Commun. Comput. Phys.
doi: 10.4208/cicp.020515.250716a

Vol. **21**, No. 2, pp. 313-357
February 2017

The Landau-Zener Transition and the Surface Hopping Method for the 2D Dirac Equation for Graphene

Ali Faraj[1,2] and Shi Jin[3,4,*]

[1] *Institute of Natural Sciences, Shanghai Jiao Tong University, Shanghai 200240, P.R. China.*
[2] *Grenoble INP, ESISAR, 26902 Valence Cedex 9, France.*
[3] *Department of Mathematics, Institute of Natural Sciences, MOE-LSEC and SHL-MAC, Shanghai Jiao Tong University, Shanghai 200240, P.R. China.*
[4] *Department of Mathematics, University of Wisconsin, Madison, WI 53706, USA.*

Received 2 May 2015; Accepted (in revised version) 25 July 2016

Abstract. A Lagrangian surface hopping algorithm is implemented to study the two dimensional massless Dirac equation for Graphene with an electrostatic potential, in the semiclassical regime. In this problem, the crossing of the energy levels of the system at Dirac points requires a particular treatment in the algorithm in order to describe the quantum transition—characterized by the Landau-Zener probability—between different energy levels. We first derive the Landau-Zener probability for the underlying problem, then incorporate it into the surface hopping algorithm. We also show that different asymptotic models for this problem derived in [O. Morandi, F. Schurrer, J. Phys. A: Math. Theor. 44 (2011) 265301] may give different transition probabilities. We conduct numerical experiments to compare the solutions to the Dirac equation, the surface hopping algorithm, and the asymptotic models of [O. Morandi, F. Schurrer, J. Phys. A: Math. Theor. 44 (2011) 265301].

AMS subject classifications: 35Q41, 37M05, 65M70, 65Z05, 81-08, 81Q20, 81V99

Key words: Dirac equation, Wigner transform, semiclassical model, band crossing, Landau-Zener formula, surface hopping algorithm, spectral methods.

1 Introduction

We are interested in the description of the transport of electrons in a single graphene layer. This material is a two-dimensional flat monolayer of carbon atoms which displays unusual and interesting electronic properties arising from the bi-conically shaped Fermi

*Corresponding author. *Email addresses:* ali.faraj@esisar.grenoble-inp.fr (A. Faraj), jin@math.wisc.edu (S. Jin)

surfaces near the Brillouin zone corners (Dirac points). The electrons propagate as massless Dirac Fermions moving with the Fermi velocity v_F, which is 300 times smaller than the speed of light $v_F \approx \frac{c}{300} \approx 10^6 m.s^{-1}$, and their behavior reproduces the physics of quantum electrodynamics but at much smaller energy scale. Although this model has been studied for a long time, see [5] for a bibliography, it has remained theoretical until the work of [32] where the graphene was produced for the first time. After these results, the interest of researchers on this material has shown a remarkable increase including applications in carbon-based electronic devices [26] and numerical simulations, see e.g. [12] and references therein.

In this paper, we will consider a model of a two-dimensional Dirac equation [2,5,31] of a graphene sheet in the presence of an external potential. This model consists of a small parameter h directly related to the Planck constant. We are interested in the design of an efficient numerical method—the surface hopping method—for the graphene Dirac equation in the semiclassical regime where $h \ll 1$. In this regime, the solution of the Dirac equation is highly oscillatory thus a huge computational cost is required to give accurate wave functions or physical observables for either finite difference methods [4,16] or time-splitting spectral method [18], since one needs to resolve the high frequency both spatially and temporally.

The development of efficient numerical methods for the related Schrödinger equation in the semiclassical regime has motivated many works in the last decade, see the review paper [20] and references therein. In the semiclassical regime, one often uses asymptotic analysis, such as the WKB analysis and the Wigner transform to help to reduce the computational costs and to develop efficient computational methods based on the asymptotic models. In the framework of Wigner transform, the idea is to construct a measure on the phase space, called the Wigner measure, when $h \to 0$, to obtain the physical observables (such as density, flux, and energy) with a computational cost far less than a direct quantum simulation. When the gap between different energy levels is of order one (the so-called *adiabatic* case), the Wigner measure technique provides a simple description of the motion: it can be well approximated by a fully diagonalized system, one classical Liouville equation for each energy level [13]. However, in the graphene Dirac equation, the energy levels *cross* at the Dirac points, where *non-adiabatic* transfers are observed and the particles can tunnel from one band to the other. The standard Wigner approach then needs to be revised to describe the non-adiabatic phenomena.

One of the widely used approaches to simulate the non-adiabatic dynamics is the surface hopping method initially proposed by Tully and Preston [39] as an efficient computational method to go beyond the classical Born-Oppenheimer approximation. This method is widely used in chemistry and molecular dynamics, see for examples [7,35,38, 39]. The basic idea is to combine classical transport of the system on individual potential energy surfaces with instantaneous transitions from one energy surface to the other. The transition rates for this band-to-band hopping are given by the well known Landau-Zener formula [40]. From the mathematical point of view, the first rigorous analysis of non-adiabatic transfer using Landau-Zener formula dates back to Hagedorn [15]. More