Quantum energy-transport and drift-diffusion models for electron transport in graphene: an approach by the wigner function

Vito Dario Camiola\textsuperscript{1} · Giovanni Mascali\textsuperscript{2,3} · Vittorio Romano\textsuperscript{1}

Received: 31 May 2021 / Accepted: 11 September 2021 / Published online: 11 November 2021
© The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2021

Abstract
The present work aims at formulating quantum energy-transport and drift-diffusion equations for charge transport in graphene from a quantum hydrodynamic model proposed in Luca and Romano (Ann. Phys. 406:30–53, 2019), obtained from the Wigner-Boltzmann equation via the moment method. Here, we only sketch the main ideas and show the most relevant formulas. Further developments are under current investigation by the authors. The interested reader can find the omitted details in the references. In analogy with the semiclassical case, we are confident that the energy-transport and drift-diffusion models have mathematical properties which allow an easier numerical treatment.

Keywords  Wigner equation · Graphene · Wigner equilibrium function

1 Introduction
Graphene, a monolayer of $sp^2$-bonded carbon atoms, is not only the basis for graphite but also a new material with immense potential in microelectronics for its exceptional electrical transport properties, like high conductivity and high charge mobility. As a result of its promising properties, it seems to be an ideal candidate to take over from silicon for the next generation of faster and smaller electronic devices.

If the length of the active area is of the order of few nanometers, quantum phenomena must be taken into account and a semiclassical description of charge transport is no longer adequate. The present work aims at formulating quantum energy-transport and drift-diffusion models for a proper description of charge transport in graphene, which is extremely important for the growing technological development in CAD tools.

In [1], a quantum hydrodynamic model for charge transport in graphene is derived from a moment expansion of the Wigner-Boltzmann equation, and the needed closure relations are obtained by adding quantum corrections based on the equilibrium Wigner function to the semiclassical model formulated in [2–6] by exploiting the Maximum Entropy Principle. The expression of the equilibrium Wigner function which takes into account the form of the energy band of graphene has been obtained by solving the corresponding Bloch equation. In the present work, from this hydrodynamic model, a quantum energy-transport and a quantum drift-diffusion model are deduced in the long time asymptotic limit.

The plan of the paper is as follows. In Sect. 2, the main features of the energy bands in graphene are recalled. In Sect. 3, the Wigner equation in graphene is introduced, and a quantum hydrodynamic model is obtained as associated moment system. The last section is devoted to the deduction of a quantum energy-transport and a quantum drift-diffusion model.

2 Band structure on graphene
Graphene is a two-dimensional crystal made of carbon atoms arranged into a honeycomb lattice structure. Solving the one-electron Schrödinger equation including only the periodic potential due to the charges of the crystal in the
tight-binding approximation yields the relation (see [7] for a comprehensive review on the topic)

\[ \delta_\pm(k) = \pm i \sqrt{3} + f(k) - tf(k). \]

The function \( f \) reads

\[ f(k) = 4 \cos \left( \frac{3a}{2} k_x \right) \cos \left( \frac{a \sqrt{3}}{2} k_y \right) + 2 \cos \left( a \sqrt{3} k_y \right), \]

where \( k \) being the two dimensional electron quasi-wave vector with respect to the center of the first Brillouin zone. The sign \(+\) refers to the conduction band, while the sign \(-\) refers to the valence band. The constant \( a \) is the interatomic distance (of the order of one Angstrom); \( t \approx 2.7 \) eV is the hopping parameter between the first nearest-neighbour orbitals, while \( t' \) is the hopping parameter between the second nearest-neighbour orbitals, and its value is still matter of debate. The function \( 3 + f(k) \) is zero at the vertices, named Dirac points, of the Brillouin zone. By neglecting \( t' \) and by choosing in the \( k \)-space a reference frame centered in the considered Dirac point, for \( |k| a \ll 1 \), that is near the Dirac points, one gets the following linear dispersion relation (see Fig. 1)

\[ \delta_\pm(p) = \pm v_F p. \]

(1)

where \( p = h k \) is the electron quasi-momentum with \( h \) the reduced Planck constant.

A nonzero value of \( t' \) breaks the symmetry with respect to \( \delta' = 0 \) and shifts the energy at the conical point from \( \delta' = 0 \) to \( \delta' = 3t' \).

In order to include the presence of a small gap between the conduction and the valence band, we assume \( t' \neq 0 \) in the tight-binding approximation. Therefore, the Hamiltonian describing the energy in the proximity of the Dirac points can be written in the form

\[ H = v_F \begin{pmatrix} \alpha & p_x + ip_y \\ p_x - ip_y & -\alpha \end{pmatrix}, \]

which has eigenvalues

\[ \delta_\pm(p) = \pm v_F \sqrt{a^2 + p^2}, \]

where \( \alpha \) is a small parameter related to the nearest-neighbour hopping energy. A similar regularization has been also adopted in [8] and can be also useful for describing charge behavior in double layer graphene and graphene nanoribbons.

3 Wigner equation for charge transport in graphene

From now on, for the sake of simplicity, we will consider only electrons in the conduction band. The inclusion of holes can be done straightforwardly. A way to formulate a quantum transport description is that of introducing a single electron Wigner quasi-distribution \( w(x, p, t) \), depending on the position \( x \), momentum \( p \) and time \( t \). Its evolution is governed by the Wigner-Poisson system for \( w \) and the electrostatic potential \( \Phi \)

\[ \frac{\partial w(x, p, t)}{\partial t} + S[\delta] w(x, p, t) - q[\Phi] w(x, p, t) = C[w], \]

\[ \nabla \cdot (\epsilon \nabla \Phi) = -q(N_D - n), \]

where \( q \) is the elementary (positive) charge, \( N_D \) is donor carrier concentration, \( \epsilon \) is the dielectric constant, \( C[w] \) is the collision term representing the electron-phonon scattering while \( S[\delta] \) and \( \theta[\delta] \) represent the pseudo-differential operators

\[ S[\delta](x, p, t) = \frac{i}{\hbar(2\pi)^2} \int_{\mathbb{R}^2} \left[ \delta(p + \hbar \frac{\nu}{2} \nu, t) - \delta(p - \hbar \frac{\nu}{2} \nu, t) \right] w(x, p', t) e^{-i(x-x')\nu} d\nu \]

\[ \theta[\delta](x, p, t) = \frac{i}{\hbar(2\pi)^2} \int_{\mathbb{R}^2} \left[ \delta(x + \hbar \frac{\eta}{2} \eta, t) - \delta(x - \hbar \frac{\eta}{2} \eta, t) \right] w(x, p', t) e^{i(x-x')\eta} d\eta \]

In the semiclassical limit \( \hbar \to 0 \), the Wigner equation reduces to the semiclassical Boltzmann one. The direct numerical solution of the Wigner equation is a daunting computational task [9]. However, the appealing aspect of quantum transport in terms of the Wigner function is that one can define the macroscopic quantities of interest as expectation values (moments) like in the semiclassical case although the Wigner function is real but not defined in sign. For example, a 6-moment model can be formulated by considering the following moments which have a direct physical meaning.

\[ \mathbb{E} \] Springer
where the factor four takes into account the spin and valley degeneration.

The corresponding evolution equations are given by

$$\frac{\partial}{\partial t} n(x, t) + \frac{\partial}{\partial x_i} \left( n(x, t) V_i \right) - \frac{\partial^2}{\partial x_i \partial x_k} \left( n(x, t) T^{(0)}_{ijk} \right) = 0,$$

$$\frac{\partial}{\partial t} (n(x, t) W) + \frac{\partial}{\partial x_i} \left( n(x, t) S_i \right) - \frac{\partial}{\partial x_i} \Phi(x) n(x, t) V_i + \frac{q^2}{24} \frac{\partial^3}{\partial x_i \partial x_j \partial x_k} n(x, t) T^{(0)}_{ijk}$$

$$= nC_w[w],$$

$$\frac{\partial}{\partial t} \left( n(x, t) V_i \right) + \frac{\partial}{\partial x_j} \left( n(x, t) F^{(0)}_{ij} \right) - \frac{\partial^2}{\partial x_i \partial x_j} \left( n(x, t) H^{(0)}_{ijkl} \right)$$

$$= nC_{V_i}[w],$$

$$\frac{\partial}{\partial t} \left( n(x, t) S_i \right) + \frac{\partial}{\partial x_j} \left( n(x, t) F^{(1)}_{ij} \right) - \frac{\partial^2}{\partial x_i \partial x_j} \left( n(x, t) H^{(1)}_{ijkl} \right)$$

$$= nC_{S_i}[w]$$

that must be expressed as functions of the basic variables $n$, $W$, $V$, $S$. Therefore, the so-called closure problem arises. In the semiclassical case, explicit closure relations have been obtained by resorting to the Maximum Entropy Principle (MEP) [10]. The analogous formulation of MEP for the Wigner function is not straightforward mainly because $w$ is not a probability density function. In [1], a hydrodynamic model has been obtained under the following assumptions (see also [11]):

1. A regime in which quantum effects can be considered only a perturbation of the semiclassical model;
2. The collision term has the same form as in the semiclassical case, an approximation widely discussed in [12].

For simplicity, we will skip all details and refer the interested reader to [1], but underline some critical point of the
theory. For the calculation of the collisional term \( C[w] \), the following argumentation is used.

We suppose that the expansion
\[
w = w^0 + \hbar^2 w^{(1)} + O(\hbar^4)
\]
holds. By proceeding in a formal way, as \( \hbar \to 0 \), the Wigner equation gives the semiclassical Boltzmann equation; therefore, we identify \( w^{(0)}(x, p, t) \) with the semiclassical distribution. As a consequence of (6), the following expansion for the collision term is obtained
\[
C[w] \approx C_0[w^{(0)}] + \hbar^2 C_1[w^{(1)}],
\]
where \( C_0[w^{(0)}] \) is identified with the semiclassical collision operator while, according to [11], the second term is modelled as
\[
C_1[w^{(1)}] = -\frac{1}{\tau} \left( w^{(1)} - w^{(1)}_{eq} \right),
\]
where \( w^{(1)}_{eq} \) is the first order term in \( \hbar^2 \) of the equilibrium Wigner function, and \( 1/\tau \) plays the role of a collision frequency that in general depends on \( p \).

Since, in the limit \( \frac{1}{\tau} \to +\infty \) one formally gets \( w^{(1)} = w^{(1)}_{eq} \), we suppose that \( w^{(1)} = w^{(1)}_{eq} \), with a good approximation (a similar assumption was made also in [13]). Therefore, it is necessary to find out the expression of \( w^{(1)}_{eq} \).

It can be obtained by using the Jaynes approach [14] of maximizing the entropy under suitable constraints on the expectation values, a crucial issue being the expression of the entropy in the quantum case. In [11, 2], the standard prescription proposed by von Neumann has been adopted, which leads to a semiclassical limit represented by the Maxwell-Boltzmann distribution. That is, with this assumption, the zero-order term of the equilibrium Wigner function does not coincide with the Fermi-Dirac distribution but gives the Boltzmann-Maxwell low density limit.

To avoid this problem, it is needed to consider a different function for the entropy. For this purpose, it is also important to observe that, as pointed out in recent papers [15, 16], in a closed system the entropy must be conserved because the evolution of the system is described by unitary operators. Instead, in an open system, like a semiconductor electron device, there is a fast decay of the off-diagonal terms and practically only the diagonal contribution survives. Arguing on such a remark, in [16] it has been suggested to use as entropy only the diagonal contribution of the density operator, and it has been proved that it increases in time according to the second law of thermodynamics. A suggested expression, already considered in [17], more recently pointed out in [15] and employed in [18], could be the following one
\[
-\kappa B \sum_k \left[ \langle \hat{\rho}_{kk} \rangle \log \langle \hat{\rho}_{kk} \rangle + \varphi(1 \pm \langle \hat{\rho}_{kk} \rangle) \log(1 \pm \langle \hat{\rho}_{kk} \rangle) \right]
\]
where the \( \langle \hat{\rho}_{kk} \rangle \)'s are the expectation values of the diagonal elements of the density operator, which can be interpreted as occupation numbers, the upper sign being valid for Bosons and the lower one for Fermions. This could solve the problem of the limit of the equilibrium Wigner function, but the needed calculations become much more involved to carry out analytically [16]. We are confident that the quantum correction given in [1] is good enough for determining the quantum extension of the semiclassical hydrodynamic model. These issues are under current investigation [19], and the consequence for the transport theory by the Wigner equation will be the subject of a forthcoming article.

Remark: It is customary in the literature to try to recover some form of Bohm potential. A standard way (see [13]) is that of introducing the approximation
\[
\nabla \log n \approx \beta q \nabla \phi,
\]
into the closure relations. Strictly, such a relation is valid only at equilibrium in the case of low densities. However, for high values of the quasi-Fermi potential \( \phi_F \) (\( \phi_F \gg k_B T \)), the above approximation has no rationale (see [1]). Therefore, we prefer to avoid the introduction of relation (9). Bohm like terms naturally arise from the closure relations.

4 Energy-transport and drift-diffusion limit models

It is possible to deduce an energy-transport model from the hydrodynamic one under a suitable scaling. In the semiclassical case, the advantages of the energy-transport formulation are a better regularity of the solutions and the possibility of applying efficient numerical schemes like the Scharfetter-Gummel one [20]. In the presence of quantum corrections, we expect also better features of solutions and a better performance of the numerical scheme. If we consider a long time scaling, the evolution Eqs. (4–5) tend to the stationary case. In particular, the equations for \( n \nabla \) and \( nS \) become a linear system for these variables
\[
\begin{pmatrix}
c_{11} & c_{12} \\
c_{21} & c_{22}
\end{pmatrix}
\begin{pmatrix}
nV_i \\
nS_i
\end{pmatrix}
= \begin{pmatrix}
b_{i}^{(0)} \\
b_{i}^{(1)}
\end{pmatrix},
\]
where the coefficients \( c_{ij} \) depend on the energy \( W \) (for explicit expressions see [1]) while
\[ b_i^{(0)} = \frac{\partial}{\partial x_j} \left( n(x, t) E_{\gamma j}^{(0)} - \frac{\hbar^2}{24} \frac{\partial^2}{\partial x_j \partial x_k} (n(x, t) H_{\gamma kl}^{(0)}) \right) \\
- q \frac{\partial}{\partial x_j} \Phi(x) n(x, t) C_{\gamma j}^{(0)} \\
+ q \hbar^2 \frac{3}{24} \Phi(x) - n(x, t) L_{\gamma j}^{(0)}, \]

\[ b_i^{(1)} = \frac{\partial}{\partial x_j} \left( n(x, t) E_{\gamma j}^{(1)} - \frac{\hbar^2}{24} \frac{\partial^2}{\partial x_j \partial x_k} (n(x, t) H_{\gamma kl}^{(1)}) \right) \\
- q \frac{\partial}{\partial x_j} \Phi(x) n(x, t) C_{\gamma j}^{(1)} \\
+ q \hbar^2 \frac{3}{24} \Phi(x) - n(x, t) L_{\gamma j}^{(1)}. \]

One gets

\[
\begin{pmatrix}
  n V_i \\
  n S_i
\end{pmatrix} = \frac{1}{c_{11} c_{22} - c_{12} c_{21}} \begin{pmatrix}
  c_{22} & -c_{12} \\
  -c_{21} & c_{11}
\end{pmatrix}
\begin{pmatrix}
  n(x, t) E_{\gamma j}^{(0)} \\
  n(x, t) E_{\gamma j}^{(1)}
\end{pmatrix}
\]

(10)

and by inserting these relations into the equations for \( n \) and \( n W \), one obtains the following stationary quantum energy-transport model

\[
\frac{\partial}{\partial x_i} \left( \frac{1}{c_{11} c_{22} - c_{12} c_{21}} \left( c_{22} b_i^{(0)} - c_{21} b_i^{(1)} \right) \right) \\
- q \frac{\partial}{\partial x_i} \Phi(x) n(x, t) V_i \\
+ q \hbar^2 \frac{3}{24} \Phi(x) n(x, t) T_{\gamma k}^{(0)} = C_W[w].
\]

(11)

Moreover, let us model the energy collision term in the relaxation approximation form

\[
C_W[w] = - \frac{W - W_0}{\tau_W},
\]

with \( \tau_W \) the energy relaxation time and \( W_0 \) the equilibrium energy. In the limit for the scaled \( \tau_W \) tending to zero, from Eq. (12) one formally has \( W = W_0 \) and only the Eq. (11) remains which is equivalent to the conservation of the total current \( J_i \), i.e.

\[
J_i = \frac{1}{c_{11} c_{22} - c_{12} c_{21}} \left( c_{22} b_i^{(0)} - c_{21} b_i^{(1)} \right) - q \hbar^2 \frac{3}{24} \Phi(x) n(x, t) T_{\gamma k}^{(0)} = J_i, \quad i = 1, 2,
\]

(13)

\( J_i \) being constant values. Equation (13) coupled with the Poisson equation for the electrostatic potential constitutes the limiting stationary drift-diffusion model deduced from the energy-transport one. It is a generalization of the standard quantum model based on the Bohm potential (see [21] for a review of the current models known in the literature).

The quantities involved in (13) can be explicitly evaluated in terms of the Fermi energy \( \delta_F \) and the electrostatic potential \( \Phi \) (we omit the details of the derivation, the interested reader can get them starting from the results in [1]).

### 5 Conclusion/summary

Quantum energy-transport and drift-diffusion equations for charge transport in graphene sheets have been found by suitably scaling a quantum hydrodynamic model on its turn obtained by means of the Wigner-Boltzmann equation via the moment method. We are confident that these models have mathematical properties which allow an easier numerical treatment as happens in the semiclassical case for silicon ([14]).

Acknowledgements This research was funded by INdAM (GNFM) and from Università degli Studi di Catania, Piano della Ricerca 2020/2022 Linea d’intervento 2 “QICT” and by the project AIM 1893589, Mobilità dei Ricercatori Asse I del PON R&I 2014–2020. The paper was written within the activity of the Interdipartimental Center for Mathematics in Industry, University of Catania.

### References

1. Luca, L., Romano, V.: Quantum corrected hydrodynamic models for charge transport in graphene. Ann. Phys. 406, 30–53 (2019)
2. Luca, L., Romano, V.: Comparing linear and nonlinear hydrodynamical models for charge transport in graphene based on the Maximum Entropy Principle. Int. J. Non-Linear Mech. 104, 39–58 (2018)
3. Luca, L., Romano, V.: Hydrodynamical models for charge transport in graphene based on the Maximum Entropy Principle: The case of moments based on energy powers. Atti della Accademia Peloritana dei Pericolanti 96(S1), A5 (2018)
4. Camiola, V.D., Romano, V.: Hydrodynamical model for charge transport in graphene. J. Stat. Phys. 157, 114–1137 (2014)
5. Mascali, G., Romano, V.: Charge Transport in graphene including thermal effects. SIAM J. Appl. Math. 77, 593–613 (2017)
6. Barletti, L.: Hydrodynamic equations for electrons in graphene obtained from the maximum entropy principle. J. Math. Phys. 55(8), 083303 (2014)
7. Castro Neto, A.H., Guinea, F., Peres, N.M.R., Novoselov, K.S., Geim, A.K.: The electronic properties of graphene. Rev. Modern Phys. 81, 109 (2009)
8. Morandi, O., Schürrer, F.: Wigner model for quantum transport in graphene. J. Phys. A: Math. Theor. 44, 265301 (2011)
9. Muscato, O., Wagner, W.: A stochastic algorithm without time discretization error for the Wigner equation. Kin. Rel. Models 12(1), 59–77 (2019)
10. Mascali, G., Romano, V.: Exploitation of the maximum entropy principle in mathematical modeling of charge transport in semiconductors. Entropy 19(1), 36 (2017). https://doi.org/10.3390/e19010036. (open access article)
11. Romano, V.: Quantum corrections to the semiclassical hydrodynamical model of semiconductors based on the maximum entropy principle. J. Math. Physics 48, 123504 (2007)
12. Querlioz, D., Dollfus, P.: The Wigner Monte Carlo Method for Nanoelectronic Devices. ISTE Wiley, Hoboken (2010)
13. Gardner, C.L.: The quantum hydrodynamic model for semiconductor devices. SIAM J. Appl. Math. 54(2), 409 (1994)
14. Camiola, V.D., Mascali, G., Romano, V.: Charge Transport in Low Dimensional Semiconductor Structures. Springer, Cham (2020)
15. Snoke, D.W., Liu, G., Girvin, S.M.: The basis of the second law of thermodynamics in quantum field theory. Ann. Phys. 327, 1825–1851 (2012)
16. Polkovnikov, A.: Microscopic diagonal entropy and its connection to basic thermodynamic relations. Ann. Phys. 326, 486 (2011)
17. Jaynes, E.T.: Information theory and statistical mechanics II. Phys. Rev. 108, 171 (1957)
18. Barletti, L., Cintolesi, C.: Derivation of isothermal quantum fluid equations with Fermi-Dirac and Bose-Einstein statistics. J. Stat. Phys. 148, 353–386 (2012)
19. Camiola, V.D., Luca, L., Romano, V.: Equilibrium Wigner function for Fermions and Bosons in the case of a general energy dispersion relation. Entropy 22, 1023 (2020)
20. Romano, V.: 2D numerical simulation of the MEP energy-transport model with a finite difference scheme. J. Comput. Phys. 221, 439–468 (2007)
21. Jüngel, A.: Transport Equations for Semiconductors. Springer, Berlin (2009)

**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.