

# Quantum Navier–Stokes equations for electrons in graphene

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The Chapman–Enskog method, in combination with the quantum maximum entropy principle (QMEP), is applied to the Wigner equation in order to obtain quantum Navier–Stokes equations for electrons in graphene in the isothermal case. The derivation is based on the quantum version of the maximum entropy principle and follows the lines of Ringhofer–Degond–Méhats’ theory (*J. Stat. Phys.* **112**, 2003 and *Z. Angew. Math. Mech.* **90**, 2010). The model obtained in this way is then semiclassically expanded up to  $\mathcal{O}(\epsilon^2)$ .

## 1 | INTRODUCTION

Graphene is a two-dimensional material that displays unusual electronic properties due to the conical shape of the energy bands in the proximity of the so-called Dirac points. For this reason, charge transport in graphene attracts a lot of interest from the scientific community. In the literature, there are several papers describing electron hydrodynamics with semiclassical or quantum models [1–7]. In particular, the viscous hydrodynamic regime, which is only possible in a time-scale where electron–electron collisions are dominant, has been deeply investigated both theoretically [3, 5, 6] and experimentally [8]. In refs. [3–6], the author reports a derivation of the viscous hydrodynamic equations based on a semiclassical Boltzmann equation, that is, a kinetic description that is classical except for some key elements such as the conical energy bands and the use of Fermi statistics. On the other hand, quantum-corrected hydrodynamic equations (obtained from a quantum kinetic description based on the Wigner equation) have been obtained only in the case of an inviscid regime and assuming regularized energy bands [2]. This is because the singular behavior of the bands at the conical intersection causes the appearance of divergent integrals when computing quantum corrections to the transport coefficients.

The aim of the present work is to explore the possibility of deriving fully-quantum and quantum-corrected hydrodynamic equations in both the inviscid and viscous regimes. Hence, we are implicitly assuming a time scale where the momentum conserving electron–electron collisions are dominant with respect to the electron–phonon (or electron–impurity) collisions [3]. For the sake of simplicity, we only consider the isothermal case, since the nonisothermal case would only bring more calculation but no methodological differences. We also work with regularized bands, by introducing a regularization parameter  $\alpha$  (with the physical meaning of an energy gap); however, the conical limit  $\alpha \rightarrow 0$  is considered whenever possible.

Quantum hydrodynamic models date back to the early period of quantum mechanics. The Schrödinger equation can be formulated in a hydrodynamic form, the so-called Madelung equations [9], which represent an isothermal Euler system with an additional  $\hbar^2$  term, called Bohm potential [10, 11]. Madelung’s approach is restricted to pure states, and so it is not suitable to introduce statistical concepts, such as equilibrium states, which are needed in the derivation of more

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general quantum fluid models. A more systematic way to derive quantum hydrodynamic models was proposed by Degond, Ringhofer, and Méhats [12, 13] by introducing the quantum maximum entropy principle (QMEP) to close the systems of the macroscopic moments. In refs. [12, 13], the authors, similarly to the classical maximum entropy principle [14, 15] and to Levermore's method [16], close the moment system by means of a quantum distribution function which maximizes the entropy with given moments. This approach is fairly general and can be applied to different systems and different regimes.

Our derivation starts from the one-particle Wigner equation [17, 18] with a BGK collisional term, which describes the relaxation of the system to the local equilibrium. Here, we are interested in the isothermal fluid equations for the particle density  $n$  and for the momentum density  $n_p$ . Following the lines of Ringhofer–Degond–Méhats' theory, we obtain the local equilibrium Wigner function by using the QMEP, which determines the local equilibrium by maximizing an entropy functional with the constraints given by the macroscopic moments. The equilibrium Wigner function  $g$  can be formally derived and it contains an implicit dependence upon the moments  $n$  and  $n_p$  through the dependence on a set of three Lagrange multipliers,  $A$  and  $\mathbf{B} = (B_1, B_2)$ . The quantum Navier–Stokes equations for graphene are then obtained by performing the limit of the Wigner equation as the mean free path converges to zero, by using the Chapman–Enskog expansion.

At order 0 in the collision-time parameter, we obtain the quantum analog of the classical Euler equations, while at order 1 the viscous corrections to the Euler model are obtained. Finally, we determine the expression of macroscopic moments as functions of the Lagrange multipliers in the semiclassical case (namely, at second-order in  $\hbar$ ) and then compute the approximated quantum Navier–Stokes equations. We also discuss the case of nonregularized (conical) energy bands, letting the regularization parameter  $\alpha$  go to 0, and show that, remarkably, the Euler equations remain nonsingular in this limit.

We remark that our approach is analogous to the one used in ref. [19], also based on the QMEP, where the authors derive for the first time quantum isothermal Navier–Stokes equations for a standard particle (i.e., with a quadratic energy band). In that paper, the authors compute, in a purely formal way, the viscous correction terms for their model. Inspired by this idea, our work positions itself in the framework of mathematical models for the inclusion of viscous effects in graphene, the existing works being focused on the Euler equations. The novelty of our paper is the theoretical calculation of the quantum corrections to the viscous terms for a fluid of electrons in graphene, with the aim of a mathematical study of their form and possibly their numerical estimation (left for future work).

The outline of the paper is the following. In Section 2 we introduce the model recalling the form of the energy bands for graphene and their regularization and write down the Wigner equation with a BGK collisional operator. In Section 3 we perform the Chapman–Enskog expansion and derive quantum Euler equations and quantum Navier–Stokes equations. In Section 4 we compute the semiclassical expansion up to  $\mathcal{O}(\hbar^2)$  for the equilibrium distribution and consequently for the Navier–Stokes equations. Section 5 contains our conclusions.

## 2 | GRAPHENE ENERGY BANDS AND KINETIC EQUATIONS

Graphene is a monolayer crystal consisting of a honeycomb lattice of carbon atoms. In the tight-binding approximation, the valence and conduction bands have conical intersections at the vertices of the Brillouin zone (the so-called Dirac points), where they touch each other with a null gap [20]. This leads to consider the carriers as “massless fermions.” In this work, we restrict our model to the conduction band, for which the explicit expression

$$\mathcal{E}(\mathbf{k}) = \hbar v_F k, \quad k = |\mathbf{k}|, \quad (1)$$

holds for  $\mathbf{k}$  in a neighborhood of a given Dirac point. Here,  $v_F$  is the Fermi speed and  $\hbar$  is the reduced Planck constant. It is customary in the models involving the graphene bands to place the origin of the Brillouin zone at the Dirac point, so the crystal vector  $\mathbf{k}$  in Equation (1) is measured from the Dirac point. The band profile given by Equation (1) presents a singular point at the origin, which causes certain integrals appearing in the kinetic formulations to diverge. However, one can introduce a very small gap related to the first and second neighbor hopping energy; this assumption provides a smooth version of the energy band [2, 20] given by

$$\mathcal{E}(\mathbf{k}) = v_F \sqrt{\hbar^2 k^2 + \alpha_0^2}, \quad (2)$$

where  $\alpha_0$  is a small parameter, physically related to the nearest-neighbor and next nearest-neighbor hopping energies.

Let  $w(\mathbf{x}, \mathbf{k}, t)$  be the single electron Wigner function [18, 21–23], which is the Wigner transform of the electron density matrix  $\rho(\mathbf{x}, \mathbf{y}, t)$

$$w(\mathbf{x}, \mathbf{k}, t) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \rho\left(\mathbf{x} + \frac{\boldsymbol{\xi}}{2}, \mathbf{x} - \frac{\boldsymbol{\xi}}{2}\right) e^{-i\boldsymbol{\xi} \cdot \mathbf{k}} d\boldsymbol{\xi}. \quad (3)$$

We suppose that the carrier population lives mainly near the Dirac point of the Brillouin zone, which we have chosen as our origin of the  $\mathbf{k}$  space. This allows to effectively enlarge the Brillouin zone to the whole of  $\mathbb{R}^2$  when integrating over  $\mathbf{k}$ , and thus to identify the crystal momentum  $\epsilon\mathbf{k}$  with the Wigner canonical momentum  $\mathbf{p}$  so that the Wigner function is viewed as a function of  $\mathbf{p}$  (instead of  $\mathbf{k}$ ), that is,  $w = w(\mathbf{x}, \mathbf{p}, t)$ .

Let us introduce reference length  $x_0$ , time  $t_0$ , energy  $E_0$ , temperature  $T_0$  and density  $n_0$ . From now on, we shall switch to dimensionless variables, by making the following substitutions:

$$x \rightarrow x_0 x, \quad t \rightarrow t_0 t, \quad p \rightarrow p_0 p, \quad \mathcal{E} \rightarrow E_0 \mathcal{E}, \quad w \rightarrow n_0 w,$$

where, for the sake of simplicity, the new dimensionless quantities are denoted by the same symbols as the old ones. Moreover, we assume that the following relations hold

$$E_0 = k_B T_0, \quad t_0 = \frac{x_0 p_0}{E_0} = \frac{x_0 p_0}{k_B T_0}, \quad (4)$$

where  $k_B$  is the Boltzmann constant. Consequently, the dimensionless energy band reads as follows:

$$\mathcal{E}(\mathbf{p}) = c \sqrt{p^2 + \alpha^2}, \quad (5)$$

where  $p = |\mathbf{p}|$  is the dimensionless momentum and

$$c = \frac{v_F p_0}{k_B T_0}, \quad \alpha = \frac{\alpha_0}{p_0}.$$

A crucial quantity associated with the energy band is the semiclassical velocity, which is defined according to the classical Hamiltonian picture:

$$\mathbf{v}(\mathbf{p}) = \nabla_{\mathbf{p}} \mathcal{E}(\mathbf{p}) = \frac{c}{\sqrt{p^2 + \alpha^2}} \mathbf{p}. \quad (6)$$

For the sake of simplicity, in this paper we consider an isothermal electron gas, so we only need the first two hydrodynamic moments, namely the charge density  $n(\mathbf{x}, t)$  and the momentum density  $n_{\mathbf{p}}(\mathbf{x}, t)$ :

$$n(\mathbf{x}, t) = \int_{\mathbb{R}^2} w(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} \equiv \langle w \rangle, \quad (7)$$

$$n_{\mathbf{p}}(\mathbf{x}, t) = \int_{\mathbb{R}^2} w(\mathbf{x}, \mathbf{p}, t) \mathbf{p} d\mathbf{p} \equiv \langle \mathbf{p} w \rangle. \quad (8)$$

With a more compact notation, we define the monomials

$$\psi_0(\mathbf{p}) = 1, \quad \psi_1(\mathbf{p}) = p_1, \quad \psi_2(\mathbf{p}) = p_2 \quad (9)$$

and the corresponding moments

$$n_s = \langle \psi_s w \rangle, \quad s = 0, 1, 2, \quad (10)$$

so that

$$n = n_0 \quad n_{\mathbf{p}} = (n_1, n_2). \quad (11)$$

In the Wigner (phase-space) formalism, the operator product translates into the Moyal product between two phase space functions  $u(\mathbf{x}, \mathbf{p}), v(\mathbf{x}, \mathbf{p})$ :

$$u \# v = \sum_{k=0}^{\infty} \epsilon^k u \#_k v, \tag{12}$$

where

$$u \#_k v = \frac{1}{(2i)^k} \sum_{|\alpha|+|\beta|=k} \frac{(-1)^{|\alpha|}}{\alpha! \beta!} \nabla_{\mathbf{x}}^{\alpha} \nabla_{\mathbf{p}}^{\beta} u \nabla_{\mathbf{p}}^{\alpha} \nabla_{\mathbf{x}}^{\beta} v \tag{13}$$

and

$$\epsilon = \frac{\hbar}{x_0 p_0} \tag{14}$$

is the dimensionless Planck constant. It is important to note that

$$u \#_k v = (-1)^k v \#_k u. \tag{15}$$

The time evolution of a single particle is governed by the Wigner equation with collisions [2]

$$\partial_t w + \Lambda[\mathcal{E}]w + \Theta[V]w = \frac{1}{\tau}(g - w). \tag{16}$$

The left-hand side of this equation accounts for the Hamiltonian dynamics of the electrons and is equivalent to the von Neumann equation for the density matrix. Here,  $\Lambda[\mathcal{E}]$  and  $\Theta[V]$  are pseudo-differential operators describing the effect of the crystal lattice and the (dimensionless) external potential  $V(\mathbf{x})$ . In terms of the Moyal product we have [24]:

$$\begin{aligned} \Lambda[\mathcal{E}]w &= \frac{i}{\epsilon} \{\mathcal{E}, w\}_{\#} = \frac{i}{\epsilon} (\mathcal{E} \# w - w \# \mathcal{E}) \\ &= \sum_{k=0}^{\infty} \frac{(-1)^k \epsilon^{2k}}{2^{2k}} \sum_{|\alpha|=2k+1} \frac{1}{\alpha!} \nabla_{\mathbf{p}}^{\alpha} \mathcal{E} \nabla_{\mathbf{x}}^{\alpha} w, \end{aligned} \tag{17}$$

$$\begin{aligned} \Theta[V]w &= \frac{i}{\epsilon} \{V, w\}_{\#} = \frac{i}{\epsilon} (V \# w - w \# V) \\ &= - \sum_{k=0}^{\infty} \frac{(-1)^k \epsilon^{2k}}{2^{2k}} \sum_{|\alpha|=2k+1} \frac{1}{\alpha!} \nabla_{\mathbf{x}}^{\alpha} V \nabla_{\mathbf{p}}^{\alpha} w \end{aligned} \tag{18}$$

(note that our sign convention for  $\Theta$  is opposite to that of ref. [2]). In the following, we will also encounter the symmetric version of  $\Theta[V]$ , namely

$$\Theta_{+}[V]w = \frac{1}{2}(V \# w + w \# V) = \sum_{k=0}^{\infty} \frac{(-1)^k \epsilon^{2k}}{2^{2k}} \sum_{|\alpha|=2k} \frac{1}{\alpha!} \nabla_{\mathbf{x}}^{\alpha} V \nabla_{\mathbf{p}}^{\alpha} w. \tag{19}$$

Definitions (17), (18), and (19) in terms the Fourier integral representation become:

$$\Lambda[\mathcal{E}]w = \frac{i}{\epsilon} \frac{1}{(2\pi)^2} \int \delta \mathcal{E}(\mathbf{p}, \nu) \tilde{w}(\nu, \mathbf{p}) e^{i\nu \cdot \mathbf{x}} d\nu, \tag{20}$$

$$\Theta[V]w = \frac{i}{\epsilon} \frac{1}{(2\pi)^2} \int \delta V(\mathbf{x}, \eta) \hat{w}(\mathbf{x}, \eta) e^{i\eta \cdot \mathbf{p}} d\eta, \tag{21}$$

$$\Theta_{+}[V]w = \frac{i}{\epsilon} \frac{1}{(2\pi)^2} \int \delta_{+} V(\mathbf{x}, \eta) \hat{w}(\mathbf{x}, \eta) e^{i\eta \cdot \mathbf{p}} d\nu, \tag{22}$$

where  $\tilde{w}(\boldsymbol{\nu}, \mathbf{p})$  is the Fourier transform of  $w(\mathbf{x}, \mathbf{p})$  with respect to  $\mathbf{x}$  and  $\hat{w}(\mathbf{x}, \boldsymbol{\eta})$  is the Fourier transform of  $w(\mathbf{x}, \mathbf{p})$  with respect to  $\mathbf{p}$ , with the symbols

$$\delta\mathcal{E}(\mathbf{p}, \boldsymbol{\nu}) = \mathcal{E}\left(\mathbf{p} + \frac{\boldsymbol{\nu}}{2}\right) - \mathcal{E}\left(\mathbf{p} - \frac{\boldsymbol{\nu}}{2}\right),$$

$$\delta V(\mathbf{x}, \boldsymbol{\eta}) = V\left(\mathbf{x} + \frac{\boldsymbol{\eta}}{2}\right) - V\left(\mathbf{x} - \frac{\boldsymbol{\eta}}{2}\right),$$

$$\delta_+ V(\mathbf{x}, \boldsymbol{\eta}) = V\left(\mathbf{x} + \frac{\boldsymbol{\eta}}{2}\right) + V\left(\mathbf{x} - \frac{\boldsymbol{\eta}}{2}\right),$$

for  $\mathbf{x}, \mathbf{p}, \boldsymbol{\nu} \in \mathbb{R}^2$ .

The right-hand side of Equation (16) accounts for the effect of collisions. According to Ringhofer–Degond–Méhats' theory [12, 13, 19], collisions in a quantum system can be represented by means of an operator of BGK type [25], describing the relaxation of the system toward a local equilibrium  $g$  in a characteristic (dimensionless) time  $\tau$ . The classical BGK operators share some aspects with the Boltzmann collision operator, like for example local conservation of mass, momentum, and energy. What changes in the quantum case is that the local equilibrium state  $g$  is represented by a suitable Wigner function that maximizes quantum entropy. Since we are considering isothermal hydrodynamics, only mass and momentum conservation will be imposed. The local equilibrium Wigner function  $g$  will be described in detail in Section 3.2.

### 3 | THE CHAPMAN–ENSKOG EXPANSION

In this section, we derive formally the hydrodynamic equations in a fully quantum picture by using the Chapman–Enskog procedure (see ref. [26] for the classical case and, for example, see ref. [13] for the quantum case).

#### 3.1 | Chapman–Enskog expansion and moments

The starting point of the Chapman–Enskog method is the formal expansion of the Wigner function in a series of powers of the collision time  $\tau$ :

$$w = w_0 + \tau w_1 + \tau^2 w_2 + \dots \quad (23)$$

As we said before, we are supposed to work in the isothermal case, and that the moments  $n_s$  (i.e.,  $n$  and  $n_p$ ) are locally conserved hydrodynamic quantities, so we assume that

$$n_s = \langle \psi_s w \rangle = \langle \psi_s g \rangle, \quad s = 0, 1, 2. \quad (24)$$

(a condition that guarantees that the BGK operator conserves  $n$  and  $n_p$ ).

The second step of the Chapman–Enskog procedure is to expand the time-derivative of the macroscopic moments (not the macroscopic moments themselves) in powers of  $\tau$ :

$$\partial_t n_s = \partial_t^0 n_s + \tau \partial_t^1 n_s + \dots \quad (25)$$

By substituting the expansion (23) in the Wigner equation (16), we obtain

$$w_0 = g \quad (26)$$

$$w_1 = -T w_0 - \partial_t^0 w_0 = -T g - \partial_t^0 g \quad (27)$$

where  $T = \Lambda[\mathcal{E}] + \Theta[V]$  and  $\partial_t^0$  stands for the time-derivatives of  $g$  approximated at order 0, as it results from the expansion (25). Indeed, the function  $g$  depends on time only through the dependence on the macroscopic quantities  $n$  and  $n_p$ , so

that

$$\partial_t g = \sum_{s=0}^2 \frac{\delta g}{\delta n_s} \frac{\partial n_s}{\partial t} = \sum_{s=0}^2 \frac{\delta g}{\delta n_s} (\partial_t^0 n_s + \tau \partial_t^1 n_s + \dots). \tag{28}$$

Note that we used the symbol of functional derivative because, as we shall see, the dependence of  $g$  on the moments  $n_s$  is deeply nonlocal. Also note that Equations (24) and (26) entail

$$\langle \psi_s w_k \rangle = 0, \quad s = 0, 1, 2, \quad k \geq 1.$$

Multiplying the Wigner equation (16) by  $\psi_s$  and integrating over  $\mathbf{p}$  we obtain

$$\partial_t n_s + \langle \psi_s T w_0 \rangle + \tau \langle \psi_s T w_1 \rangle = \mathcal{O}(\tau^2). \tag{29}$$

Then, by using expression (27), we obtain up to  $\mathcal{O}(\tau^2)$ ,

$$\partial_t n_s + \langle \psi_s T g \rangle = \tau \langle \psi_s T T g \rangle + \tau \langle \psi_s T \partial_t^0 g \rangle, \quad s = 0, 1, 2. \tag{30}$$

We have therefore identified

$$\partial_t^0 n_s = -\langle \psi_s T g \rangle, \quad \partial_t^1 n_s = \langle \psi_s T T g \rangle + \langle \psi_s T \partial_t^0 g \rangle. \tag{31}$$

The  $\mathcal{O}(1)$  equations,

$$\partial_t n_s + \langle \psi_s T g \rangle = 0, \quad s = 0, 1, 2, \tag{32}$$

are the equations of the inviscid hydrodynamics and are the quantum analog of the Euler equations of classical hydrodynamics, while the  $\mathcal{O}(\tau)$  Equations (30) give the quantum analog of the classical Navier–Stokes equations. The meaning of  $\partial_t^0$  is that the time-derivatives of moments are given by Euler equations (32).

### 3.2 | Equilibrium

In order to proceed with the Chapman–Enskog expansion, the equilibrium distribution  $g$  must be made explicit. As already mentioned in Section 2,  $g$  is a Wigner function that satisfies the QMEP. More precisely, according to the QMEP,  $g$  is the (unique) maximizer of the von Neumann entropy subject to the constraint that the observed macroscopic moments  $n$  and  $n_p$  are determined by Equation (10). We do not repeat here the derivation of the form of  $g$  (which can be found e.g., in refs. [12, 13, 24]) and we limit ourselves to state the result that one obtains assuming that the entropy is compatible with Fermi–Dirac statistics:

$$g = \text{Op}^{-1} \left( \frac{1}{e^{\text{Op}(\mathcal{E} - \mathbf{B} \cdot \mathbf{p} - A)} + 1} \right) \tag{33}$$

where we have taken into account Equation (4). Here,  $\text{Op}$  represents the Weyl quantization and is defined, for a phase space function  $a = a(\mathbf{x}, \mathbf{p})$ , by

$$[\text{Op}(a)\varphi](\mathbf{x}) = \frac{1}{(2\pi\epsilon)^2} \int a\left(\frac{\mathbf{x} + \mathbf{y}}{2}, \mathbf{p}\right) \varphi(\mathbf{y}) e^{i(\mathbf{x} - \mathbf{y}) \cdot \mathbf{p} / \epsilon} d\mathbf{y} d\mathbf{p}. \tag{34}$$

We recall [18, 22, 23] that the inverse transform  $\text{Op}^{-1}$  coincides with the Wigner transform up to the identification of the operator  $\text{Op}(a)$  with its integral kernel  $a$ . To this extent, the Wigner transform (3) and the Weyl transform (34) are the inverse of each other.

The definition of  $g$  is completed by imposing the constraints (24). In (33) the scalar function  $A$  and the vector function  $\mathbf{B} = (B_1, B_2)$ , both real-valued, are the Lagrange multipliers that provide the necessary degrees of freedom for  $g$  to fulfill such constraints.

### 3.3 | Quantum Euler equations

We now express the quantum Euler equations (32) in terms of the Lagrange multipliers.

For the operator  $\Lambda[\mathcal{E}]$  we have

$$\begin{aligned}\Lambda[\mathcal{E}]g &= \frac{i}{\epsilon}\{\mathcal{E}, g\}_{\#} = \frac{i}{\epsilon}\{\mathcal{E} - \mathbf{B} \cdot \mathbf{p} - A, g\}_{\#} + \frac{i}{\epsilon}\{\mathbf{B} \cdot \mathbf{p} + A, g\}_{\#} \\ &= \frac{i}{\epsilon}\{\mathbf{B} \cdot \mathbf{p} + A, g\}_{\#} = \frac{i}{\epsilon}\{\mathbf{B} \cdot \mathbf{p}, g\}_{\#} + \Theta[A]g,\end{aligned}$$

where we used the fact that  $\{\mathcal{E} - \mathbf{B} \cdot \mathbf{p} - A, g\}_{\#} = 0$ , since  $g$  is a function of (and therefore commutes with)  $\mathcal{E} - \mathbf{B} \cdot \mathbf{p} - A$  (see (33)). Moreover (using the convention of summing over repeated indices  $\mathbf{B} \cdot \mathbf{p} = B_j p_j$ ),

$$\begin{aligned}\frac{i}{\epsilon}\{B_j p_j, g\}_{\#} &= \frac{2i}{\epsilon} \sum_{\text{odd } k} \epsilon^k (B_j p_j)_{\#k} g \\ &= \frac{2i}{\epsilon} \sum_{k=0}^{\infty} \frac{\epsilon^{2k+1}}{(2i)^{2k+1}} \sum_{|\alpha|+|\beta|=2k+1} \frac{(-1)^{|\alpha|}}{\alpha! \beta!} \nabla_x^\alpha B_j \nabla_p^\beta p_j \nabla_p^\alpha \nabla_x^\beta g.\end{aligned}$$

In the last expression, only the terms with  $\beta = 0$  and  $\beta = 1$  are nonzero in the factor  $\nabla_p^\beta p_j$  and we obtain:

$$\begin{aligned}\frac{i}{\epsilon}\{B_j p_j, g\}_{\#} &= - \sum_{k=0}^{\infty} \frac{(-1)^k \epsilon^{2k}}{4^k} \sum_{|\alpha|=2k+1} \frac{1}{\alpha!} p_j \nabla_x^\alpha B_j \nabla_p^\alpha g \\ &\quad + \sum_{k=0}^{\infty} \frac{(-1)^k \epsilon^{2k}}{4^k} \sum_{|\alpha|=2k} \frac{1}{\alpha!} \nabla_x^\alpha B_j \nabla_p^\alpha \frac{\partial g}{\partial x_j}.\end{aligned}$$

Comparing with (18) and (19) yields

$$\frac{i}{\epsilon}\{B_j p_j, g\}_{\#} = p_j \Theta[B_j]g + \Theta_+[B_j] \frac{\partial g}{\partial x_j}$$

and, therefore,

$$\Lambda[\mathcal{E}]g = p_j \Theta[B_j]g + \Theta_+[B_j] \frac{\partial g}{\partial x_j} + \Theta[A]g.$$

Then,

$$Tg = \Lambda[\mathcal{E}]g + \Theta[V]g = p_j \Theta[B_j]g + \Theta_+[B_j] \frac{\partial g}{\partial x_j} + \Theta[A + V]g. \quad (35)$$

Here and in the following section we shall use the identities

$$\begin{aligned}\langle \Theta[V]w \rangle &= 0, & \langle p_j \Theta[V]w \rangle &= \frac{\partial V}{\partial x_j} \langle w \rangle, \\ \langle \Theta_+[V]w \rangle &= V \langle w \rangle, & \langle p_j \Theta_+[V]w \rangle &= V \langle p_j w \rangle.\end{aligned} \quad (36)$$

Thanks to (36) we obtain from (35):

$$\langle Tg \rangle = \langle \Lambda[\mathcal{E}]g + \Theta[V]g \rangle = \frac{\partial}{\partial x_j} (B_j \langle g \rangle) = \frac{\partial}{\partial x_j} (B_j n_0) \quad (37)$$

and, for  $i = 1, 2$ ,

$$\begin{aligned}
 \langle p_i Tg \rangle &= \langle p_i \Lambda[\mathcal{E}]g + p_i \Theta[V]g \rangle \\
 &= \frac{\partial B_j}{\partial x_i} \langle p_j g \rangle + \frac{\partial}{\partial x_j} (B_j \langle p_i g \rangle) + \frac{\partial(A+V)}{\partial x_i} \langle g \rangle \\
 &= \frac{\partial B_j}{\partial x_i} n_j + \frac{\partial}{\partial x_j} (B_j n_i) + \frac{\partial(A+V)}{\partial x_i} n_0.
 \end{aligned} \tag{38}$$

Hence, Equation (32) reads as follows:

$$\begin{cases} \partial_t n_0 + \frac{\partial(B_j n_0)}{\partial x_j} = 0 \\ \partial_t n_i + \frac{\partial B_j}{\partial x_i} n_j + \frac{\partial(B_j n_i)}{\partial x_j} + \frac{\partial(A+V)}{\partial x_i} n_0 = 0, \quad i = 1, 2. \end{cases} \tag{39}$$

As discussed in Section 3, Equations (39) are the quantum Euler equations for electrons in graphene. The form of Equation (39) is similar to that of the quantum Euler equations found in other contexts [24, 27].

### 3.4 | Quantum Navier–Stokes equations

The next order in the Chapman–Enskog expansion,  $\mathcal{O}(\tau)$ , provides the quantum Navier–Stokes equations which include viscosity terms. From Equation (30) we see that these terms are given by  $\tau \langle \psi_s T T g \rangle + \tau \langle \psi_s T \partial_t^0 g \rangle$ , for  $s = 0, 1, 2$ . We have

$$TTg = (\Lambda[\mathcal{E}] + \Theta[V]) \left( p_j \Theta[B_j]g + \Theta_+[B_j] \frac{\partial g}{\partial x_j} + \Theta[A^*]g \right).$$

where  $A^* = A + V$ . Then, by using (36), we obtain

$$\langle TTg \rangle = \left\langle \Lambda[\mathcal{E}] \left( p_j \Theta[B_j]g + \Theta_+[B_j] \frac{\partial g}{\partial x_j} + \Theta[A^*]g \right) \right\rangle \tag{40}$$

and

$$\begin{aligned}
 \langle p_i T T g \rangle &= \left\langle \Lambda[\mathcal{E}] \left( p_i p_j \Theta[B_j]g + p_i \Theta_+[B_j] \frac{\partial g}{\partial x_j} + p_i \Theta[A^*]g \right) \right\rangle \\
 &\quad + \frac{\partial V}{\partial x_i} \frac{\partial(B_j n_0)}{\partial x_j}.
 \end{aligned} \tag{41}$$

Unfortunately, no simplifying identities like (36) are available for  $\Lambda[\mathcal{E}]$ . Moreover, the nonpolynomial form of the energy band  $\mathcal{E}$  makes the Navier–Stokes terms (40) and (41) much less treatable than the corresponding terms for quadratic bands [19].

Turning to the expression  $\langle \psi_s T \partial_t^0 g \rangle$ , we recall that  $\partial_t^0$  means that the time-derivatives of the moments  $n_s$  are approximated by the Euler equations (39). The term  $\langle \psi_s T \partial_t^0 g \rangle$  cannot be made more explicit, given the lack of a general explicit form for the dependence of the Lagrange multipliers on the moments  $n_s$ . This can only be done in the semiclassical approximation that will be discussed in Section 4. For the moment, we shall just improve a little bit the expression by using Equations (37) and (38):

$$\langle T \partial_t^0 g \rangle = \partial_t^0 \langle Tg \rangle = \partial_t^0 \left( \frac{\partial(B_j n_0)}{\partial x_j} \right) \tag{42}$$

and, for  $i = 1, 2$ ,

$$\langle p_i T \partial_t^0 g \rangle = \partial_t^0 \left( \frac{\partial B_j}{\partial x_i} n_j + \frac{\partial (B_j n_i)}{\partial x_j} + \frac{\partial A^*}{\partial x_i} n_0 \right). \quad (43)$$

In conclusion we get:

$$\begin{aligned} \partial_t n_0 + \frac{\partial (B_j n_0)}{\partial x_j} &= \tau \partial_t^0 \left( \frac{\partial (B_j n_0)}{\partial x_j} \right) \\ &+ \tau \left\langle \Lambda[\mathcal{E}] \left( p_j \Theta[B_j] g + \Theta_+[B_j] \frac{\partial g}{\partial x_j} + \Theta[A^*] g \right) \right\rangle \end{aligned} \quad (44)$$

and, for  $i = 1, 2$ ,

$$\begin{aligned} \partial_t n_i + \frac{\partial B_j}{\partial x_i} n_j + \frac{\partial (B_j n_i)}{\partial x_j} + \frac{\partial A^*}{\partial x_i} n_0 &= \\ \tau \partial_t^0 \left( \frac{\partial B_j}{\partial x_i} n_j + \frac{\partial (B_j n_i)}{\partial x_j} + \frac{\partial A^*}{\partial x_i} n_0 \right) &+ \tau \frac{\partial V}{\partial x_i} \frac{\partial (B_j n_0)}{\partial x_j} \\ + \tau \left\langle \Lambda[\mathcal{E}] \left( p_i p_j \Theta[B_j] g + p_i \Theta_+[B_j] \frac{\partial g}{\partial x_j} + p_i \Theta[A^*] g \right) \right\rangle. \end{aligned} \quad (45)$$

which are the quantum Navier–Stokes equations for electrons in graphene. Here,  $\partial_t^0$  means that every time-derivative of the moments  $n_0$ ,  $n_1$ , and  $n_2$  must be computed by using

$$\begin{aligned} \partial_t^0 n_0 &= - \frac{\partial (B_j n_0)}{\partial x_j}, \\ \partial_t^0 n_i &= - \frac{\partial B_j}{\partial x_i} n_j - \frac{\partial (B_j n_i)}{\partial x_j} - \frac{\partial (A + V)}{\partial x_i} n_0, \quad i = 1, 2. \end{aligned} \quad (46)$$

Equations (44) and (45) are still in implicit form, since we need to express the Lagrange multipliers  $A$  and  $\mathbf{B}$  in terms of the densities  $n_0$ ,  $n_1$ , and  $n_2$ . We shall address this point in the next section, by adopting a semiclassical approach. This will allow us to obtain a closed-form set for Equations (44) and (45). We also note that, once this issue has been solved, the equations can directly be used for a numerical approach and thus for applications to real systems.

#### 4 | SEMICLASSICAL EXPANSION

In this section we introduce the semiclassical approximation, by expanding all quantities and equations to second-order in  $\epsilon$ . To this aim, we introduce the phase space function  $h(\mathbf{x}, \mathbf{p})$  given by

$$h := -\mathcal{E} + \mathbf{B} \cdot \mathbf{p} + A. \quad (47)$$

where the energy band  $\mathcal{E} = \mathcal{E}(\mathbf{p})$  is given by (2);  $A = A(\mathbf{x})$  and  $\mathbf{B} = \mathbf{B}(\mathbf{x})$  are the Lagrange multipliers. For the sake of simplicity, let us assume that the Fermi–Dirac distribution can be approximated with the Maxwell–Boltzmann one. The Fermi–Dirac is certainly more appropriate to the physical regime under consideration but we preferred to avoid technical complications in order to better illustrate the method. Equation (33) then becomes

$$g = \text{Op}^{-1} (e^{\text{Op}(h)}), \quad (48)$$

which is the so-called *quantum exponential* of  $h$  [12, 13, 24, 27]. The quantum exponential admits the semiclassical expansion

$$g = g^{(0)} + \epsilon^2 g^{(2)} + \mathcal{O}(\epsilon^4), \quad (49)$$

where

$$g^{(0)} = e^h \tag{50}$$

is the classical exponential and [13, 22, 24, 27]

$$g^{(2)} = \frac{1}{8} e^h \left\{ -\frac{\partial^2 h}{\partial x_i \partial x_j} \frac{\partial^2 h}{\partial p_i \partial p_j} + \frac{\partial^2 h}{\partial x_i \partial p_j} \frac{\partial^2 h}{\partial p_i \partial x_j} - \frac{1}{3} \frac{\partial^2 h}{\partial x_i \partial x_j} \frac{\partial h}{\partial p_i} \frac{\partial h}{\partial p_j} + \frac{2}{3} \frac{\partial^2 h}{\partial x_i \partial p_j} \frac{\partial h}{\partial p_i} \frac{\partial h}{\partial x_j} - \frac{1}{3} \frac{\partial^2 h}{\partial p_i \partial p_j} \frac{\partial h}{\partial x_i} \frac{\partial h}{\partial x_j} \right\}, \tag{51}$$

where summation convention over repeated indices is adopted. In our case, recalling (6), we have

$$\begin{aligned} \frac{\partial h}{\partial x_i} &= \frac{\partial(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i}, & \frac{\partial h}{\partial p_i} &= B_i - v_i, \\ \frac{\partial^2 h}{\partial x_i \partial x_j} &= \frac{\partial^2(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i \partial x_j}, & \frac{\partial^2 h}{\partial p_i \partial p_j} &= -\frac{\partial v_i}{\partial p_j}, & \frac{\partial^2 h}{\partial x_i \partial p_j} &= \frac{\partial B_j}{\partial x_i}. \end{aligned}$$

Substituting into (51) yields

$$g^{(2)} = \frac{1}{8} e^h \left\{ \frac{\partial^2(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i \partial x_j} \frac{\partial v_i}{\partial p_j} + \frac{\partial B_j}{\partial x_i} \frac{\partial B_i}{\partial x_j} - \frac{1}{3} \frac{\partial^2(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i \partial x_j} (B_i - v_i)(B_j - v_j) + \frac{2}{3} \frac{\partial B_j}{\partial x_i} \frac{\partial(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_j} (B_i - v_i) + \frac{1}{3} \frac{\partial(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i} \frac{\partial(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_j} \frac{\partial v_i}{\partial p_j} \right\}. \tag{52}$$

### 4.1 | Semiclassical expansion of the constraints

In order to proceed with the semiclassical approximation, we need to expand the constraints (24) up to order  $\epsilon^2$ , that is,

$$\langle g^{(0)} \rangle + \epsilon^2 \langle g^{(2)} \rangle = n_0, \quad \langle \mathbf{p} g^{(0)} \rangle + \epsilon^2 \langle \mathbf{p} g^{(2)} \rangle = n_{\mathbf{p}}. \tag{53}$$

We begin with the leading order,  $g^{(0)} = e^h$ . By using the polar representations

$$\mathbf{p} = \rho(\cos \theta, \sin \theta), \quad \mathbf{B} = b(\cos \theta_B, \sin \theta_B),$$

we obtain

$$\begin{aligned} \langle e^h \rangle &= \int_{\mathbb{R}^2} e^{-\mathcal{E} + \mathbf{B} \cdot \mathbf{p} + A} d\mathbf{p} = e^A \int_0^\infty \rho e^{-c\sqrt{\rho^2 + \alpha^2}} \int_{-\pi}^\pi e^{b\rho \cos(\theta - \theta_B)} d\theta d\rho. \\ &= e^A \int_0^\infty \rho e^{-c\sqrt{\rho^2 + \alpha^2}} \int_{-\pi}^\pi e^{b\rho \cos(\theta)} d\theta d\rho = 2\pi e^A \int_0^\infty \rho e^{-c\sqrt{\rho^2 + \alpha^2}} I_0(b\rho) d\rho \\ &= 2\pi e^A \int_\alpha^\infty s e^{-cs} I_0(b\sqrt{s^2 - \alpha^2}) ds = 2\pi e^A \alpha^2 \int_1^\infty t e^{-c\alpha t} I_0(b\alpha\sqrt{t^2 - 1}) dt \\ &= -2\pi e^A \frac{\partial}{\partial c} \left( \alpha \int_1^\infty e^{-c\alpha t} I_0(b\alpha\sqrt{t^2 - 1}) dt \right) \end{aligned}$$

where  $I_0$  is the zeroth-order modified Bessel function of the first kind. Since

$$\alpha \int_1^\infty e^{-c\alpha t} I_0(b\alpha\sqrt{t^2-1}) dt = \frac{e^{-\alpha\sqrt{c^2-b^2}}}{\sqrt{c^2-b^2}}$$

for  $b < c$  (see Remark 1 and e.g., ref. [28]), we obtain

$$\langle e^h \rangle = -2\pi\alpha e^A \frac{\partial}{\partial c} \left( \frac{e^{-\alpha\sqrt{c^2-b^2}}}{\sqrt{c^2-b^2}} \right) = \frac{2\pi c e^A e^{-\alpha\sqrt{c^2-b^2}} (\alpha\sqrt{c^2-b^2} + 1)}{(c^2-b^2)^{3/2}} \quad (54)$$

Now,

$$\nabla_{\mathbf{p}} e^h = -\mathbf{v}e^h + \mathbf{B}e^h$$

and so we have

$$\langle \mathbf{v}e^h \rangle = \mathbf{B}\langle e^h \rangle.$$

Moreover,

$$\begin{aligned} \langle \mathbf{p}e^h \rangle &= \langle \nabla_{\mathbf{B}} e^h \rangle = \nabla_{\mathbf{B}} \langle e^h \rangle = \nabla_{\mathbf{B}} \left( \frac{2\pi c e^A e^{-\alpha\sqrt{c^2-b^2}} (\alpha\sqrt{c^2-b^2} + 1)}{(c^2-b^2)^{3/2}} \right) \\ &= \frac{2\pi c e^A e^{-\alpha\sqrt{c^2-b^2}} (\alpha^2(c^2-b^2) + 3\alpha\sqrt{c^2-b^2} + 3)}{(c^2-b^2)^{5/2}} \mathbf{B} \\ &= \left( \frac{3}{c^2-b^2} + \frac{\alpha^2}{\alpha\sqrt{c^2-b^2} + 1} \right) \langle e^h \rangle \mathbf{B}. \end{aligned} \quad (55)$$

It is convenient to define  $\mathbf{j}$  such that

$$n_{\mathbf{p}} = n_0 \mathbf{j} \quad (56)$$

and to introduce the semiclassical current  $\mathbf{u}$  as

$$n_0 \mathbf{u} := \langle \mathbf{v}e^h \rangle. \quad (57)$$

Hence, from the preceding computations, we see that the following relations between the Lagrange multipliers  $A$  and  $\mathbf{B}$  and the hydrodynamic moments  $n_0$ ,  $\mathbf{u}$  and  $n_{\mathbf{p}}$  hold true at leading-order:

$$\begin{aligned} n_0 &= \frac{2\pi c e^A e^{-\alpha\sqrt{c^2-u^2}} (\alpha\sqrt{c^2-u^2} + 1)}{(c^2-u^2)^{3/2}}, \\ \mathbf{u} &= \mathbf{B}, \\ \mathbf{j} &= \left( \frac{3}{c^2-u^2} + \frac{\alpha^2}{\alpha\sqrt{c^2-u^2} + 1} \right) \mathbf{u}, \end{aligned} \quad (58)$$

where, as usual,  $u := |\mathbf{u}|$ .

*Remark 1.* Since  $e^h/n_0$  is a nonconstant probability distribution in  $\mathbf{p}$ , and since  $|\mathbf{v}| \leq c$  (for  $\alpha \geq 0$ ), then from Jensen's inequality we have

$$|\mathbf{u}| = \frac{1}{n_0} |\langle \mathbf{v}e^h \rangle| < \frac{1}{n_0} \langle |\mathbf{v}|e^h \rangle \leq c,$$

with the strict inequality sign, which ensures that the consistency relation  $u < c$  is fulfilled (also for  $\alpha = 0$ ).

*Remark 2.* For  $\alpha = 0$  we obtain the relations

$$n_0 = \frac{2\pi c e^A}{(c^2 - u^2)^{3/2}}, \quad \mathbf{u} = \mathbf{B}, \quad \mathbf{j} = \frac{3\mathbf{u}}{c^2 - u^2} \quad (59)$$

which are known to hold true for the conical band (with Maxwell–Boltzmann statistics), see for example, ref. [6].

To write down the constraints (53) at second-order, we need to compute  $\langle g^{(2)} \rangle$  and  $\langle \mathbf{p}g^{(2)} \rangle$ , that is,  $\langle \psi_s g^{(2)} \rangle$  for  $s = 0, 1, 2$ . From (52) we have:

$$\begin{aligned} \langle \psi_s g^{(2)} \rangle &= \frac{1}{8} \left\{ \left\langle \psi_s \frac{\partial^2(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i \partial x_j} \frac{\partial v_i}{\partial p_j} e^h \right\rangle + \frac{\partial B_j}{\partial x_i} \frac{\partial B_i}{\partial x_j} n_s \right. \\ &\quad - \frac{1}{3} \left\langle \psi_s \frac{\partial^2(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i \partial x_j} (B_i - v_i)(B_j - v_j) e^h \right\rangle \\ &\quad + \frac{2}{3} \frac{\partial B_j}{\partial x_i} \left\langle \psi_s \frac{\partial(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_j} (B_i - v_i) e^h \right\rangle \\ &\quad \left. + \frac{1}{3} \left\langle \psi_s \frac{\partial(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_i} \frac{\partial(\mathbf{B} \cdot \mathbf{p} + A)}{\partial x_j} \frac{\partial v_i}{\partial p_j} e^h \right\rangle \right\} \quad (60) \end{aligned}$$

for  $s = 0, 1, 2$ .

The moments (i.e., the expressions in angular brackets) in Equation (60), can be (in principle) computed explicitly as functions of  $n_0$  and  $\mathbf{u}$  by using techniques similar to those employed to obtain the relations (58), but the resulting expressions are much more cumbersome.

Note that all the moments appearing in (60) are finite also for  $\alpha = 0$  (because the only singularity comes from  $\partial v_i / \partial p_j$ , which behaves like  $p^{-1}$ , and thus integrable in dimension two). This implies that the semiclassical expansion of the Lagrange multipliers has no singularities, at least to second-order. On the other hand, the quantum Euler equations (39) have been proven to depend only on the Lagrange multipliers. Hence, we obtain the remarkable result that, in our approach, the second-order semiclassical Euler equations contain no singularities, even without band regularization.

## 4.2 | Inversion of the constraint system

Equations (58) and (60) are the expressions of the hydrodynamic moments as functions of the Lagrange multipliers to second-order (first-order in  $\epsilon^2$ ). However, in order to get explicit semiclassical Navier–Stokes equations, it is necessary to express the Lagrange multipliers in terms of the hydrodynamic moments in the quantum Navier–Stokes equations (44) and (45). Then, our next task is to invert the  $\mathcal{O}(\epsilon^2)$  constraint system (53).

To better understand this point, let us schematically indicate by  $\mathbf{A} = (A, \mathbf{B})$  the vector of Lagrange multipliers, and by  $\mathbf{N} = (n_0, \mathbf{j})$  the vector of hydrodynamic moments. In the previous section, we have expressed  $\mathbf{N}$  as a function of  $\mathbf{A}$  up to order  $\epsilon^2$ :

$$\mathbf{N} = \mathbf{F}^{(0)}(\mathbf{A}) + \epsilon^2 \mathbf{F}^{(2)}(\mathbf{A}) + \mathcal{O}(\epsilon^4), \quad (61)$$

where  $\mathbf{F}^{(0)}(\mathbf{A})$  and  $\mathbf{F}^{(2)}(\mathbf{A})$  are given by Equations (58) and (60), respectively. Inverting these relations at order  $\epsilon^2$  means writing

$$\mathbf{A} = \mathbf{A}^{(0)}(\mathbf{N}) + \epsilon \mathbf{A}^{(1)}(\mathbf{N}) + \epsilon^2 \mathbf{A}^{(2)}(\mathbf{N}) + \mathcal{O}(\epsilon^3). \quad (62)$$

To determine the functions  $\mathbf{A}^{(0)}$ ,  $\mathbf{A}^{(1)}$ , and  $\mathbf{A}^{(2)}$ , we insert (62) into (61), which yields (by Taylor expansion)

$$\begin{aligned} \mathbf{N} &= \mathbf{F}^{(0)}(\mathbf{A}^{(0)}) + \epsilon \frac{\partial \mathbf{F}^{(0)}}{\partial \mathbf{A}}(\mathbf{A}^{(0)}) \mathbf{A}^{(1)} \\ &\quad + \epsilon^2 \mathbf{A}^{(1)} \frac{\partial^2 \mathbf{F}^{(0)}}{\partial \mathbf{A}^2}(\mathbf{A}^{(0)}) \mathbf{A}^{(1)} + 2\epsilon^2 \frac{\partial \mathbf{F}^{(0)}}{\partial \mathbf{A}}(\mathbf{A}^{(0)}) \mathbf{A}^{(2)} + 2\epsilon^2 \mathbf{F}^{(2)}(\mathbf{A}^{(0)}) + \mathcal{O}(\epsilon^3). \quad (63) \end{aligned}$$

At leading-order we obtain

$$\mathbf{A}^{(0)} = (\mathbf{F}^{(0)})^{-1}(\mathbf{N}) \quad (64)$$

corresponding to the inversion of (58), that is,

$$A^{(0)} = a(n_0, u) = \log \left( \frac{(c^2 - u^2)^{3/2} n_0}{2\pi c e^{-\alpha\sqrt{c^2 - u^2}} (\alpha\sqrt{c^2 - u^2} + 1)} \right), \quad (65)$$

$$\mathbf{B}^{(0)} = \mathbf{u},$$

where the link with  $\mathbf{j}$  is given by the leading-order relation

$$\mathbf{j} = \left( \frac{3}{c^2 - u^2} + \frac{\alpha^2}{\alpha\sqrt{c^2 - u^2} + 1} \right) \mathbf{u}. \quad (66)$$

From the first-order equation

$$\frac{\partial \mathbf{F}^{(0)}}{\partial \mathbf{A}}(\mathbf{A}^{(0)}) \mathbf{A}^{(1)} = \mathbf{0} \quad (67)$$

we immediately obtain  $\mathbf{A}^{(1)} = \mathbf{0}$ , so that the second-order inversion reduces to the linear system

$$\frac{\partial \mathbf{F}^{(0)}}{\partial \mathbf{A}}(\mathbf{A}^{(0)}) \mathbf{A}^{(2)} = -\mathbf{F}^{(2)}(\mathbf{A}^{(0)}) \quad (68)$$

for the unknown  $\mathbf{A}^{(2)}$  (see also ref. [24]), where

$$\frac{\partial \mathbf{F}^{(0)}}{\partial \mathbf{A}}(\mathbf{A}^{(0)})$$

is the Jacobian matrix of the mapping (58) evaluated at  $A = A^{(0)}$ ,  $\mathbf{B} = \mathbf{B}^{(0)}$  (given by (65)), and  $\mathbf{F}^{(2)}(\mathbf{A}^{(0)})$  is given by (60), also evaluated at  $A = A^{(0)}$ ,  $\mathbf{B} = \mathbf{B}^{(0)}$ . More explicitly, using (54) and (55),

$$\frac{\partial \mathbf{F}^{(0)}}{\partial \mathbf{A}}(\mathbf{A}^{(0)}) = \left( \begin{array}{cc} \frac{\partial \langle e^h \rangle}{\partial A} & \frac{\partial \langle e^h \rangle}{\partial \mathbf{B}} \\ \frac{\partial \langle \mathbf{p} e^h \rangle / n_0}{\partial A} & \frac{\partial \langle \mathbf{p} e^h \rangle / n_0}{\partial \mathbf{B}} \end{array} \right) \Big|_{A=A^{(0)}, \mathbf{B}=\mathbf{B}^{(0)}} = \begin{pmatrix} n_0 & n_0 \mathbf{j} \\ \mathbf{0} & M(n_0, \mathbf{u}) \end{pmatrix} \quad (69)$$

where  $M(n_0, \mathbf{u})$  is the  $2 \times 2$  matrix

$$M(n_0, \mathbf{u}) = \frac{\alpha}{\sqrt{c^2 - u^2} (\alpha\sqrt{c^2 - u^2} + 1)} \mathbf{B} \otimes \mathbf{B} \quad (70)$$

$$+ \left( \frac{3}{c^2 - u^2} + \frac{\alpha^2}{\alpha\sqrt{c^2 - u^2} + 1} \right) I. \quad (70)$$

Moreover,

$$\mathbf{F}^{(2)}(\mathbf{A}^{(0)}) = \begin{pmatrix} f_1^{(2)}(n_0, \mathbf{u}) \\ f_p^{(2)}(n_0, \mathbf{u}) \end{pmatrix}$$

where  $f_1^{(2)}(n_0, \mathbf{u})$  and  $f_p^{(2)}(n_0, \mathbf{u})$  are given by the right-hand side of (60), for  $s = 0, 1, 2$ , with  $A, \mathbf{B}$  substituted by their leading-order expressions (65), and  $\mathbf{j}$  is still given by the leading-order relation (66). Hence, the second-order corrections to the relations (65) are obtained by solving the linear system

$$\begin{pmatrix} n_0 & n_0 \mathbf{j} \\ \mathbf{0} & M(n_0, \mathbf{u}) \end{pmatrix} \begin{pmatrix} A^{(2)} \\ \mathbf{B}^{(2)} \end{pmatrix} = - \begin{pmatrix} f_1^{(2)}(n_0, \mathbf{u}) \\ f_p^{(2)}(n_0, \mathbf{u}) \end{pmatrix} \quad (71)$$

(together with the relation (66) between  $\mathbf{j}$  and  $\mathbf{u}$ ).

### 4.3 | Semiclassical expansion of the quantum Navier–Stokes equations

In the semiclassical approximation, the hydrodynamic equations for electrons in graphene can be summarized in the following theorem.

**Theorem 1.** *The quantum corrected semiclassical model for a regularized energy band, in the isothermal case, reads as*

$$\partial_t n_i + E_i^{(0)} + \epsilon^2 E_i^{(2)} = \tau S_i^{(0)} + \tau \epsilon^2 S_i^{(2)}, \quad i = 0, 1, 2 \tag{72}$$

where the Euler terms are

$$E_0^{(0)} = \frac{\partial(n_0 u_j)}{\partial x_j}, \tag{73}$$

$$E_i^{(0)} = n_j \frac{\partial u_j}{\partial x_i} + \frac{\partial(n_i u_j)}{\partial x_j} + n_0 \frac{\partial(a + V)}{\partial x_i}, \quad i = 1, 2$$

$$E_0^{(2)} = \frac{\partial(n_0 B_j^{(2)})}{\partial x_j}, \tag{74}$$

$$E_i^{(2)} = n_j \frac{\partial B_j^{(2)}}{\partial x_i} + \frac{\partial(n_i B_j^{(2)})}{\partial x_j} + n_0 \frac{\partial A^{(2)}}{\partial x_i}, \quad i = 1, 2$$

where  $a = A^{(0)}$ ,  $A^{(2)}$ ,  $B_j^{(2)}$  are given by (65), (71), and are functions of the macroscopic moments  $n_0$  and  $\mathbf{u} = |\mathbf{u}|$ , while the viscosity terms have the expressions

$$S_0^{(0)} = -\frac{\partial}{\partial x_j} \left[ \left( u_j + n_0 \frac{\partial u_j}{\partial n_0} \right) E_0^{(0)} + \frac{\partial u_j}{\partial j_k} E_k^{(0)} \right] + \frac{\partial}{\partial x_k} \left( \frac{\partial u_j}{\partial x_l} \left\langle \frac{\partial(v_k p_j)}{\partial p_l} g^{(0)} \right\rangle + u_j \frac{\partial(n_0 u_k)}{\partial x_j} + \frac{\partial(a + V)}{\partial x_l} \left\langle \frac{\partial v_k}{\partial p_l} g^{(0)} \right\rangle \right), \tag{75}$$

$$S_i^{(0)} = -\left[ n_j \frac{\partial}{\partial x_i} \frac{\partial u_j}{\partial n_0} + \frac{\partial}{\partial x_i} \left( n_i \frac{\partial u_j}{\partial n_0} \right) + n_0 \frac{\partial}{\partial x_i} \frac{\partial a}{\partial n_0} + \frac{\partial a}{\partial x_i} \right] E_0^{(0)} - \left[ n_k \frac{\partial}{\partial x_i} \frac{\partial u_j}{\partial n_k} + \frac{\partial u_j}{\partial x_k} + \frac{\partial}{\partial x_j} \left( u_j \delta_{ik} + n_i \frac{\partial u_j}{\partial n_k} \right) + n_0 \frac{\partial}{\partial x_i} \frac{\partial a}{\partial n_k} \right] E_k^{(0)} + \frac{\partial}{\partial x_k} \left[ \frac{\partial u_j}{\partial x_l} \left\langle \frac{\partial(v_k p_i p_j)}{\partial p_l} g^{(0)} \right\rangle + u_j \frac{\partial \langle v_k p_i g^{(0)} \rangle}{\partial x_j} + \frac{\partial(a + V)}{\partial x_l} \left\langle \frac{\partial(v_k p_i)}{\partial p_l} g^{(0)} \right\rangle \right] \tag{76}$$

(for  $i = 1, 2$ ).

$$S_0^{(2)} = \partial_t^0 \left( \frac{\partial(n_0 B_j^{(2)})}{\partial x_j} \right) + \sum_{\alpha+\beta+\gamma+\delta=2} \left\langle \Lambda^{(\alpha)}[\mathcal{E}] \left( \Theta^{(\beta)}[p_j B_j^{(\gamma)} + A_*^{(\gamma)}] g^{(\delta)} + \Theta_+^{(\beta)}[B_j^{(\gamma)}] \frac{\partial g^{(\delta)}}{\partial x_j} \right) \right\rangle \tag{77}$$

and, for  $i = 1, 2$ ,

$$S_i^{(2)} = \partial_t^0 \left( \frac{\partial B_j^{(2)}}{\partial x_i} n_j + \frac{\partial(n_i B_j^{(2)})}{\partial x_j} + \frac{\partial A^{(2)}}{\partial x_i} n_0 \right) + \frac{\partial V}{\partial x_i} \frac{\partial(n_0 B_j^{(2)})}{\partial x_j} + \sum_{\alpha+\beta+\gamma+\delta=2} \left\langle \Lambda^{(\alpha)}[\mathcal{E}] \left( \Theta^{(\beta)}[p_i p_j B_j^{(\gamma)} + p_i A_*^{(\gamma)}] g^{(\delta)} + \Theta_+^{(\beta)}[p_i B_j^{(\gamma)}] \frac{\partial g^{(\delta)}}{\partial x_j} \right) \right\rangle. \tag{78}$$

*Proof.* The derivation of the model is reported in Appendix.  $\square$

Note that  $E_i^{(0)}$  and  $E_i^{(2)}$  provide the leading-order and second-order approximations of the quantum Euler equations, while  $S_i^{(0)}$  and  $S_i^{(2)}$  are the analogous approximation of the “viscous” terms. The  $\epsilon^2$  quantum corrections  $E_i^{(2)}$  and  $S_i^{(2)}$  depend on the second-order Lagrange multipliers  $A^{(2)}$  and  $B_j^{(2)}$ , but the dependence of the latter on the hydrodynamic unknowns  $n_i$  is complicated and it is not explicitly written down here: it can be deduced starting from Equation (71).

The high complexity of the model and the cumbersome equations require a numerical implementation to better understand the role of the terms involved. In ref. [29] a calculation of the bulk and shear viscosity of the electron liquid in a doped graphene sheet is reported. In ref. [30] the authors show a quantitative calculation of the electronic shear and Hall viscosities in graphene. In ref. [5] the authors determine the ratio of the shear viscosity to the entropy density, also discussing the possible consequences of the low viscosity. In this framework, as a natural continuation of our work, it could be desirable to perform a numerical estimation of the viscosity terms derived in the paper and consequently discuss a comparison with the quantities mentioned above.

#### 4.4 | The small current regime

A simplified model can be obtained by assuming a regime of small current, namely,

$$\mathbf{j} = \mathcal{O}(\epsilon).$$

We recall that

$$\mathbf{g}^{(0)} = \mathbf{e}^h = \exp(-\mathcal{E} + \mathbf{p} \cdot \mathbf{B} + A),$$

and (see (58))

$$\begin{aligned} \langle \mathbf{e}^h \rangle &= \frac{1 + \alpha \sqrt{c^2 - b^2}}{e^{\alpha \sqrt{c^2 - b^2}}} \frac{2\pi c e^A}{(c^2 - b^2)^{3/2}}, \\ \langle \mathbf{v} \mathbf{e}^h \rangle &= \langle \mathbf{e}^h \rangle \mathbf{B}, \\ \langle \mathbf{p} \mathbf{e}^h \rangle &= \left( \frac{3}{c^2 - b^2} + \frac{\alpha^2}{\alpha \sqrt{c^2 - b^2} + 1} \right) \langle \mathbf{e}^h \rangle \mathbf{B}. \end{aligned} \quad (79)$$

where  $b = |\mathbf{B}|$ . As in Section 4.2, let

$$A = A^{(0)} + \epsilon A^{(1)} + \epsilon^2 A^{(2)} + \dots, \quad \mathbf{B} = \mathbf{B}^{(0)} + \epsilon \mathbf{B}^{(1)} + \epsilon^2 \mathbf{B}^{(2)} + \dots.$$

Since now

$$\mathbf{N}^{(0)} = (n, \mathbf{0}), \quad \mathbf{N}^{(1)} = (0, \mathbf{j})$$

following the procedure of Section 4.2, the leading-order Equation (64) yields

$$\mathbf{B}^{(0)} = \mathbf{0}, \quad \frac{2\pi(1 + c\alpha)}{e^{c\alpha} c^2} e^{A^{(0)}} = n. \quad (80)$$

In particular,

$$A^{(0)} = \log \left( \frac{e^{c\alpha} c^2 n}{2\pi(1 + c\alpha)} \right). \quad (81)$$

The first-order Equation (67) has now a nonvanishing  $\mathbf{N}^{(1)}$  at the right-hand side and the Jacobian matrix is given by

$$\begin{aligned} \frac{\partial \langle e^h \rangle}{\partial A} &= \langle e^h \rangle, & \frac{\partial \langle e^h \rangle}{\partial B_i} &= \left\langle \frac{\partial e^h}{\partial B_i} \right\rangle = \langle p_i e^h \rangle \\ \frac{\partial \langle p_i e^h \rangle}{\partial A} &= \langle p_i e^h \rangle, & \frac{\partial \langle p_i e^h \rangle}{\partial B_j} &= \left\langle p_i \frac{\partial e^h}{\partial B_j} \right\rangle = \langle p_i p_j e^h \rangle \end{aligned} \tag{82}$$

By evaluating such matrix (82) at  $A = A^{(0)}$  and  $\mathbf{B} = \mathbf{B}^{(0)}$ , we see that the first-order equation is

$$\begin{pmatrix} n & 0 \\ 0 & C_1 n \end{pmatrix} \begin{pmatrix} A^{(1)} \\ \mathbf{B}^{(1)} \end{pmatrix} = \begin{pmatrix} 0 \\ \mathbf{j} \end{pmatrix}, \tag{83}$$

where

$$C_1 = \langle p_i^2 e^{-\mathcal{E}} \rangle = \frac{1}{2} \langle |\mathbf{p}|^2 e^{-\mathcal{E}} \rangle = \frac{2\pi}{c^4} (c^2 \alpha^2 + 3c\alpha + 3).$$

This leads to

$$A^{(1)} = 0, \quad \mathbf{B}^{(1)} = \frac{1}{C_1 n} \mathbf{j}. \tag{84}$$

The second-order inversion equation, given by (63), requires the evaluation of  $g^{(2)}$  at  $A = A^{(0)}$  and  $\mathbf{B} = \mathbf{B}^{(0)} = \mathbf{0}$ , which leads to the much simpler expression

$$g^{(2)} \approx \frac{1}{8} e^{A^{(0)}} e^{-\mathcal{E}} \left( \frac{\partial^2 A^{(0)}}{\partial x_i \partial x_j} \frac{\partial v_i}{\partial p_j} - \frac{1}{3} \frac{\partial^2 A^{(0)}}{\partial x_i \partial x_j} v_i v_j + \frac{1}{3} \frac{\partial A^{(0)}}{\partial x_i} \frac{\partial A^{(0)}}{\partial x_j} \frac{\partial v_i}{\partial p_j} \right). \tag{85}$$

Hence, by using (80) and obvious symmetry reasons,

$$\langle g^{(2)} \rangle \approx C_2 n \left( \frac{2}{3} \Delta A^{(0)} + |\nabla A^{(0)}|^2 \right), \quad \langle \mathbf{p} g^{(2)} \rangle = \mathbf{0}, \tag{86}$$

where

$$C_2 = \frac{1}{16} \frac{e^{c\alpha} c^2}{2\pi(1+c\alpha)} \langle |\mathbf{v}|^2 e^{-\mathcal{E}} \rangle = \frac{1}{16} \frac{e^{c\alpha} c^4}{(1+c\alpha)} \int_{\alpha}^{+\infty} \frac{s^2 - \alpha^2}{s} e^{-cs} ds. \tag{87}$$

The last ingredient we need to invert in (63) at second-order are the Hessian matrices of  $\langle e^k \rangle$  and  $\langle p_i e^h \rangle$  evaluated at  $A^{(0)}$  and  $\mathbf{B}^{(0)}$ . Exploiting symmetries, we readily see that the first one is given by

$$\begin{pmatrix} n & 0 \\ 0 & C_1 n \delta_{ij} \end{pmatrix}$$

and the second one vanishes. Hence, according to (63),  $A^{(2)}$  and  $\mathbf{B}^{(2)}$  are given by

$$\begin{pmatrix} C_1 |\mathbf{j}|^2 \\ \mathbf{0} \end{pmatrix} + 2 \begin{pmatrix} 1 & 0 \\ 0 & C_1 \end{pmatrix} \begin{pmatrix} A^{(2)} \\ \mathbf{B}^{(2)} \end{pmatrix} + 2C_2 \begin{pmatrix} \frac{2}{3} \Delta A^{(0)} + |\nabla A^{(0)}|^2 \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} 0 \\ \mathbf{0} \end{pmatrix},$$

that is,

$$A^{(2)} = -C_2 \left( \frac{2}{3} \Delta A^{(0)} + |\nabla A^{(0)}|^2 \right) - \frac{C_1}{2} |\mathbf{j}|^2, \quad \mathbf{B}^{(2)} = \mathbf{0}, \tag{88}$$

A further simplification is given by the fact that the terms  $S_i^{(2)}$  are of third-order with respect to the small parameters  $\tau$  and  $\epsilon$  and so one can decide to neglect them in a suitable regime. All such simplifications result in a system of Navier–Stokes-like

equations of the form

$$\partial_t n_i + E_i^{(0)} + \epsilon^2 E_i^{(2)} = \tau S_i^{(0)}, \quad i = 0, 1, 2, \quad (89)$$

where the semiclassical Euler terms  $E_i^{(0)}$  are given by (73), the semiclassical viscosity terms  $S_i^{(0)}$  are given by (75) and (76) and the quantum corrections  $E_i^{(2)}$  are given by

$$E_0^{(2)} = -n_0 \frac{\partial}{\partial x_i} \left( \frac{2C_2}{3} \Delta A^{(0)} + C_2 |\nabla A^{(0)}|^2 + \frac{C_1}{2} |\mathbf{j}|^2 \right), \quad (90)$$

$$E_i^{(2)} = 0, \quad i = 1, 2,$$

$A^{(0)}$  being given by (81). Note that  $E_0^{(2)}$  is the Bohm potential for our system [10, 11, 22, 24]. We remark that in the case of nonsmoothed cones, that is for  $\alpha = 0$ , the model is nonsingular, since the coefficients  $C_1$  and  $C_2$  remain finite. This was expected, as we already remarked that the singular terms are all in  $S_i^{(2)}$ .

## 5 | CONCLUSIONS

In this work, we have obtained the hydrodynamic equations for a population of conduction electron carriers in graphene, by using a regularized form for the energy band and by assuming a isothermal regime. The macroscopic equation include the inviscid Euler equations and the viscosity terms. The underlying kinetic model is given by the Wigner-function approach, in which the effect of the periodic potential is accounted for by a pseudo-differential operator with the symbol given by the band shape. We use the Chapman–Enskog procedure accompanied by the quantum maximum energy principle, which provides the Wigner equilibrium function in terms of a set of Lagrange multipliers. The relationship between the hydrodynamic quantities and the Lagrange multipliers cannot be inverted in general, thus we obtain hydrodynamic equations which, in their general quantum form, are left implicit. Subsequently, we expand the hydrodynamic equations together with all relevant quantities to second-order in  $\epsilon$ , thus obtaining the semiclassical approximation for the inviscid and viscous hydrodynamic equations. It is worth to remark that, in contrast with previous studies, the semiclassical Euler equations that we obtain by applying the QMEP are nonsingular in the zero-gap limit  $\alpha \rightarrow 0$ .

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## APPENDIX A: PROOF OF THEOREM 1

We compute the expressions  $E_i^{(m)}$  and  $S_i^{(m)}$  one by one. To this aim, we recall from Section 2 that the pseudo-differential operator admit the expansions:

$$\Lambda[\mathcal{E}] \approx \Lambda^{(0)}[\mathcal{E}] + \epsilon^2 \Lambda^{(2)}[\mathcal{E}] = \mathbf{v} \cdot \nabla_x - \frac{\epsilon^2}{4} \sum_{|\alpha|=3} \frac{1}{\alpha!} \nabla_p^\alpha \mathcal{E} \cdot \nabla_x^\alpha, \quad (\text{A1})$$

$$\Theta[V] \approx \Theta^{(0)}[V] + \epsilon^2 \Theta^{(2)}[V] = -\nabla_x V \cdot \nabla_p + \frac{\epsilon^2}{4} \sum_{|\alpha|=3} \frac{1}{\alpha!} \nabla_x^\alpha V \cdot \nabla_p^\alpha, \quad (\text{A2})$$

$$\Theta_+[V] \approx \Theta_+^{(0)}[V] + \epsilon^2 \Theta_+^{(2)}[V] = V - \frac{\epsilon^2}{4} \sum_{|\alpha|=2} \frac{1}{\alpha!} \nabla_x^\alpha V \cdot \nabla_p^\alpha. \quad (\text{A3})$$

These expansions, together with the expansions of the equilibrium and of the Lagrange multipliers obtained in Section 4.2 will now be used in Equations (44) and (45) to obtain the  $\mathcal{O}(\varepsilon^2)$  model (72). From Equations (44) and the leading-order expansion (65) of the Lagrange multipliers, we immediately obtain for the Euler terms  $E_i^{(0)}$  and  $E_i^{(2)}$  the expressions (73) and (74).

Let us now turn to the viscosity terms, starting from the leading-order. From (44), (65) and (A1)–(A3) we obtain

$$S_0^{(0)} = \partial_t^0 \frac{\partial(n_0 u_j)}{\partial x_j} + \frac{\partial}{\partial x_k} \left[ -\frac{\partial u_j}{\partial x_l} \left\langle v_k p_j \frac{\partial g^{(0)}}{\partial p_l} \right\rangle + u_j \frac{\partial \langle v_k g^{(0)} \rangle}{\partial x_j} - \frac{\partial(a+V)}{\partial x_l} \left\langle v_k \frac{\partial g^{(0)}}{\partial p_l} \right\rangle \right],$$

where  $g^{(0)}$  is the local equilibrium at leading-order, that is,

$$g^{(0)} = \exp(-\mathcal{E} + \mathbf{u} \cdot \mathbf{p} + a).$$

Keeping in mind the relationships (56) and (66) between  $\mathbf{u}$ ,  $\mathbf{j}$ ,  $n_0$  and  $n_p$ , we have

$$\frac{\partial(n_0 u_j)}{\partial n_0} = u_j + n_0 \frac{\partial u_j}{\partial n_0}$$

and, for  $i = 1, 2$ ,

$$\frac{\partial(n_0 u_j)}{\partial n_i} = \frac{\partial(n_0 u_j)}{\partial j_k} \frac{\partial j_k}{\partial n_i} = n_0 \frac{\partial u_j}{\partial j_k} \frac{1}{n_0} = \frac{\partial u_j}{\partial j_k},$$

where  $\partial u_j / \partial j_k$  is to be computed from Equation (66). Note that here, at variance with Section 3.1, we are using ordinary derivatives with respect to the moments  $n_i$ : this is because, in the semiclassical expansion, the Lagrange multipliers depend locally on the moments. Therefore, performing integrations by parts and also recalling that  $\langle v_k g^{(0)} \rangle = n_0 u_k$  and

$$\partial_t^0 n_i = -E_i^{(0)}, \quad i = 0, 1, 2,$$

we obtain the expression for  $S_0^{(0)}$  as shown in the theorem. By similar procedures, we first obtain from Equation (45)

$$S_i^{(0)} = \partial_t^0 \left( \frac{\partial u_j}{\partial x_i} n_j + \frac{\partial(n_i u_j)}{\partial x_j} + \frac{\partial(a+V)}{\partial x_i} n_0 \right) + \frac{\partial V}{\partial x_i} \frac{\partial(n_0 u_j)}{\partial x_j} + \frac{\partial}{\partial x_k} \left[ -\frac{\partial u_j}{\partial x_l} \left\langle v_k p_i p_j \frac{\partial g^{(0)}}{\partial p_l} \right\rangle + u_j \frac{\partial \langle v_k p_i g^{(0)} \rangle}{\partial x_j} - \frac{\partial(a+V)}{\partial x_l} \left\langle v_k p_i \frac{\partial g^{(0)}}{\partial p_l} \right\rangle \right]$$

and then the expression (76) where the terms

$$-\frac{\partial V}{\partial x_i} E_0^{(0)} \quad \text{and} \quad \frac{\partial V}{\partial x_i} \frac{\partial(n_0 u_j)}{\partial x_j}$$

have canceled. The viscous quantum corrections  $S_i^{(2)}$  originate from collecting all the  $\mathcal{O}(\varepsilon^2)$  terms appearing at the right-hand sides of (44) and (45), and taking into account the expansions (A1), (A2), and (A3). This yields the expressions (77) and (78). Working out more explicitly these terms would lead to very cumbersome expressions and therefore we decided to limit ourselves to report the overall form without entering into further details.