goto, Y. Ootuka, K. Tsukagoshi, S. Moriyama, E. Watanabe, and D. Tsuya, *Appl. Phys. Express* **4**, 075102 (2011).

⁹T. Georgiou, L. Britnell, P. Blake, R. V. Gorbachev, A. Gholinia, A. K. Geim, C. Casiraghi, and K. S. Novoselov, *Appl. Phys. Lett.* **99**, 093103 (2011).

¹⁰R. Decker, Y. Wang, V. W. Brar, W. Regan, H. Tsai, Q. Wu, W. Gannett, A. Zettl, and M. F. Crommie, *Nano Lett.* **11**, 2291 (2011).

¹¹K. K. Gomes, W. Mar, W. Ko, F. Guinea, and H. C. Manoharan, *Nature (London)* **483**, 306 (2012).

¹²N. N. Klimov, S. Jung, S. Zhu, T. Li, C. A. Wright, S. D. Solares, D. B. Newell, N. B. Zhitenev, and J. A. Stroscio, *Science* **336**, 1557 (2012).

- ¹³H. Suzuura and T. Ando, *Phys. Rev. B* **65**, 235412 (2002).
- ¹⁴N. Levy, S. A. Burke, K. L. Meaker, M. Panlasigui, A. Zettl, F. Guinea, A. H. Castro Neto, and M. F. Crommie, *Science* **329**, 544 (2010).
- ¹⁵F. Guinea, M. I. Katsnelson, and A. G. Geim, *Nat. Phys.* **6**, 30 (2010).
- ¹⁶F. Guinea, A. G. Geim, M. I. Katsnelson, and K. S. Novoselov, *Phys. Rev. B* **81**, 035408 (2010).
- ¹⁷G. Gui, J. Li, and J. Zhong, *Phys. Rev. B* **78**, 075435 (2008).
- ¹⁸V. M. Pereira and A. Castro-Neto, *Phys. Rev. Lett.* **103**, 046801 (2009).
- ¹⁹T. Low, F. Guinea, and M. I. Katsnelson, *Phys. Rev. B* **83**, 195436 (2011).
- ²⁰F. de Juan, A. Cortijo, M. A. H. Vozmediano, and A. Cano, *Nat. Phys.* **7**, 811 (2011).
- ²¹Y. Chang, T. Albash, and S. Haas, *Phys. Rev. B* **86**, 125402 (2012).
- ²²D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).
- ²³B. Wunsch, F. Guinea, and F. Sols, *New J. Phys.* **10**, 103027 (2008).
- ²⁴A. L. Kitt, V. M. Pereira, A. K. Swan, and B. B. Goldberg, *Phys. Rev. B* **85**, 115432 (2012).
- ²⁵M. Oliva-Leyva and G. G. Naumis, arXiv:1212.1760.
- ²⁶J. González, F. Guinea, and M. A. H. Vozmediano, *Phys. Rev. Lett.* **69**, 172 (1992).
- ²⁷J. González, F. Guinea, and M. A. H. Vozmediano, *Nucl. Phys. B* **406**, 771 (1993).
- ²⁸A. Cortijo and M. A. H. Vozmediano, *Eur. Phys. Lett.* **77**, 47002 (2007).
- ²⁹A. Cortijo and M. A. H. Vozmediano, *Nucl. Phys. B* **763**, 293 (2007).
- ³⁰F. de Juan, A. Cortijo, and M. A. H. Vozmediano, *Phys. Rev. B* **76**, 165409 (2007).
- ³¹F. de Juan, M. Sturla, and M. A. H. Vozmediano, *Phys. Rev. Lett.* **108**, 227205 (2012).
- ³²F. Guinea, B. Horovitz, and P. L. Doussal, *Phys. Rev. B* **77**, 205421 (2008).
- ³³P. M. Chaikin and T. C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge, UK, 1995).
- ³⁴As a consequence of the extra i , the vector field Γ_i is odd under time reversal and couples with equal signs at the two Fermi points.
- ³⁵See for example Ref. 44 where the dependence of the pseudomagnetic field on the lattice orientation was explored.
- ³⁶C. Hwang, C. Park, D. A. Siegel, A. V. Fedorov, S. G. Louie, and A. Lanzara, *Phys. Rev. B* **84**, 125422 (2011).
- ³⁷A. L. Walter, A. Bostwick, F. Speck, M. Ostler, K. S. Kim, Y. J. Chang, L. Moreschini, D. Innocenti, T. Seyller, K. Horn, and E. Rotenberg, *New J. Phys.* **15**, 023019 (2013).
- ³⁸V. M. Pereira, R. M. Ribeiro, N. M. R. Peres, and A. H. Castro Neto, *Eur. Phys. Lett.* **92**, 67001 (2011).
- ³⁹J. L. Mañes, *Phys. Rev. B* **76**, 045430 (2007).
- ⁴⁰R. Winkler and U. Zulicke, *Phys. Rev. B* **82**, 245313 (2010).
- ⁴¹T. L. Linnik, *J. Phys.: Condens. Matter* **24**, 205302 (2012).
- ⁴²F. de Juan, J. L. Mañes, M. Sturla, and M. A. H. Vozmediano (unpublished).
- ⁴³Note that the magnetic fields shown in Ref. 24 were computed with the full strain tensor rather than its in-plane part, which is incorrect. The magnetic field is zero by construction (Ref. 45).
- ⁴⁴M. Mucha-Kruczycki and V. I. Fal'ko, *Solid State Commun.* **152**, 1442 (2012).
- ⁴⁵A. L. Kitt, V. M. Pereira, A. K. Swan, and B. B. Goldberg, arXiv:1111.4871.