Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2022-0011

Vol. **34**, No. 1, pp. 235-260
July 2023

Inverse Design of Strained Graphene Surfaces for Electron Control

François Fillion-Gourdeau[1], Emmanuel Lorin[2,3,1] and Steve Maclean[1]

[1] *Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada, N2L 3G1.*
[2] *School of Mathematics and Statistics, Carleton University, Ottawa, Canada, K1S 5B6.*
[3] *Centre de Recherches Mathématiques, Université de Montréal, Montréal, Canada, H3T 1J4.*

Received 11 January 2022; Accepted (in revised version) 29 August 2022

Abstract. This paper is devoted to the inverse design of strained graphene surfaces for the control of electrons in the semi-classical optical-like regime. Assuming that charge carriers are described by the Dirac equation in curved-space and exploiting the fact that wave propagation can be described by ray-optics in this regime, a general computational strategy is proposed in order to find strain fields associated with a desired effective refractive index profile. The latter is first determined by solving semi-classical trajectories and by optimizing a chosen objective functional using a genetic algorithm. Then, the graded refractive index corresponding to the strain field is obtained by using its connection to the metric component in isothermal coordinates. These coordinates are evaluated via numerical quasiconformal transformations by solving the Beltrami equation with a finite volume method. The graphene surface deformation is finally optimized, also using a genetic algorithm, to reproduce the desired index of refraction. Some analytical results and numerical experiments are performed to illustrate the methodology.

AMS subject classifications: 35Q41, 81Q05, 81Q20, 78A05

Key words: Graphene, isothermal coordinates, Beltrami equation, gravitational lens, waveguide, finite volume method, genetic algorithm, Dirac equation.

1 Introduction

Straintronics, the control of electronic states by straining graphene and other 2D materials, has seen a surge of interest in the last decade because it promises new interesting

[1]Corresponding author. *Email addresses:* `francois.fillion@inrs.ca` (F. Fillion-Gourdeau), `elorin@math.carleton.ca` (E. Lorin), `steve.maclean@inrs.ca` (S. Maclean)

physics [1–6] and because it has potential for applications, such as the Dirac fermion microscope [7]. When graphene is deformed or stretched, the interatomic distance is locally modified which in turn, changes the tight-binding description since the value of overlap integrals depends on the atomic position. Remarkably, this theoretical framework reduces to the 2D curved-space Dirac equation in the low-energy limit [8–12], allowing for analogies between matter-gravity coupling theories and material science [13–15].

Understanding the behaviour of electrons in strained graphene is a challenging task, even in the low energy limit, because it requires a solution to the curved-space Dirac equation coupled to an emergent pseudo-electromagnetic field. This equation has been solved in the time-independent case to characterize static properties of charge carriers [16–19]. In particular, this approach, along with other ones based on the tight-binding model [20], applied to homogeneously strained graphene has led to the discovery of Landau-like energy levels generated by large pseudo-magnetic fields that can reach up to 300 T [21]. The dynamic case, on the other hand, has not been investigated as thoroughly, in part because obtaining solutions to the time-dependent curved-space Dirac equation is more challenging (see [22]). Nevertheless, some recent studies have tackled this challenge and demonstrated that wave packets can be manipulated by scattering on strained regions [17,23,24]. For example, using numerical approaches, it was shown that electron wave packets can be confined [25] or focused [26,27].

In this work, we consider electron scattering over strained regions in the semi-classical and low-energy ($\lesssim$2 eV) limit. The main goal is the inverse design of specific strain fields to steer and control charge carriers for applications in graphene nanoelectronics. To reach this goal, a set of numerical techniques is developed. Throughout the article, the effect of the pseudomagnetic field is neglected, allowing us to introduce isothermal coordinates to describe the strained surface. The interest of working in isothermal coordinates is that its metric components can be interpreted physically as a graded index of refraction in the semi-classical approximation. The counterpart is that the construction of the metric tensor in isothermal coordinates requires the solution to the Beltrami equation, a first order system of partial differential equations. In this paper, this equation is numerically solved using a least-square cell-centered finite volume method, which offers a simple and flexible framework to solve partial differential equations with a reasonable accuracy. More importantly, however, is that it offers a direct connection between the strain field and the refractive index via semi-classical trajectories. We demonstrate that this feature can be exploited to inverse design strain fields by combining this approach with a standard metaheuristic optimization technique.

The paper is organized as follows. In Section 2, the curved-space Dirac equation in isothermal coordinates and its semi-classical limit are reviewed. In Section 3, we present the general strategy used for the inverse design of strained surfaces. Section 4 is devoted to the optimization algorithm allowing to construct a desired graded index of refraction. A numerical scheme to solve the Beltrami equation is introduced in Section 5. We then propose an original optimization method for parameterizing the surface corresponding to the desired index of refraction in Section 6. In Section 7, we propose some numerical