Quantum transmission conditions for drift-diffusion equations describing charges in graphene with steep potentials

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Abstract

We present a formal derivation of a drift-diffusion model for stationary electron transport in graphene, in presence of sharp potential profiles, such as barriers and steps. Assuming the electric potential to have steep variations within a strip of vanishing width on a macroscopic scale, such strip is viewed as a quantum interface that couples the classical regions at its left and right sides. In the two classical regions, where the potential is assumed to be smooth, electron and hole transport is described in terms of semiclassical kinetic equations. The diffusive limit of the kinetic model is derived by means of a Hilbert expansion and a boundary layer analysis, and consists of drift-diffusion equations in the classical regions, coupled by quantum diffusive transmission conditions through the interface. The boundary layer analysis leads to the discussion of a four-fold Milne (half-space, half-range) transport problem.

1 Introduction

Theoretical prediction and experimental demonstration of striking quantum phenomena manifested by electrons in graphene, such as Klein paradox [17, 24] and Veselago lensing [11, 18], are among the most important achievements of solid-state physics in the last decade, and offer interesting opportunities to nano-electronics and opto-electronics. All such phenomena are intimately related to the chiral nature of electrons in graphene [10] and take place in presence of electric potential steps or barriers, that can be realised by means of suitable electric gates or doping profiles. On the other hand, such effects depend on the quantum coherence of the electrons and their neat manifestation is only possible in idealised situations, or at least in very controlled experimental settings, where the transport is essentially ballistic. Collisional and diffusive transport, instead, is a more realistic regime but tends to increase the decoherence, which results in blurred versions of the purely ballistic pictures. It is therefore important to offer a mathematical instrument to describe and analyse such more realistic situation.

We propose here a hybrid model where a thin “active” quantum region, containing to the rapid potential variations, is viewed as a “quantum interface” that couples the surrounding “classical” regions, where the transport regime is diffusive and incoherent. The coupling is firstly described at the kinetic level, where the classical-quantum matching is more natural, and then the diffusive limit is performed by means of the Hilbert expansion method [12]. This first, theoretical paper is devoted to the derivation of the model, which will be numerically tested in a subsequent work. We remark that part of the contents of the present paper have been anticipated in Ref. [5].

A hybrid kinetic-quantum model for standard particles (i.e. scalar particles with parabolic energy-band, as opposed to chiral particles with conical energy-band, as electrons in graphene) has been firstly considered by Ben Abdallah [7, 8]. The central idea in Ben Abdallah’s construction is that a scattering problem is solved in the quantum region, that is a thin strip around the steep potential variations, and the resulting scattering states (incident/reflected/transmitted waves) are identified with inflow/outflow particles in/from the classical regions. This leads to a hybrid model where *transmission conditions*, of quantum nature, are imposed to classical kinetic equations.

The diffusive limit of Ben Abdallah’s model is studied by Degond and El Ayyadi in Ref. [13]. Here, the kinetic model of Ref. [7] is expanded in powers of the scaled collision time (Hilbert expansion), which leads to classical Drift-Diffusion (D-D) equations in the classical regions. The Hilbert expansion of the kinetic transmission condition yields purely classical diffusive transmission conditions at leading order. However, a boundary-layer analysis shows that there is a first-order quantum correction of the diffusive transmission conditions under the form of an “extrapolation coefficient” (somehow analogous to the extrapolation length of neutron transport theory [2]), which depends on the reflection and transmission coefficients coming from the quantum scattering problem.

An intermediate (between kinetic and diffusive) hybrid classical-quantum model has been studied in Ref. [14], where two SHE (Spherical Harmonic Expansion) models are coupled via suitable interface conditions.

As explained above, our goal is to construct a diffusive model of the electron transport in a graphene device where a small (compared to a macroscopic scale) region, containing the steep potential variations, is the “active” zone where quantum coherence is exploited. Although our construction is inspired by the quoted works [7, 13, 14], nevertheless we have to deal here with a rather different situation. First of all, electrons in graphene have a chirality, which is an additional, discrete degree of freedom, denoted by s; this implies that, in each classical region, two populations of electrons (corresponding to $s = 1$ and $s = -1$) have to be considered. The two populations, in absence of other coupling mechanisms in the bulk, are coupled by the quantum interface. The second aspect is that electrons have a conical dispersion relation (energy band), which requires the use of a semiclassical[1] transport equation and a non-standard Fermi-Dirac (F-D) distribution. Finally, electrons with negative

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[1] According to the terminology adopted, e.g., in [1], we call “semiclassical” classical transport (or Boltzmann) equation where elements of quantum nature are retained, e.g. a non-parabolic dispersion relation.

chirality have a negative energy cone which is unbounded from below; this fact forces us to describe such electrons in terms of holes (electron vacancies). This is not a novelty, of course, but the fact that positive-energy and negative-energy electrons are coupled by the quantum interface makes the introduction of holes a delicate issue.

The content of the present paper is the following. After a brief review of the basic facts about the quantum dynamics of electrons in graphene (Section 2), the construction of the model begins, at the kinetic level, in Sec. 3. If (x, y) are the coordinates on the graphene sheet, we assume that the electric potential is a sum $V(x) + U(x, y)$, where $V(x)$ has steep variations within a tiny strip around $x = 0$ and tends to a constant potential difference δV outside. This is the potential which is responsible for the quantum effects and is treated by means of the stationary Schrödinger equation. The second term, U is the smooth part of the potential: it is treated semiclassically and produces the drift term of the D-D equations. Assuming that the width of the quantum strip vanishes on a macroscopic scale, this picture corresponds to a configuration where $x = 0$ is a quantum interface separating the classical regions $x < 0$ and $x > 0$ (see Figure 3). In Sec. 3.1 we write down the stationary transport equations in the classical regions and the kinetic transmission conditions (KTC) at $x = 0$. The KTC express the fact that inflowing/outflowing classical particles correspond to the incoming/outgoing plane waves described by by the scattering problem across the interface. In Sec. 3.2, in view of the diffusive limit, we add to the transport equation a relaxation term towards two local Fermi-Dirac distributions (one for each value of chirality). In Sec. 3.3, the KTC are reformulated in terms of electrons and holes and are proven to conserve the total charge flux across the interface.

Section 4 is devoted to the diffusive limit of the kinetic model and contains the main results of the paper. In Sec. 4.1 we study the diffusion limit in the bulk, that is in the classical regions. By means of a Hilbert expansion [12, 22] in powers of the typical collision time τ, we obtain semiclassical, stationary, D-D equations for electrons and holes. In Sec. 4.2 the we expand the KTC. At leading-order we immediately obtain diffusive transmission conditions (DTC) as a relation between the chemical potential at the two sides of the interface. Such leading-order DTC couple electrons and holes but are not "quantum", to the extent that they are independent on the solution of the scattering problem. In Sec. 4.3 it is shown that the introduction of a boundary-layer corrector in the Hilbert expansion is necessary to obtain the first-order DTC. Such corrector is associated to a system of four Milne (half-space, half-range) transport equation coupled by non-homogeneous KTC. The mathematical properties of such four-fold Milne problem are stated in Theorem 4.4, which is the first of the two main results of the paper. The layer analysis leads to the first-order correction to the DTC (Theorem 4.5), which is the second main result of the paper. The correction is expressed as a relation between left and right chemical potentials and involves the asymptotic densities associated to the Milne problem. Such densities, which are a generalization of the extrapolation coefficients of Ref. [13], depend on the scattering coefficients and, therefore, the first-order DTC contain information coming from the quantum physics of the interface. In Sec. 4.4 it is examined the special case where the F-D distribution is approximated by the Maxwell-Boltzmann distribution. Finally, in Sec. 5, we summarize our results by writing down a diffusive model with DTC for a prototypical graphene device.

2 Quantum and semiclassical dynamics of electrons in graphene

We briefly review here some basic facts about the dynamics of electrons in a graphene sheet. For an exhaustive introduction to the subject we address the reader to Ref. [10].

Due to its remarkable mechanical, thermal, optical and electronic properties, graphene has attracted a lot of scientific attention in the last years, and is thought to have several possible technological applications, as for example in the design of electronic devices. It is a two-dimensional crystal of carbon atoms, arranged in a honeycomb lattice. Since every fundamental cell of the associated Bravais lattice contains two carbon atoms, the honeycomb can be decomposed into two inequivalent sublattices. This property implies the existence of two energy-bands having conical intersections at exactly two points (Dirac points) of the reciprocal fundamental cell [10, 23]. Assuming that the so-called inter-valley scattering is negligible, one can consider just a single Dirac point and approximately conical energy bands (Dirac cones) around that point. Graphene is therefore a zero-gap semi-conductor with linear, rather than quadratic, dispersion relation.

As graphene is a 2-dimensional crystal, we shall use the 2-dimensional variable $\boldsymbol{x} = (x, y)$ to identify the electron position. In the vicinity of a Dirac point the dynamics of the electron envelope wave-function is determined by the Dirac-like Hamiltonian

$$\mathcal{H} = c\,\boldsymbol{P}\cdot\boldsymbol{\sigma} + V\,\sigma_0\,, \tag{2.1}$$

where $c \approx 10^6$ m/s is the Fermi velocity (often indicated by v_F in literature), $\boldsymbol{P} = (P_x, P_y) = -i\hbar\nabla$ is the pseudomomentum operator, $V = V(\boldsymbol{x})$ is the potential energy,[2] and σ_0 as well as the Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are given by

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

The stationary Schrödinger equation associated to the Hamiltonian (2.1) is the following eigenvalue problem:

$$\begin{pmatrix} V & c\,(P_x - iP_y) \\ c\,(P_x + iP_y) & V \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \tag{2.2}$$

where E is the energy eigenvalue. Since the wave-function $\Psi = (\psi_1, \psi_2)^t$ is a two-component (bi-spinor) wave-function, we can associate to electrons (besides the usual 1/2-spin which is neglected here) an additional discrete degree of freedom. This is the *chirality*, which is analogous to photon helicity and is represented by the operator

$$S = \frac{1}{|\boldsymbol{P}|} \begin{pmatrix} 0 & P_x - iP_y \\ P_x + iP_y & 0 \end{pmatrix},$$

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[2] We remark that we are using the potential energy V instead of the electric potential $-V/q$ (where $q > 0$ is the elementary charge).

possessing the two eigenvalues $s = 1$ and $s = -1$. This quantity can be interpreted as the projection of the pseudospin $\boldsymbol{\sigma}$ on the direction of the pseudomomentum. For constant V, it is readily seen that the solution to the stationary Schrödinger equation (2.2) exists for any given $E \in \mathbb{R}$ and is given by plane-wave-like functions parametrised by $\boldsymbol{p} = (p_x, p_y) \in \mathbb{R}^2$ and $s \in \{+1, -1\}$, namely:

$$\Psi_{\boldsymbol{p},s}(\boldsymbol{x}) = \begin{pmatrix} 1 \\ s\, e^{i\,\phi} \end{pmatrix} \mathrm{e}^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}}, \tag{2.3}$$

where

$$|\boldsymbol{p}| = \frac{E - V}{c}, \qquad s = \operatorname{sign}(E - V), \qquad \phi = \arg(p_x + ip_y).$$

Note that:

1. $\Psi_{\boldsymbol{p},s}(\boldsymbol{x})$ is a simultaneous (generalised) eigenvector of $\mathcal{H}$, $\boldsymbol{P}$ and S and, therefore, it corresponds to a state with defined energy, E, pseudomomentum $\boldsymbol{p}$ and chirality s;
2. the energy E has a degeneracy corresponding to rotations in the two-dimensional $\boldsymbol{p}$-space;
3. the sign of $E - V$ is equal to the chirality s, which can be interpreted as the pseudospin being parallel ($s = 1$) or antiparallel ($s = -1$) to the wave direction $\boldsymbol{p}$.

The energy dispersion relation, i.e. the energy as a function of $\boldsymbol{p}$ and s when $V = 0$, is, therefore

$$E_s(\boldsymbol{p}) = sc|\boldsymbol{p}|, \tag{2.4}$$

which corresponds to the positive and negative Dirac cones. Using a slightly sloppy terminology, we shall also refer to $E_s(\boldsymbol{p})$ as the "energy bands" of the electron.

In the semiclassical limit, the electron wave function collapses into states of defined pseudomomentum $\boldsymbol{p} = (p_x, p_y) \in \mathbb{R}^2$ and chirality $s = \pm 1$, and the dynamics is described by the Hamiltonian system

$$\begin{cases} \dot{\boldsymbol{x}} = \nabla_{\boldsymbol{p}} E_s(\boldsymbol{p}), \\ \dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{x}} V(\boldsymbol{x}), \end{cases} \tag{2.5}$$

where the energy-band derivatives,

$$\nabla_{\boldsymbol{p}} E_s(\boldsymbol{p}) = \frac{sc\boldsymbol{p}}{|\boldsymbol{p}|}, \tag{2.6}$$

are the associated semiclassical velocities. From a semiclassical point of view, it is apparent that electrons in graphene behave as if they were massless charged particles. They move with constant speed c and the direction of motion is either parallel to the pseudomomentum, for electrons with positive chirality/energy, or anti-parallel, for electrons with negative chirality/energy, and the changes of direction are determined by the electric force. Note that positive and negative electrons are completely decoupled in the semiclassical picture, which corresponds to the absence of quantum interference between the two chirality states (see also Ref. [20]).

Remark 2.1 In the following, $s = \pm 1$ or $s = \pm$ will be used indifferently.

3 Hybrid kinetic-quantum model

In this section we introduce a hybrid kinetic-quantum model of electron transport on a graphene sheet in presence of steep potentials. By this we mean that the behaviour of the electrons in proximity of an abrupt potential variation is described by a fully-quantum scattering problem, while, in the regions where the potential is smooth, it is described by a semiclassical transport , or “kinetic” equation. Such description will be the starting point of the derivation of a hybrid *diffusive*-quantum model, which will be carried out in Sec. 4.

For the sake of simplicity, we make the following assumptions on the electric potential energy (see Figure 1).

H1. $V = V(x)$ depends only on the variable x (which implies that it conserves p_y);

H2. $V(x) \to 0$ on the left and $V(x) \to \delta V$ on the right of a “quantum strip”, around $x = 0$, having vanishing width on a macroscopic length scale.

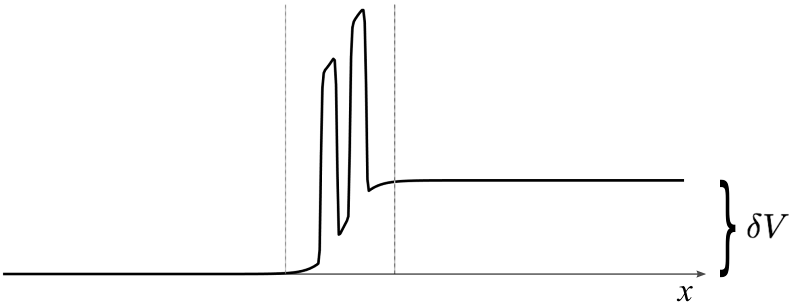

Figure 1: Example of an electric potential profile $V(x)$ satisfying assumptions **H1** and **H2** above. The “quantum active region” lies between the two vertical lines, and V is asymptotically constant with values 0 and δV outside.

For a potential $V(x)$ satisfying **H1** and **H2**, the stationary Schrödinger equation (2.2) has the character of a scattering problem. In particular, Eq. (2.2) is explicitly solvable outside the quantum-strip and the solutions are recognized to be superpositions of plane waves (2.3) with pseudomementum $\boldsymbol{p}$ and chirality s. Imposing the continuity of the two-component wave function inside the quantum strip with the outside plane-wave solutions, yields the scattering (reflection and transmission) coefficients as functions of energy, which constitute the most relevant information associated to the scattering problem. The fact that the plane-wave exterior solutions have defined $\boldsymbol{p}$ and s allows, as explained below, to interpret such waves as particles flowing in and out from the classical regions, which permits to match the two classical regions via the reflection and transmission coefficients.

It is here important to remark that if the left wave (i.e. at $x < 0$) is characterized by $(\boldsymbol{p}, s)$ and the right wave (i.e. at $x > 0$) is characterized by $(\boldsymbol{p}', s')$ (recall, however, that p_y is conserved, meaning $p_y = p'_y$), then the parameters p_x, s, p'_x, s' are related by the conservation of energy

$$sc|\boldsymbol{p}| = s'c|\boldsymbol{p}'| + \delta V, \tag{3.1}$$

as exemplified in Figure 2.

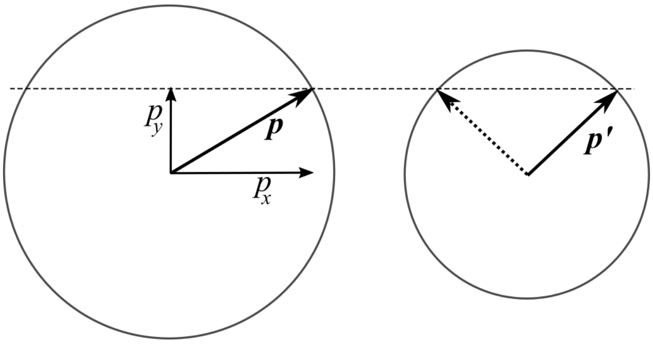

Figure 2: Representation of the conservation of energy $sc|\boldsymbol{p}| = s'c|\boldsymbol{p}'| + \delta V$, and y-momentum $p_y = p'_y$. We assume that an electron with energy $E > 0$ is scattered from the left to the right of the quantum strip. The two circles in the $\boldsymbol{p}$-space correspond, respectively, to the sections $c|\boldsymbol{p}| = E$ and $cs'|\boldsymbol{p}'| + \delta V = E$ of the left and right cones, and the horizontal dashed line represents conservation of p_y. Assuming $\delta V > 0$, the continuous arrow at the right represents the scattered pseudomomentum $\boldsymbol{p}'$ in the case $E > \delta V$ ($s = +1$), while the dashed arrow represents $\boldsymbol{p}'$ in the case $0 < E < \delta V$ ($s = -1$). Recall, in fact, that negative chirality is characterized by the pseudomeomentum being antiparallel to the direction of motion.

3.1 Kinetic transmission conditions (KTC)

Solving the eigenvalue problem (2.2) with the potential V satisfying conditions **H1** and **H2** above, provides us with the scattering data, i.e. the transmission and reflection coefficients. For $i = 1, 2$, we denote by $T^i_s(\boldsymbol{p}, s)$ and $R^i_s(\boldsymbol{p}, s)$ the transmission and reflection coefficients from the left ($i = 1$) and from the right ($i = 2$). They satisfy the following properties:

- **P1.** unitarity: $T^i_s(\boldsymbol{p}) \geq 0$ and $R^i_s(\boldsymbol{p}) \geq 0$, with $T^i_s(\boldsymbol{p}) + R^i_s(\boldsymbol{p}) = 1$;
- **P2.** energy-dependence: $T^i_s(\boldsymbol{p})$ and $R^i_s(\boldsymbol{p})$ depend on $\boldsymbol{p}$ and s only through the energy $sc|\boldsymbol{p}|$;
- **P3.** reciprocity: $T^1_s(\boldsymbol{p}) = T^2_{s'}(\boldsymbol{p}')$, whenever $(\boldsymbol{p}, s)$ and $(\boldsymbol{p}', s')$ are related by the conservation of energy (3.1).

If the potential $V(x)$ is piecewise constant, as in some cases of importance for applications, such as for the potential step [11] or the potential barrier [17, 19], then the solution to (2.2) can be explicitly computed by gluing up, with continuity, solutions of the form (2.3), procedure which allows to obtain explicit expressions of the scattering coefficients. For example, for a potential step of height δV it is easy to check that the transmission coefficient for an electron incident from the left with energy $E = sc|\boldsymbol{p}|$, is given by

$$T_s^1(\boldsymbol{p}) = \begin{cases} \dfrac{2\cos(\phi)\cos(\theta)}{1+\cos(\phi+\theta)}, & \text{if } |E\sin(\phi)| < |E-\delta V|, \\ 0, & \text{otherwise,} \end{cases} \tag{3.2}$$

where $\phi \in (-\frac{\pi}{2}, \frac{\pi}{2})$ is the incidence angle and $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$ is the transmission angle (both measured from an axis perpendicular to the step, so that $\phi = 0$ and $\theta = 0$ correspond, respectively, to perpendicular incidence and transmission). The two angles are constrained by

$$E\sin(\phi) = (E - \delta V)\sin(\theta). \tag{3.3}$$

Note that (3.3) is a "signed Snell law": when $0 < E < \delta V$ the angles ϕ and θ have opposite signs and $E - \delta V$ is like a negative refractive index, which produces the electronic equivalent of the so-called Veselago lens [11].

We now come to the kinetic part of the model, the quantum part being fully represented by the scattering reflection and transmission coefficients $T_s^i(\boldsymbol{p}, s)$ and $R_s^i(\boldsymbol{p}, s)$. On the macroscopic scale, the quantum strip has a vanishing width and becomes a one-dimensional interface between two classical regions. Let us assume that, in addition to the quantum active potential $V(x)$ considered so far, there is a smooth potential $U(x, y)$, which can be neglected at the microscopic scale but becomes important in the classical regions (where, conversely, V is constant). The kinetic description is expressed in terms of the phase-space distributions $w_s(\boldsymbol{x}, \boldsymbol{p})$ of electrons with positive ($s = +$) and negative ($s = -$) chirality/energy. They are assumed to satisfy a semiclassical, stationary transport equation of the form

$$\left(s\,\frac{c\boldsymbol{p}}{|\boldsymbol{p}|} \cdot \nabla_{\boldsymbol{x}} - \nabla_{\boldsymbol{x}} U \cdot \nabla_{\boldsymbol{p}} \right) w_s = \mathcal{C}_s(w_s), \tag{3.4}$$

where the left-hand side corresponds to the Hamiltonian dynamics (2.5) (with V replaced by U) and $\mathcal{C}_s(w_s)$ is a suitable collisional term to be specified later on. The semiclassical kinetic equation (3.4) is assumed to hold in the two classical regions, $x > 0$ and $x < 0$, for the two populations of electrons with positive and negative chirality. It is worth to remark that Eq. (3.4) has been introduced here in a heuristic way but it could be deduced as the semiclassical limit of the von Neumann (quantum Liouville) equation via Wigner transform [3, 6].

Following Ref. [7], we introduce a kinetic-quantum coupling in terms of *kinetic transmission conditions* (KTC) between the two classical regions through the quantum interface $x = 0$. The fundamental idea is that an incident/transmitted/reflected plane wave at the quantum interface, characterized by $(\boldsymbol{p}, s)$, is identified with a corresponding particle in the classical regions inflowing/outflowing at $x = 0$. More precisely, since the direction of motion of an electron with pseudomomentum $\boldsymbol{p}$ and chirality s is $s\boldsymbol{p}/|\boldsymbol{p}|$ (see Eqs. (2.5) and (2.6)), then such an electron is entering the left region (or leaving the right region) if $sp_x < 0$, and is leaving the left region (or entering the right region) if $sp_x > 0$.

With this in mind, in order to express the KTC, let us first of all introduce a suitable notation.

Definition 3.1 *An upper index $i = 1, 2$ denotes the left/right limits at $x = 0$ of an x-dependent quantity $u(x)$:*

$$u^1 := \lim_{x \to 0^-} u(x), \qquad u^2 := \lim_{x \to 0^+} u(x).$$

Then, according to what was discussed above, we write down the KTC as follows:

$$\begin{cases} w_s^1(p_x) = R_s^1(\boldsymbol{p}) w_s^1(-p_x) + T_{s'}^2(\boldsymbol{p}') w_{s'}^2(p'_x), & sp_x,\ s'p'_x < 0, \\ w_{s'}^2(p'_x) = R_{s'}^2(\boldsymbol{p}) w_{s'}^2(-p'_x) + T_s^1(\boldsymbol{p}) w_s^1(p_x), & s'p'_x,\ sp_x > 0, \end{cases} \tag{3.5}$$

where only the relevant variable p_x has been explicitly indicated, and we recall that $(\boldsymbol{p}, s)$ and $(\boldsymbol{p}', s')$ are uniquely determined each other by (3.1) together with the indication of the sign of p_x (this is enough, since $p_y = p'_y$). In (3.5) we also used the fact that the reflection and transmission coefficients depend on $\boldsymbol{p}$ and $\boldsymbol{p}'$ only through $|\boldsymbol{p}|$ and $|\boldsymbol{p}'|$ (property 2 of the scattering coefficients).

Recalling that the products sp_x and $s'p'_x$ determine the outflow or the inflow direction, it is easy to give the following interpretation of the conditions (3.5): at each side of the quantum interface, the inflow into the classical region is given in part by the reflected outflow from the same side and in part by the transmitted outflow from the opposite side.

3.2 Electrons and holes

The final goal of this work is to derive a diffusive limit of the hybrid kinetic model introduced in the previous section. This still needs a further step in the kinetic description, namely the specification of a suitable collision operator in Eq. (3.4), and the consequent introduction of the hole population.

To simplify the derivation of the diffusive equations we assume that the collisional term $\mathcal{C}_s(w_s)$ is of Bhatnagar-Gross-Krook (BGK) type, which expresses the relaxation of w_s towards a local Fermi-Dirac (F-D) distribution having the same density as w_s. Thus, we assume

$$\mathcal{C}_s(w_s) = \frac{w_s^{\mathrm{eq}} - w_s}{\tau}, \tag{3.6}$$

where

$$w_s^{\mathrm{eq}} = \frac{1}{\mathrm{e}^{s(\beta c|\boldsymbol{p}| - A_s)} + 1}. \tag{3.7}$$

Here, τ is the relaxation time and $\beta := 1/k_B T$, where k_B is the Boltzmann constant and T is the given temperature. Moreover, the sign of the chemical potentials A_s has been chosen for later convenience.[3]

Now, the equilibrium w_s^{eq} should be related to the unknown distribution w_s by the requirement that they have the same density. However, since the lower energy cone is unbounded from below (see Eq. (3.20)), w_-^{eq} cannot have finite moments, and such requirement does not

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[3] Note that here we are using non-dimensional chemical potentials, while the dimensional chemical potentials, that have the dimensions of a energy, are given by $\beta^{-1} A_s$.

make any sense for $s = -1$. In order to fix this, we have to describe negative-energy/chirality electrons in term of electron vacancies *(holes)*. Let us therefore introduce the distributions f_+ (electrons) and f_- (holes) defined by

$$f_+(\boldsymbol{x}, \boldsymbol{p}) = w_+(\boldsymbol{x}, \boldsymbol{p}), \qquad f_-(\boldsymbol{x}, \boldsymbol{p}) = 1 - w_-(\boldsymbol{x}, -\boldsymbol{p}). \tag{3.8}$$

Note that the definition of f_- contains a change in the sign of $\boldsymbol{p}$, so that holes move parallel to $\boldsymbol{p}$.

By applying the transformation (3.8) to Eq. (3.4), with $\mathcal{C}_s$ given by (3.6), we obtain

$$\left(\frac{c\boldsymbol{p}}{|\boldsymbol{p}|} \cdot \nabla_{\boldsymbol{x}} - s \nabla_{\boldsymbol{x}} U \cdot \nabla_{\boldsymbol{p}} \right) f_s = \frac{f_s^{\mathrm{eq}} - f_s}{\tau}, \tag{3.9}$$

where

$$f_s^{\mathrm{eq}} = \frac{1}{\mathrm{e}^{\beta c |\boldsymbol{p}| - A_s} + 1}, \tag{3.10}$$

are now F-D distributions both with *positive* energies, so that they possess finite moments. In particular, we can ask that f_s^{eq} and f_s have the same densities, i.e. we impose the constraint

$$\langle f_s^{\mathrm{eq}} \rangle = \langle f_s \rangle := n_s, \tag{3.11}$$

where we have introduced the bracket notation for the normalized[4] integrals

$$\langle \cdot \rangle = \frac{1}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \cdot \, d\boldsymbol{p}. \tag{3.12}$$

Equation (3.9) with the constraint (3.11), is the stationary, semiclassical transport equation which shall be used for the description of electrons and holes transport in the semiclassical regions.

By using polar coordinates it is not difficult to see that the constraint (3.11) fixes the chemical potentials A_s as functions of the densities n_s, via the following formula (see [3]):

$$\phi_2(A_s) = \frac{n_s}{n_0}, \tag{3.13}$$

where

$$\phi_k(z) := \frac{1}{\Gamma(k)} \int_0^\infty \frac{t^{k-1}}{e^{t-z} + 1} \, dt \tag{3.14}$$

and

$$n_0 := \frac{2\pi}{(2\pi\hbar c\beta)^2} = \frac{(k_B T)^2}{2\pi\hbar^2 c^2}. \tag{3.15}$$

The function $\phi_k : \mathbb{R} \to (0, +\infty)$ is the Fermi integral of order $k > 0$, and can be proved to be strictly increasing. It will be convenient to denote by $A(n)$ the chemical potential corresponding to the density n, i.e.

$$A(n) = \phi_2^{-1} \left(\frac{n}{n_0} \right), \tag{3.16}$$

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[4] The normalization constant is required in order to get the the correct moments of a non-dimensional Wigner function [3].

and to introduce the notation

$$F_n(\boldsymbol{p}) = \frac{1}{\mathrm{e}^{\beta c|\boldsymbol{p}| - A(n)} + 1}\,, \tag{3.17}$$

for the F-D distribution with density n. Then we shall rewrite the transport equation (3.9) as

$$\tau\left(\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} - s\nabla_{\boldsymbol{x}}U\cdot\nabla_{\boldsymbol{p}}\right) f_s = F_{\langle f_s\rangle} - f_s, \tag{3.18}$$

which incorporates the constraint (3.11) and where we adopted the notation

$$\boldsymbol{v}(\boldsymbol{p}) := \frac{c\boldsymbol{p}}{|\boldsymbol{p}|} \tag{3.19}$$

for the semiclassical velocity. Note that, at variance with negative-energy electrons, the velocity of holes has the same direction as $\boldsymbol{p}$.

3.3 Kinetic transmission conditions for electrons and holes

We now need to express the KTC (3.5) in terms of the distributions f_s, i.e. in terms of electrons and holes. Let us begin by introducing more handy notations. We define the "state variable"

$$\boldsymbol{z} = (\boldsymbol{p}, s) = (p_x, p_y, s) \in \mathbb{R}^2 \times \{-1, +1\},$$

and express all the quantities that depend on $\boldsymbol{p}$ and s as functions of $\boldsymbol{z}$, e.g. the Dirac cones,

$$E(\boldsymbol{z}) = E_s(\boldsymbol{p}) = sc|\boldsymbol{p}|, \tag{3.20}$$

and the electron/hole densities

$$f(\boldsymbol{x}, \boldsymbol{z}) = f_s(\boldsymbol{x}, \boldsymbol{p}). \tag{3.21}$$

Moreover, for $i = 1, 2$ we define the following sets

$$\Theta := \mathbb{R}^2 \times \{-1, +1\}, \quad \Theta^i_{\text{in}} := \{\boldsymbol{z} \in \Theta \mid (-1)^i p_x > 0\}, \quad \Theta^i_{\text{out}} := \{\boldsymbol{z} \in \Theta \mid (-1)^i p_x < 0\}. \tag{3.22}$$

Note that Θ^i_{in} and Θ^i_{out} correspond, respectively, to the inflow and the outflow ranges of the pseudomomentum at $x = 0$, pertaining to the left ($i = 1$) and right ($i = 2$) regions. The integration with respect to $\boldsymbol{z}$ will stand for a sum with respect to s and an integration with respect to $\boldsymbol{p}$, for example:

$$\int_\Theta f(\boldsymbol{z})\, d\boldsymbol{z} = \sum_{s=\pm1} \int_{\mathbb{R}^2} f_s(\boldsymbol{p}) d\boldsymbol{p}.$$

Instead, recall that $\langle\cdot\rangle$ (definition (3.12)) is just a normalized integration with respect to $\boldsymbol{p}$ and, therefore, is a quantity that depends on $\boldsymbol{x}$ and s:

$$\langle f\rangle(\boldsymbol{x}, s) = \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2} f(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{p} = \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2} f_s(\boldsymbol{x}, \boldsymbol{p}) d\boldsymbol{p}. \tag{3.23}$$

We also introduce the reflection transformation

$$\sim\!\boldsymbol{z} := (-p_x, p_y, s), \tag{3.24}$$

for $\boldsymbol{z} = (\boldsymbol{p}, s)$, which exchanges Θ^i_{in} and Θ^i_{out}. Note that the properties **P1**–**P3** of the scattering coefficients imply the following identities:

1. $T^i(\boldsymbol{z}) + R^i(\boldsymbol{z}) = 1$;
2. $T^i(\sim\boldsymbol{z}) = T^i(\boldsymbol{z})$ and $R^i(\sim\boldsymbol{z}) = R^i(\boldsymbol{z})$;
3. $T^i(\boldsymbol{z}) = T^j(\boldsymbol{z}')$, if $E(\boldsymbol{z}) = E(\boldsymbol{z}') + (-1)^j \delta V$, with $j \neq i$.

Now, by applying the transformation (3.8) to Eq. (3.5), and using the notation just introduced, we can express the transmission conditions for the electron/hole distributions as follows:

$$f^i(\boldsymbol{z}) = R^i(\boldsymbol{z}) f^i(\sim\boldsymbol{z}) + T^j(\boldsymbol{z}') \left(ss' f^j(\boldsymbol{z}') + \epsilon_{ss'} \right), \quad \boldsymbol{z} \in \Theta^i_{\text{in}},\ \boldsymbol{z}' \in \Theta^j_{\text{out}}, \tag{3.25}$$

where $j \neq i$, and $\boldsymbol{z}'$ is constrained to $\boldsymbol{z}$ by the conservation of the energy and of the y-component of the pseudomomentum, namely

$$E(\boldsymbol{z}) = E(\boldsymbol{z}') + (-1)^j \delta V, \qquad p_y = p'_y, \tag{3.26}$$

for $\boldsymbol{z} = (\boldsymbol{p}, s)$ and for $\boldsymbol{z}' = (\boldsymbol{p}', s')$. The symbol $\epsilon_{ss'}$ is defined as

$$\epsilon_{ss'} = \begin{cases} 0, & \text{if } s = s', \\ 1, & \text{if } s \neq s'. \end{cases} \tag{3.27}$$

The KTC in the form (3.25) express very clearly the fact that the inflow at $\boldsymbol{z} \in \Theta^i_{\text{in}}$ is partly due to the reflected outflow $\sim\boldsymbol{z} \in \Theta^i_{\text{out}}$ from the same side i, and partly given by the transmitted outflow $\boldsymbol{z}' \in \Theta^j_{\text{out}}$ from the opposite side j. The inhomogeneous term $\epsilon_{ss'}$ comes from the inhomogeneous relation (3.8) between f_s and w_s. Moreover, Eqs. (3.25) and (3.26), together with the reciprocity property of the scattering coefficients, make the symmetry of the transmission conditions evident: the equation for the i-side is is transformed in the equation for the j-side by changing the sign of δV. In particular, when $\delta V = 0$, the two equations are identical and (since in this case $\boldsymbol{z} = \boldsymbol{z}'$) take the simple form

$$f^i(\boldsymbol{z}) = R^i(\boldsymbol{z}) f^i(\sim\boldsymbol{z}) + T^j(\boldsymbol{z}) f^j(\boldsymbol{z}), \qquad \boldsymbol{z} \in \Theta^i_{\text{in}}. \tag{3.28}$$

Proposition 3.2 (Flux conservation) *For all* $\delta V \in \mathbb{R}$ *the KTC* (3.25) *conserve the total charge flux across the quantum interface* $x = 0$*, i.e.*

$$J^1_{+,x} - J^1_{-,x} = J^2_{+,x} - J^2_{-,x}, \tag{3.29}$$

where, recalling definitions (3.12) *and* (3.19)*,* $\boldsymbol{J}_s = (J_{s,x}, J_{s,y})$ *is the current, defined by*

$$\boldsymbol{J}_s := \langle \boldsymbol{v} f_s \rangle. \tag{3.30}$$

If $\delta V = 0$*, then the conservation of the flux is valid separately for each population*

$$J^1_{+,x} = J^2_{+,x}, \qquad J^1_{-,x} = J^2_{-,x}, \tag{3.31}$$

which means that there is no particle exchange between the upper and lower cone.

Proof. In order to incorporate more explicitly in the transmission conditions the conservation properties (3.26), let us rewrite (3.25) as follows:

$$f^i(\boldsymbol{z}) = R^i(\boldsymbol{z}) f^i(\sim\boldsymbol{z}) + \int_{\Theta^j_{\text{out}}} T^j(\boldsymbol{z}') \left(ss' f^j(\boldsymbol{z}') + \epsilon_{ss'} \right) k^j(\boldsymbol{z},\boldsymbol{z}') |\mu(\boldsymbol{z}')| d\boldsymbol{z}', \quad \boldsymbol{z} \in \Theta^i_{\text{in}}, \tag{3.32}$$

where $j \neq i$ and where we defined

$$k^j(\boldsymbol{z},\boldsymbol{z}') = \delta\big(E(\boldsymbol{z}) - E(\boldsymbol{z}') - (-1)^j \delta V\big)\, \delta(p_y - p_y'), \tag{3.33}$$

$$\mu(\boldsymbol{z}) = v_x(\boldsymbol{p}) = \frac{c p_x}{|\boldsymbol{p}|}. \tag{3.34}$$

Note that $|\mu(\boldsymbol{z})|$ is the Jacobian determinant of the transformation

$$\boldsymbol{z} \mapsto (E(\boldsymbol{z}), p_y),$$

which is bijective from Θ^i_{in} (or Θ^i_{out}) to $\{(E,p_y) \in \mathbb{R}^2 \mid |E| \geq c|p_y|\}$. By using $R^i = 1 - T^i$, we can also rewrite (3.32) in the following form:

$$f^i(\boldsymbol{z}) - f^i(\sim\boldsymbol{z}) = -T^i(\boldsymbol{z}) f^i(\sim\boldsymbol{z}) + \int_{\Theta^j_{\text{out}}} T^j(\boldsymbol{z}') \left(ss' f^j(\boldsymbol{z}') + \epsilon_{ss'} \right) k^j(\boldsymbol{z},\boldsymbol{z}') |\mu(\boldsymbol{z}')| d\boldsymbol{z}'. \tag{3.35}$$

Let us multiply both sides by $s\mu(\boldsymbol{z})$ and integrate over $\boldsymbol{z} \in \Theta^i_{\text{in}}$. At the left-hand side we obtain

$$\begin{aligned} \int_{\Theta^i_{\text{in}}} s \left[f^i(\boldsymbol{z}) - f^i(\sim\boldsymbol{z}) \right] \mu(\boldsymbol{z})\, d\boldsymbol{z} &= \int_{\Theta^i_{\text{in}}} s f^i(\boldsymbol{z}) \mu(\boldsymbol{z})\, d\boldsymbol{z} + \int_{\Theta^i_{\text{out}}} s f^i(\boldsymbol{z}) \mu(\boldsymbol{z})\, d\boldsymbol{z} \\ &= \int_{\Theta} s f^i(\boldsymbol{z}) \mu(\boldsymbol{z})\, d\boldsymbol{z} = \int_{\mathbb{R}^2} f^i_+(\boldsymbol{p}) \frac{c p_x}{|\boldsymbol{p}|}\, d\boldsymbol{p} - \int_{\mathbb{R}^2} f^i_-(\boldsymbol{p}) \frac{c p_x}{|\boldsymbol{p}|}\, d\boldsymbol{p}, \end{aligned}$$

which is equal to $J^i_{+,x} - J^i_{-,x}$ upon multiplying by $(2\pi\hbar)^{-2}$. At the right-hand side we obtain

$$\begin{aligned} - \int_{\Theta^i_{\text{in}}} T^i(\boldsymbol{z}) s f^i(\sim\boldsymbol{z}) \mu(\boldsymbol{z}) d\boldsymbol{z} + \int_{\Theta^i_{\text{in}}} \int_{\Theta^j_{\text{out}}} T^j(\boldsymbol{z}') \left(s' f^j(\boldsymbol{z}') + s\epsilon_{ss'} \right) k^j(\boldsymbol{z},\boldsymbol{z}') |\mu(\boldsymbol{z}')| \mu(\boldsymbol{z}) d\boldsymbol{z}' d\boldsymbol{z} \\ = \int_{\Theta^i_{\text{out}}} T^i(\boldsymbol{z}) s f^i(\boldsymbol{z}) \mu(\boldsymbol{z}) d\boldsymbol{z} + \int_{\Theta^j_{\text{out}}} T^j(\boldsymbol{z}') s' f^j(\boldsymbol{z}') \mu(\boldsymbol{z}') d\boldsymbol{z}' + C_j, \end{aligned} \tag{3.36}$$

where we used the fact that $|\mu(\boldsymbol{z}')|\mu(\boldsymbol{z}) = \mu(\boldsymbol{z}')|\mu(\boldsymbol{z})|$ for if $\boldsymbol{z} \in \Theta^i_{\text{in}}$ and $\boldsymbol{z}' \in \Theta^j_{\text{out}}$, and the identity

$$\int_{\Theta^i_{\text{in}}} k^j(\boldsymbol{z},\boldsymbol{z}') |\mu(\boldsymbol{z})| d\boldsymbol{z} = 1. \tag{3.37}$$

The constant C_j is[5]

$$\begin{aligned} C_j = \int_{\Theta^i_{\text{in}}} \int_{\Theta^j_{\text{out}}} T^j(\boldsymbol{z}') s \epsilon_{ss'} k^j(\boldsymbol{z},\boldsymbol{z}') |\mu(\boldsymbol{z}')| \mu(\boldsymbol{z}) d\boldsymbol{z}' d\boldsymbol{z} \\ = \int_{\Theta^i_{\text{out}}} \int_{\Theta^j_{\text{in}}} T^i(\boldsymbol{z}) s' \epsilon_{s's}\, k^i(\boldsymbol{z}',\boldsymbol{z}) \mu(\boldsymbol{z}') |\mu(\boldsymbol{z})| d\boldsymbol{z}' d\boldsymbol{z} = C_i\,, \end{aligned}$$

---

[5] Note that the constant C_i is finite because conservation of energy holds with different signs of s and s' only in a finite energy interval, which corresponds to a bounded $\boldsymbol{p}$-region.

where we used the properties

$$k^j(\boldsymbol{z},\boldsymbol{z}') = k^i(\boldsymbol{z}',\boldsymbol{z}), \qquad s\epsilon_{ss'} = -s'\epsilon_{s's}$$

and made the change of variables $\boldsymbol{z} \mapsto \sim\boldsymbol{z}$, $\boldsymbol{z}' \mapsto \sim\boldsymbol{z}'$. Hence, we see that the right-hand side expression (3.36) is identical for $(i,j) = (1,2)$ and $(i,j) = (2,1)$, which proves Eq. (3.29).
In the particular case $\delta V = 0$, the KTC reduce to the form (3.28) and, by rewriting them as

$$f^i(\boldsymbol{z}) - f^i(\sim\boldsymbol{z}) = -T^i(\boldsymbol{z})f^i(\sim\boldsymbol{z}) + T^j(\boldsymbol{z})f^j(\boldsymbol{z}),$$

the verification of (3.31) is immediate. □

Proposition 3.3 (KTC for Fermi-Dirac distributions) *Let n_+ and n_- be two assigned functions of $\boldsymbol{x}$. Then, the KTC* (3.25) *(or their equivalent formulation* (3.32)*) are satisfied for the F-D distributions*

$$f(\boldsymbol{x},\boldsymbol{z}) = f_s(\boldsymbol{x},\boldsymbol{p}) = F_{n_s(\boldsymbol{x})}(\boldsymbol{p}), \qquad s = \pm,$$

if and only if

$$sA(n_s^1) = s'A(n_{s'}^2) + \beta\delta V, \tag{3.38}$$

for all "admissible" couples (s,s'), i.e. such that

$$sc|\boldsymbol{p}| = s'c|\boldsymbol{p}'| + \delta V, \tag{3.39}$$

for some $\boldsymbol{p} \neq 0$ and $\boldsymbol{p}' \neq 0$ with $T^1(\boldsymbol{p}) \neq 0$.

Proof. We recall that (3.25) are the KTC (3.5) after the transformation (3.8). If $f_s(\boldsymbol{x},\boldsymbol{p}) = F_{n_s(\boldsymbol{x})}(\boldsymbol{p})$, then the corresponding w_s's are given by

$$w_s(\boldsymbol{x},\boldsymbol{p}) = \frac{1}{\mathrm{e}^{s\beta c|\boldsymbol{p}| - sA(n_s(\boldsymbol{x}))} + 1}.$$

Substituting these F-D distributions in Eq. (3.5) with $i = 1$, using $R^1(\boldsymbol{z}) = 1 - T^1(\boldsymbol{z})$ and $T^1(\boldsymbol{z}) = T^2(\boldsymbol{z}')$, and the fact that $w_s(\boldsymbol{x},\boldsymbol{p}) = w_s(\boldsymbol{x},-\boldsymbol{p})$ (for such particular w_s's), we obtain the condition

$$T_s^1(\boldsymbol{p})\left[w_s^1(\boldsymbol{p}) - w_{s'}^2(\boldsymbol{p}')\right] = 0$$

(note that for $i = 2$ one would obtain to the same condition). Hence, we find that the equality

$$\frac{1}{\mathrm{e}^{s\beta c|\boldsymbol{p}| - sA(n_s^1)} + 1} = \frac{1}{\mathrm{e}^{s'\beta c|\boldsymbol{p}'| - s'A(n_{s'}^2)} + 1}$$

must hold for all $(\boldsymbol{p},s)$ and $(\boldsymbol{p}',s')$ that satisfy (3.39) with $T_s^1(\boldsymbol{p}) \neq 0$. This defines the admissible couples (s,s'), provided that $\boldsymbol{p} \neq 0$ and $\boldsymbol{p}' \neq 0$ (otherwise s or s' are undefined). Substituting $s'c|\boldsymbol{p}'| = -sc|\boldsymbol{p}| + \delta V$, we get the equality

$$\frac{1}{\mathrm{e}^{s\beta c|\boldsymbol{p}| - sA(n_s^1)} + 1} = \frac{1}{\mathrm{e}^{s\beta c|\boldsymbol{p}| - \beta\delta V - s'A(n_{s'}^2)} + 1},$$

which implies Eq. (3.38). □

Remark 3.4 It is readily seen that, apart from degenerate situations, the admissible couples (s,s') are $(+,+),(+,-),(-,-)$ if $\delta V > 0$; $(+,+),(-,-)$ if $\delta V = 0$; $(+,+),(-,+),(-,-)$, if $\delta V < 0$.

4 Diffusion limit

In this section we study the diffusion limit of the hybrid kinetic-quantum model (3.18), (3.25), by assuming $\tau \ll 1$. We divide the derivation, which is based on the Hilbert expansion method, into the "bulk" part (i.e. the semiclassical regions) and the "interface" part (i.e., close to the quantum interface).

4.1 Diffusion limit in the semiclassical regions

Let us consider the Hilbert expansion (HE) of the unknown $f(\boldsymbol{x}, \boldsymbol{z}) = f_s(\boldsymbol{x}, \boldsymbol{p})$ in (3.18), in powers of the relaxation time τ, to be considered as a small parameter:

$$f = f^{(0)} + \tau f^{(1)} + \tau^2 f^{(2)} + \cdots \tag{4.1}$$

When substituting this expansion into the transport equation (3.18) we have to be aware of the fact that the BGK operator is nonlinear, due to the use of F-D statistics $F_{\langle f \rangle}$. A linearization of the collision operator is thus necessary, which requires to expand the F-D distribution around the equilibrium density, i.e.

$$F_{n^{(0)}+\tau n^{(1)}+\tau^2 n^{(2)}+\mathcal{O}(\tau^3)} = F_{n^{(0)}} + \tau F'_{n^{(0)}} n^{(1)} + \tau^2 \big[F'_{n^{(0)}} n^{(2)} + \frac{1}{2} F''_{n^{(0)}} (n^{(1)})^2\big] + \mathcal{O}(\tau^3), \tag{4.2}$$

where the primes denote the derivatives of F_n with respect to n. By using (3.16) and the property $\phi'_k = \phi_{k-1}$, we obtain

$$F'_n(\boldsymbol{p}) = \frac{F_n(\boldsymbol{p})^2 \mathrm{e}^{\beta c|\boldsymbol{p}| - A(n)}}{n_0 \phi_1(A(n))}, \tag{4.3}$$

while the explicit form of F''_n is not important. Moreover, note that

$$\langle F'_n \rangle = \frac{d}{dn} \langle F_n \rangle = \frac{d}{dn} n = 1 \tag{4.4}$$

and, for the same reason, one has

$$\langle F''_n \rangle = 0. \tag{4.5}$$

The linearisation of our BGK collision operator

$$\mathcal{Q}(f) := F_{\langle f \rangle} - f\,, \tag{4.6}$$

around the equilibrium $f^{(0)}$ is hence defined as

$$\mathcal{L}_{\langle f^{(0)} \rangle}(g) := F'_{\langle f^{(0)} \rangle} \langle g \rangle - g. \tag{4.7}$$

In order to be able to find some information about the distribution functions $f^{(0)}, f^{(1)}, \ldots$, we shall need to study in more details this linear collision operator. Note that $\mathcal{L}_{\langle f^{(0)} \rangle}$ is an operator acting on functions of $\boldsymbol{p}$, and the $(\boldsymbol{x}, s)$-dependence is just parametric, through the real parameter $n = \langle f^{(0)} \rangle(\boldsymbol{x}, s)$. The properties of $\mathcal{L}_n$ are summarised in the following Lemma, whose proof is rather standard and can be easily adapted from [22].

Lemma 4.1 (Properties of the linearised collision operator $\mathcal{L}_n$) *Let $n \geq 0$ be a fixed real number, and let $\mathcal{L}_n : \mathcal{H} \to \mathcal{H}$ be the operator defined by $\mathcal{L}_n(g) := F'_n\langle g\rangle - g$ and acting on the Hilbert-space*

$$\mathcal{H} := \left\{ f \in \mathrm{L}^2(\mathbb{R}^2) \;\middle|\; \int_{\mathbb{R}^2} |f|^2 \, (F'_n)^{-1} \, d\boldsymbol{p} < \infty \right\}, \qquad (f,g)_{\mathcal{H}} := \int_{\mathbb{R}^2} fg \, (F'_n)^{-1} \, d\boldsymbol{p}.$$

(i) $\mathcal{L}_n$ is a well-defined, linear, bounded, symmetric and non-negative operator with kernel given by

$$\ker \mathcal{L}_n := \left\{ g \in \mathcal{H} \;\middle|\; g = F'_n\langle g\rangle \right\} \, .$$

(ii) The orthogonal of the kernel is nothing else than the range of $\mathcal{L}_n$ and is given by

$$(\ker \mathcal{L}_n)^{\perp} = \operatorname{imag} \mathcal{L}_n = \left\{ g \in \mathcal{H} \;\middle|\; \langle g\rangle = 0 \right\} \, .$$

(iii) Coercivity: for any $f \in \operatorname{imag} \mathcal{L}_n$,

$$- \int_{\mathbb{R}^2} \mathcal{L}_n(f) \, f \, (F'_n)^{-1} \, d\boldsymbol{p} \geq \|f\|^2_{\mathcal{H}} \, .$$

(iv) Invertibility: the operator $\mathcal{L}_n$ is a one-to-one mapping, if defined as

$$\mathcal{L}_n : (\ker \mathcal{L}_n)^{\perp} \to (\ker \mathcal{L}_n)^{\perp} \, ,$$

such that the equation $\mathcal{L}_n(f) = g$ has a unique solution $f \in (\ker \mathcal{L}_n)^{\perp}$ if and only if $g \in (\ker \mathcal{L}_n)^{\perp}$.

Plugging now the HE (4.1) into Eq. (3.18), one obtains, at second order in τ,

$$\tau \left(\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} - s \nabla_{\boldsymbol{x}} U \cdot \nabla_{\boldsymbol{p}} \right) \left(f^{(0)} + \tau f^{(1)} \right) = \mathcal{Q}(f^{(0)}) + \tau \mathcal{L}_{\langle f^{(0)} \rangle}(f^{(1)}) \\ + \tau^2 \mathcal{L}_{\langle f^{(0)} \rangle}(f^{(2)}) + \frac{\tau^2}{2} F''_{\langle f^{(0)} \rangle} \langle f^{(1)} \rangle^2 + \mathcal{O}(\tau^3) \quad (4.8)$$

(we recall that $f^{(k)}$ and $\langle f^{(k)} \rangle$ are s-dependent quantities). Comparing the terms of the same power in τ permits to get step by step some information on $f^{(0)}$, $f^{(1)}$,..., and finally to obtain the Drift-Diffusion model in the limit $\tau \to 0$.

Step 1: order τ^0. At order τ^0 we obtain the condition $\mathcal{Q}(f_s^{(0)}) = 0$ meaning $F_{\langle f_s^{(0)} \rangle} = f_s^{(0)}$, which implies that the equilibrium is a F-D distribution function

$$f^{(0)}(\boldsymbol{x}, \boldsymbol{z}) = f_s^{(0)}(\boldsymbol{x}, \boldsymbol{p}) = F_{n_s(\boldsymbol{x})}(\boldsymbol{p}), \quad (4.9)$$

with $n_+(\boldsymbol{x})$ and $n_-(\boldsymbol{x})$ still to be determined.

Step 2: Order τ^1. At order τ^1 we obtain the equation

$$\mathcal{L}_{\langle f^{(0)}\rangle}(f^{(1)}) = (\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} - s\nabla_{\boldsymbol{x}}U\cdot\nabla_{\boldsymbol{p}})\, f^{(0)}.$$

By indicating the s-dependence explicitly and using (4.3) and (4.9), this equation can be rewritten as

$$\mathcal{L}_{n_s}(f_s^{(1)}) = F'_{n_s}\boldsymbol{v}\cdot(\nabla n_s + s\beta n_0\,\phi_1(A_s)\nabla U) =: -\boldsymbol{\ell}_s\cdot\boldsymbol{j}_s, \tag{4.10}$$

where, for later convenience, we have denoted

$$\boldsymbol{\ell}_s := \frac{2}{c^2}F'_{n_s}\boldsymbol{v} \tag{4.11}$$

and

$$\boldsymbol{j}_s := -\frac{c^2}{2}\left(\nabla n_s + s\beta n_0\,\phi_1(A_s)\nabla U\right). \tag{4.12}$$

Owing to the properties of the linearised BGK operator (see Lemma 4.1), Eq. (4.10) has the general solution

$$f_s^{(1)} = \boldsymbol{\ell}_s\cdot\boldsymbol{j}_s + \sigma_s F'_{n_s}, \tag{4.13}$$

for any σ_s constant with respect to $\boldsymbol{p}$. Without loss of generality we can take $\sigma_s = 0$, meaning that $f_s^{(1)} \in (\ker\mathcal{L}_{n_s})^\perp$, because the addition of $\sigma_s F'_{n_s}$ does not affect the subsequent steps. By using the the identity

$$\langle\boldsymbol{v}\otimes\boldsymbol{v}F_n\rangle = \frac{c^2 n}{2}I\,,$$

where I is the 2×2 identity matrix (see e.g. Ref. [3]), one obtains

$$\langle\boldsymbol{v}\otimes\boldsymbol{v}F'_n\rangle = \frac{d}{dn}\langle\boldsymbol{v}\otimes\boldsymbol{v}F_n\rangle = \frac{c^2}{2}I\,,$$

leading to

$$\langle\boldsymbol{v}\otimes\boldsymbol{\ell}_s\rangle = I. \tag{4.14}$$

Equation (4.14), together with the obvious identities $\langle\boldsymbol{v}F_{n_s}\rangle = \langle\boldsymbol{v}F'_{n_s}\rangle = 0$, has the important implication that the current $\boldsymbol{J}_s = \langle\boldsymbol{v}\,f_s\rangle$ is given by $\tau\boldsymbol{j}_s$ up to higher orders, namely

$$\boldsymbol{J}_s = \tau\boldsymbol{j}_s + \mathcal{O}(\tau^2). \tag{4.15}$$

Step 3: Order τ^2. Going on with the HE (4.8), at order τ^2 we get the equation

$$\mathcal{L}_{\langle f^{(0)}\rangle}(f^{(2)}) = F'_{\langle f^{(0)}\rangle}\langle f^{(2)}\rangle - f^{(2)} = (\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} - s\nabla_{\boldsymbol{x}}U\cdot\nabla_{\boldsymbol{p}})\, f^{(1)} - \frac{1}{2}F''_{\langle f^{(0)}\rangle}\langle f^{(1)}\rangle^2.$$

The solvability condition of this equation with respect to $f^{(2)}$ is

$$\begin{aligned}\langle(\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} - s\nabla_{\boldsymbol{x}}U\cdot\nabla_{\boldsymbol{p}})\, f^{(1)} - \frac{1}{2}F''_{\langle f^{(0)}\rangle}\langle f^{(1)}\rangle^2\rangle &= \\ \langle(\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} - s\nabla_{\boldsymbol{x}}U\cdot\nabla_{\boldsymbol{p}})\, f^{(1)}\rangle &= \langle\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}f^{(1)}\rangle = 0,\end{aligned}$$

where the first equality comes from (4.5). This solvability condition is nothing else than the stationary[6]. Drift-Diffusion equation, whose explicit form, thanks to (4.14), is

$$\operatorname{div}\left[\nabla n_s + s\beta n_0\, \phi_1(A_s)\nabla U\right] = 0 \tag{4.16}$$

Note that $n_0\,\phi_1(A_s)$ is a nonlinear function of the density n_s, which reduces to n_s in the Maxwell-Boltzmann approximation (see Sec. 4.4).

The results of this section are summarised in the following Proposition.

Proposition 4.2 *Supposing the solution $f(\boldsymbol{x},\boldsymbol{z}) = f_s(\boldsymbol{x},\boldsymbol{p})$ of the transport equation* (3.18) *to admit a Hilbert expansion of the form*

$$f = F + \tau G + \mathcal{O}(\tau^2), \tag{4.17}$$

then the highest order terms are given by

$$F(\boldsymbol{x},\boldsymbol{z}) = F_{n_s(\boldsymbol{x})}(\boldsymbol{p}) \qquad \text{and} \qquad G(\boldsymbol{x},\boldsymbol{z}) = \boldsymbol{\ell}_s(\boldsymbol{x},\boldsymbol{p})\cdot \boldsymbol{j}_s(\boldsymbol{x}), \tag{4.18}$$

where the functions $F_{n_s(\boldsymbol{x})}(\boldsymbol{p})$, $\ell_s(\boldsymbol{x},\boldsymbol{p})$ and $\boldsymbol{j}_s(\boldsymbol{x})$ are given, respectively, by (3.17), (4.11) *and* (4.12)*. Moreover, up to terms of order τ^2, the density $n_s(\boldsymbol{x})$ satisfies the Drift-Diffusion equation* (4.16) *in the semiclassical regions $x > 0$ and $x < 0$.*

4.2 Diffusion limit at the quantum interface: leading order

We have now to deal with the diffusion limit of the transmission conditions. This means that we have to perform the Hilbert expansion of the left and right boundary values of $f(\boldsymbol{x},\boldsymbol{z})$, i.e. of $f^1(\boldsymbol{z})$ and $f^2(\boldsymbol{z})$.

To this aim, let us introduce a concise notation for the Transmission Conditions (3.32). We put

$$f^i_{\rm in} = f^i_{|\Theta^i_{\rm in}}, \qquad f^i_{\rm out} = f^i_{|\Theta^i_{\rm out}} \tag{4.19}$$

(see definition (3.22)), and rewrite the KTC (3.32) in a short form as

$$f^i_{\rm in} = \mathcal{B}^i(f^i_{\rm out}, f^j_{\rm out}), \tag{4.20}$$

where the boundary operator $\mathcal{B}^i$ is defined as

$$\mathcal{B}^i(f^i_{\rm out}, f^j_{\rm out})(\boldsymbol{z}) = R^i(\boldsymbol{z}) f^i_{\rm out}(\sim\!\boldsymbol{z}) + T^j(\boldsymbol{z}')\left(ss' f^j_{\rm out}(\boldsymbol{z}') + \epsilon_{ss'}\right), \qquad \boldsymbol{z}\in\Theta^i_{\rm in}, \tag{4.21}$$

with $\boldsymbol{z}' \in \Theta^j_{\rm out}$ defined by (3.26) and with the usual convention that $j \neq i$. It is important to remark that $\mathcal{B}^i$ is not a linear but rather an affine transformation, so that

$$\mathcal{B}^i\left((f+g)^i_{\rm out}, (f+g)^j_{\rm out}\right) = \mathcal{B}^i(f^i_{\rm out}, f^j_{\rm out}) + \mathcal{K}^i(g^i_{\rm out}, g^j_{\rm out}), \tag{4.22}$$

the linear part $\mathcal{K}^i$ being, of course,

$$\mathcal{K}^i(f^i_{\rm out}, f^j_{\rm out})(\boldsymbol{z}) = R^i(\boldsymbol{z}) f^i_{\rm out}(\sim\!\boldsymbol{z}) + T^j(\boldsymbol{z}') f^j_{\rm out}(\boldsymbol{z}'). \tag{4.23}$$

---

[6] See Ref. [3] for the time-dependent version of (4.16)

We recall that the first two terms of the Hilbert Expansion $f = F + \tau G + o(\tau)$, far from the interface, are given in Proposition 4.2. Therefore, the KTC at leading order are

$$F^i_{\text{in}} = \mathcal{B}^i\big(F^i_{\text{out}}, F^j_{\text{out}}\big),$$

where $F(\boldsymbol{x}, \boldsymbol{z})$ is the Fermi-Dirac distribution $F_{n_s(\boldsymbol{x})}(\boldsymbol{p})$. But, then, Proposition 3.3 applies, and leads to the following result.

Proposition 4.3 (Diffusive transmission conditions (DTC) at leading order) *Up to terms of order τ, the left and right densities at the interface $x = 0$, n^1_s and n^2_s, are constrained by the condition*

$$sA(n^1_s) = s'A(n^2_{s'}) + \beta\delta V, \tag{4.24}$$

that must hold for all admissible couples (s, s').

The leading-order DTC (4.24) are not “quantum”, to the extent that they do not depend on the scattering coefficients. In the next section we shall see that the first-order correction introduces such dependence.

4.3 Diffusion limit at the quantum interface: first order

In order to search for a quantum correction, we require that the kinetic transmission conditions are satisfied by $f = F + \tau G + o(\tau)$ also at the first order in τ and, therefore, we impose the condition

$$F^i_{\text{in}} + \tau G^i_{\text{in}} = \mathcal{B}^i\big(F^i_{\text{out}} + \tau G^i_{\text{out}}, F^j_{\text{out}} + \tau G^j_{\text{out}}\big). \tag{4.25}$$

However here we step into a difficulty, since, while $F^i_{\text{in}} = \mathcal{B}^i\big(F^i_{\text{out}}, F^j_{\text{out}}\big)$ can be satisfied with the suitable choice (4.24) of the chemical potentials, in general no chemical potentials exists such that Eq. (4.25) is also satisfied. This means that the HE ansatz is incorrect at order τ in the proximity of the interface. This difficulty is not new and similar situations are considered in literature. In general, one can overcome this burden by introducing a suitable boundary layer corrector [13, 14], which will lead to the well-known Milne-problems, permitting finally to couple the two Drift-Diffusion models on both sides of the interface.

Let us present in more details how to obtain these Milne problems. Instead of using the Hilbert expansion (4.1), we shall slightly modify it by inserting a layer corrector at the order τ, in the following manner

$$f(x, y, \boldsymbol{z}) = F(x, y, \boldsymbol{z}) + \tau\left[G(x, y, \boldsymbol{z}) - H\Big(\frac{x}{\tau}, y, \boldsymbol{z}\Big)\right] + \tau^2 f^{(2)}(x, y, \boldsymbol{z}) + \cdots, \tag{4.26}$$

where $F(\boldsymbol{x}, \boldsymbol{z})$ and $G(\boldsymbol{x}, \boldsymbol{z})$ are still given by Eq. (4.18), and $H(\xi, y, \boldsymbol{z})$ is the corrector term, which is a function of the boundary-layer variable by $\xi = x/\tau$. The corrector is to be chosen in such a manner to satisfy the following two requirements:

R1. the corrector should not affect the HE in the bulk, i.e. $F + \tau G - \tau H$, should be still a solution to the transport equation (3.18) up to $\mathcal{O}(\tau^2)$ far from the interface;

R2. at the interface, the corrector has to be constructed such that the transmission conditions at first-order are satisfied for a suitable choice of chemical potentials.

Substituting now the modified Hilbert-Ansatz (4.26) into Eq. (3.18) and denoting, for simplicity reasons, the transport term by $\mathcal{T} := \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} - s\nabla_{\boldsymbol{x}} U \cdot \nabla_{\boldsymbol{p}}$, yields

$$\tau\mathcal{T}(F + \tau G) - \tau\mu \frac{\partial H}{\partial \xi} = \mathcal{Q}(F) + \tau\mathcal{L}_{\langle F\rangle}(G) - \tau\mathcal{L}_{\langle F\rangle}(H) + \mathcal{O}(\tau^2)\,, \tag{4.27}$$

where μ, $\mathcal{Q}$ and $\mathcal{L}$ are defined in (3.34), (4.6) and (4.7), respectively. Using now the identities satisfied by F and G, i.e. $Q(F) = 0$ and $\mathcal{T}F = \mathcal{L}_{\langle F\rangle}(G)$, one remains, up to $\mathcal{O}(\tau^2)$, with the equation

$$\mu \frac{\partial H}{\partial \xi} = F'_{\langle F\rangle}\langle H\rangle - H.$$

Recalling that

$$\langle F\rangle(\boldsymbol{x}, s) = n_s(x, y) = n_s(\tau\xi, y),$$

we expect to introduce just an error of order τ^2 in (4.27), if we substitute $n_s(x, y)$ with its boundary values $n_s^i(y)$, where we recall that $n_s^i(y)$ denotes the limit of $n_s(x, y)$ as x tends to 0 from the i-th side (Definition 3.1). Thus, we expect that requirement **R1** is fulfilled if H satisfies the equation

$$\mu \frac{\partial H}{\partial \xi} = F'_{n_s^i}\langle H\rangle - H \tag{4.28}$$

on the i-th side of the interface (this is nothing else than a half-space, stationary transport equation). We shall see below that a corrector satisfying (4.28) and such that also requirement **R2** is satisfied, can be constructed by means of four auxiliary functions

$$\theta^i(\xi, y, \boldsymbol{z}) = \theta^i_s(\xi, y, \boldsymbol{p}), \quad (-1)^i\xi > 0, \quad y \in \mathbb{R}, \quad \boldsymbol{z} = (\boldsymbol{p}, s) \in \Theta, \quad i = 1, 2,$$

that satisfy (4.28) associated with the linear non-homogeneous KTC

$$\theta^i_{\text{in}} - G^i_{\text{in}} = \mathcal{K}^i\big(\theta^i_{\text{out}} - G^i_{\text{out}}, \theta^j_{\text{out}} - G^j_{\text{out}}\big),$$

(recall (4.22) and (4.23)). Hence, let us consider the problem

$$\begin{cases} \mu \dfrac{\partial \theta^i}{\partial \xi} = F'_{n_s^i}\langle \theta^i\rangle - \theta^i, & (-1)^i\xi > 0, \\ \theta^i_{\text{in}} - \mathcal{K}^i\big(\theta^i_{\text{out}}, \theta^j_{\text{out}}\big) = G^i_{\text{in}} - \mathcal{K}^i\big(G^i_{\text{out}}, G^j_{\text{out}}\big), & \xi = 0, \end{cases} \tag{4.29}$$

Note that in n_s^i, the upper index i refers to the interface limit of n_s, but in θ^i it is used to label the side where the problem is posed (and not the limit). Note also that the coordinate y is just an overall parameter in the problem.

Equation (4.29) is a system of four half-space, half-range Milne problems [15], for the functions θ^1_+, θ^1_-, θ^2_+, θ^2_-, coupled via non-homogenous transmission conditions. The following theorem, whose proof is deferred to Appendix A, is fundamental for the construction of the layer corrector.

Theorem 4.4 (Solution to the coupled Milne problems) *Problem* (4.29) *admits a solution* (θ^1, θ^2) *with*

$$\theta^i_s \in \mathrm{L}^\infty\big((-1)^i[0,+\infty)\times\Theta, (F'_{n^i_s})^{-1}d\xi d\boldsymbol{p}\big), \qquad i=1,2, \quad s=\pm,$$

if and only if the flux conservation condition holds:

$$\begin{cases} j^1_+ - j^1_- = j^2_+ - j^2_-, & \text{if } \delta V \neq 0, \\ j^1_s = j^2_s, \quad s=\pm 1, & \text{if } \delta V = 0. \end{cases} \tag{4.30}$$

Such solution is unique up to the addition of any solution of the homogeneous problem (i.e., problem (4.29) *with* $G=0$*). Moreover, four constants* $n^{1,\infty}_+$, $n^{1,\infty}_-$, $n^{2,\infty}_+$, $n^{2,\infty}_-$ *(depending on the parameter* y*) exist such that*

$$\theta^i(\xi,y,\boldsymbol{z}) \to \theta^{i,\infty}(y,\boldsymbol{z}) := n^{i,\infty}_s(y)F'_{n^i_s}(\boldsymbol{p}), \quad \text{as } \xi\to(-1)^i\infty, \tag{4.31}$$

and the convergence is exponentially fast; in particular,

$$|\langle\theta^i_s\rangle - n^{i,\infty}_s| \leq C\mathrm{e}^{-\alpha|\xi|}, \tag{4.32}$$

for some constants $C>0$ *and* $\alpha>0$ *(possibly depending on the parameter* y*).*

Thanks to Theorem 4.4 we can now construct the corrector H, which we define as follows:

$$H(\xi,y,\boldsymbol{z}) = \begin{cases} \theta^1(\xi,y,\boldsymbol{z}) - \theta^{1,\infty}(y,\boldsymbol{z}), & \text{if } \xi<0, \\ \theta^2(\xi,y,\boldsymbol{z}) - \theta^{2,\infty}(y,\boldsymbol{z}), & \text{if } \xi>0, \end{cases} \tag{4.33}$$

where the functions θ^i, are the solution to the coupled Milne problem (4.29) and $\theta^{i,\infty}$ are their asymptotic distributions (4.31). As we shall see below, although the solution to (4.29) is only determined up to the addition of an arbitrary solution of the homogeneous problem, such addition does not affect the final result, namely Theorem 4.5.

Let us now verify that the corrector function H given by (4.33) satisfies the two requirements **R1** and **R2**.

First of all, from Theorem 4.4 it follows immediately that H vanishes exponentially fast away from the interface, with

$$|\langle H\rangle| \leq C\mathrm{e}^{-\alpha|x|/\tau}. \tag{4.34}$$

Moreover, H satisfies Eq. (4.28), since both θ^i_s and $n^{i,\infty}_s F'_{n^i_s}$ do. Then, we already know that $F+\tau(G-H)$ satisfies the transport equation up to terms of order τ^2 if the error that is made by substituting in (4.27) $F'_{n_s}\langle H\rangle$ with the boundary limit $F'_{n^i_s}\langle H\rangle$ is of order τ. But, indeed, from the Taylor expansion of n_s (assumed regular enough) and from inequality (4.34), we have that

$$|(F'_{n^i_s} - F'_{n_s})\langle H\rangle| \leq M|x|\mathrm{e}^{-\alpha|x|/\tau} \leq \frac{M\tau}{\alpha}\mathrm{e}^{-\alpha|x|/\tau},$$

for some constant $M>0$. This proves **R1**.

Coming to requirement **R2**, when evaluating the transmission conditions on the modified HE (4.26), Eq. (4.25) is replaced by

$$\begin{aligned} F^i_{\text{in}} + \tau(G-H)^i_{\text{in}} &= \mathcal{B}^i\left(F^i_{\text{out}} + \tau(G-H)^i_{\text{out}}, F^j_{\text{out}} + \tau(G-H)^j_{\text{out}}\right) \\ &= \mathcal{B}^i\left(F^i_{\text{out}}, F^j_{\text{out}}\right) + \tau\mathcal{K}^i\left((G-H)^i_{\text{out}}, (G-H)^j_{\text{out}}\right), \end{aligned} \tag{4.35}$$

where we used (4.22). But

$$(G-H)^i_{\text{in}} - \mathcal{K}^i\left((G-H)^i_{\text{out}}, (G-H)^j_{\text{out}}\right) = \theta^{i,\infty}_{\text{in}} - \mathcal{K}^i(\theta^{i,\infty}_{\text{out}}, \theta^{j,\infty}_{\text{out}}),$$

because of the definition of H (4.33) and the boundary conditions in (4.29). Then, (4.35) becomes

$$F^i_{\text{in}} + \tau\theta^{i,\infty}_{\text{in}} = \mathcal{B}^i\left(F^i_{\text{out}} + \tau\theta^{i,\infty}_{\text{out}}, F^j_{\text{out}} + \tau\theta^{j,\infty}_{\text{out}}\right). \tag{4.36}$$

Now, we recall that $F^i_s = F_{n^i_s}$, $\theta^{i,\infty}_s = n^{i,\infty}_s F'_{n^i_s}$, and, from (4.2),

$$F_{n^i_s} + \tau n^{i,\infty}_s F'_{n^s_i} = F_{n^i_s + \tau n^{i,\infty}_s} + \mathcal{O}(\tau^2).$$

Hence, Eq. (4.36) is, up to $\mathcal{O}(\tau^2)$, a KTC condition for Fermi-Dirac distributions with densities $n^i_s + \tau n^{i,\infty}_s$ and Proposition 3.3 immediately leads to our principal result.

Theorem 4.5 (Diffusive transmission conditions at first order) *Assume that the current conservation* (4.30) *holds. Then, up to errors of order τ^2, the left and right densities at the interface $x = 0$, n^1_s and n^2_s, are constrained by the condition*

$$sA(n^1_s + \tau n^{1,\infty}_s) = s'A(n^2_{s'} + \tau n^{2,\infty}_{s'}) + \beta\delta V, \tag{4.37}$$

that must hold for all admissible couples (s, s'), where $n^{i,\infty}_s$ are the asymptotic densities[7] *of the solution θ^i_s to the Milne problem* (4.29) *(see* (4.31)*).*

Equation (4.37) gives the DTC at first order for the electron/hole densities n_s across the interface. They are a first order correction to the leading order conditions (4.24) and can be considered as a "quantum correction" since they depend upon the scattering data T^i_s through the asymptotic densities $n^{i,\infty}_s$ associated to the solutions of the Milne problem (4.29).

Remark 4.6 The solutions θ^i_s and, consequently, the asymptotic densities $n^{i,\infty}_s$ are unique only up to the addition of a solution to the homogeneous Milne problem. However, since the addition of such a solution does not change Eq. (4.36) (by definition), then Eq. (4.37) is not affected by the particular choice of the solutions θ^i_s.

---

[7] Since we are using dimensionless phase-space distributions, the physical dimensions of $n^{i,\infty}_s$ are actually those of a frequency.

4.4 Maxwell-Boltzmann approximation

For large energies, the F-D distribution (3.17) is asymptotically approximated by the Maxwell-Boltzmann (M-B) distribution $nM(\boldsymbol{p})$, where

$$M(\boldsymbol{p}) = \frac{\mathrm{e}^{-\beta c|\boldsymbol{p}|}}{n_0} \tag{4.38}$$

is the normalised Maxwellian and the constant n_0 is given by (3.15). Correspondingly, the Fermi integrals (3.14) are asymptotically approximated by

$$\phi_k(A) \sim \mathrm{e}^A$$

(independently on $k > 0$) and, in particular, Eq. (3.16) is approximated by

$$\mathrm{e}^{A(n)} \sim \frac{n}{n_0}.$$

Then, it is readily seen that the M-B approximation of the Drift-Diffusion equation (4.16) is given by

$$\operatorname{div}\left[\nabla n_s + s\beta n_s \nabla U\right] = 0, \tag{4.39}$$

and the M-B approximation of the first-order DTC (4.37) writes

$$\Big(\frac{n_s^1 + \tau n_s^{1,\infty}}{n_0}\Big)^s = \Big(\frac{n_{s'}^2 + \tau n_{s'}^{2,\infty}}{n_0}\Big)^{s'} \mathrm{e}^{\beta\delta V}, \tag{4.40}$$

for all admissible couples (s, s'). Moreover, the asymptotic densities $n_s^{i,\infty}$ are calculated, as functions of $\boldsymbol{j}_s^i$, from the Milne problem (4.29) with

$$F'_{n_s^i} \sim M, \qquad \boldsymbol{\ell}_s^i \sim \frac{2}{c^2} M\boldsymbol{v}. \tag{4.41}$$

Note that in the M-B approximation the dependence of F'_n (and, consequently, $\boldsymbol{\ell}$) on n disappears and then the approximated quantities become independent on the indices s and i. It is instructive to write down (4.40) more explicitly for $\delta V > 0$. In this case, the admissible couples (s, s') are $(+,+), (+,-), (-,-)$ and we obtain therefore:

$$\begin{cases} n_+^1 - \mathrm{e}^{\beta\delta V} n_+^2 = \tau\big(\mathrm{e}^{\beta\delta V} n_+^{2,\infty} - n_+^{1,\infty}\big), \\ \big(n_+^1 + \tau n_+^{1,\infty}\big)\big(n_-^2 + \tau n_-^{2,\infty}\big) = \mathrm{e}^{\beta\delta V}(n_0)^2, \\ n_-^1 - \mathrm{e}^{-\beta\delta V} n_-^2 = \tau\big(\mathrm{e}^{-\beta\delta V} n_-^{2,\infty} - n_-^{1,\infty}\big). \end{cases} \tag{4.42}$$

We note that the first equations is identical (in form) to the first-order DTC found in Refs. [13, 14] for the case of a single, parabolic energy band, and the third one is its hole version (the potential changes sign). The second equation is a quantum correction to the semiconductor mass-action law $n_+^1 n_-^2 = \mathrm{e}^{\beta\delta V}(n_0)^2$. Clearly, it can be approximated at order τ as follows:

$$n_+^1 n_-^2 - e^{\beta\delta V}(n_0)^2 = -\tau\big(n_+^1 n_-^{2,\infty} + n_-^2 n_+^{1,\infty}\big). \tag{4.43}$$

5 Hybrid Drift-Diffusion-quantum model

We now summarize the results obtained in the present work, by writing down the hybrid diffusive-quantum model describing the electron transport in a graphene device.

Let our hypothetic graphene device be represented by the rectangle $(x, y) \in (-L, L) \times (-l, l)$ (see Fig. 3), where the steep potential variations are concentrated in $x = 0$ (on a macroscopic scale), and the two classical regions are

$$\Omega^1 = (-L, 0) \times (-l, l), \qquad \text{and} \qquad \Omega^2 = (0, L) \times (-l, l).$$

For the sake of simplicity, we shall work in the M-B approximation (see Sec. 4.4). Then, in Ω^1 and Ω^2 the stationary drift-diffusion equation (4.39) is assumed to hold. At the external boundary of the device standard conditions can be imposed, e.g. non homogeneous Dirichlet conditions at $x = -L$ and $x = L$ (representing ohmic contacts) and homogeneous Robin conditions at $y = -l$ and $y = l$ (representing an insulating boundary). At the quantum-classical interface, $x = 0$, the DTC (4.40) are imposed.

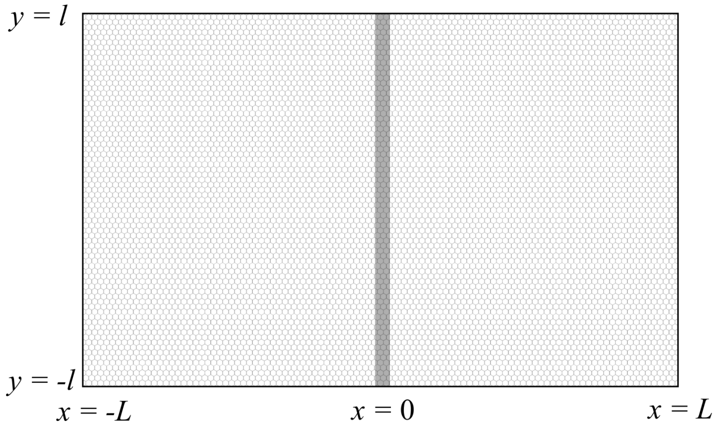

Figure 3: Geometry of a prototypical graphene device: the central strip represents the quantum active region, where the DTC are imposed. On the remaining boundaries, classical Dirichlet and Robin conditions can be imposed.

If $\delta V > 0$, the DTC are explicitly given by (4.42), where the second equation can be substituted by (4.43). This is a rank-3 condition and we still need a further condition, which is given by the total flux conservation $(4.30)_1$ across the interface. We stress the fact that the flux conservation is also required to ensure existence of $n_s^{i,\infty}$, according to Theorem 4.4.

Hence, the resulting hybrid diffusive-quantum model reads as follows:

$$
\begin{aligned}
&\left.\begin{aligned} \operatorname{div} \boldsymbol{j}_s = 0 \\ \boldsymbol{j}_s = -\big(\nabla n_s + s\beta n_s \nabla U\big) \end{aligned}\right\}, && \text{in the semiclassical regions } \Omega^1 \cup \Omega^2, \\
&\qquad n_s = n_s^{\pm L}, && \text{at the Ohmic boundary } x = \pm L, \\
&\qquad j_{s,y} = 0, && \text{at the insulating boundary } y = \pm l, \\
&\left.\begin{aligned} n_+^1 - \mathrm{e}^{\beta\delta V} n_+^2 = \tau\big(\mathrm{e}^{\beta\delta V} n_+^{2,\infty} - n_+^{1,\infty}\big) \\ n_+^1 n_-^2 + \tau\big(n_+^1 n_-^{2,\infty} + n_-^2 n_+^{1,\infty}\big) = \mathrm{e}^{\beta\delta V}(n_0)^2 \\ n_-^1 - \mathrm{e}^{-\beta\delta V} n_-^2 = \tau\big(\mathrm{e}^{-\beta\delta V} n_-^{2,\infty} - n_-^{1,\infty}\big) \\ j_{+,x}^1 - j_{-,x}^1 = j_{+,x}^2 - j_{-,x}^2 = 0 \end{aligned}\right\}, && \text{across the quantum interface } x = 0,
\end{aligned}
\tag{5.1}
$$

where $n_s^{\pm L}$ are the given densities of electrons and holes at the contacts. The quantities $n_s^{i,\infty}$ are the asymptotic densities associated to the system of Milne equations

$$
\begin{cases}
\mu \dfrac{\partial \theta_s^i}{\partial \xi} = M\langle \theta_s^i \rangle - \theta_s^i, & (-1)^i \xi > 0, \\
\theta_{\text{in}}^i - \mathcal{K}^i\big(\theta_{\text{out}}^i, \theta_{\text{out}}^j\big) = G_{\text{in}}^i - \mathcal{K}^i\big(G_{\text{out}}^i, G_{\text{out}}^j\big), & \xi = 0.
\end{cases}
\tag{5.2}
$$

where

$$
G_s^i = M \boldsymbol{v} \cdot \boldsymbol{j}_s^i. \tag{5.3}
$$

Note that the functions $n_s^{i,\infty}(y)$ depend on $\boldsymbol{j}_s$ and, therefore, the DTC couple the four (left/right, electrons/holes) drift-diffusion equations in (5.1). We also remark that the $n_s^{i,\infty}$'s embody the quantum part of the model, represented by the scattering problem (2.2).

Remark 5.1 As it can be seen by comparing (5.3) with (4.41) and (4.18), here $\boldsymbol{j}$ has been conveniently redefined as the drift-diffusion current divided by $c^2/2$.

If $\delta V = 0$, then the second DTC equations (4.42) disappears and we are left with a rank-2 condition. On the other hand, in this case, the current conservation holds *separately* for electrons and holes (see Eq. $(4.30)_2$) and we gain one more condition on the current. If $\delta V = 0$, therefore, the diffusion model is still given by (5.1) but the conditions across the interface must be substituted by

$$
\left.\begin{aligned}
n_+^1 - \mathrm{e}^{\beta\delta V} n_+^2 = \tau\big(\mathrm{e}^{\beta\delta V} n_+^{2,\infty} - n_+^{1,\infty}\big) \\
n_-^1 - \mathrm{e}^{-\beta\delta V} n_-^2 = \tau\big(\mathrm{e}^{-\beta\delta V} n_-^{2,\infty} - n_-^{1,\infty}\big) \\
j_{+,x}^1 = j_{+,x}^2 \\
j_{-,x}^1 = j_{-,x}^2
\end{aligned}\right\}. \tag{5.4}
$$

We note that, in this case, also the asymptotic densities $n_s^{i,\infty}$ are decoupled with respect to s. This is an immediate consequence of the fact that, when $\delta V = 0$, the KTC for electrons and holes are decoupled and, consequently, electrons and holes are also decoupled in the Milne problem (4.29), or (5.2) in the M-B case. Hence, if no additional coupling mechanisms are introduced, if $\delta V = 0$ electrons and holes are completely independent, both in the kinetic and in the diffusive models.

Of course, solving numerically the coupled Milne equations (4.29) or (5.2) is in general a hard task, and the advantage of the diffusive-quantum model (5.1), with respect to the kinetic-quantum one, is far from being evident. It is therefore necessary to reduce the complexity of problem (4.29). This can be done by assuming that the outflow distribution θ^i_{out} is an equilibrium distribution (e.g. a Maxwellian, for problem (5.2)), so that the only unknowns of the albedo problems are four albedo densities (see Ref. [13] for the case of standard particles). Another possibility is the application of the iterative procedure proposed by Golse and Klar in Ref. [16]. This will be the subject of a subsequent work, devoted to numerics for real applications.

We finally remark that, in the present formulation, the quantum part of the problem is independent of the semiclassical one, to the extent that the scattering problem (2.2) is solved, self-consistently and once for all, in order to get the scattering data. However, a more complicate nonlinear coupling can be introduced by assuming that the quantum potential V depends in part on the densities n_s through a Poisson equation [7, 13].

A Proof of Theorem 4.4

In order to streamline the notation, let us put

$$L^i(\boldsymbol{z}) = L^i_s(\boldsymbol{p}) := F'_{n^i_s}(\boldsymbol{p}), \tag{A.1}$$

and rewrite the Milne problem (4.29) accordingly:

$$\begin{cases} \mu \dfrac{\partial \theta^i}{\partial \xi} = L^i \langle \theta^i \rangle - \theta^i, & (-1)^i \xi > 0, \\ \theta^i_{\text{in}} - \mathcal{K}^i\big(\theta^i_{\text{out}}, \theta^j_{\text{out}}\big) = G^i_{\text{in}} - \mathcal{K}^i\big(G^i_{\text{out}}, G^j_{\text{out}}\big), & \xi = 0. \end{cases} \tag{A.2}$$

We recall that in problem (A.2) the y-variable is just a parameter, which shall be omitted throughout the proof.
The proof is inspired by the ideas of Ref. [14] and is divided into three steps for the reader's convenience.

Step 1: reduction to a $|\boldsymbol{p}|$-averaged problem. Let us consider the uncoupled version of (A.2), with assigned inflows g^i:

$$\begin{cases} \mu \dfrac{\partial \theta^i}{\partial \xi}(\xi, \boldsymbol{z}) = L^i(\boldsymbol{z}) \langle \theta^i \rangle - \theta^i(\xi, \boldsymbol{z}), & (-1)^i \xi > 0, \quad \boldsymbol{z} \in \Theta, \\ \theta^i_{\text{in}}(\boldsymbol{z}) = g^i(\boldsymbol{z}), & \xi = 0, \quad \boldsymbol{z} \in \Theta^i_{\text{in}} \end{cases} \tag{A.3}$$

(recall definitions (A.1), (3.23) and (4.19)). We introduce the $|\boldsymbol{p}|$-average

$$\tilde{\theta}^i(\xi,\varphi,s) := \frac{1}{2\pi\hbar^2}\int_0^{+\infty} \theta^i(\xi, |\boldsymbol{p}|\cos\varphi, |\boldsymbol{p}|\sin\varphi, s)\, |\boldsymbol{p}|\, d|\boldsymbol{p}|, \tag{A.4}$$

where the normalisation constant is chosen so that

$$\langle\theta^i\rangle(\xi,s) = \frac{1}{2\pi}\int_0^{2\pi} \tilde{\theta}^i(\xi,\varphi,s)\, d\varphi \quad \text{and} \quad \tilde{L}^i_s = 1,$$

where $\langle\theta^i\rangle$ is defined in (3.12). We introduce the analogous of the sets (3.22) for the averaged quantities:

$$\tilde{\Theta} := [0,2\pi) \times \{-1,+1\}, \quad \tilde{\Theta}^i_{\text{in/out}} := \{(\varphi,s) \in \Theta \mid (-1)^i \cos\varphi \gtrless 0\} \tag{A.5}$$

and extend, in the obvious way, to $\tilde{\theta}^i$ the notations $\tilde{\theta}^i_{\text{in}}$ and $\tilde{\theta}^i_{\text{out}}$. Taking the $|\boldsymbol{p}|$-average of (A.3), we obtain that $\tilde{\theta}^i_s$ satisfies

$$\begin{cases} \mu \dfrac{\partial\tilde{\theta}^i}{\partial\xi}(\xi,\varphi,s) = \dfrac{1}{2\pi}\displaystyle\int_0^{2\pi} \tilde{\theta}^i(\xi,\varphi,s)\, d\varphi - \tilde{\theta}^i(\xi,\varphi,s), & (-1)^i\xi > 0, \quad (\varphi,s) \in \tilde{\Theta}, \\ \tilde{\theta}^i_{\text{in}}(\varphi,s) = \tilde{g}^i(\varphi,s), & \xi = 0, \quad (\varphi,s) \in \tilde{\Theta}^i_{\text{in}}, \end{cases} \tag{A.6}$$

where we recall that

$$\mu = \frac{cp_x}{|\boldsymbol{p}|} = c\cos\varphi.$$

Conversely, it is easy to check that, if $\tilde{\theta}^i$ is a solution of (A.6), then

$$\theta^i := L^i\tilde{\theta}^i + \begin{cases} \mathrm{e}^{-\xi/\mu}\left(g^i - L^i\tilde{g}^i\right), & (-1)^i\mu > 0, \\ 0, & (-1)^i\mu < 0, \end{cases} \tag{A.7}$$

is solution of (A.3). The equations (A.6) are four ($s = \pm 1$, $i = 1,2$) independent Milne problems having the form of a Milne problem for neutron transport, to the extent that the kernel of the collision operator coincides with the functions that are constant with respect to φ [2, 15]. About such problem the following facts are known [2, 14, 22]:

(i) If $\tilde{g}^i \in \mathrm{L}^\infty(\tilde{\Theta}^i_{\text{in}})$, the solution $\tilde{\theta}^i$ of (A.6) exists and is unique in $\mathrm{L}^\infty\big((-1)^i[0,+\infty) \times \tilde{\Theta}\big)$. Moreover, one has the positivity, i.e. $\tilde{\theta}^i \geq 0$ if $\tilde{g}^i \geq 0$.

(ii) A constant $n^{i,\infty}_s$ (depending on $\tilde{g}^i$) exists such that $\tilde{\theta}^i(\xi,\varphi,s) \to n^{i,\infty}_s$, as $\xi \to (-1)^i\infty$, and the convergence is exponentially fast; in particular

$$\left|\int_0^{2\pi} \tilde{\theta}^i(\xi,\varphi,s)\, d\varphi - n^{i,\infty}_s\right| \leq C\mathrm{e}^{-\alpha|\xi|},$$

for some constants $C > 0$ and $\alpha > 0$. Moreover, $n^{i,\infty} \geq 0$ if $\tilde{g}^i \geq 0$.

(iii) The *Albedo operator*, that associates the inflow to the outflow, i.e. $\tilde{\theta}^i_{\text{in}} \equiv \tilde{g}^i \mapsto \tilde{\theta}^i_{\text{out}}$, is a compact linear operator from $\mathrm{L}^\infty(\tilde{\Theta}^i_{\text{in}})$ to $\mathrm{L}^\infty(\tilde{\Theta}^i_{\text{out}})$.

Step 2: formulation as a Fredholm problem. Thanks to the explicit formula (A.7), it is easy to extend the above results to the $|\boldsymbol{p}|$-dependent problem (A.3). Let us define the weighted spaces

$$X^i := \mathrm{L}^\infty\big(\Theta, (L^i)^{-1} d\boldsymbol{p}\big), \quad X^i_{\text{in}} := \mathrm{L}^\infty\big(\Theta^i_{\text{in}}, (L^i)^{-1} d\boldsymbol{p}\big), \quad X^i_{\text{out}} := \mathrm{L}^\infty\big(\Theta^i_{\text{out}}, (L^i)^{-1} d\boldsymbol{p}\big).$$

Note that $g \in X^i$ implies that $g \in \mathrm{L}^p(\Theta)$ for all $p \in [0,\infty]$. Then, from the results of Step 1, we have the following facts about problem (A.3):

(i) If $g^i \in X^i_{\text{in}}$, the solution θ^i of problem (A.3) exists and is unique in $\mathrm{L}^\infty\big((-1)^i[0,+\infty), X^i\big)$. Moreover, $\theta^i \geq 0$ if $g^i \geq 0$.

(ii) A constant $n_s^{i,\infty}$ (depending on g^i) exists such that $\theta^i(\xi,\boldsymbol{z}) \to n_s^{i,\infty} L^i_s(\boldsymbol{p})$, as $\xi \to (-1)^i\infty$, and the convergence is exponentially fast; in particular

$$\left|\langle\theta^i_s\rangle(\xi) - n_s^{i,\infty}\right| \leq C\mathrm{e}^{-\alpha|\xi|},$$

for some constants $C > 0$ and $\alpha > 0$. Moreover, $n^{i,\infty} \geq 0$ if $g^i \geq 0$.

(iii) The Albedo operator, associating the inflow $\theta^i_{\text{in}} \equiv g^i$ to the outflow θ^i_{out},

$$\mathcal{A}^i : X^i_{\text{in}} \to X^i_{\text{out}}, \qquad \mathcal{A}^i\theta^i_{\text{in}} := \theta^i_{\text{out}},$$

is a compact linear operator.

We now come to the coupled Milne problem (A.2). Thanks to the Albedo operator just introduced, we can reformulate (A.2) as a Fredholm problem in $X^1_{\text{in}} \times X^2_{\text{in}}$ for the unknown inflow data $(\theta^1_{\text{in}}, \theta^2_{\text{in}})$, namely:

$$\begin{pmatrix} \theta^1_{\text{in}} \\ \theta^2_{\text{in}} \end{pmatrix} - \mathcal{K} \begin{pmatrix} \mathcal{A}^1\theta^1_{\text{in}} \\ \mathcal{A}^2\theta^2_{\text{in}} \end{pmatrix} = \begin{pmatrix} \Gamma^1 \\ \Gamma^2 \end{pmatrix} \tag{A.8}$$

where, recalling definition (4.23),

$$\mathcal{K} \begin{pmatrix} \theta^1_{\text{out}} \\ \theta^2_{\text{out}} \end{pmatrix} = \begin{pmatrix} \mathcal{K}^1\big(\theta^1_{\text{out}}, \theta^2_{\text{out}}\big) \\ \mathcal{K}^2\big(\theta^2_{\text{out}}, \theta^1_{\text{out}}\big) \end{pmatrix},$$

and the components of the non-homogeneous term are

$$\Gamma^i = G^i_{\text{in}} - \mathcal{K}^i\big(G^i_{\text{out}}, G^j_{\text{out}}\big). \tag{A.9}$$

Let us now show that $\mathcal{K} : X^1_{\text{out}} \times X^2_{\text{out}} \to X^1_{\text{in}} \times X^2_{\text{in}}$ is a linear, continuous operator. In fact, for $\boldsymbol{z} \in \Theta^i_{\text{in}}$ we can write

$$\frac{\theta^i_{\text{in}}(\boldsymbol{z})}{L^i(\boldsymbol{z})} = \frac{\mathcal{K}^i(\theta^i_{\text{out}}, \theta^j_{\text{out}})(\boldsymbol{z})}{L^i(\boldsymbol{z})} = R^i(\boldsymbol{z})\frac{\theta^i_{\text{out}}(\sim\boldsymbol{z})}{L^i(\boldsymbol{z})} + T^j(\boldsymbol{z}')\frac{ss'\theta^j_{\text{out}}(\boldsymbol{z}')}{L^i(\boldsymbol{z})},$$

where $\boldsymbol{z}' \in \Theta^j_{\text{out}}$ is constrained to $\boldsymbol{z}$ by the conservation laws (3.26). Recalling definitions (4.3) and (A.1), and using (4.24) and the identity

$$\frac{\mathrm{e}^h}{(\mathrm{e}^h+1)^2} = \frac{\mathrm{e}^{-h}}{(\mathrm{e}^{-h}+1)^2},$$

it is not difficult to show that the following relation holds

$$\phi_1(A(n^i_s))\, L^i_s(\boldsymbol{p}) = \phi_1(A(n^j_{s'}))\, L^j_{s'}(\boldsymbol{p}'), \tag{A.10}$$

for all $\boldsymbol{z} = (\boldsymbol{p}, s)$ and $\boldsymbol{z}' = (\boldsymbol{p}', s')$ related as above. Then, the previous equality can be rewritten as

$$\frac{\theta^i_{\text{in}}(\boldsymbol{z})}{L^i(\boldsymbol{z})} = R^i(\boldsymbol{z}) \frac{\theta^i_{\text{out}}(\sim\boldsymbol{z})}{L^i(\boldsymbol{z})} + T^j(\boldsymbol{z}') \frac{ss' c^i_s \theta^j_{\text{out}}(\boldsymbol{z}')}{c^j_{s'} L^j(\boldsymbol{z}')},$$

where

$$c^i(\boldsymbol{z}) = c^i_s := \phi_1(A(n^i_s)) \tag{A.11}$$

are positive constants that only depend on s (and not on $\boldsymbol{p}$). Using Jensen inequality we can write

$$\left|\frac{\theta^i_{\text{in}}(\boldsymbol{z})}{L^i(\boldsymbol{z})}\right|^2 \le R^i(\boldsymbol{z}) \left|\frac{\theta^i_{\text{out}}(\sim\boldsymbol{z})}{L^i(\boldsymbol{z})}\right|^2 + T^j(\boldsymbol{z}') \left|\frac{c^i_s}{c^j_{s'}}\right|^2 \left|\frac{\theta^j_{\text{out}}(\boldsymbol{z}')}{L^j(\boldsymbol{z}')}\right|^2,$$

(we adopt the redundant notation $|\cdot|^2$ for the square, just to improve readability), which shows the continuity of $\mathcal{K}$, since the scattering coefficients are bounded by 1.

Hence, the composition of $\mathcal{K}$, which is continuous, with the $\mathcal{A}^i$'s, which are compact, is a compact operator on $X^1_{\text{in}} \times X^2_{\text{in}}$ and, therefore, (A.8) is a Fredholm equation with compact operator. The proof of Theorem 4.4 is thus reduced to a Fredholm alternative, which will be discussed in the next two steps.

Step 3: the homogeneous problem. We now consider the homogeneous version of the Milne problem (A.2), corresponding to $G = 0$:

$$\begin{cases} \mu \dfrac{\partial \theta^i}{\partial \xi} = L^i \langle \theta^i \rangle - \theta^i, & (-1)^i \xi > 0, \\[2ex] \theta^i_{\text{in}} - \mathcal{K}^i(\theta^i_{\text{out}}, \theta^j_{\text{out}}) = 0, & \xi = 0. \end{cases} \tag{A.12}$$

Let (θ^1, θ^2) be a solution of such a problem in the space $X^1 \times X^2$. It is convenient to introduce the functions (ψ^1, ψ^2) as follows:

$$\theta^i(\xi, \boldsymbol{z}) = \sqrt{L^i(\boldsymbol{z})}\, \psi^i(\xi, \boldsymbol{z}), \qquad i = 1, 2,$$

so that $\psi^i/\sqrt{L^i}$ is bounded and ψ^i satisfies the equation

$$\mu \frac{\partial \psi^i}{\partial \xi} = \sqrt{L^i}\, \langle \sqrt{L^i}\, \psi^i \rangle - \psi^i. \tag{A.13}$$

It is immediate to verify that

$$\int_{\mathbb{R}^2} \left(\sqrt{L^i_s} \left\langle \sqrt{L^i_s}\, \psi^i_s \right\rangle - \psi^i_s \right) \psi^i \, d\boldsymbol{p} \le 0, \tag{A.14}$$

and that the equality holds if and only if ψ^i_s is in the kernel of the collision operator, i.e. $\psi^i_s = \sqrt{L^i_s}\,\gamma_s$, for some γ_s constant with respect to $\boldsymbol{p}$. By multiplying by ψ^i both sides of (A.13), integrating over $\boldsymbol{p} \in \mathbb{R}^2$ we obtain

$$\frac{1}{2}\frac{\partial}{\partial\xi}\int_{\mathbb{R}^2} \left|\psi^i_s(\xi,\boldsymbol{p})\right|^2 \mu(\boldsymbol{p})\, d\boldsymbol{p} = \int_{\mathbb{R}^2} \left(\sqrt{L^i_s}\left\langle\sqrt{L^i_s}\,\psi^i_s\right\rangle - \psi^i_s\right)\psi^i_s\, d\boldsymbol{p} \leq 0. \tag{A.15}$$

From (ii) of Step 2 we know that $\psi^i_s(\xi,\boldsymbol{p})$ tends to a function of the form $\sqrt{L^i_s(\boldsymbol{p})}\,\gamma^i_s(\xi)$, as $\xi \to (-1)^i\infty$ and, therefore, by integrating the previous inequality over $\xi \in (-1)^i[0,+\infty)$ and recalling that μ is an odd function of $\boldsymbol{p}$, we obtain

$$\int_{\mathbb{R}^2} \left|\psi^1_s(0,\boldsymbol{p})\right|^2 \mu(\boldsymbol{p})\, d\boldsymbol{p} \leq 0 \leq \int_{\mathbb{R}^2} \left|\psi^2_s(0,\boldsymbol{p})\right|^2 \mu(\boldsymbol{p})\, d\boldsymbol{p}. \tag{A.16}$$

On the other hand, (θ^1,θ^2) satisfy the homogeneous KTC

$$\theta^i(0,\boldsymbol{z}) = R^i(\boldsymbol{z})\theta^i(0,\sim\!\boldsymbol{z}) + T^j(\boldsymbol{z}')ss'\theta^j(0,\boldsymbol{z}')$$

and, correspondingly, (ψ^1,ψ^2) satisfy

$$\sqrt{L^i(\boldsymbol{z})}\,\psi^i(0,\boldsymbol{z}) = R^i(\boldsymbol{z})\sqrt{L^i(\boldsymbol{z})}\,\psi^i(0,\sim\!\boldsymbol{z}) + T^j(\boldsymbol{z}')ss'\sqrt{L^j(\boldsymbol{z}')}\,\psi^j(0,\boldsymbol{z}'),$$

where $\boldsymbol{z} \in \Theta^i_{\text{in}}$ and $\boldsymbol{z}' \in \Theta^j_{\text{out}}$ are constrained by the conservation of energy (3.26). By using (A.10) and (A.11), we obtain

$$\sqrt{c^i(\boldsymbol{z})}\,\psi^i(0,\boldsymbol{z}) = R^i(\boldsymbol{z})\sqrt{c^i(\boldsymbol{z})}\,\psi^i(0,\sim\!\boldsymbol{z}) + T^j(\boldsymbol{z}')ss'\sqrt{c^j(\boldsymbol{z}')}\,\psi^j(0,\boldsymbol{z}'), \tag{A.17}$$

and then, using Jensen inequality,

$$c^i(\boldsymbol{z})\left|\psi^i(0,\boldsymbol{z})\right|^2 \leq R^i(\boldsymbol{z})c^i(\boldsymbol{z})\left|\psi^i(0,\sim\!\boldsymbol{z})\right|^2 + T^j(\boldsymbol{z}')c^j(\boldsymbol{z}')\left|\psi^j(0,\boldsymbol{z}')\right|^2$$

or, equivalently,

$$c^i(\boldsymbol{z})\left(\left|\psi^i(0,\boldsymbol{z})\right|^2 - \left|\psi^i(0,\sim\!\boldsymbol{z})\right|^2\right) \leq -T^i(\boldsymbol{z})c^i(\boldsymbol{z})\left|\psi^i(0,\sim\!\boldsymbol{z})\right|^2 + T^j(\boldsymbol{z}')c^j(\boldsymbol{z}')\left|\psi^j(0,\boldsymbol{z}')\right|^2.$$

We now multiply both sides by $\mu(\boldsymbol{z})$, $\boldsymbol{z} \in \Theta^i_{\text{in}}$, which is negative (or zero) for $i = 1$ and positive (or zero) for $i = 2$, so that

$$\begin{aligned} c^1(\boldsymbol{z})\left(\left|\psi^1(0,\boldsymbol{z})\right|^2 - \left|\psi^1(0,\sim\!\boldsymbol{z})\right|^2\right)\mu(\boldsymbol{z}) \geq{}& -T^1(\boldsymbol{z})c^1(\boldsymbol{z})\left|\psi^1(0,\sim\!\boldsymbol{z})\right|^2\mu(\boldsymbol{z}) \\ &+ T^2(\boldsymbol{z}')c^2(\boldsymbol{z}')\left|\psi^2(0,\boldsymbol{z}')\right|^2\mu(\boldsymbol{z}), \end{aligned}$$

$$\begin{aligned} c^2(\boldsymbol{z})\left(\left|\psi^2(0,\boldsymbol{z})\right|^2 - \left|\psi^2(0,\sim\!\boldsymbol{z})\right|^2\right)\mu(\boldsymbol{z}) \leq{}& -T^2(\boldsymbol{z})c^2(\boldsymbol{z})\left|\psi^2(0,\sim\!\boldsymbol{z})\right|^2\mu(\boldsymbol{z}) \\ &+ T^1(\boldsymbol{z}')c^1(\boldsymbol{z}')\left|\psi^1(0,\boldsymbol{z}')\right|^2\mu(\boldsymbol{z}). \end{aligned}$$

If we now integrate the first inequality over $\boldsymbol{z} \in \Theta^1_{\text{in}}$, and the second one over $\boldsymbol{z} \in \Theta^2_{\text{in}}$, by following the same passages as in the proof of Proposition 3.2 we arrive at

$$\begin{aligned}\int_\Theta c^1(\boldsymbol{z}) \left|\psi^1(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z}) d\boldsymbol{z} \geq \int_{\Theta^1_{\text{out}}} & T^1(\boldsymbol{z}) c^1(\boldsymbol{z}) \left|\psi^1(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z})\, d\boldsymbol{z} \\ & + \int_{\Theta^2_{\text{out}}} T^2(\boldsymbol{z}') c^2(\boldsymbol{z}') \left|\psi^2(0,\boldsymbol{z}')\right|^2 \mu(\boldsymbol{z}')\, d\boldsymbol{z}'\end{aligned}$$

$$\begin{aligned}\int_\Theta c^2(\boldsymbol{z}) \left|\psi^2(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z}) d\boldsymbol{z} \leq \int_{\Theta^2_{\text{out}}} & T^2(\boldsymbol{z}') c^2(\boldsymbol{z}') \left|\psi^2(0,\boldsymbol{z}')\right|^2 \mu(\boldsymbol{z}')\, d\boldsymbol{z}' \\ & + \int_{\Theta^1_{\text{out}}} T^1(\boldsymbol{z}) c^1(\boldsymbol{z}) \left|\theta^1(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z})\, d\boldsymbol{z}\end{aligned}$$

(where in the last integral of both inequalities, $\boldsymbol{z}$ and $\boldsymbol{z}'$ are related by $E(\boldsymbol{z}) = E(\boldsymbol{z}') + \delta V$), which immediately leads to

$$\int_\Theta c^1(\boldsymbol{z}) \left|\psi^1(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z}) d\boldsymbol{z} \geq \int_\Theta c^2(\boldsymbol{z}) \left|\psi^2(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z}) d\boldsymbol{z}. \tag{A.18}$$

If we now come back to (A.16), multiply the right and the left sides by the positive constants $c^1(\boldsymbol{z}) = c^1_s$ and $c^2(\boldsymbol{z}) = c^2_s$, respectively, and sum up with respect to s, we obtain

$$\int_\Theta c^1(\boldsymbol{z}) \left|\psi^1(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z}) d\boldsymbol{z} \leq 0 \leq \int_\Theta c^2(\boldsymbol{z}) \left|\psi^2(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z}) d\boldsymbol{z}. \tag{A.19}$$

By comparing (A.18) with (A.19) we see that, necessarily,

$$\int_\Theta c^1(\boldsymbol{z}) \left|\psi^i(0,\boldsymbol{z})\right|^2 \mu(\boldsymbol{z}) d\boldsymbol{z} = 0, \qquad i = 1,2.$$

Multiplying (A.15) by $c^i(\boldsymbol{z}) = c^i_s$, summing up with respect to s and integrating with respect to ξ yields, therefore,

$$\int_0^{(-1)^i\infty} \int_\Theta c^i \left(\sqrt{L^i} \left\langle \sqrt{L^i}\, \psi^i \right\rangle - \psi^i \right) \psi^i \, d\boldsymbol{z}\, d\xi = 0.$$

Since c^i are positive constants that only depend on s, and the integrals with respect to $\boldsymbol{p}$ are definite in sign (see (A.14)), this implies that

$$\int_{\mathbb{R}^2} \left(\sqrt{L^i_s} \left\langle \sqrt{L^i_s}\, \psi^i_s \right\rangle - \psi^i_s \right) \psi^i_s \, d\boldsymbol{p} = 0$$

for all $\xi \in (-1)^i[0,+\infty)$. This equality can only hold when $\psi^i(\xi,\cdot)$ is in the kernel of the collision operator, which implies that $\theta^i(\xi,\boldsymbol{p})$ is necessarily of the form

$$\theta^i(\xi,\boldsymbol{z}) = \theta^i_s(\xi,\boldsymbol{p}) = L^i_s(\boldsymbol{p}) \gamma^i_s(\xi).$$

Finally, the substitution of this expression in the first of equations (A.12) immediately yields that γ^i_s is constant, so that

$$\theta^i_s(\xi,\boldsymbol{p}) = L^i_s(\boldsymbol{p}) \gamma^i_s. \tag{A.20}$$

Substituting (A.20) in the second of equations (A.12) and using (A.10) leads to the following necessary and sufficient condition for (A.20) to be solution of the homogeneous Milne problem (A.12):

$$c^j_{s'}\gamma^i_s = c^i_s\gamma^j_{s'} \tag{A.21}$$

where c^i_s is defined by (A.11), and i, j and s, s' are related as usual. Recalling that the conservation of energy is satisfied by three couples (s, s') if $\delta V \neq 0$ and just by two couples in the case if $\delta V = 0$ (see Remark 3.4), we notice that (A.21) is a rank-3 condition if $\delta V \neq 0$ and a rank-2 condition if $\delta V = 0$.

Step 4: the inhomogeneous problem. Let us finally return to the complete, inhomogeneous problem (A.2). Let (θ^1, θ^2) be a bounded solution of (A.2). The integration in $\boldsymbol{p}$ of the first equation in (A.2) yields

$$\frac{d}{d\xi}\langle\mu\theta^i_s\rangle = 0,$$

and the integration in $\boldsymbol{p}$ after multiplication by μ yields

$$\frac{d}{d\xi}\langle\mu^2\theta^i_s\rangle = -\langle\mu\theta^i_s\rangle.$$

Hence, $\langle\mu\theta^i_s\rangle$ is a constant, and this constant must be zero, otherwise $|\langle\mu^2\theta^i_s\rangle|$ would grow linearly with ξ, in contradiction with the boundedness assumption. So we have

$$\int_{\mathbb{R}^2}\theta^i_s(\xi,\boldsymbol{p})\,\mu(\boldsymbol{p})\,d\boldsymbol{p} = 0, \tag{A.22}$$

for all $\xi \in (-1)^i[0, +\infty)$, $i = 1, 2$ and $s = \pm 1$. If we now rewrite the boundary conditions as

$$\theta^i_{\text{in}} - G^i_{\text{in}} - \mathcal{K}^i\big(\theta^i_{\text{out}} - G^i_{\text{out}}, \theta^j_{\text{out}} - G^j_{\text{out}}\big) = 0,$$

then, from Proposition 3.2 (that applies also to the linear KTC), we have that the conservation of charge flux holds:

$$\int_\Theta s(\theta^1(0,\boldsymbol{z}) - G^1(\boldsymbol{z}))\mu(z)\,d\boldsymbol{z} = \int_\Theta s(\theta^2(0,\boldsymbol{z}) - G^2(\boldsymbol{z}))\mu(\boldsymbol{z})\,d\boldsymbol{z}.$$

But then, since (A.22) implies that the charge flux associated to θ^i vanishes, we obtain that the flux conservation for G^i must hold:

$$\int_\Theta s\,G^1(\boldsymbol{z})\mu(\boldsymbol{z})\,d\boldsymbol{z} = \int_\Theta s\,G^2(\boldsymbol{z})\mu(\boldsymbol{z})\,d\boldsymbol{z}. \tag{A.23}$$

Equation (A.23) is therefore a necessary condition for the existence of a bounded solution to the Milne problem (A.2) or, equivalently, to the Fredholm problem (A.8) when Γ^i has the form (A.9). Using (4.14), it is immediate to verify that the G^i's, given by (4.18), satisfy this condition if and only if (4.30) holds.

Now, from Step 3 we know that the kernel of the Fredholm operator at the left-hand side of (A.8) is spanned by the functions of the form $L^i_s(\boldsymbol{p})\gamma^i_s$, with γ^i_s satisfying (A.21), and is therefore a subspace of $X^1_{\text{in}}, \times X^2_{\text{in}}$ of dimension d, where $d = 1$ if $\delta V \neq 0$, and $d = 2$ if $\delta V = 0$.

Hence, the range of the Fredholm operator is a closed subspace of codimension d. But (A.23) also defines a subspace of codimension d, and then it describes the condition of existence of the solution to the Fredholm equation when Γ^i is of the form (A.9). We conclude that (4.30) is a necessary and sufficient condition for the existence of a solution to the Fredholm equation (A.8) (and, therefore, of the Milne problem (A.2)), up to a solution of the associated homogeneous problem. This proves the first part of Theorem 4.4.

The second part of the theorem, that is the existence of the asymptotic densities $n_s^{i,\infty}$ and the exponential estimate (4.32), follows from (ii) of Step 2. In fact, once the coupled Milne problem is solved, the inflow of each component θ_s^i is determined (up to the addition of a term of the form (A.20)–(A.21)), and point (ii) of Step 2 applies.[8]

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