

## Discrete differential geometry and the properties of conformal two-dimensional materials



Salvador Barraza-Lopez

Department of Physics, University of Arkansas, Fayetteville, AR 72701, USA

### ARTICLE INFO

#### Article history:

Received 24 January 2015

Received in revised form 24 June 2015

Accepted 28 June 2015

Available online 19 July 2015

#### Keywords:

Discrete geometry

Graphene

Two-dimensional materials

### ABSTRACT

Two-dimensional materials were first isolated no longer than ten years ago, and a comprehensive understanding of their properties under non-planar shapes is still being developed. Strictly speaking, the theoretical study of the properties of graphene and other two-dimensional materials is the most complete for planar structures and for structures with small deformations from planarity. The opposite limit of large deformations is yet to be studied comprehensively but that limit is extremely relevant because it determines material properties near the point of failure. We are exploring uses for discrete differential geometry within the context of graphene and other two-dimensional materials, and these concepts appear promising in linking materials properties to shape regardless of how large a given material deformation is. A brief account of additional contributions arising from our group to two-dimensional materials that include graphene, stanene and phosphorene is provided towards the end of this manuscript.

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Geometry is a pillar of Science, and many physical theories are decidedly geometric [1]. This manuscript provides an overview of recent developments towards linking the properties of two-dimensional materials to a given arbitrary shape, where *shape* is understood as the local two-dimensional geometry of atom-thin materials that are embedded on a three-dimensional space. The unifying point of the description concerns the introduction of a discrete geometry to deal with two-dimensional materials while fully preserving their atomistic information.

Thus, we showcase here a set of geometrical principles that apply to nets, where a *net* is a discrete surface or a mesh. We identify two-dimensional materials with *meshes*, and apply precepts from a branch of Mathematics [2] that deals with discrete surfaces. We have presented a number of results in linking this geometry to materials properties already [3–7]. This subject has contributions from other teams as well [8–10].

I acknowledge Drs. Pacheco SanJuan, Wang, Harriss, Rivero, Vanević, and Terrones' contributions to this ongoing work. I also thank students Sloan, Horvath, Utt, Pour-Imani, Mehboudi, and Klee for their contributions at different stages. I am grateful to many colleagues for their observations and encouragement; most particularly to María A.H. Vozmediano.

Graphene and other 2-D materials provide a stage to further our understanding of Physics. Perhaps the most natural

connection to be studied concerns the creation of gauge fields on effective Dirac particles in 2+1 dimensions as the geometry evolves from a reference, planar shape [11–13], to be addressed next.

The starting point for us was the analysis of strain created by a scanning tunneling microscope (STM) on graphene [18]. There is a theory laid out on a structural continuum [22,11–17] that correlates structural deformations to mechanically-induced gauges on Dirac fermions in 2+1 dimensions. These effective Dirac fermions arise from a first nearest neighbor tight-binding description of  $\pi$ -electrons on graphene at low energies. Changes in distances arising from a structural deformation are estimated from a continuum model of the distortion, and these changes in distances alter the magnitude of the tight-binding hopping terms locally.

The formulation is inherently semi-classical, in the sense that the underlying dynamics is that of pseudospins (which strictly speaking are only valid on the ideal non-deformed crystalline structure) and the gauge fields produced by mechanical deformations induce local modifications to the  $\pi$ -electron pseudospin Hamiltonian. We estimated gauge fields employing that formalism [11–13] but this question quickly came up:

1. An STM can tell individual atoms. Can one rewrite the theory expressed on a continuum structure to reflect such atomistic nature? What do we learn when the theory is laid out this way that is different from the continuum formalism?

E-mail address: [sbarraza@uark.edu](mailto:sbarraza@uark.edu)

This paper contains three sections that are somehow independent: (1) Its main thrust is the description of the coupling of finite displacements to a semiclassical pseudospin dynamics of  $\pi$ -electrons on graphene in which we attempt to provide an answer to the question above (pages 2–5). (2) We then provide a description of a discrete geometry that applies to arbitrary two-dimensional materials (pages 5–7). (3) The document ends by briefly mentioning other developments in graphene and other materials in which we have been involved (pages 8–10).

## 1. A lattice gauge field theory for Dirac fermions in graphene

The interplay among the electronic and mechanical properties of graphene membranes remains under experimental and theoretical investigation [11–13,19–23], and an insightful picture of the effects of deformations employs gauge fields that influence the dynamics of charge carriers [11–13,21,22].

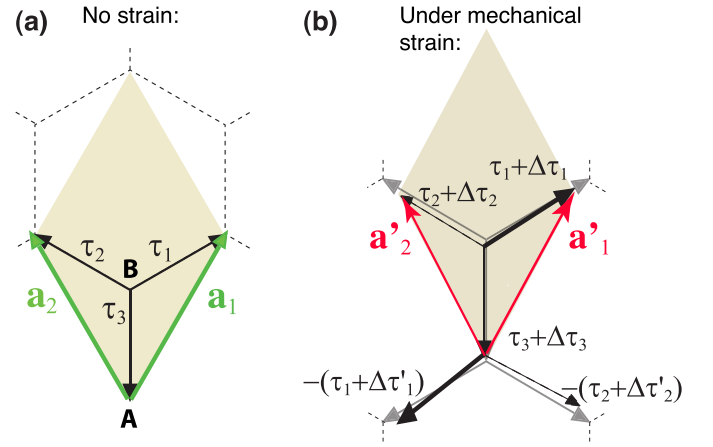
The formulation is inherently semi-classical and takes pseudospin hamiltonians as the main object, which strictly speaking are only valid on the ideal non-deformed crystalline structure, with gauge fields arising from slow-varying mechanical deformations providing local modifications to the said Hamiltonian.

But graphene can sustain elastic deformations as large as 20% [24] and using this picture, the resulting pseudo-magnetic fields are much larger than those magnetic fields available in state-of-the-art experimental facilities. The presence of a pseudo-magnetic field is observed via broad Landau levels (LLs) in strained graphene nanobubbles on a metal substrate [25]. In addition to the pseudo-magnetic vector potential  $\mathbf{A}_s$ , strain also induces a scalar deformation potential  $E_s$  [22,26,27] that affects the electron dynamics in non-trivial ways. Part of our motivation was to reconcile the experimental results that can be obtained when the lattice is largely deformed, with a theory that by construction applies to small deformations. What we accomplished is a close view at the inner workings of this theory that has led to unique insights, and a quantitative understanding of “slowly varying deformations” within the context of this theory. Our formulation brings to the spotlight some of the inherent assumptions on the prevailing theoretical framework.

The underlying assumptions of the theory expressed on a structural continuum are expressed in the following sentence: “If a mechanical strain varies smoothly on the scale of interatomic distances, it does not break sublattice symmetry but rather deforms the Brillouin zone in such a way that the Dirac cones located in graphene at points  $K$  and  $K'$  are shifted in opposite directions [12].”

Previous statement tells us that – *provided strain preserves sublattice symmetry* – one can understand the effects of mechanical strain on the electronic structure in terms of a semiclassical approach, in which mechanical strain induces the spatially-varying gauge fields  $B_s(\mathbf{r}) = \nabla \times \mathbf{A}_s(\mathbf{r})$  and  $E_s(\mathbf{r})$  into a spatially-varying pseudospin Hamiltonian  $\mathcal{H}_{ps}(\mathbf{q}, \mathbf{r})$ , where  $\mathcal{H}_{ps}(\mathbf{q})$  is the low-energy expansion of the Hamiltonian in reciprocal space in the absence of strain. This semiclassical approximation is justified when the strain extends over many unit cells and it preserves sublattice symmetry [12,13,22], and many of the equations on this Section will help us keep track of said sublattice symmetry.

Evidently, it is possible to determine the electronic properties directly from a tight-binding Hamiltonian  $\mathcal{H}$  in real space, without resorting to the semiclassical approximation and without imposing a sublattice symmetry *a priori*. That is, while the semiclassical  $\mathcal{H}_{ps}(\mathbf{q}, \mathbf{r})$  is defined in reciprocal space (thus assuming some reasonable preservation of crystalline order), the tight-binding Hamiltonian  $\mathcal{H}$  in real space is more general and can be used for



**Fig. 1.** (a) Definitions of geometrical parameters in a unit cell. (b) Sublattice symmetry relates to how pairs of nearest-neighbor vectors (either in thick, or dashed lines) are modified due to strain. These vectors change by  $\Delta\tau_j$  and  $\Delta\tau'_j$  upon strain ( $j = 1, 2$ ). Relative displacements of neighboring atoms lead to modified lattice vectors; the choice of renormalized lattice vectors will be unique *only* to the extent to which sublattice symmetry is preserved:  $\Delta\tau'_j \simeq \Delta\tau_j$ .

membranes with arbitrary spatial distribution and magnitude of the strain.

In the previous formulation of the theory both  $\mathbf{A}_s$  and  $E_s$  are expressed in terms of a *continuous* displacement field  $\mathbf{u}(x, y)$  obtained within first-order continuum elasticity (CE) [11–13,22]. It is not possible to assess sublattice symmetry on a continuum media, and therefore proper phase conjugation of pseudospin Hamiltonians becomes an implicit assumption of that theory.

But the only way to know whether the strain preserves sublattice symmetry [12] implies analyzing relative atomic displacements in arbitrary structural distortions that could be captured directly from experiment [28], or from molecular dynamics simulations.

Let us start by considering the unit cell before (Fig. 1(a)) and after arbitrary strain has been applied (Fig. 1(b)). The lattice vectors and the vectors joining atoms are given by (Fig. 1(a)):

$$\mathbf{a}_1 = (1/2, \sqrt{3}/2)a_0, \quad \mathbf{a}_2 = (-1/2, \sqrt{3}/2)a_0, \quad (1)$$

$$\boldsymbol{\tau}_1 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \frac{a_0}{\sqrt{3}}, \quad \boldsymbol{\tau}_2 = \left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \frac{a_0}{\sqrt{3}}, \quad \boldsymbol{\tau}_3 = (0, -1) \frac{a_0}{\sqrt{3}}, \quad (2)$$

before the deformation takes place. When a deformation is applied (Fig. 1(b)) the two off-diagonal terms making up the pseudospin tight-binding Hamiltonian will be:

$$-\sum_{j=1}^3 (t + \delta t_j(\Delta\tau_j)) e^{i(\boldsymbol{\tau}_j + \Delta\tau_j) \cdot \mathbf{k}},$$

and

$$-\sum_{j=1}^3 (t + \delta t'_j(\Delta\tau'_j)) e^{i(\boldsymbol{\tau}'_j + \Delta\tau'_j) \cdot \mathbf{k}},$$

where  $t$  is the hopping term,  $\delta t$  is its change upon strain to be explicitly defined later on, and  $\mathbf{k}$  is the crystal momentum.

Each local pseudospin Hamiltonian will only have physical meaning when it is properly conjugated, which implies sublattice symmetry holds. This happens at unit cells where:

$$\Delta\tau'_j \simeq \Delta\tau_j \quad (j = 1, 2). \quad (3)$$

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