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A kinetic model for the transport of electrons in a graphene layer ☆

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ABSTRACT

In this article, we propose a new numerical scheme for the computation of the transport of electrons in a graphene device. The underlying quantum model for graphene is a massless Dirac equation, whose eigenvalues display a conical singularity responsible for non-adiabatic transitions between the two modes. We first derive a kinetic model which takes the form of two Boltzmann equations coupled by a collision operator modeling the non-adiabatic transitions. This collision term includes a Landau–Zener transfer term and a jump operator whose presence is essential in order to ensure a good energy conservation during the transitions. We propose an algorithmic realization of the semi-group solving the kinetic model, by a particle method. We give analytic justification of the model and propose a series of numerical experiments studying the influences of the various sources of errors between the quantum and the kinetic models.

1. Introduction

1.1. Graphene structures

Recently, graphene based structures have been the object of intensive research in nanoelectronics, see for instance the reviews [4,9] and references therein. Graphene is a single 2D sheet of carbon atoms in a honeycomb lattice and, differently from conventional semiconductors, the most important aspect of graphene's energy dispersion is its linear energy–momentum relationship. Electrons behave as massless relativistic particles, the conduction and valence bands intersecting at the zero energy point, with no energy gap (see [31]). These features enable to observe at low energy some physical phenomena of quantum electrodynamics, such as Klein tunneling that is, the fact that Dirac fermions can be transmitted through a classically forbidden region.

We are here interested in numerical schemes describing the transport of electrons in a graphene device via a kinetic model. Kinetic models are usually easier to implement numerically and have a cheaper numerical cost, compared to out-of-equilibrium full quantum models. Indeed, they are compatible with the Lagrangian approach while the natural treatment

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of the quantum model requires small discretization steps, due to the smallness of physical parameters. In this paper, we will use a particle method to solve numerically the kinetic model. Moreover, the treatment of boundary conditions is simpler in this framework, which also enables to enrich the description by adding collisional effects via Boltzmann-like terms. However, due to the absence of gap between the conduction and valence bands, it is not correct to describe separately the electrons and the holes, which remain coupled even at the semiclassical limit. The objective of this paper is to introduce a kinetic model for ballistic transport, which treats the possible transitions between bands and allows for an easy numerical realizations. This kinetic model is derived rigorously in a linear setting and leads to algorithmic realizations which are tested numerically.

Previous kinetic models have been discussed by O. Morandi and F. Schürrer in [30] and a quite similar strategy as ours has been developed at the same moment where we were writing this paper by A. Faraj and S. Jin in [10]. We refer to Section 1.6 below for further details.

1.2. The quantum model

The kinetic model that will be introduced below consists in a system of approximate equations based on the Wigner counterpart of an underlying quantum transport model. At the quantum level, the ensemble of particles is described by its density matrix $\varrho(T)$. This trace-class operator allows to describe the system by computing expectation values of observables at time T. Let A be an observable, such as impulsion operators $-i\partial_{X_j}$, $j=\{1,2\}$, or position operators $\widehat{X}_j$ (the operators of multiplication by X_j), the expectation value at time T of the observable A for the system described by the matrix density ϱ is given by $\langle A\rangle = \mathrm{tr}(A\varrho(T))$. Matrix densities $\varrho(T)$ solve a von Neumann equation

$$i\hbar\partial_T\varrho = [\mathcal{H},\varrho],$$

where the Hamiltonian $\mathcal{H}$ takes into account the physical properties of the system. As observed in [24] and references therein, the electronic Hamiltonian $\mathcal{H}$ for graphene can be approximated for low energies by the Dirac-like Hamiltonian

$$\mathcal{H} = -i\hbar v_F\sigma\cdot\nabla_X + eU = v_F\hbar\begin{pmatrix}0 & -i\partial_{X_1}-\partial_{X_2}\\ -i\partial_{X_1}+\partial_{X_2} & 0\end{pmatrix} + eU,$$

where $X\in\mathbf{R}^2$, v_F is the Fermi velocity, $\sigma=(\sigma_{X_1},\sigma_{X_2})$ denotes the Pauli matrices vector and $U=U(X)$ is a smooth bounded potential with bounded derivatives (see also [4,9,30] for physical references).

Let us first put this equation in dimensionless form. We introduce a characteristic space length L, a characteristic energy $\overline{E}$ and a characteristic density $\overline{n}$, then define the associated characteristic time by $\overline{t}=\frac{\hbar}{\overline{E}}$ and denote

$$x=\frac{X}{L},\quad t=\frac{T}{\overline{t}},\quad V=\frac{eU}{\overline{E}},\quad \varrho^\varepsilon=\frac{\varrho}{\overline{n}L^2}.$$

The system in dimensionless form reads

$$i\varepsilon\partial_t\varrho^\varepsilon = [(A(\varepsilon D)+V),\varrho^\varepsilon], \tag{1.1}$$

where the semiclassical dimensionless parameter is

$$\varepsilon=\frac{\hbar v_F}{\overline{E}L}\ll 1,$$

the applied potential $V(x)$ is supposed to be smooth, bounded with bounded derivatives, as the function $U(x)$ above, $D=-i\nabla_x$ and A is the matrix

$$A(\xi)=\begin{pmatrix}0 & \xi_1-i\xi_2\\ \xi_1+i\xi_2 & 0\end{pmatrix}.$$

The matrix $A(\xi)$ has two eigenvalues $|\xi|$ and $-|\xi|$. The singularity of these eigenvalues at the point $\xi=0$ is called *conical singularity*. The associated eigenprojectors Π^+ and Π^- satisfy

$$\Pi^\pm(\xi)=\frac{1}{2}\mathrm{Id}\pm\frac{1}{2|\xi|}A(\xi)$$

where Id is the identity matrix. They help to distinguish between the *plus*-particles and the *minus*-particles of this two-level system: the expectation of the number of $\pm$-particles at time t is given by $n^\pm(t)=\mathrm{tr}(\Pi^\pm(\varepsilon D)\rho^\varepsilon(t))$.

We shall assume that for any $\varepsilon>0$, the initial data $\varrho^\varepsilon(0)$ is a nonnegative trace-class operator. We shall denote by $\mathcal{L}^1(L^2(\mathbf{R}^2;\mathbf{C}^2))$ the set of trace-class operators on the set of vector-valued square-integrable functions $L^2(\mathbf{R}^2;\mathbf{C}^2)$. We shall assume that the family of operators $\left(\varrho^\varepsilon(0)\right)_{\varepsilon>0}$ is a bounded family of $\mathcal{L}^1(L^2(\mathbf{R}^2;\mathbf{C}^2))$, that is

$$\exists C>0,\ \ \forall\varepsilon>0,\ \ \|\varrho^\varepsilon(0)\|_{\mathcal{L}^1(L^2(\mathbf{R}^2;\mathbf{C}^2))}\leqslant C. \tag{1.2}$$

Note that under these assumptions, we obtain

$$\forall t\in\mathbf{R},\ \ \forall\varepsilon>0,\ \ \|\varrho^\varepsilon(t)\|_{\mathcal{L}^1(L^2(\mathbf{R}^2;\mathbf{C}^2))}\leqslant C.$$