Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2024-0103

Vol. **37**, No. 4, pp. 1055-1084
April 2025

Uncertainty Quantification for Charge Transport in GNRs Through Particle Galerkin Methods for the Semiclassical Boltzmann Equation

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Received 30 April 2024; Accepted (in revised version) 12 November 2024

Abstract. In this article, we investigate some issues related to the quantification of uncertainties associated with the electrical properties of graphene nanoribbons. The approach is suited to understand the effects of missing information linked to the difficulty of fixing some material parameters, such as the band gap, and the strength of the applied electric field. In particular, we focus on the extension of particle Galerkin methods for kinetic equations in the case of the semiclassical Boltzmann equation for charge transport in graphene nanoribbons with uncertainties. To this end, we develop an efficient particle scheme which allows us to parallelize the computation and then, after a suitable generalization of the scheme to the case of random inputs, we present a Galerkin reformulation of the particle dynamics, obtained by means of a generalized Polynomial Chaos approach, which allows the reconstruction of the kinetic distribution. As a consequence, the proposed particle-based scheme preserves the physical properties and the positivity of the distribution function also in the presence of a complex scattering in the transport equation of electrons. The impact of the uncertainty of the band gap and applied field on the electrical current is analysed.

AMS subject classifications: 82D37, 82C70, 65C05, 82M31

Key words: Charge transport, graphene, uncertainty quantification, semiclassical Boltzmann equation, stochastic Galerkin, particle methods.

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1 Introduction

Low dimensional materials are investigated in electronics with the aim to reduce the dimensions of the future electronic devices. One of the most prominent 2D materials is graphene for its very peculiar electronic properties. The absence of an energy gap limits the use of graphene in field effect transistors (FETs) because there exists a restricted current-off region. A possible way to overcome such a drawback is to consider narrow strips of graphene, called graphene nanoribbons (GNRs), see e.g. [11]. In fact, the spatial confinement induces a band gap, even if the mobility reduces with respect to the large area graphene sheet.

An accurate description of charge transport in large area graphene and in GNRs can be obtained by solving in the physical space the semiclassical Boltzmann equations (BE) [29,33] – also called quantum Boltzmann equations – for charge transport by resorting to direct simulation Monte Carlo (DSMC) [50] or deterministic approach as WENO scheme [46] or discontinuous Galerkin (DG) methods [12,13,15,32,41,42,53,54]. Other approaches present in the literature include the adoption of drift-diffusion models, hydrodynamical models [2,7,31,34] (for a comprehensive review see [6]) or the Wigner equation [8,38–40].

In order to reduce the computational complexity of the problem, we have adopted an effective model with reduced dimensionality obtained by integrating with respect to the transversal direction (y-component in Fig. 1) and, as also done in [21], reformulating the effect of the edge as a further scattering. After the homogenization with respect to the y-variable, since the material is homogeneous with respect to the longitudinal direction as well, also the dependence on the x-variable is dropped. We remark that the effect of the finite width of the nanoribbon is still present in the effectively adopted model as a scattering term and as a parameter in the energy dispersion relation.

Despite the very huge literature on these topics, to quantify the impact of deviations from the classical deterministic modelling setting to include uncertain geometries and molecular mechanics properties of the materials, new approaches based on uncertainty quantification (UQ) methods should be developed. Indeed, to ensure performance reliability it is important to develop a predictive framework that is robust with respect to inevitable fabrication errors and initial conditions parameterizing the molecular dynamics that are based on nanoscale experiments. In the present paper we will tackle issues of uncertainty quantification related to the electrical properties of graphene but a similar analysis can be performed for the mechanical features as well, see e.g. [22,51].

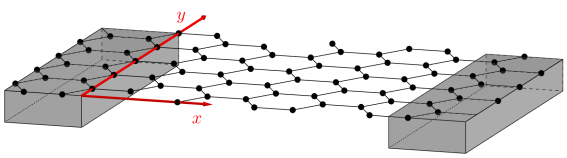

Figure 1: Schematic representation of a graphene nanoribbon. Note the irregular edges.