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Deformation of a graphene sheet: Interaction of fermions with phonons

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We construct an effective low-energy Hamiltonian, which describes fermions dwelling on a deformed honeycomb lattice with dislocations and disclinations, and with arbitrary hopping parameters of the corresponding tight binding model. Despite the presence of dislocations and disclinations, the tight binding Hamiltonian preserves the connectivity number 3 at each lattice site. This construction is related to fermions with a two-dimensional gravity. The effective theory has a local SU(2) gauge invariance of the group of rotations. We reformulate the model by fermions interacting with the deformation as a fermion lattice model with a phonon field and calculate the response of the fermion currents to the external deformation or phonon field. This indicates a Z_2 anomaly. This can be detected experimentally.

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Introduction. The physics of electronic properties of strained [1–8] or lattice deformed graphene [9–15] is an interesting problem, which reveals how concepts of two-dimensional (2D) gravity can penetrate into the condensed matter area. Usually, one argues that deformations and strains give rise to the curvature of the surface of a 2D crystal, which is equivalent to the presence of gravity in a two-dimensional world [16–18]. Moreover, it was argued by Vozmediano *et al.* [9–12] that besides the metric (or gravitational) field, a U(1) gauge field emerges as well. The dynamics of elastic deformations, dislocations, and disclinations of lattices was studied and an effective action for phonons was derived in Refs. [19,21]. In [19], a crumpling phase transition was analyzed. The appearance of 2D gravity in similar problems is not surprising. It is based on the paradigm that any reasonable definition of physical observables on random lattices should be covariant under the appointment of a coordinate system. In other words, the system should be invariant under reparametrization, which leads to the emergence of 2D gravity. Moreover, any other degree of freedom, based on distortions, disclinations, dislocations, and other lattice irregularities, should be governed by reparametrization invariance and the fields describing them should have appropriate transformation properties.

It is known from differential geometry [22] that each random surface can be uniquely parametrized by a field of normal vectors $\hat{n}(\hat{\xi})$, where $\hat{\xi}$ are elements of a two-dimensional coordinate system, and a three-component metric field $g_{\alpha\beta}$, which can be combined into the so-called conformal factor $\rho(\hat{\xi})$. The surface normal vector has two degrees of freedom, which together with $\rho(\hat{\xi})$ give a dual version of three degrees of freedom, $\vec{X}(\hat{\xi})$, of the surface. The normal vector $\hat{n}(\hat{\xi})$ can be identified by the factor SU(2)/U(1) of 3D rotations over O(2) rotations around normal. Therefore, one could expect that the fermions living on the surface should have the reparametrization (2D gravity) and 3D rotational symmetries.

In Refs. [23,24], such theory of Dirac particles, induced from the Clifford algebra in 3D, was constructed. The appearance of SU(2) gauge symmetry in Refs. [23,24] essentially differs from the approach developed in Refs. [9–15] where, besides the gravity, only a U(1) gauge group is present.

We used the induced Dirac action in [25] to study the transport properties of fermions on arbitrary surfaces. However, no formal arguments were given there that the Dirac action is linked to a hopping model on arbitrary bipartite lattices embedded in three spatial dimensions. In this Letter, we will argue that the physics of fermions hopping with arbitrary parameters on a deformed bipartite lattice leads indeed to a Dirac theory [23,24], using an arbitrary lattice with connectivity number 3 at all sites as an example. Considering deformations, disclinations [see Fig. 1(a) as an example], and dislocations [Fig. 1(b)] of a bipartite lattice as an elastic field of phonons, we reduce the problem to the interaction of fermions with phonons and define the corresponding Hamiltonian. We analyze the emerging Z_2 anomaly [34,35,36,39] of this model and show how phonons may produce an anomalous current, which, in principle, can be detected experimentally [26,27].

Model for random deformations of a graphene sheet. We depart from an arbitrary deformation of the honeycomb lattice. For our consideration, it is not important to have an exact honeycomb lattice. We consider a deformed surface which consists of sites with three attached links everywhere, while facets are not necessarily hexagons (there can be all possible \hat{n} -polygons); see Fig. 2

as an example. At each vertex, we consider three independent hopping parameters $t^j(\hat{\xi})$, $j = 1, 2, 3$ for the fermions with the Hamiltonian

$$H = \sum_{j,\hat{\xi}} t^j \{ \psi_A^\dagger[\vec{X}(\hat{\xi} + \hat{\mu}_j)] \psi_B[\vec{X}(\hat{\xi})] + \psi_B^\dagger[\vec{X}(\hat{\xi}^\alpha)] \psi_A[\vec{X}(\hat{\xi} + \hat{\mu}_j)] \}, \quad (1)$$

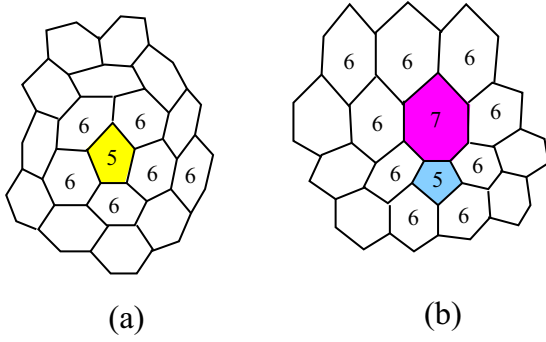


FIG. 1. (a) A disclination leading to the appearance of a pentagon and (b) a dislocation created by a pentagon/heptagon pair.

where A and B refer to the natural partition of the honeycomb lattice into sublattices and $\vec{X}(\hat{\xi})$ is a 3D coordinate vector of 2D lattice site $\hat{\xi}$. Vector $\hat{\mu}_j$ connects neighboring sites on the parametric space and represents the difference of the coordinates of neighboring sites in a patch. Because we are going to consider arbitrarily deformed lattices, it is not possible to introduce any unique 2D Cartesian coordinate system for the entire lattice. As for the manifolds, we cover the whole lattice by a system of patches U_a , in which each of them envelops three neighboring sites. They may have an overlap region $U_a \cap U_b$ covering neighboring links or a single site. An example of such coverings U_1, U_2 is presented in Fig. 2. Inside of each U_a , we have Cartesian coordinate systems which are connected by differentiable functions, $\hat{\xi}^{(a)} = f^{(ab)}[\hat{\xi}^{(b)}]$. This reparametrization transformation defines the gluing rules of the points in the overlap region. Because we are going to formulate a reparametrization invariant theory, it will have a well-defined Hamiltonian, which depends on points, but not on the coordinate system. This also means that we will have a 2D gravity theory. An important remark is in order here: In place of the honeycomb lattice, other bipartite lattices can be considered within this very formalism. The Hamiltonian (1) can be generalized for this case using an arbitrary connectivity l , i.e., the number of lattice links associated with lattice site $\hat{\xi}$, which is not necessarily 3 as for the honeycomb lattice. Then the sum over j in Eq. (1) and in all the formulas below should run from 1 to l . In the subsequent discussion, however, we will focus on the honeycomb lattice.

It is clear that by two local rotations in 3D along the hopping links, we can make triangles in each patch paral-

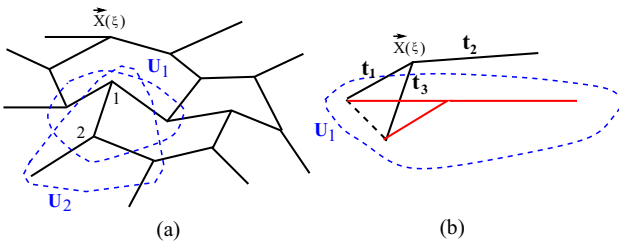


FIG. 2. (a) An example of a random honeycomb lattice in 3D with two patches U_1 and U_2 , which cover neighboring vertices 1 and 2. The link (1,2) is common for two patches. (b) Three-dimensional vertex $\vec{X}(\hat{\xi})$ (black) and its projection on a flat space by rotation (red).

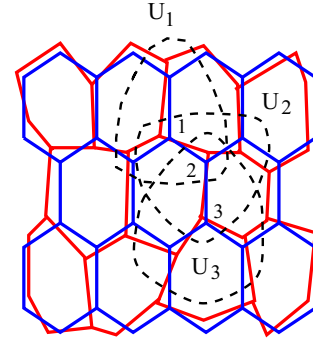


FIG. 3. Flattened random honeycomb lattice (red) and its reparametrization (deformation) to a regular one (blue). Dotted black lines emphasize patches U_1, U_2, U_3 , which cover vertices 1, 2, 3 together with associated links.

lel to the (x, y) plain. Each of such links contains a pair of fermions, $\Psi[\vec{X}(\hat{\xi})] = \{\psi_A[\vec{X}(\hat{\xi})], \psi_B[\vec{X}(\hat{\xi})]\}$, in the corresponding U_a . As pairs of complex numbers, $\psi_{A,B}$ form the space of spinor representations of the rotation group $SU(2)$, where group elements $\Omega_a[\vec{X}(\hat{\xi})]$ act in each patch a . Generally, the rotations on different patches are different. But in the overlap region, they are connected by rotations $\Omega_{ab} = \Omega_b[\vec{X}(\hat{\xi}^{(b)})]\Omega_a^{-1}[\vec{X}(\hat{\xi}^{(a)})]$, which gives rules of gluing of the tangential vectors on different patches. For some types of disclinations and dislocations, which locally break the (A,B) -bipartite division of the lattice, i.e., when the (A,B) -notion of the sites 1 and 2 of the common link of patches U_1 and U_2 [see Fig. 1(a)] becomes incompatible, the gluing field $\Omega_1[\vec{X}(\hat{\xi}^{(1)})]$ will contain a 3D rotation $e^{i\pi\sigma_1/2} = i\sigma_1$, which changes the helicity on the 2D patch and ensures the correct gluing. Therefore, besides the reparametrization symmetry, our Hamiltonian should also have a local gauge $SU(2)$ symmetry. In Fig. 3, we visualize the flat projection of the random lattice surface in 3D (marked red), which can be reparametrized as a regular honeycomb lattice (marked blue). Black dotted lines emphasize the open disk patches of the Cartesian coordinate systems.

After a rotation, the 3D lattice becomes a flat but deformed lattice in 2D with connectivity 3, while our Hamiltonian (1) in a 2D basis space becomes

$$H = \frac{1}{2} \sum_{\hat{\xi}} \sum_{j=1}^3 t^j \Psi'^{\dagger}(\hat{\xi}) \Omega^+[\vec{X}(\hat{\xi})] \sigma_1 \times [e^{-\overleftarrow{\partial} \cdot \hat{\mu}_j \sigma_3} + e^{\sigma_3 \hat{\mu}_j \cdot \overrightarrow{\partial}}] \Omega[\vec{X}(\hat{\xi})] \Psi'(\hat{\xi}), \quad (2)$$

where left/right arrows above the partial derivative operators point into the direction of their action and $\sigma_{1,3}$ are Pauli matrices. It is important to emphasize here that fermions in (1) live in three dimensions and, after the rotation of A and B sublattice points on a surface in 3D with coordinates $\vec{X}(\hat{\xi})$, they become $\Psi[\vec{X}(\hat{\xi})] = \Omega[\vec{X}(\hat{\xi})] \Psi'(\hat{\xi})$ (below we omit the notion prime in Ψ'). Any deformation of the surface from $X_1(\hat{\xi})$ to $X_2(\hat{\xi})$ in Eq. (2) can be expressed by the transformation

$$\Psi[\vec{X}_2(\hat{\xi})] = \Omega[\vec{X}_1(\hat{\xi}), \vec{X}_2(\hat{\xi})] \Psi[\vec{X}_1(\hat{\xi})] \quad (3)$$

of the fermionic fields, with

$$\Omega[\vec{X}_1(\hat{\xi}), \vec{X}_2(\hat{\xi})] = \Omega[\vec{X}_2(\hat{\xi})]\Omega^{-1}[\vec{X}_1(\hat{\xi})]. \quad (4)$$

This demonstrates the presence of hidden SU(2) invariance of the Hamiltonian (1). In general, a conditional expression for the existence of a pair of Dirac nodes on such random lattice reads

$$\sum_{j=1}^3 t^j e^{i\hat{\mu}_j \cdot \vec{K}} = 0, \quad (5)$$

with the local, patch-dependent momentum \vec{K} . In the Supplemental Material [20], we demonstrate, by an explicit calculation, the existence of \vec{K} for a randomly deformed honeycomb lattice. The analysis presented there can also be extended to larger connectivity.

The local definition (5) can be approximated by assuming only small deformations. Then we could expand around the \vec{K} and \vec{K}' points of the regular honeycomb lattice [9–15]. In the following, we will not employ such an approximation, but expand the fermion field in low-energy modes around the nodes defined in Eq. (5). Then we shift the derivatives in the exponents in (2) by $\theta_j = \hat{\mu}_j \cdot \vec{K}$ and replace $\hat{\mu}_j \cdot \vec{\partial} \rightarrow i\theta_j + \hat{\mu}_j \cdot \vec{\partial}$ and $-\hat{\mu}_j \cdot \vec{\partial} \rightarrow i\theta_j - \hat{\mu}_j \cdot \vec{\partial}$. By doing this and taking into account that the vectors $\hat{\mu}_j$ are proportional to the minimal length scale of the lattice ε , we can expand the translation operators $e^{-\vec{\partial} \cdot \hat{\mu}_j}$ and $e^{\vec{\partial} \cdot \hat{\mu}_j}$ and keep only the linear terms.

In order to expand the exponent, one should first decouple in the exponential term θ_j from the derivatives by using the Campbell-Hausdorff formula [22]. Then a commutator term will appear. However, the commutator terms from the two exponents cancel each other. Eventually, by taking into account that the constant term in this expansion is zero due to Eq. (5), the low-energy Hamiltonian becomes

$$H = \frac{i}{2} \sum_{j, \hat{\xi}} \Psi^+(\hat{\xi}) \Omega^+[\vec{X}(\hat{\xi})] t^j (\cos \theta_j \sigma_2 - \sin \theta_j \sigma_1) \times [\hat{\mu}_j \cdot \vec{\partial} - \vec{\partial} \cdot \hat{\mu}_j] \Omega[\vec{X}(\hat{\xi})] \Psi(\hat{\xi}), \quad (6)$$

which depends on the nodes of the randomly deformed honeycomb lattice θ_j . The θ_j -dependent terms can be cast into the new parameters

$$\begin{aligned} \varepsilon \hat{e}^2 &= \sum_j t^j \hat{\mu}_j \cos \theta_j, \\ \varepsilon \hat{e}^1 &= - \sum_j t^j \hat{\mu}_j \sin \theta_j, \end{aligned} \quad (7)$$

where we can consider elements of \hat{e}^a , $a = 1, 2$ as tetrads of 2D gravity. Then the fermionic Hamiltonian reads

$$H = \frac{i\varepsilon}{2} \sum_{\hat{\xi}} e \Psi^+(\hat{\xi}) \Omega^+[\vec{X}(\hat{\xi})] \sigma^\alpha \times (\vec{\partial}_\alpha - \overleftarrow{\partial}_\alpha) \Omega[\vec{X}(\hat{\xi})] \Psi(\hat{\xi}), \quad (8)$$

where e is the determinant of the tetrads element $e^{\alpha a}$ and ε is the minimal length scale of the lattice and $\sigma^\alpha = e^{\alpha a} \sigma_a$. By using an ambiguity of the coordinate vectors $\hat{\mu}_j$, one can

associate tetrads $e^{\alpha a}$ with the induced metric of the surface, $g_{\alpha\beta} = \partial_\alpha \vec{X} \partial_\beta \vec{X}$. Namely, we can fix the coordinate vectors $\hat{\mu}_j$ in such a way that

$$\partial_\alpha \vec{X} \partial_\beta \vec{X} = \sum_{a=1,2} e_a^\alpha e_a^\beta, \quad (9)$$

where $e_a^\alpha = [e^{\alpha a}]^{-1}$, defined in Eq. (7).

The Hamiltonian (8) coincides with the Hamiltonian of the Dirac theory on 2D random surfaces induced from 3D flat Dirac theory with an Euclidean metric defined in Refs. [23,24]. It was shown that by defining the induced gamma matrices as $\hat{\gamma}_\alpha = \partial_\alpha \vec{X} \hat{\gamma}$ ($\hat{\gamma}$ are 3D Dirac γ -matrices) and a 3D rotation, one arrives at the simpler Hamiltonian

$$H = \frac{i}{2} \int d\hat{\xi} \sqrt{g} \Psi^+(\hat{\xi}) \hat{\gamma}^\alpha (\vec{\partial}_\alpha - \overleftarrow{\partial}_\alpha) \Psi(\hat{\xi}), \quad (10)$$

where $g = \det[g_{\alpha\beta}]$. This expression shows that besides 2D gravity, we also have local 3D rotations, which induce a non-Abelian SU(2) gauge field. Transforming the left differential in (10) to the right one, we obtain

$$H = i \int d\hat{\xi} \sqrt{g} \Psi^+(\hat{\xi}) \left(\hat{\gamma}^\alpha \partial_\alpha + \frac{1}{2} \nabla_\alpha \hat{\gamma}^\alpha \right) \Psi(\hat{\xi}), \quad (11)$$

where ∇_α is a covariant derivative defined by Christoffel symbols [22]. The term $\nabla_\alpha \hat{\gamma}^\alpha = \sqrt{g} h_\alpha^\alpha \hat{n}$ is connected with the second quadratic form $h_{\alpha\beta} = \vec{n} \nabla_\alpha \partial_\beta \vec{X}$, where $\vec{n} = \sqrt{g} \partial_1 \vec{X} \times \partial_2 \vec{X}$ is the vector normal to the surface at $\hat{\xi}$. In Ref. [25], Hamiltonian (11) was used to calculate the optical conductivity of the fermions on a random surface.

Phonon-fermion interaction. Our goal is to understand how the Hamiltonian (11) on a deformed lattice can be related to static phonons, interacting with fermions on a graphene sheet. The phonon field is the field of elastic deformations of the graphene sheet, $\vec{X}(\hat{\xi})$ [11,12,28]. On a flat regular honeycomb lattice background, we write

$$\vec{X}(\hat{\xi}) = \xi^a \vec{a}_a + \vec{u}(\hat{\xi}), \quad (12)$$

where \vec{a}_a , ($a = 1, 2$) are two basic vectors on a flat plane and $\vec{u}(\hat{\xi})$ is the phonon field. The differential operator $\mathcal{D} = \hat{\gamma}^\alpha \partial_\alpha + \frac{1}{2} \nabla_\alpha \hat{\gamma}^\alpha$, which appears between fermionic fields in the Hamiltonian (11), reads, in lowest order of the phonon field,

$$\sqrt{g} \mathcal{D} = iT \sigma_a \partial_a + iT_a^j \sigma_j \partial_a + \sigma_a A_a + \sigma_3 M. \quad (13)$$

Here the coefficient T reads

$$T = 1 + u_{aa} + \frac{1}{2} (u_a^3)^2 + \frac{1}{2} (u_a^a u_b^b - u_b^a u_a^b) + \mathcal{O}(u^3), \quad (14)$$

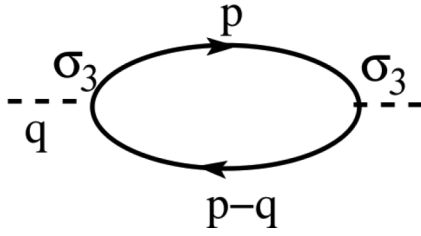
and the middle term with the gradient deformation tensor is

$$T_a^j = (1 + u_b^b) \partial_a u^j - u_b^j (\partial_a u_b^b + u_b^a) + \mathcal{O}(u^3), \quad (15)$$

while $\sqrt{g} = 1 + u_{aa}$.

The covariant derivatives of Eq. (13) coincide with those proposed in the model of electron-phonon interaction in Refs. [29,30]. Here and below, the repeated indices denote summations over $a, b = 1, 2$ and $i, j = 1, 2, 3$, respectively.

Formally, M can be considered as a mass term, while A_a , $a = 1, 2$ are components of a U(1) gauge field that

FIG. 4. One-loop Feynman diagram for $\langle j_3 j_3 \rangle$ correlator.

emerged due to the deformations of the honeycomb lattice. These quantities read, up to second order in the field u ,

$$M = \frac{1}{2} [\partial_a^2 u^3 + \partial_a u^a \partial_a^2 u^3 - \partial_a^2 u^b u_b^3], \quad (16)$$

$$A_a = -\frac{1}{2} [\partial_a u^3 \partial_b^2 u^3 + \partial_b^2 u^\sigma (\partial_a u^\sigma + \partial_\sigma u^a)]. \quad (17)$$

One recognizes that the lowest linear order in the phonon field u contributes only to the mass term, while the emerging U(1) gauge field appears in quadratic order of u .

The mass term $M\sigma_3$ in Eq. (13) can be interpreted as a current j_3 that couples to the fermions. In order to get an effective functional integral for the phonon field, we integrate over the fermion field. Adopting the dimensional regularization scheme, one obtains, in one-loop order (cf. Fig. 4 [31–33]),

$$S_N(M) = \frac{1}{8} \int \frac{d^3 k}{(2\pi)^3} \sqrt{k_0^2 + \mathbf{k}^2} M_k M_{-k}. \quad (18)$$

In deriving this expression, one has to keep in mind that σ_3 does not commute with the fermionic propagator; cf. the Supplemental Material [20]. Plugging the Fourier transformed M from (16) into (18), we get the contribution to the phonon action induced by the fermion-phonon interaction. The leading order in this action is quadratic in phonon field u coming from the linear term in (16). Another contribution to the effective action of phonons from quantum fluctuations comes from the anomalous current-current correlators $\langle j_a j_b \rangle$, corresponding to the remaining two spacelike components of the gauge field $A_{a=1,2}$. According to the seminal works of Redlich [31,34], Semenoff [35], and Jackiw [36], the effective action reads

$$S_A(A) = -i \text{sgn}(m) \epsilon_{ab} \int d\tau d^2 x A_a \partial_\tau A_b, \quad (19)$$

where $\text{sgn}(m)$ refers to an infinitesimally small, bare mass parameter m , which was introduced to regularize the infrared divergence and sent to zero after the integration. Plugging (17) into $S_A(A)$, we will get another term in the effective action of phonons, which is quartic in u , coming from the leading

quadratic order of A_a . This term is generated by a chiral Z_2 anomaly. The variation of the action given by Eq. (19) with respect to A_a creates an anomalous current,

$$j_a = -i \text{sgn}(m) \epsilon_{ab} \partial_\tau A_b. \quad (20)$$

The sign (or Z_2) ambiguity of the mass reflects the fact that the mass parameter must not necessarily be positive. As is always the case with anomalies in perturbative approaches, the anomalous current given by Eq. (20) appears because the regulator violates the chiral symmetry of the model given by Eq. (11) explicitly. Due to the finite bandwidth of our lattice model, there is no need for an ultraviolet regularization here. In this case, the chiral symmetry is preserved and the anomalous currents cancel each other due to fermion species doubling [37]. However, if the dynamics of the phonons is included in the model, the breaking of the chiral symmetry can occur spontaneously, provided that the phonon-phonon interaction strength exceeds a certain critical value. Then there will be no cancellations between the \vec{K} and \vec{K}' points. This mechanism was recently investigated by two of us in Refs. [29,30,38].

Conclusions. In this Letter, we construct a low-energy theory of fermions interacting with deformations of the honeycomb lattice. In contrast to similar studies reported recently in Refs. [9–15], where fermions are bound to the flat but distorted sheets, we investigate the case when the effective gauge fields are induced by embedding of a two-dimensional surface into a three-dimensional Euclidean space [23,24]. In addition to the U(1) gauge fields and interaction with 2D gravity of the former approaches, our effective theory reveals a non-Abelian SU(2) gauge field. We reduce the 2D gravity (metric) field to deformations of the 3D lattice, which forms three-dimensional phononic fields. The calculation of a Z_2 anomaly links the current of the fermions with phononic field strength, which, in principle, can be detected experimentally. It remains for the future to extend the formalism presented here to the curved spaces. The ultimate goal may be to establish an effective low-energy field theory of phonons in the spirit of effective Liouville actions [16,40] accompanied by induced topological (Chern-Simons or Hopf) terms [23,24]. To an extent, a number of intermediate ideas in terms of mathematical modeling and its effect on transport were successfully realized in [25].

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