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Frozen Gaussian Approximation for the Dirac Equation in Curved Space with Application to Strained Graphene

Lihui Chai[1], Lorin Emmanuel[2,*] and Xu Yang[3]

[1] *School of Mathematics, Sun Yat-sen University, Guangzhou, China.*
[2] *School of Mathematics and Statistics, Carleton University, Ottawa, Canada. Centre de Recherches Mathématiques, Université de Montréal, Montréal, Canada.*
[3] *Department of Mathematics, University of California, Santa Barbara, USA.*

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Abstract. In this paper, we derive the frozen Gaussian approximation (FGA) for computing the solution to the Dirac equation in curved space in the semi-classical regime. The latter equation is used in particular for modeling electronic scattering on strained graphene surfaces. We present numerical comparisons of the Dirac solutions on curved and flat spaces, illustrating the focusing effect of graphene surfaces, as well as qualitative comparisons with a tight-binding model. A CPU-time comparison shows that FGA becomes more efficient than an IMEX pseudospectral method when the semiclassical parameter is small.

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

Key words: Dirac equation, semi-classical regime, frozen Gaussian approximation, strained graphene.

1 Introduction

In this paper, we are interested in computing the solution of a massless two-dimensional Dirac equation in curved space in the low energy limit (semi-classical regime), modeling electron motions on strained graphene surfaces [5, 9, 22, 25, 26]. Some connections with refractive optics can also be obtained through Evans' model [13]. Mathematically, the Dirac equation in curved space is a non-conservative first-order hyperbolic system.

*Corresponding author. *Email addresses:* chailihui@mail.sysu.edu.cn (L. Chai), elorin@math.carleton.ca (E. Lorin), xuyang@math.ucsb.edu (X. Yang)

Although the Dirac equation under consideration is linear, it has non-constant (space-dependent) coefficients and possesses, compared to the Dirac equation in flat space, additional order-zero terms (corresponding physically to spin connections); see [14]. The latter is, however, perturbative in the semi-classical regime.

The Frozen Gaussian Approximation (FGA) is one of the most accurate and efficient methods for computing the solution to wave equations, including the Dirac equation, in the semi-classical regime. FGA was first developed by Herman-Kluk (HK) [16] for computing the solution to the Schrödinger equation in the semi-classical regime, and it was mathematically analyzed in [27]. More recently, the HK-formalism was used and analyzed to derive fast numerical solvers in the semi-classical regime for different classes of partial differential equations: the Schrödinger equation [32], the classical wave equation [19,20] and general linear hyperbolic systems of conservation laws [21]. The analysis of FGA for the Dirac equation in flat space was given in [7], and an alternative efficient Gaussian beam method was proposed in [31] for solving the Dirac equation in flat space in the semi-classical regime.

The objective of this work is to describe the trajectories of electrons on a given strained graphene surface. To achieve this goal, we will proceed as follows:

- Establish the two-dimensional (2D) massless Dirac equation in curved space ($\mathcal{S}$) and in semi-classical regime.
- Solve this Dirac equation in curved space by FGA.
- Compute the classical or semi-classical electron trajectories thanks to the Hamiltonian flow used in FGA. In particular, we shall present focusing effects of strained graphene.

Let us first discuss the interest in using FGA for the Dirac equation modeling strained graphene surfaces. The most advanced models, beyond ab initio calculations (which are not realistic for a large number of atoms), are based on density functional theory (and Kohn-Sham equations). These models are very computationally complex, so that for graphene, tight-binding models are usually preferred as they allow for far more efficient computations, while still keeping a good modeling accuracy. Moreover, it is well-known that interesting properties of 2D materials often occur at low energy; from the effective Hamiltonian obtained by Bloch transform on the tight-binding operator [6, 17], the expansion of the dispersion relation about the so-called Dirac points (zeros of effective Hamiltonian eigenvalues) allows to obtain a continuum theory-based massless 2D Dirac equation, and with non-constant coefficients in the case of strained graphene). In graphene, the distance between Carbon atoms is typically much smaller than the scale of the deformation, so that the semi-classical regime (denoting ε as the small parameter) is usually considered [24]. However, the direct numerical computation of the Dirac equation in the semi-classical regime requires mesh size typically in $\mathcal{O}(\varepsilon)$ or even smaller, therefore the computational time is inversely proportional to ε on a fine grid, leading to expensive or unaffordable computational cost. In addition, non-constant coefficients