Adiabatic quantum-fluid transport models

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Abstract

Coupled quantum-fluid models are derived by means of a diffusion approximation from adiabatic quantum-kinetic models. These models describe the electron transport of a bidimensional electron gas. Particles are confined in one direction (denoted by z) while transport occurs in an orthogonal direction (denoted by x). The length-scale in the z direction is comparable to the de Broglie wavelength, while the x-length scale is much bigger. The aim of this paper is to investigate the diffusion limit from quantum-kinetic to quantum-fluid models, which are numerically more interesting. Transitions between sub-bands are considered in the Fermi Golden rule setting.

Keywords : Schrödinger equation; Boltzmann equation; Subband model; Collision operator; Diffusion limit; Spherical Harmonic Expansion model; Energy-Transport model.

1 Introduction

Directionally coupled quantum/classical models are suited for the description of the electron transport in devices in which the electron gas is confined in one direction and the transport is allowed in the remaining directions. This situation arises for example in MOSFET transistors, nanotubes, nanowires, etc. In such devices the length-scale of the confinement direction is of the order of the electron de Broglie wavelength, such that quantum transport models have to be adopted in this direction. The length-scale in the transport direction is several times bigger than the de Broglie wavelength, allowing thus the use of classical models for the electron transport description.

Such type of subband models are subject of recent work. In [6] a quantum/kinetic subband model is derived by a partially semi-classical limit from a fully quantum model. The study of the limit model is then presented in [5, 7], analyzing the existence of weak or classical solutions for the Schrödinger-Vlasov system, coupled with the Poisson equation. The starting model of the present paper is a similar quantum/kinetic model, which describes the electron evolution in the confinement direction by the Schrödinger equation, whereas the transport direction is governed by the Boltzmann equation.

Quantum kinetic models are computationally rather expensive. In this aim the derivation of quantum fluid adiabatic models has an important significance for the semiconductor device simulation. A coupled Schrödinger/Drift-Diffusion system is investigated in [8]. The purpose of this paper is to derive coupled quantum mesoscopic models, which are computationally less expensive than the Schrödinger/Boltzmann system and provide a physically more accurate description of the electron transport than the Schrödinger/Drift-Diffusion system.

Depending on the particular choice of the dominant collision mechanism, we show that the Schrödinger/Boltzmann system tends in the diffusion limit either towards a coupled Schrödinger/SHE model (Spherical Harmonic Expansion) or towards a coupled Schrödinger/ET model (Energy-Transport). Considering firstly an elastic impurity collision operator, which accounts also for the transitions between the subbands, a diffusion limit $\alpha \to 0$ is carried out formally and rigorously. The parameter α represents the ratio of the mean free path (between collisions) to the typical macroscopic device size. The limit model is shown to be a coupled system constituted of the Schrödinger equation in the confinement direction and the SHE model in the transport one, the latter being a diffusion equation for the energy-dependent distribution function. In a second part, we assume that the dominant scattering operator consists of the sum of the elastic operator and the electron-electron collision operator. In a formal asymptotic approach, the corresponding Schrödinger/Boltzmann system is shown to relax towards a coupled Schrödinger/ET system. The resulting ET model in the transport direction is constituted of a balance law for the electron density and an energy balance equation.

In the pure classical framework, the derivation of fluid models from kinetic ones has been amply investigated, using moment methods or Hilbert expansions. An overview of these transport models can be found in [2, 10, 17, 19] as well as in the following non-exhaustive list of references for the derivation of the SHE model [11, 14], ET model [3, 4, 13, 20] and DD model [20, 22, 24, 25, 27]. The models derived in the present paper differ from their classical counterparts in that the energy subbands depend on the time and the position variables. Moreover the involvement of these energy subbands in the coefficients of the fluid models, reflects the coupling with the quantum model in the confinement direction.

The subband models introduced and derived in this paper are based on the fact that quantum effects and collision mechanisms occur separately in different directions, due to the geometry of the device. When such an assumption cannot be adopted, our approach is not relevant and one has to follow a different route. In [9], several SHE models incorporating quantum effects (in both longitudinal and transversal directions) are proposed. Let us briefly summarize this approach in order to put our paper into perspective. In a first step, a quantum SHE model is derived as the diffusive limit of a Wigner-Boltzmann system. The disadvantage of this approach is the fact that collisions are modeled in a classical setting, which means that the collision operator is local in the position variable and does not mix position and momentum. Then, in a second step, a fully quantum SHE model is proposed, whose derivation is based on the concept of the "local quantum equilibrium", introduced in [18], and using an entropy minimization procedure. The idea consists in replacing the classical elastic Boltzmann operator by a relaxation operator whose kernel consists of these quantum equilibrium states (this approach was previously used in [15] in order to get quantum Drift-Diffusion and quantum Energy-Transport systems; see also [16, 21]). Unfortunately the so-obtained model presents a complicated non local structure – it is not a partial differential system – and its numerical implementation is not an easy task. Consequently, it seems reasonable to define firstly an approximate model which would be local in space : such a procedure is proposed in [9] in the semi-classical scaling ($\mathcal{O}(\hbar^4)$-approximations are also proposed for the QDD, QET and QHD models in [15] as well as in [23], $\hbar$ being the reduced Planck constant). The present article proposes a complementary strategy: the collisional Wigner equation is *firstly* (formally) approximated via a semi-classical limit in the longitudinal directions (the confined direction remaining quantized), leading thus to our collisional subband model. *Then* the diffusive approximation is performed to obtain a SHE model (or an ET model).

This paper is organized as follows. Section 2 is devoted to the diffusion limit towards the adiabatic Schrödinger/SHE model. Firstly the properties of the elastic collision operator are studied and a formal diffusive limit is performed, based on a Hilbert expansion. The formal result is given in Theorem 2.7. Then a mathematical rigorous proof is carried out in Section 2.4, the principal rigorous result being presented in Theorem 2.11. Section 3 deals with the formal diffusion limit towards the adiabatic Schrödinger/ET model. This formal result is stated in Theorem 3.6.
The rigorous derivation of the Schrödinger/ET model is beyond the aim of this paper, due to the complexity of the problem, and is deferred to an ulterior work. In the classical case, the rigorous limit from the Boltzmann equation towards the ET model was carried out in [4].

2 The diffusion limit towards the SHE model

2.1 The diffusion scaling

Let us consider an electron ensemble in the slab $\mathbb{R}^2 \times (0,1)$ of $\mathbb{R}^3$. The first two directions, called x, correspond to the classical degrees of freedom of the electrons, whereas in the third direction z, quantum effects take place. For a given electrostatic potential, the electron ensemble can be described by a sequence (f_n) of distribution functions (for the classical directions $x \in \mathbb{R}^2$ and the corresponding velocities $v \in \mathbb{R}^2$) and a sequence (χ_n) of wave functions (for the quantum direction z). The electron density is written then as

$$n(t,x,z) = \sum_{n \geq 1} \left(\int_{\mathbb{R}^2} f_n(t,x,v)\, dv \right) |\chi_n(t,x,z)|^2 \ .$$

In dimensionless variables, the problem consists in finding for $t \in (0,T)$, $x \in \mathbb{R}^2$, $z \in (0,1)$ and $v \in \mathbb{R}^2$ the unknowns $(\epsilon_n(t,x), \chi_n(t,x,z), f_n(t,x,v))_{n\in\mathbb{N}^*}$, where the potential $V(t,x,z)$ is assumed to be given. The wave functions χ_n depend parametrically on t and x, and form a complete sequence of eigenfunctions of the one dimensional Schrödinger operator $-\frac{1}{2}\, d^2/dz^2 + V$. More precisely, χ_n are solutions of the eigenvalue problem

$$\begin{cases} -\dfrac{1}{2}\,\partial_{zz}\chi_n + V\chi_n = \epsilon_n\chi_n\,, \\ \chi_n(t,x,\cdot) \in H_0^1(0,1), \qquad \displaystyle\int_0^1 \chi_n\,\chi_m\,dz = \delta_{nm}\,, \end{cases} \tag{2.1}$$

where ϵ_n are the corresponding eigenvalues. It is known that the eigenvalues are simple and that they form an increasing sequence tending to $+\infty$ $(\epsilon_1 < \epsilon_2 < \cdots)$ [5, 26]. These functions represent the potential energy of the different electron subbands in the confined z-direction and the index n stands for the n-th subband.

The distribution function f_n of the subband n is solution of the rescaled Boltzmann equation

$$\begin{cases} \partial_t f_n + \dfrac{1}{\alpha}\,(v\cdot\nabla_x f_n - \nabla_x\epsilon_n\cdot\nabla_v f_n) = \dfrac{1}{\alpha^2}Q(f)_n \\ f_n(0,x,v) = f_{in,n}(x,v)\,, \end{cases} \tag{2.2}$$

where the operator Q accounts for collisions in the subband n, as well as for transitions between the subbands. We shall denote by f the collection of all the subband distribution functions, $f = (f_n)_{n\in\mathbb{N}^*}$. The collision operator Q is taken under the following form

$$Q(f)_n := \sum_{m\in\mathbb{N}^*}\int_{\mathbb{R}^2} \left[\sigma(t,x;m,v'\to n,v)f_m(t,x,v') - \sigma(t,x;n,v\to m,v')f_n(t,x,v)\right]\,dv'\,. \tag{2.3}$$

The first term on the right hand side is the gain term, describing the particles "jumping" from the subband m with a longitudinal velocity v', towards the subband n and possessing there the longitudinal velocity v. The second term is the usual loss term. The transition rates $\sigma(t,x;m,v'\to n,v)$ are computed in the Fermi Golden rule approximation and depend on the nature of the considered collisions.

In the first part of this paper, impurity collisions are considered, such that the transition rates take the following form

$$\sigma(t,x;m,v'\to n,v) = \alpha_{mn}(t,x,v',v)\delta(\epsilon_n(t,x) + \frac{|v|^2}{2} - \epsilon_m(t,x) - \frac{|v'|^2}{2})\,,$$

where α_{mn} are the so-called scattering cross sections. The elastic impurity collision operator Q_0 reads then

$$Q_0(f)_n = \sum_{m\in\mathbb{N}^*}\int_{\mathbb{R}^2} \alpha_{nm}(t,x,v,v')\delta(\epsilon_n + \frac{|v|^2}{2} - \epsilon_m - \frac{|v'|^2}{2})\,[f_m(t,x,v') - f_n(t,x,v)]\,dv'\,, \tag{2.4}$$

and we shall assume in the sequel the fundamental hypothesis:

Hypothesis 1 The coefficients α_{nm} satisfy the following positivity, boundedness and symmetry properties, with λ_0 and λ_1 two positive constants

$$0 < \lambda_0 < \alpha_{nm} N(t, x, \epsilon_n + \frac{|v|^2}{2}) < \lambda_1 < +\infty \quad , \quad \alpha_{nm}(t, x, v, v') = \alpha_{mn}(t, x, v', v),$$

where the weight function N, the density of states, which is introduced in Definition 2.3.

Generally, the potential is not a priori known, but is computed self-consistently by means of the charge density. Denoting by V_{ext} the exterior potential and by V_s the self-consistent one, then $V = V_{ext} + V_s$, where V_s is solution of the Poisson equation

$$-\Delta V_s(t, x, z) = n(t, x, z) \, ,$$

subject to appropriate boundary conditions. In order to keep this paper as simple as possible, we consider the potential as given. The extension to the self-consistent case changes nothing to the formal analysis.

2.2 Properties of the collision operator Q_0

In this section, we study the elastic collision operator Q_0. In particular, we determine its kernel, prove that it is a Fredholm operator and show that it is dissipative. We begin by recalling the coarea formula.

Lemma 2.1 (Coarea formula) *Let $d \in \mathbb{N}$, $\mathcal{B} \subset \mathbb{R}^d$, $\mathcal{R} \subset \mathbb{R}$. Then for every function $f \in C(\mathbb{R}^d)$ and $g \in C^1(\mathcal{B}, \mathcal{R})$ we have*

$$\int_{\mathcal{B}} f(v) dv = \int_{\mathcal{R}} \left(\int_{S_\varepsilon} f(v) dN_\varepsilon(v) \right) d\varepsilon \, ,$$

where $S_\varepsilon := \{v \in \mathcal{B} \; ; \; g(v) = \varepsilon\}$ is the surface of constant energy ε, and

$$dN_\varepsilon(v) := \frac{d\sigma_\varepsilon(v)}{|\nabla g(v)|} \, ,$$

is the coarea measure, with $d\sigma_\varepsilon(v)$ being the surface measure on the sphere S_ε.

Remark 2.2 *In this paper, we shall consider the parabolic band approximation and take thus $g(v) := \frac{|v|^2}{2}$, leading to $dN_\varepsilon(v) = \frac{d\sigma_\varepsilon(v)}{|v|}$. Moreover the surface*

$$S_{\varepsilon - \epsilon_n}(t, x) = \left\{ v \in \mathbb{R}^2 \; / \; \frac{|v|^2}{2} + \epsilon_n(t, x) = \varepsilon \right\} ,$$

represents the ensemble of possible velocities of electrons belonging to the n-th subband and having the total energy ε.

Let us now introduce some notations.

Definition 2.3 *The following definitions are used all along the paper:*

- *We define the function* $\mathcal{N}(t,x,\varepsilon) := \max\{n \in \mathbb{N}^* \ / \ \epsilon_n(t,x) \leq \varepsilon\}$ *with the convention* $\mathcal{N}(t,x,\varepsilon) = 0$ *if* $\varepsilon < \epsilon_1(t,x)$*. This represents the number of subbands lying beneath the energy value* ε *at* (t,x)*. The density of states is thus defined as*

$$N(t,x,\varepsilon) := \sum_{n\in\mathbb{N}^*} \int_{S_{\varepsilon-\epsilon_n}} dN_{\varepsilon-\epsilon_n}(v) = 2\pi\mathcal{N}(t,x,\varepsilon)\,. \tag{2.5}$$

  Remark that in the 2D case we have

$$\int_{S_{\varepsilon-\epsilon_n}} dN_{\varepsilon-\epsilon_n}(v) = 2\pi\mathcal{H}(\varepsilon-\epsilon_n)\,,$$

  with $\mathcal{H}$ *the Heaviside function.*

- *We introduce the Hilbert space*

$$\mathbb{L}^2 := \{f = (f_n)_{n\in\mathbb{N}^*}, \quad \sum_{n=1}^{+\infty} \int_{\mathbb{R}^2} |f_n(v)|^2\, dv < +\infty\}\,,$$

  with the $\mathbb{L}^2$ *scalar product defined by*

$$\langle f, g\rangle := \sum_{n\in\mathbb{N}^*} \int_{\mathbb{R}^2} f_n g_n\, dv\,.$$

- *Let* H *denote a Lipschitz continuous function on* $\mathbb{R}$ *with* $H(0) = 0$*. Then, for all* $f \in \mathbb{L}^2$*,* $H(f)$ *defined by* $[H(f)]_n = H(f_n)$ *is an element of* $\mathbb{L}^2$*.*

- *The total energy of an electron, belonging to the* n*-th subband and having the velocity* v*, is shortly denoted by*

$$\mathbf{e}_n(t,x,v) := \epsilon_n(t,x) + \frac{|v|^2}{2}\,.$$

With the notations introduced above, we have for some function ψ

$$\sum_n \int_{\mathbb{R}^2} \psi_n(v)\, dv = \sum_n \int_{\epsilon_n}^{+\infty} \left(\int_{S_{\varepsilon-\epsilon_n}} \psi_n(v) dN_{\varepsilon-\epsilon_n}(v) \right) d\varepsilon\,,$$

$$\sum_n \int_{\mathbb{R}^2} \psi_n(v)\delta(\epsilon_n + \frac{v^2}{2} - \varepsilon)\, dv = \sum_n \int_{S_{\varepsilon-\epsilon_n}} \psi_n(v) dN_{\varepsilon-\epsilon_n}(v)\,.$$

We can pass now to the study of the elastic collision operator Q_0. The variables t and x are considered in the following of this section as parameters and are thus omitted for simplicity.

Proposition 2.4 *Under Hypothesis 1, the operator Q_0 satisfies the following properties :*
(i) The linear operator $Q_0 : \mathbb{L}^2 \to \mathbb{L}^2$ is a bounded, symmetric, non-positive operator.
(ii) For any increasing Lipschitz continuous function H with $H(0) = 0$, we have the dissipative inequality

$$\langle Q_0(f), H(f) \rangle \leq 0 , \quad \forall f \in \mathbb{L}^2. \tag{2.6}$$

(iii) For any bounded function $\psi : \mathbb{R} \to \mathbb{R}$ we denote by $\psi(\mathbf{e})$ the sequence $(\psi(\mathbf{e}))_n(v) = \psi(\frac{|v|^2}{2} + \epsilon_n)$. Defining $\psi(\mathbf{e})f$ by $(\psi(\mathbf{e})f)_n(v) = \psi(\frac{|v|^2}{2} + \epsilon_n) f_n(v)$, we have

$$Q_0(\psi(\mathbf{e})f) = \psi(\mathbf{e}) Q_0(f) \quad \forall f \in \mathbb{L}^2 .$$

(iv)The Kernel of Q_0 is the set

$$\mathcal{A} := \{ f \in \mathbb{L}^2 \quad / \quad \exists \psi : \mathbb{R} \to \mathbb{R} \ \textit{with} \ f = \psi(\mathbf{e}) \} ,$$

and $f \in \mathcal{A}$ if and only if $\langle Q_0(f), H(f) \rangle = 0$ for some strictly increasing Lipschitz continuous function H. In particular, the collision operator Q_0 conserves the mass and the total energy.

Proof Let us first prove (i). Like in the scalar case, the symmetry of the operator Q_0 is a direct consequence of the symmetry of the cross sections α_{nm}, while the negativity is a consequence of the positivity of these cross sections. Namely, it is immediately seen that

$$\langle Q_0 f, g \rangle = -\frac{1}{2} \sum_{m,n=1}^{+\infty} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \alpha_{m,n}(v', v) \delta(\epsilon_m + |v'|^2/2 - \epsilon_n - |v|^2/2)(f'_m - f_n)(g'_m - g_n) \, dv' \, dv , \tag{2.7}$$

where we have dropped the (t, x) dependence for notational simplicity and where we have used the usual notation $f'_m = f_m(v')$, $f_n = f_n(v)$. The right-hand side being invariant when the roles of f and g are exchanged, the operator Q_0 is symmetric. The negativity of Q_0 is also immediate as well as item (ii). Let us now prove that Q_0 is bounded on $\mathbb{L}^2$. To this aim, it is enough to prove that

$$|\langle Q_0 f, g \rangle| \leq C \|f\| \, \|g\| \quad \forall f, g \in \mathbb{L}^2 .$$

From (2.7), a simple Cauchy-Schwarz inequality leads to

$$|\langle Q_0 f, g \rangle| \leq A(f) A(g) ,$$

where

$$
\begin{aligned}
A(h)^2 &= \frac{1}{2}\lambda_1 \sum_{m,n} \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \frac{1}{N(\epsilon_n + \frac{|v|^2}{2})} \delta(\epsilon_m + \frac{|v'|^2}{2} - \epsilon_n - \frac{|v|^2}{2})(h'_m - h_n)^2 dv\, dv' \\
&\le \lambda_1 \sum_{m,n} \int\int \frac{1}{N(\epsilon_n + \frac{|v|^2}{2})} \delta(\mathbf{e}'_m - \mathbf{e}_n)((h'_m)^2 + h_n^2) dv\, dv' \\
&= 2\lambda_1 \sum_{m,n} \int\int \frac{1}{N(\epsilon_n + \frac{|v|^2}{2})} \delta(\mathbf{e}'_m - \mathbf{e}_n) h_n^2 dv\, dv' \\
&= 2\lambda_1 \sum_n \int_{\epsilon_1}^{\infty} \int_{S_{\varepsilon-\epsilon_n}} \left(\sum_m \int_{S_{\varepsilon-\epsilon_m}} dN_{\varepsilon-\epsilon_m}(v') \right) \frac{1}{N(\varepsilon)} h_n^2(v) dN_{\varepsilon-\epsilon_n}(v) d\varepsilon \\
&= 2\lambda_1 \sum_n \int_{\epsilon_1}^{\infty} \int_{S_{\varepsilon-\epsilon_n}} h_n^2(v) dN_{\varepsilon-\epsilon_n}(v) d\varepsilon = 2\lambda_1 \|h\|^2,
\end{aligned}
$$

which finishes the proof of item (i). Besides, item (iii) is immediate. Let us now prove item (iv). It is clear that $\mathcal{A}$ is a subset of $\ker(Q_0)$. Let now H be strictly increasing and such that $\langle Q_0(f), H(f)\rangle = 0$. From (2.7), we deduce that $f_m(v') = f_n(v)$ whenever $\epsilon_m + \frac{|v'|^2}{2} = \epsilon_n + \frac{|v|^2}{2}$. This is satisfied if and only if f is a function of the energy, $f = \psi(\mathbf{e})$. □

Let us now prove that $-Q_0$ is coercive on the orthogonal to its kernel.

Proposition 2.5 *The operator Q_0 satisfies the following properties:*
(i) The orthogonal to the kernel of Q_0 is given by

$$
\ker(Q_0)^\perp := \{f \in \mathbb{L}^2, \quad \textit{such that} \quad \sum_n \int_{S_{\varepsilon-\epsilon_n}} f_n(v) dN_{\varepsilon-\epsilon_n}(v) = 0 \quad \textit{for a.a.} \quad \varepsilon \ge \epsilon_1\}.
$$

(ii) There exists a constant $C > 0$, such that

$$
-\langle Q_0(f), f\rangle \ge C\|f\|^2, \quad \forall\ f \in \ker(Q_0)^\perp. \tag{2.8}
$$

(iii) The range $R(Q_0)$ is closed and coincides with $\ker(Q_0)^\perp$.

Proof Item (i) is immediate and item (iii) is a direct consequence of item (ii). It remains to show (ii). The starting point is

$$
\begin{aligned}
-\langle Q_0(f), f\rangle &= \frac{1}{2} \sum_{m,n=1}^{+\infty} \int_{\mathbb{R}^2\times\mathbb{R}^2} \alpha_{m,n}(v', v) \delta(\epsilon_m + \frac{|v'|^2}{2} - \epsilon_n - \frac{|v|^2}{2})(f'_m - f_n)^2\, dv'\, dv \\
&\ge \frac{1}{2}\lambda_0 \sum_{m,n=1}^{+\infty} \int_{\mathbb{R}^2\times\mathbb{R}^2} \frac{1}{N(\epsilon_n + \frac{|v|^2}{2})} \delta(\mathbf{e}'_m - \mathbf{e}_n)(f'^2_m - 2f_n f'_m + f_n^2)\, dv'\, dv\,.
\end{aligned}
$$

Using the fact, that $f \in \ker(Q_0)^\perp$, we have

$$
\sum_{m,n=1}^{+\infty} \int_{\mathbb{R}^2\times\mathbb{R}^2} \frac{1}{N(\mathbf{e}_n)} \delta(\mathbf{e}'_m - \mathbf{e}_n) f_n f'_m\, dv'\, dv = 0\,,
$$

implying

$$
\begin{aligned}
-\langle Q_0(f), f\rangle &\geq \frac{1}{2}\lambda_0 \sum_{m,n=1}^{+\infty} \int_{\mathbb{R}^2\times\mathbb{R}^2} \frac{1}{N(\mathbf{e}_n)}\delta(\mathbf{e}'_m - \mathbf{e}_n)(f'^2_m + f^2_n)\, dv'\, dv \\
&= \lambda_0 \sum_{m,n=1}^{+\infty} \int_{\mathbb{R}^2\times\mathbb{R}^2} \frac{1}{N(\mathbf{e}_n)}\delta(\mathbf{e}'_m - \mathbf{e}_n) f^2_n\, dv'\, dv \\
&= \lambda_0 \sum_{n=1}^{+\infty} \int_{\epsilon_1}^{\infty} \int_{S_{\varepsilon-\epsilon_n}} |f_n(v)|^2 dN_{\varepsilon-\epsilon_n}(v) d\varepsilon = \lambda_0 \|f\|^2 .
\end{aligned}
$$

□

Remark 2.6 *Defining by*

$$
\mathcal{P} : \mathbb{L}^2 \to \ker(Q_0) \qquad ; \qquad \mathcal{P}^\perp : \mathbb{L}^2 \to \quad \ker(Q_0)^\perp ,
$$

the projections on the kernel respectively on the orthogonal of the kernel of Q_0, such that $\mathcal{P}^\perp(f) = (Id - \mathcal{P})(f)$, we can express the coercivity inequality (2.8) as

$$
-\langle Q_0(f), f\rangle \geq C\|f - \mathcal{P}f\|^2, \quad \forall\ f \in \mathbb{L}^2 . \tag{2.9}
$$

2.3 The diffusion limit $\alpha \to 0$: formal approach

We investigate in this section the formal limit $\alpha \to 0$ in order to derive from the above model a quantum-fluid subband model, corresponding to the chosen elastic collision operator Q_0. The limit model will be quantum in the confined z-direction, and in the transport direction x we shall get the SHE model. This diffusion approximation is based upon the Hilbert expansion

$$
f^\alpha = f^0 + \alpha f^1 + \alpha^2 f^2 + \cdots \tag{2.10}
$$

Inserting this expansion in (2.2) and identifying equal powers of α, leads to the equations

$$
Q_0(f^0)_n = 0, \tag{2.11}
$$

$$
Q_0(f^1)_n = v\cdot\nabla_x f^0_n - \nabla_x\epsilon_n\cdot\nabla_v f^0_n, \tag{2.12}
$$

$$
Q_0(f^2)_n = \partial_t f^0_n + v\cdot\nabla_x f^1_n - \nabla_x\epsilon_n\cdot\nabla_v f^1_n. \tag{2.13}
$$

The first equation and Proposition 2.4 imply the existence of an energy dependent function $F(t,x,\varepsilon)$, such that

$$
f^0_n(t,x,v) = F(t,x,\frac{|v|^2}{2} + \epsilon_n) . \tag{2.14}
$$

The second equation can then be rewritten as

$$Q_0(f^1)_n(t,x,v) = v \cdot (\nabla_x F)(t,x,\frac{|v|^2}{2} + \epsilon_n)\,.$$

Denoting

$$G(t,x,\varepsilon) := \nabla_x F(t,x,\varepsilon)\,,$$

we have

$$Q_0(f^1) = v\psi(\mathbf{e}) \cdot \frac{G}{\psi}(\mathbf{e})\,,$$

where $\psi : \mathbb{R} \to \mathbb{R}$ is a function, such that $v\psi(\mathbf{e}) \in \mathbb{L}^2$. It is then readily seen that $v\psi(\mathbf{e}) \in \ker(Q_0)^\perp$, so that the equation

$$-Q_0(h) = v\psi(\mathbf{e})\,,$$

admits a unique solution in $\ker(Q_0)^\perp$, that we write $h = \vartheta\psi(\mathbf{e})$. Therefore, the only solution $f^1 \in \ker(Q_0)^\perp$ of (2.12) is defined by

$$f^1 = -\vartheta \cdot G(\mathbf{e}). \tag{2.15}$$

This last equation has to be understood as follows

$$f^1_n(t,x,v) = -\vartheta_n(t,x,v) \cdot G(t,x,\epsilon_n + \frac{|v|^2}{2})\,,$$

where ϑ_n is a vector-valued function in $\mathbb{R}^2$ (as well as $G(\cdot) \in \mathbb{R}^2$). Remark that ϑ is independent from the choice of the function ψ.
Now in order to assure the solvability of equation (2.13), it is necessary and sufficient that the right-hand side belongs to $\ker(Q_0)^\perp$. This leads to the solvability condition

$$\sum_n \int_{S_{\varepsilon-\epsilon_n}} (\partial_t f^0_n + v \cdot \nabla_x f^1_n - \nabla_x \epsilon_n \cdot \nabla_v f^1_n)\, dN_{\varepsilon-\epsilon_n}(v) = 0\,, \quad \text{for a.a.} \quad \varepsilon \geq \epsilon_1\,.$$

Multiplication with an arbitrary energy-dependent test function $\varphi \in C_0(\mathbb{R})$ and integration with respect to the energy variable ε, yields

$$\int_{\epsilon_1}^\infty \sum_n \int_{S_{\varepsilon-\epsilon_n}} (\partial_t f^0_n + v \cdot \nabla_x f^1_n - \nabla_x \epsilon_n \cdot \nabla_v f^1_n)\, dN_{\varepsilon-\epsilon_n}(v)\, \varphi(\varepsilon)\, d\varepsilon = 0\,. \tag{2.16}$$

The first term gives

$$\begin{aligned}\int_{\epsilon_1}^\infty \sum_n \int_{S_{\varepsilon-\epsilon_n}} \partial_t f^0_n\, dN_{\varepsilon-\epsilon_n}(v)\, \varphi(\varepsilon)\, d\varepsilon &= \int_{\epsilon_1}^\infty \sum_n \int_{S_{\varepsilon-\epsilon_n}} (\partial_t F + \partial_\varepsilon F \partial_t \epsilon_n)\, dN_{\varepsilon-\epsilon_n}(v)\, \varphi(\varepsilon)\, d\varepsilon \\ &= \int_{\epsilon_1}^\infty \partial_t F\ N\ \varphi(\varepsilon)\, d\varepsilon + \int_{\epsilon_1}^\infty \partial_\epsilon F \left(\sum_n \partial_t \epsilon_n \int_{S_{\varepsilon-\epsilon_n}} dN_{\varepsilon-\epsilon_n}(v) \right) \varphi(\varepsilon)\, d\varepsilon\,.\end{aligned}$$

Using (2.15) we can deduce furthermore

$$\int_{\epsilon_1}^{\infty} \sum_n \int_{S_{\varepsilon-\epsilon_n}} v \cdot \nabla_x f_n^1 \; dN_{\varepsilon-\epsilon_n}(v) \; \varphi(\varepsilon) \; d\varepsilon = \sum_n \int_{\mathbb{R}^2} \nabla_x \cdot (v \; f_n^1) \; \varphi(\mathbf{e}_n) \; dv =$$
$$= \nabla_x \cdot \left[\sum_n \int_{\mathbb{R}^2} v \; f_n^1 \; \varphi(\mathbf{e}_n) \; dv \right] - \sum_n \int_{\mathbb{R}^2} f_n^1 \; v \cdot \nabla_x \epsilon_n \; \varphi'(\mathbf{e}_n) \; dv$$
$$= - \int_{\epsilon_1}^{\infty} \nabla_x \cdot \left[\sum_n \int_{S_{\varepsilon-\epsilon_n}} v \otimes \vartheta_n \; dN_{\varepsilon-\epsilon_n}(v) \cdot \nabla_x F \right] \; \varphi(\varepsilon) \; d\varepsilon - \sum_n \int_{\mathbb{R}^2} f_n^1 \; v \cdot \nabla_x \epsilon_n \; \varphi'(\mathbf{e}_n) dv \,,$$

and for the last term of (2.16)

$$- \int_{\epsilon_1}^{\infty} \sum_n \int_{S_{\varepsilon-\epsilon_n}} \nabla_x \epsilon_n \cdot \nabla_v f_n^1 \; dN_{\varepsilon-\epsilon_n}(v) \; \varphi(\varepsilon) \; d\varepsilon = - \sum_n \int_{\mathbb{R}^2} \nabla_v \cdot (f_n^1 \; \nabla_x \epsilon_n) \; \varphi(\mathbf{e}_n) \; dv =$$
$$= \sum_n \int_{\mathbb{R}^2} f_n^1 \; \nabla_x \epsilon_n \cdot v \; \varphi'(\mathbf{e}_n) \; dv \,.$$

Concluding, the solvability condition for equation (2.13) reads for all test functions $\varphi \in C_0(\mathbb{R})$

$$\int_{\epsilon_1}^{\infty} \partial_t F \; N \; \varphi \; d\varepsilon + \int_{\epsilon_1}^{\infty} \partial_\varepsilon F \; \kappa \; \varphi \; d\varepsilon + \int_{\epsilon_1}^{\infty} \nabla_x \cdot J \; \varphi \; d\varepsilon = 0 \,,$$

where we used the notations

$$J(t,x,\varepsilon) \;\; := \;\; \sum_n \int_{S_{\varepsilon-\epsilon_n}} v f_n^1 \; dN_{\varepsilon-\epsilon_n}(v) = - \sum_n \int_{S_{\varepsilon-\epsilon_n}} (v \otimes \vartheta_n) dN_{\varepsilon-\epsilon_n}(v) \cdot \nabla_x F \,, \tag{2.17}$$

with

$$D(t,x,\varepsilon) := \sum_n \int_{S_{\varepsilon-\epsilon_n}} v \otimes \vartheta_n \; dN_{\varepsilon-\epsilon_n}(v) \,, \tag{2.18}$$

the so-called diffusion matrix. Moreover we denoted

$$\kappa(t,x,\varepsilon) := \sum_n \partial_t \epsilon_n \int_{S_{\varepsilon-\epsilon_n}} dN_{\varepsilon-\epsilon_n}(v) = -2\pi \partial_t \left(\sum_n (\varepsilon - \epsilon_n)^+ \right) \,. \tag{2.19}$$

Recalling the definition of the density of states

$$N(t,x,\varepsilon) = \sum_{n \in \mathbb{N}^*} \int_{S_{\varepsilon-\epsilon_n}} dN_{\varepsilon-\epsilon_n}(v) \,, \tag{2.20}$$

we observe that we have in a distributional sense the relation

$$\partial_t N(t,x,\varepsilon) = -\partial_\varepsilon \kappa(t,x,\varepsilon) \,.$$

Thus we deduce the following important theorem

Theorem 2.7 (Formal diffusion limit)
The system of equations (2.11)-(2.13), deduced from the Hilbert expansion (2.10), is solvable if and only if f^0 and f^1 are determined by (2.14), (2.15), and the distribution function $F(t,x,\varepsilon)$ satisfies the following diffusion equation in the position-energy space

$$N\partial_t F + \nabla_x \cdot J + \kappa\, \partial_\varepsilon F = 0\,, \tag{2.21}$$

where the current density is given by

$$J(t,x,\varepsilon) = -D(t,x,\varepsilon) \cdot \nabla_x F(t,x,\varepsilon)\,, \tag{2.22}$$

and N, D, κ are defined in (2.20), (2.18), (2.19).

This model is referred to as the SHE model. In contrast to the Boltzmann equation, the distribution function F, solution of the SHE model, is only energy dependent. Due to the elastic collisions, the angular dependence of the electron velocity is averaged in the diffusion limit.

Hereby we shall also remark, that a similar equation is obtained for the 1D case, in the diffusion limit $\alpha \to 0$ of the following rescaled Boltzmann equation

$$\begin{cases} \partial_t f + \dfrac{1}{\alpha}\left(\nabla_v \epsilon \cdot \nabla_x f - \nabla_x \epsilon \cdot \nabla_v f\right) = \dfrac{1}{\alpha^2} Q(f) \\ f(0,x,v) = f_{in}(x,v)\,, \end{cases}$$

where $\epsilon(t,x,v)$ is an arbitrary regular function, satisfying $\epsilon(t,x,v) = \epsilon(t,x,-v)$. In the limit we get the diffusion equation

$$(\partial_t F)\, N + \nabla_x \cdot J + (\partial_\varepsilon F)\, \kappa = 0\,,$$

with $J := -D \cdot \nabla_x F$ and

$$D(t,x,\varepsilon) := \int_{S_\varepsilon} \nabla_v \epsilon \otimes \vartheta \; dN_\varepsilon(v) \quad ; \quad \kappa(t,x,\varepsilon) := \int_{S_\varepsilon} \partial_t \epsilon \; dN_\varepsilon(v) \quad ; \quad N = \int_{S_\varepsilon} dN_\varepsilon(v)\,,$$

the surface of constant energy being defined as $S_\varepsilon := \{v \in \mathbb{R}^2 \;/\; \epsilon(t,x,v) = \varepsilon\}$.

Let us now state an important property of the diffusion matrix D, corresponding to the SHE model (2.21)-(2.22).

Lemma 2.8 *The diffusion matrix $D(t,x,\varepsilon)$, defined in (2.18) is a symmetric, non-negative 2×2 matrix, satisfying*

$$D(t,x,\varepsilon) \geq C \sum_n \int_{S_{\varepsilon - \epsilon_n}} v \otimes v \; dN_{\varepsilon - \epsilon_n}(v)\,, \tag{2.23}$$

with a constant $C > 0$ independent on t, x and ε.

Proof Let t and x be fixed parameters within this proof. Moreover let $\varphi \in C_0(\mathbb{R})$ be an arbitrary test function with compact support, and $\psi : \mathbb{R} \to \mathbb{R}$ a function, such that $v\psi(\mathbf{e}) \in \mathbb{L}^2$. Then using the selfadjointness of the operator Q_0, we have

$$\begin{aligned}
\int_{\epsilon_1}^{\infty} D_{ij}(\varepsilon)\varphi(\varepsilon)d\varepsilon &= \int_{\epsilon_1}^{\infty} \sum_n \int_{S_{\varepsilon-\epsilon_n}} v_i\ \vartheta_n^j\ dN_{\varepsilon-\epsilon_n}(v)\ \varphi(\varepsilon)\ d\varepsilon \\
&= \sum_n \int_{\mathbb{R}^2} (v_i\ \psi(\mathbf{e}_n)) \left(\frac{1}{\psi(\mathbf{e}_n)} \vartheta_n^j \varphi(\mathbf{e}_n) \right) dv \\
&= -\sum_n \int_{\mathbb{R}^2} Q_0(\vartheta^i\ \psi(\mathbf{e}))_n \left(\frac{1}{\psi(\mathbf{e}_n)} \vartheta_n^j \varphi(\mathbf{e}_n) \right) dv \\
&= -\sum_n \int_{\mathbb{R}^2} \left(\vartheta_n^i\ \frac{1}{\psi(\mathbf{e}_n)} \right) Q_0(\psi(\mathbf{e})\,\vartheta^j)_n\ \varphi(\mathbf{e}_n)\ dv \\
&= \sum_n \int_{\mathbb{R}^2} \vartheta_n^i\ v_j\ \varphi(\mathbf{e}_n)\ dv = \int_{\epsilon_1}^{\infty} D_{ji}(\varepsilon)\ \varphi(\varepsilon)\ d\varepsilon\,.
\end{aligned}$$

Since φ was arbitrary, we deduce the equality $D_{ij}(\varepsilon) = D_{ji}(\varepsilon)$ for a.a. $\varepsilon \in [\epsilon_1, \infty)$. The non-negativity is a direct consequence of the inequality (2.23). To prove this inequality, let $\varphi \in C_0(\mathbb{R})$ be a test function, with $\varphi \geq 0$. Note, that in this case $v\sqrt{\varphi(\mathbf{e})} \in \mathbb{L}^2$. Let $(\xi_1, \xi_2) \in \mathbb{R}^2$ be fixed, we have

$$\begin{aligned}
\int_{\epsilon_1}^{\infty} \varphi(\varepsilon) \sum_{i,j=1}^{2} D_{ij}(\varepsilon)\,\xi_i\,\xi_j\ d\varepsilon &= \int_{\epsilon_1}^{\infty} \sum_n \left(\int_{S_{\varepsilon-\epsilon_n}} \varphi(\varepsilon) \sum_{i,j} v_i\ \vartheta_n^j\ \xi_i\ \xi_j\ dN_{\varepsilon-\epsilon_n}(v) \right) d\varepsilon = \\
&= \sum_n \int_{\mathbb{R}^2} \sum_i \left(\sqrt{\varphi(\mathbf{e}_n)}\ v_i\ \xi_i \right) \sum_j \left(\sqrt{\varphi(\mathbf{e}_n)}\ \vartheta_n^j\ \xi_j \right)\ dv \\
&= -\sum_n \int_{\mathbb{R}^2} Q_0 \left(\sum_{i=1}^{2} \sqrt{\varphi(\mathbf{e})}\ \vartheta^i\ \xi_i \right)_n \left(\sum_{j=1}^{2} \sqrt{\varphi(\mathbf{e}_n)}\ \vartheta_n^j\ \xi_j \right)\ dv.
\end{aligned}$$

Using the coercivity and the boundedness of the operator Q_0, we deduce

$$\begin{aligned}
\int_{\epsilon_1}^{\infty} \varphi(\varepsilon) \sum_{i,j} D_{ij}(\varepsilon)\ \xi_i\ \xi_j\ d\varepsilon &\geq C\ \|\sum_{i=1}^{2} \vartheta^i\ \xi_i \sqrt{\varphi(\mathbf{e})}\ \|^2 \geq C\ \|Q_0 \left(\sum_{i=1}^{2} \vartheta^i\ \xi_i\ \sqrt{\varphi(\mathbf{e})} \right) \|^2 \\
&= C\ \|Q_0(\vartheta\ \sqrt{\varphi(\mathbf{e})}) \cdot \xi\|^2 = C\ \|\sqrt{\varphi(\mathbf{e})}\ v \cdot \xi\ \|^2 \\
&= C \sum_n \int_{\epsilon_1}^{\infty} \varphi(\varepsilon) \int_{S_{\varepsilon-\epsilon_n}} |v \cdot \xi|^2\ dN_{\varepsilon-\epsilon_n}(v)\ d\varepsilon \\
&= C \sum_n \int_{\epsilon_1}^{\infty} \varphi(\varepsilon) \int_{S_{\varepsilon-\epsilon_n}} \sum_{i,j} (v \otimes v)_{ij}\ \xi_i\ \xi_j\ dN_{\varepsilon-\epsilon_n}(v)\ d\varepsilon \\
&= C \int_{\epsilon_1}^{\infty} \varphi(\varepsilon) \sum_{i,j} \left[\sum_n \left(\int_{S_{\varepsilon-\epsilon_n}} (v \otimes v)_{ij}\ dN_{\varepsilon-\epsilon_n}(v) \right) \right]\ \xi_i\ \xi_j\ d\varepsilon
\end{aligned}$$

for all $\varphi \in C_0(\mathbb{R})$, $\varphi \geq 0$, which implies (2.23). □

In a simplified case, we can give the exact expression for the diffusion matrix D and show that the estimate (2.23) is sharp. Let us consider cross sections of the form

$$\alpha_{nm}(t,x,v,v') := \alpha(t,x,\epsilon_n + \frac{|v|^2}{2})\,,$$

with $\alpha(t,x,\varepsilon)$ an energy dependent function. Then we are able to determine the expression of the unique solution $h \in (\ker Q_0)^\perp$ of $-Q_0(h) = v\psi(\mathbf{e})$. Indeed

$$Q_0(h)_n(v) = \sum_m \int_{\mathbb{R}^2} \alpha(t,x,\mathbf{e}_n)\delta(\mathbf{e}_n - \mathbf{e}'_m)h'_m dv' - \sum_m \int_{\mathbb{R}^2} \alpha(t,x,\mathbf{e}_n)\delta(\mathbf{e}_n - \mathbf{e}'_m)dv' h_n\,.$$

The first term vanishes, as $h \in (\ker Q_0)^\perp$. Hence

$$-Q_0(h)_n(v) = \alpha(t,x,\mathbf{e}_n)\int_{\epsilon_1}^\infty \sum_m \int_{S_{\varepsilon-\epsilon_m}} \delta(\mathbf{e}_n - \mathbf{e}'_m)dN_{\varepsilon-\epsilon_m}(v)\,d\varepsilon\,h_n = \alpha(\mathbf{e}_n)N(\mathbf{e}_n)h_n(v)\,,$$

implying

$$h_n(t,x,v) = v\frac{\psi(\mathbf{e}_n)}{\alpha(t,x,\mathbf{e}_n)N(t,x,\mathbf{e}_n)} \quad \Rightarrow \quad \vartheta_n(t,x,v) = \frac{1}{\alpha(t,x,\mathbf{e}_n)N(t,x,\mathbf{e}_n)}v\,.$$

Consequently, the diffusion matrix D has the explicit form

$$\begin{aligned} D(t,x,\varepsilon) &= \frac{1}{\alpha(t,x,\varepsilon)N(t,x,\varepsilon)}\sum_n \int_{S_{\varepsilon-\epsilon_n}} v\otimes v\ dN_{\varepsilon-\epsilon_m}(v) \\ &= \frac{2\pi}{\alpha(t,x,\varepsilon)N(t,x,\varepsilon)}\sum_n (\varepsilon-\epsilon_n)^+ Id\,, \end{aligned}$$

with Id the identity matrix.

2.4 The rigorous approach

This section is devoted to the rigorous proof of the convergence of the solution corresponding to the adiabatic quantum/kinetic model (2.1)-(2.2) towards the solution corresponding to the quantum/fluid model (2.1), (2.21), (2.22), which was formally derived in the last section. We first claim the following existence result for the one-dimensional Schrödinger equation (2.1). Details can be found in [5].

Lemma 2.9 *Let the potential V be a fixed real-valued function belonging to $C^1([0,T];W^{1,\infty}(\mathbb{R}^2\times[0,1]))$. The eigenvalue problem (2.1) admits a unique solution $(\epsilon_n,\chi_n)_{n\in\mathbb{N}} \in C^1([0,T];W^{1,\infty}(\mathbb{R}^2)) \times C^1([0,T];W^{1,\infty}(\mathbb{R}^2\times[0,1]))$.*

To precise the right functional framework, we have to introduce some new notations.

- We shall denote by $\mathcal{L}^2$ and $L^2_{x,\epsilon_{loc}}$ the following spaces

$$\begin{aligned}\mathcal{L}^2 &:= \left\{ f = (f_n(x,v))_{n\in\mathbb{N}} \ / \ \sum_n \int_{\mathbb{R}^2\times\mathbb{R}^2} |f_n(x,v)|^2 dv dx < \infty \right\} ,\\ L^2_{x,\epsilon_{loc}} &:= \left\{ \rho : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R} \ / \ \int_{\mathbb{R}^2} \int_K |\rho(x,\epsilon)|^2 d\epsilon dx < \infty \,, \ \forall K \subset \mathbb{R} \ \text{bounded} \right\} .\end{aligned}$$

- The transport operator Λ is defined by

$$\Lambda : D(\Lambda) \to \mathcal{L}^2 \ ; \quad (\Lambda g)_n(x,v) := v \cdot \nabla_x g_n - \nabla_x \epsilon_n \cdot \nabla_v g_n \,,$$

with the domain and corresponding norm

$$D(\Lambda) := \{ g \in \mathcal{L}^2 \ / \ \Lambda g \in \mathcal{L}^2 \} \qquad ; \qquad ||g||^2_{D(\Lambda)} := ||g||^2_{\mathcal{L}^2} + ||\Lambda g||^2_{\mathcal{L}^2} \,.$$

The weak formulation of the Boltzmann equation (2.2) is given in the following

Definition 2.10 *A function $f^\alpha \in L^2(0,T,\mathcal{L}^2)$ is called a weak solution of (2.2), if f^α satisfies*

$$\begin{aligned}\sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} f_n^\alpha \partial_t \varphi_n \, dv dx dt + \frac{1}{\alpha} \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} f_n^\alpha (\Lambda\varphi)_n \, dv dx dt \\ + \frac{1}{\alpha^2} \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} Q_0(f^\alpha)_n \varphi_n \, dv dx dt = - \sum_n \int_{\mathbb{R}^2\times\mathbb{R}^2} f^\alpha_{in,n} \varphi_n(0) \, dv dx \,,\end{aligned} \tag{2.24}$$

for all test functions φ belonging to

$$\mathcal{S} := \left\{ \varphi \in W^{1,2}(0,T;\mathcal{L}^2) \cap L^2(0,T;D(\Lambda)) \ , \ \varphi(T,\cdot,\cdot) \equiv 0 \right\} \,.$$

The goal of this section is to prove the following main theorem :

Theorem 2.11 (Rigorous diffusion limit)
Let f^α be the weak solution of the Boltzmann equation (2.2) for $\alpha > 0$ and let f^α_{in} converge in $\mathcal{L}^2$ towards a function f_{in}, as $\alpha \to 0$. Then, up to a subsequence, f^α converge weakly in $L^2(0,T;\mathcal{L}^2)$ towards a function f which is only energy-dependent, that means

$$f_n(t,x,v) = F(t,x,\epsilon_n(t,x) + \frac{|v|^2}{2}) \,,$$

and the distribution function F satisfies in a weak sense the following SHE model

$$\partial_t(N\,F) + \nabla_x \cdot J + \partial_\varepsilon(F\kappa) = 0 \,, \tag{2.25}$$

with the current density given by

$$J(t,x,\varepsilon) = -D(t,x,\varepsilon) \cdot \nabla_x F(t,x,\varepsilon) \,, \tag{2.26}$$

and the initial data

$$F(0,x,\varepsilon) = F_{in}(x,\varepsilon) := \frac{1}{N(0,x,\varepsilon)} \sum_n \int_{S_{\varepsilon - \epsilon_{n(0,x)}}} f_{in,n}(x,v)\, dN_{\varepsilon-\epsilon_n}(v)\,, \tag{2.27}$$

where N, D, κ are defined in (2.20), (2.18), (2.19).

Remark 2.12 *The weak formulation of the continuity equation (2.25) reads*

$$\int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} N\, F\, \partial_t \Phi \; d\epsilon dx dt + \int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} J \cdot \nabla_x \Phi \; d\epsilon dx dt + \int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} F\, \kappa\, \partial_\epsilon \Phi \; d\epsilon dx dt =$$
$$= - \int_{\mathbb{R}^2} \int_{\mathbb{R}} N(0,x,\epsilon)\, F_{in}(x,\epsilon)\, \Phi(0,x,\epsilon)\; d\epsilon dx\,, \qquad \forall \Phi \in C_0^1([0,T) \times \mathbb{R}^2 \times \mathbb{R})\,, \tag{2.28}$$

whereas the current equation has the following weak form

$$\int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} J \cdot \Psi \; d\epsilon dx dt = \sum_n \int_0^T \int_{\mathbb{R}^2 \times \mathbb{R}^2} (\Lambda f)_n\, Q_0^{-1} (v \cdot \Psi)_n \; dv dx dt\,,$$
$$\forall \Psi \in C_0([0,T] \times \mathbb{R}^2 \times \mathbb{R})^2\,. \tag{2.29}$$

The derivation of the current weak formulation (2.29) is immediate by observing that

$$\sum_n \int_0^T \int_{\mathbb{R}^2 \times \mathbb{R}^2} (\Lambda f)_n\, Q_0^{-1} (v \cdot \Psi)_n \; dv dx dt = -\sum_n \int_0^T \int_{\mathbb{R}^2 \times \mathbb{R}^2} (\nabla_x F \cdot v)(\vartheta_n \cdot \Psi)\, dv dx dt$$
$$= - \int_0^T \int_{\mathbb{R}^2} \int_{\epsilon_1}^\infty \nabla_x F(t,x,\varepsilon) \cdot \left(\sum_n \int_{S_{\varepsilon-\epsilon_n}} v \otimes \vartheta_n dN_{\varepsilon - \epsilon_n}(v) \right) \cdot \Psi(t,x,\varepsilon) \; d\varepsilon dx dt\,.$$

To justify the existence of all these integrals, we show later on, that the involved functions belong to the right functional spaces.

The proof of Theorem 2.11 is done in several steps. Establishing a priori estimates, the sequence $\{f^\alpha\}$ of weak solutions of (2.2) is shown to be bounded in $L^2(0,T,\mathcal{L}^2)$. This implies the existence of a function $f \in L^2(0,T,\mathcal{L}^2)$ such that, up to a subsequence, $f^\alpha \to f$ weakly in $L^2(0,T,\mathcal{L}^2)$. It will be proven in a next step that this limit function is only energy-dependent. Finally, passing to the limit in the weak formulation (2.24), with special choices of test functions, enables to get the desired equation.

Lemma 2.13 *The Boltzmann equation (2.2) admits for each $\alpha > 0$ and $f_{in}^\alpha \in \mathcal{L}^2$ a unique weak solution $f^\alpha \in L^2(0,T;\mathcal{L}^2)$.*

Proof To prove this lemma, we shall use a fixed point argument. Let us define for a fixed $\alpha > 0$ the application

$$\tau : L^2(0,T;\mathcal{L}^2) \to L^2(0,T;\mathcal{L}^2) \qquad ; \qquad f^{old} \mapsto f^{new} \,,$$

with f^{new} solution of

$$\begin{cases} \partial_t f_n^{new} + \dfrac{1}{\alpha}\left(v \cdot \nabla_x f_n^{new} - \nabla_x \epsilon_n \cdot \nabla_v f_n^{new}\right) + \dfrac{1}{\alpha^2} Q_0^-(f^{new})_n = \dfrac{1}{\alpha^2} Q_0^+(f^{old})_n \\ f^{new}(0,x,v) = f_{in,n}(x,v)\,, \end{cases} \tag{2.30}$$

where Q_0^+ and Q_0^- are the gain respectively loss terms, given by

$$\begin{aligned} Q_0^+(f)_n(t,x,v) &= \sum_{m \in \mathbb{N}^*} \int_{\mathbb{R}^2} \alpha_{nm}(t,x,v,v')\delta(\mathbf{e}_n - \mathbf{e}'_m) f_m(t,x,v')dv'\,, \\ Q_0^-(f)_n(t,x,v) &= \sum_{m \in \mathbb{N}^*} \int_{\mathbb{R}^2} \alpha_{nm}(t,x,v,v')\delta(\mathbf{e}_n - \mathbf{e}'_m)dv' \; f_n(t,x,v)\,. \end{aligned}$$

The idea is to prove that this application is a contraction and admits thus a fixed point $f \in L^2(0,T,\mathcal{L}^2)$. Our first concern shall be to show that τ is well defined. For this let $f^{old} \in L^2(0,T,\mathcal{L}^2)$. By standard existence results for the transport equation, we deduce for each $n \in \mathbb{N}^*$ the existence of a weak solution $f_n^{new} \in L^\infty(0,T,L^2_{x,v})$ of (2.30), satisfying the estimate

$$||f_n^{new}(t,\cdot,\cdot)||_{L^2_{x,v}} \le ||f_{in,n}(\cdot,\cdot)||_{L^2_{x,v}} + \frac{1}{\alpha^2}\int_0^t ||(Q_0^+(f^{old}))_n(s)||_{L^2_{x,v}} ds \quad \text{for a.a. } t \in (0,T)\,.$$

This implies after a summation over n

$$||f^{new}(t,\cdot,\cdot)||^2_{L^\infty(0,T,\mathcal{L}^2)} \le 2||f_{in}||^2_{\mathcal{L}^2} + 2T\frac{1}{\alpha^4}||Q_0^+(f^{old})||^2_{L^2(0,t,\mathcal{L}^2)}\,,$$

yielding $f^{new} \in L^\infty(0,T,\mathcal{L}^2) \subset L^2(0,T,\mathcal{L}^2)$. To prove that τ is a contraction, we shall introduce a new equivalent norm in $L^2(0,T,\mathcal{L}^2)$, by

$$||g||^2_\delta := \int_0^T e^{-\delta t}||g(t,\cdot,\cdot)||^2_{\mathcal{L}^2}\, dt \qquad \forall g \in L^2(0,T,\mathcal{L}^2)\,.$$

The parameter $\delta > 0$ shall be specified later on. With this norm, we have

$$\begin{aligned} ||\tau(f_1^{old}) - \tau(f_2^{old})||_\delta &= ||f_1^{new} - f_2^{new}||_\delta = \int_0^T e^{-\delta t}||f_1^{new}(t) - f_2^{new}(t)||^2_{\mathcal{L}^2}\, dt \\ &\le \frac{2T}{\alpha^4}\int_0^T e^{-\delta t}\int_0^t ||Q_0^+(f_1^{old} - f_2^{old})(s)||^2_{\mathcal{L}^2} ds dt \\ &= \frac{2T}{\alpha^4}\int_0^T \int_s^T e^{-\delta t}||Q_0^+(f_1^{old} - f_2^{old})(s)||^2_{\mathcal{L}^2} dt ds \\ &\le \frac{2cT}{\alpha^4}\int_0^T ||f_1^{old}(s) - f_2^{old}(s)||^2_{\mathcal{L}^2}\frac{e^{-\delta s} - e^{-\delta T}}{\delta} ds \\ &\le \frac{2cT}{\alpha^4 \delta}||f_1^{old} - f_2^{old}||^2_\delta\,. \end{aligned}$$

For fixed $\alpha > 0$ and T, we can choose $\delta > 0$ in such a manner, that the application τ is a contraction in $(L^2(0,T;\mathcal{L}^2), ||\cdot||_\delta)$. Thus τ admits a fixed point $f \in L^2(0,T,\mathcal{L}^2)$, unique weak solution of the Boltzmann equation (2.2). □

Lemma 2.14 *The weak solutions f^α of the rescaled Boltzmann equation (2.2) form a bounded sequence in $L^2(0,T;\mathcal{L}^2)$, such that up to a subsequence $f^\alpha \to f$ weakly in $L^2(0,T;\mathcal{L}^2)$, as $\alpha \to 0$. Moreover there exists an energy-dependent function $F(t,x,\varepsilon)$ such that the limit function f reads*

$$f_n(t,x,v) = F(t,x,\epsilon_n + \frac{|v|^2}{2}) .$$

Proof Multiplying (2.2) with f^α and integrating with respect to (t,x,v), leads to

$$\frac{1}{2}\sum_n \int_0^t \int_{\mathbb{R}^2\times\mathbb{R}^2} \partial_t |f_n^\alpha|^2 dvdxds = \frac{1}{\alpha^2}\sum_n \int_0^t \int_{\mathbb{R}^2\times\mathbb{R}^2} Q_0(f^\alpha)_n f_n^\alpha dvdxds \, ,$$

implying

$$\frac{1}{2}||f^\alpha(t,\cdot,\cdot)||^2_{\mathcal{L}^2} = \frac{1}{2}||f^\alpha_{in}(\cdot,\cdot)||^2_{\mathcal{L}^2} + \frac{1}{\alpha^2}\sum_n \int_0^t \int_{\mathbb{R}^2\times\mathbb{R}^2} Q_0(f^\alpha)_n f_n^\alpha dvdxds \, . \qquad (2.31)$$

This procedure requires some regularity for the functions f^α. However a standard regularisation technique permits to deduce (2.31) even for $f^\alpha \in L^2(0,T,\mathcal{L}^2)$. The non-positivity of the operator Q_0 and the boundedness of the sequence f^α_{in} imply

$$||f^\alpha(t,\cdot,\cdot)||^2_{\mathcal{L}^2} \le ||f^\alpha_{in}(\cdot,\cdot)||^2_{\mathcal{L}^2} \le c\, , \quad \forall \alpha > 0\, ,$$

establishing thus the boundedness of the sequence f^α in $L^\infty(0,T;\mathcal{L}^2)$. Consequently, up to a subsequence, f^α is weakly convergent in $L^2(0,T;\mathcal{L}^2)$ as α tends to zero. It remains to prove that the limit function f is only energy dependent. For this, we multiply equation (2.31) by α^2 and pass to the limit $\alpha \to 0$. Thus, we have

$$\sum_n \int_0^t \int_{\mathbb{R}^2\times\mathbb{R}^2} Q_0(f^\alpha)_n f_n^\alpha dvdxds \to 0\, , \quad \forall t \in [0,T]\, .$$

With (2.9) this yields $\mathcal{P}^\perp f^\alpha \to 0$ in $L^2(0,T,\mathcal{L}^2)$, hence $Q_0(f^\alpha) = Q_0(\mathcal{P}^\perp f^\alpha) \to 0$. As however $f^\alpha \rightharpoonup f$ and thus $Q_0(f^\alpha) \rightharpoonup Q_0(f)$ in $L^2(0,T,\mathcal{L}^2)$, we get $Q_0(f) = 0$. Consequently, the limit function f belongs to the kernel of Q_0. □

It remains to show that the limiting distribution function F of Lemma 2.14 satisfies in a weak sense the SHE model (2.25), (2.26). For this, it will be of use to introduce the electron and the current densities associated to the statistics f^α

$$\rho^\alpha(t,x,\epsilon) := \sum_n \int_{S_{\epsilon-\epsilon_n}} f_n^\alpha(t,x,v)\, dN_{\epsilon-\epsilon_n}(v)\, , \quad J^\alpha(t,x,\epsilon) := \frac{1}{\alpha}\sum_n \int_{S_{\epsilon-\epsilon_n}} v f_n^\alpha\, dN_{\epsilon-\epsilon_n}(v)\, ,$$

as well as the terms

$$\Gamma^\alpha(t,x,\epsilon) := \sum_n \partial_t \epsilon_n \int_{S_{\epsilon-\epsilon_n}} f_n^\alpha(t,x,v)\, dN_{\epsilon-\epsilon_n}(v)\,, \quad \rho_{in}^\alpha(x,\epsilon) := \sum_n \int_{S_{\epsilon-\epsilon_{n(0,x)}}} f_{in,n}^\alpha \, dN_{\epsilon-\epsilon_n}(v)\,.$$

Using the boundedness of the distribution functions f^α in $L^2(0,T,\mathcal{L}^2)$ and choosing in (2.24) the particular test function $\varphi^1 \in \mathcal{S}$ given by

$$\varphi_n^1(t,x,v) := \Phi(t,x,\epsilon_n + \frac{|v|^2}{2})\,, \tag{2.32}$$

with $\Phi \in C_0^1([0,T) \times \mathbb{R}^2 \times \mathbb{R})$, we can show immediately:

Lemma 2.15 *(i) The energy-dependent functions* $(\rho^\alpha, J^\alpha, \Gamma^\alpha) \in L^2(0,T;L^2_{x,\epsilon_{loc}})^4$ *and the initial data* $\rho^\alpha_{in} \in L^2_{x,\epsilon_{loc}}$ *satisfy in a weak sense the following system*

$$\begin{cases} \partial_t \rho^\alpha + \nabla_x \cdot J^\alpha + \partial_\epsilon \Gamma^\alpha = 0 \\ \rho^\alpha(0) = \rho^\alpha_{in}\,. \end{cases}$$

(ii) The sequences $\rho^\alpha, J^\alpha, \Gamma^\alpha$ *as well as* ρ^α_{in} *are bounded in the corresponding spaces and thus (up to a subsequence) weakly convergent for* $\alpha \to 0$ *towards some functions* $(\rho, J, \Gamma) \in L^2(0,T;L^2_{x,\epsilon_{loc}})^4$ *and* $\rho_{in} \in L^2_{x,\epsilon_{loc}}$*. These limit functions satisfy the following equation*

$$\int_0^T \int_{\mathbb{R}^2}\int_{\mathbb{R}} \rho\, \partial_t \Phi \; d\epsilon dx dt + \int_0^T \int_{\mathbb{R}^2}\int_{\mathbb{R}} J \cdot \nabla_x \Phi \; d\epsilon dx dt + \int_0^T \int_{\mathbb{R}^2}\int_{\mathbb{R}} \Gamma\, \partial_\epsilon \Phi \; d\epsilon dx dt =$$
$$= - \int_{\mathbb{R}^2}\int_{\mathbb{R}} \rho_{in}(x,\epsilon)\, \Phi(0,x,\epsilon)\; d\epsilon dx\,, \qquad \forall \Phi \in C_0^1([0,T) \times \mathbb{R}^2 \times \mathbb{R})\,. \tag{2.33}$$

Proof It remains to show that J^α is a bounded sequence in $L^2(0,T;L^2_{x,\epsilon_{loc}})^2$. For this let us decompose f^α as follows

$$f^\alpha = h^\alpha + \alpha g^\alpha \quad \text{with} \quad h^\alpha := \mathcal{P} f^\alpha \quad ; \quad g^\alpha := \frac{1}{\alpha} \mathcal{P}^\perp f^\alpha\,. \tag{2.34}$$

Thus

$$\int_0^T \int_{\mathbb{R}^2}\int_K |J^\alpha(t,x,\epsilon)|^2 \, d\epsilon dx dt = \int_0^T \int_{\mathbb{R}^2}\int_K \left| \sum_n \int_{S_{\epsilon-\epsilon_n}} g_n^\alpha(t,x,v) v \, dN_{\epsilon-\epsilon_n}(v) \right|^2 d\epsilon dx dt$$
$$\leq \int_0^T \int_{\mathbb{R}^2}\int_K \left(\sum_n \int_{S_{\epsilon-\epsilon_n}} |g_n^\alpha(t,x,v)|^2 \, dN_{\epsilon-\epsilon_n}(v) \right) \left(\sum_n \int_{S_{\epsilon-\epsilon_n}} |v|^2 \, dN_{\epsilon-\epsilon_n}(v) \right) d\epsilon dx dt$$
$$\leq c_K < \infty\,,$$

where $c_K > 0$ is a constant independent on α. For this last estimate we used the coercivity inequality (2.8) as well as equation (2.31), and the fact, that K is a bounded set. □

In order to finish the proof of the main theorem, it remains to express the limit functions ρ, J, Γ and ρ_{in} in terms of the distribution function F.

Proof of Theorem 2.11 For the identification of the functions ρ, J, Γ and ρ_{in}, we shall use the fact that $f^\alpha \rightharpoonup f$ in $L^2(0,T,\mathcal{L}^2)$. Thus we have for some arbitrary test function $\Phi \in C_0^1([0,T) \times \mathbb{R}^2 \times \mathbb{R})$

$$\int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} \rho^\alpha(t,x,\epsilon)\Phi(t,x,\epsilon)\, d\epsilon dx dt = \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} f_n^\alpha(t,x,v)\Phi(t,x,\epsilon_n + \frac{|v|^2}{2})\, dv dx dt$$
$$\longrightarrow_{\alpha\to 0} \int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} F(t,x,\epsilon)\, N(t,x,\epsilon)\Phi(t,x,\epsilon)\, d\epsilon dx dt\,.$$

But since $\rho^\alpha \rightharpoonup \rho$ in $L^2(0,T,\mathcal{L}^2)$, we get $\rho = F\, N \in L^2(0,T; L^2_{x,\epsilon_{loc}})$. Similarly due to the fact that $f^\alpha_{in} \to f_{in}$ in $\mathcal{L}^2$, we deduce $\rho_{in} = F_{in}\, N(0) \in L^2_{x,\epsilon_{loc}}$. Furthermore

$$\int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} \Gamma^\alpha(t,x,\epsilon)\Phi(t,x,\epsilon)\, d\epsilon dx dt = \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} f_n^\alpha\, \partial_t \epsilon_n\, \Phi(t,x,\epsilon_n + \frac{|v|^2}{2})\, dv dx dt$$
$$\longrightarrow_{\alpha\to 0} \int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} F(t,x,\epsilon) \left(\sum_n \partial_t \epsilon_n \int_{S_{\varepsilon-\epsilon_n}} dN_{\varepsilon-\epsilon_n}(v) \right) \Phi(t,x,\epsilon)\, d\epsilon dx dt\,,$$

implying $\Gamma = F\,\kappa \in L^2(0,T; L^2_{x,\epsilon_{loc}})$. And finally, let us analyse the limit of the following term

$$\int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} J^\alpha \cdot \Psi\, d\epsilon dx dt = \frac{1}{\alpha} \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} f_n^\alpha(t,x,v)\, v \cdot \Psi\, dv dx dt\,,$$

for some test function $\Psi \in C_0([0,T] \times \mathbb{R}^2 \times \mathbb{R})^2$. For this, let us consider again the decomposition (2.34), implying, in view of $v \cdot \Psi \in \ker(Q_0)^\perp$, that

$$\frac{1}{\alpha} \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} f_n^\alpha\, (v\cdot\Psi)_n\, dv dx dt = \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} g_n^\alpha\, (v\cdot\Psi)_n\, dv dx dt\,.$$

As shown in the proof of Lemma 2.15, the sequence g^α is bounded in $L^2(0,T,\mathcal{L}^2)$, and thus converges weakly (up to a subsequence) towards some function $g \in L^2(0,T,\mathcal{L}^2)$, leading to

$$\sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} g_n^\alpha (v\cdot\Psi)_n\, dv dx dt \to \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} g_n (v\cdot\Psi)_n\, dv dx dt\,.$$

To finish the proof we have to express this last integral in terms of the distribution function F. For this purpose, let us insert the decompostion (2.34) in the variational formulation (2.24), where $\varphi \in \mathcal{S}$ is an arbitrary test function, deducing thus

$$\sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} h_n^\alpha (\Lambda\varphi)_n\, dv dx dt + \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} Q_0(g^\alpha)_n \varphi_n\, dv dx dt = \mathcal{O}(\alpha)\,.$$

Here we used the fact, that f^α, g^α and h^α are bounded sequences in $L^2(0,T,\mathcal{L}^2)$ and $\mathcal{O}(\alpha)$ stands for the terms of the order one in α. From (2.34), one can deduce immediately that $h^\alpha \rightharpoonup f$ in $L^2(0,T,\mathcal{L}^2)$, such that passing to the limit in the last equation yields

$$\sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} f_n(\Lambda\varphi)_n \, dvdxdt + \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} Q_0(g)_n \varphi_n \, dvdxdt = 0\,, \tag{2.35}$$

which shows that $\Lambda f = \nabla_x F \cdot v$ is a well defined function in $L^2(0,T,\mathcal{L}^2)$. Choosing at this stage the special function $\varphi^2 \in L^2(0,T,\mathcal{L}^2)$ (unique in $\ker(Q_0)^\perp$), given by

$$\varphi^2 := Q_0^{-1}(v\cdot\Psi)\,,$$

we have by using (2.35)

$$\begin{aligned}\sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} g_n(v\cdot\Psi)_n \, dvdxdt \; &= \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} g_n Q_0(\varphi^2)_n \, dvdxdt = \\ = \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} (\Lambda f)_n \varphi^2_n \, dvdxdt \; &= \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} (\Lambda f)_n (Q_0^{-1}(v\cdot\Psi))_n \, dvdxdt\,.\end{aligned}$$

Altogether we have thus $\forall \Psi \in C_0([0,T]\times\mathbb{R}^2\times\mathbb{R})^2$

$$\int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}} J^\alpha \cdot \Psi \, d\epsilon dxdt \longrightarrow_{\alpha\to 0} \sum_n \int_0^T \int_{\mathbb{R}^2\times\mathbb{R}^2} (\Lambda f)_n (Q_0^{-1}(v\cdot\Psi))_n \, dvdxdt,$$

which proves that $J \in L^2(0,T;L^2_{x,\epsilon_{loc}})$ is a solution of the weak formulation (2.29). This fact, as well as equation (2.33) permits to finish the proof of the main theorem. □

3 The diffusion limit towards the ET model

In the previous section we have derived the coupled Schrödinger/SHE model from the Schrödinger/Boltzmann system, by assuming that the elastic impurity collisions are predominant. In this section we shall perform another relaxation limit, based on a different collision mechanism, constituted of the elastic impurity scattering and the electron-electron scattering. In the limit of a vanishing rescaled free mean path $\alpha \to 0$, we shall get the coupled Schrödinger/ET model.

Starting point is the coupled model composed of the rescaled Boltzmann equation in the transport direction x

$$\left\{ \begin{aligned} &\partial_t f_n + \frac{1}{\alpha}(v\cdot\nabla_x f_n - \nabla_x \epsilon_n \cdot \nabla_v f_n) = \frac{1}{\alpha^2}(Q_0(f)_n + Q_e(f)_n) \\ &f_n(0,x,v) = f_{in,n}(x,v)\,, \end{aligned} \right. \tag{3.1}$$

whereas the confinement direction is still described by means of the 1D Schrödinger equation (2.1). The linear, elastic collision operator Q_0, describing the lattice-defect collisions, is the same as in the previous section,

$$Q_0(f)_n := \sum_{m\in\mathbb{N}^*} \int_{\mathbb{R}^2} \alpha_{mn}(t,x,v',v)\delta(\epsilon_n + \frac{|v|^2}{2} - \epsilon_m - \frac{|v'|^2}{2})(f_m(t,x,v') - f_n(t,x,v))\,dv' \,, \tag{3.2}$$

and the elastic, non-linear electron-electron collision operator Q_e is given by

$$Q_e(f)_n(v) :=$$

$$\sum_{m,r,s\in\mathbb{N}^*} \int_{(\mathbb{R}^2)^3} \beta_{nmrs}(t,x,v,v_1,v',v_1')\delta(\epsilon_n + \frac{|v|^2}{2} + \epsilon_m + \frac{|v_1|^2}{2} - \epsilon_r - \frac{|v'|^2}{2} - \epsilon_s - \frac{|v_1'|^2}{2})$$
$$\delta(v + v_1 - v' - v_1')[f_r' f_{s,1}'(1-\eta f_n)(1-\eta f_{m,1}) - f_n f_{m,1}(1-\eta f_r')(1-\eta f_{s,1}')]\,dv_1 dv' dv_1' \,, \tag{3.3}$$

where $\eta \geq 0$ is a distribution function scale and the terms $0 \leq 1 - \eta f_n \leq 1$ express the Pauli exclusion principle. We shall denote in the following the kinetic energy of the electrons belonging to the $n-th$ energy subband, by

$$\mathbf{e}_n(t,x,v) := \epsilon_n(t,x) + \frac{|v|^2}{2} \,.$$

The notations $\mathbf{e}_{m,1}$, $\mathbf{e}_r'$ and $\mathbf{e}_{s,1}'$ stand then for $\mathbf{e}_m(v_1)$, $\mathbf{e}_r(v')$ respectively $\mathbf{e}_s(v_1')$. The scattering cross sections α_{nm} satisfy Hypothesis 1, whereas β_{nmrs} are assumed to satisfy

Hypothesis 2 The coefficients β_{nmrs} satisfy the following positivity, boundedness and symmetry properties

$$0 < \lambda_2 < \beta_{nmrs} M(t,x,v,n,v_1,m) < \lambda_3 < +\infty \,,$$
$$\beta_{nmrs}(v,v_1,v',v_1') = \beta_{mnrs}(v_1,v,v',v_1') = \beta_{rsnm}(v',v_1',v,v_1).$$

The weight function M is defined as

$$M(t,x,v,n,v_1,m) := \sum_{r,s\in\mathbb{N}^*} \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \delta(\mathbf{e}_n + \mathbf{e}_{m,1} - \mathbf{e}_r' - \mathbf{e}_{s,1}')\delta(v + v_1 - v' - v_1')dv'dv_1' \,.$$

Similarly as for the elastic impurity collisions, the weight function M is a density of states. It gives the number of possible configurations the electrons can occupy after an electron-electron collision, if their configuration before the collision was (v,n,v_1,m). Using the conservation of the energy and the impulsion, the outgoing velocities are given by

$$\begin{cases} v' = \dfrac{v+v_1}{2} + \sqrt{\epsilon_n + \epsilon_m - \epsilon_r - \epsilon_s + \dfrac{1}{4}|v - v_1|^2}\;\sigma \\ v_1' = \dfrac{v+v_1}{2} - \sqrt{\epsilon_n + \epsilon_m - \epsilon_r - \epsilon_s + \dfrac{1}{4}|v - v_1|^2}\;\sigma \end{cases} , \quad |\sigma| = 1\,,\ \sigma \in \mathbb{R}^2\,,$$

such that the density of states can be written in the form

$$M(t,x,v,n,v_1,m) := 2\pi \sum_{r,s\in\mathbb{N}^*} \left(\epsilon_n + \epsilon_m - \epsilon_r - \epsilon_s + \frac{1}{4}|v-v_1|^2\right)^+ .$$

As for the derivation of the SHE model, we shall perform a Hilbert expansion

$$f^\alpha = f^0 + \alpha f^1 + \alpha^2 f^2 + \cdots \tag{3.4}$$

The electron-electron collision operator being not linear, we have to expand it around the equilibrium function f^0, as

$$Q_e(f) = Q_e(f^0) + \alpha DQ_e(f^0)(f^1) + \alpha^2 \left[DQ_e(f^0)(f^2) + \frac{1}{2}D^2Q_e(f^0)(f^1,f^1)\right] + \cdots .$$

Substituting the Hilbert expansion in the Boltzmann equation (3.1) and comparing the terms in the same order of α, yields the equations

$$Q_e(f^0)_n + Q_0(f^0)_n = 0\,, \tag{3.5}$$

$$DQ_e(f^0)(f^1)_n + Q_0(f^1)_n = v\cdot\nabla_x f_n^0 - \nabla_x\epsilon_n\cdot\nabla_v f_n^0\,, \tag{3.6}$$

$$DQ_e(f^0)(f^2)_n + Q_0(f^2)_n = \partial_t f_n^0 + v\cdot\nabla_x f_n^1 - \nabla_x\epsilon_n\cdot\nabla_v f_n^1 - \frac{1}{2}D^2Q_e(f^0)(f^1,f^1)_n\,. \tag{3.7}$$

To solve these equations we have to analyze the operators Q_e+Q_0 respectively $DQ_e(f^0)+Q_0$. In particular, we are interested in finding the kernel of Q_e+Q_0 and the orthogonal to the kernel of $DQ_e(f^0)+Q_0$. This shall be the aim of the next sections.

3.1 Properties of the operator $Q_e + Q_0$: formal approach

The purpose of this section is to derive some properties of the operator Q_e+Q_0, especially to determine its kernel, and consequently to solve the equation (3.5) in order to find the zeroth order term of the Hilbert expansion.

Proposition 3.1 *Under the Hypothesis 2, the operator Q_e satisfies the following properties:*
(i) The micro-reversibility assumption on β_{nmrs} implies immediately

$$\langle Q_e(f),g\rangle = -\frac{1}{4}\sum_{n,m,r,s}\int_{(\mathbb{R}^2)^4} \beta_{nmrs}\delta_{\mathbf{e}}\delta_v[f_r'f_{s,1}'(1-\eta f_n)(1-\eta f_{m,1}) - f_n f_{m,1}(1-\eta f_r')(1-\eta f_{s,1}')]\,[g_r' + g_{s,1}' - g_n - g_{m,1}]\,dv dv_1 dv' dv_1'\,.$$

(ii) Let the function H be defined as $H(x) := \ln\frac{x}{1-\eta x}$. Then Q_e satisfies the following dissipative inequality

$$\langle Q_e(f), H(f)\rangle \le 0\,. \tag{3.8}$$

(iii) Collision invariants

$$\left\langle Q_e(f), \begin{pmatrix} \mathbf{1} \\ v\mathbf{1} \\ \mathbf{e}(v) \end{pmatrix} \right\rangle = 0 \,. \tag{3.9}$$

Proof The proof of this proposition is immediate and similar to the proof of Proposition 2.4. It is based on the positivity and symmetry properties of the cross sections β_{nmrs}. We remark only, that with the special choice of the function H, we have

$$\langle Q_e(f), H(f) \rangle =$$

$$-\frac{1}{4} \sum_{n,m,r,s} \int_{(\mathbb{R}^2)^4} \beta_{nmrs} \delta_{\mathbf{e}} \delta_v [f'_r f'_{s,1}(1-\eta f_n)(1-\eta f_{m,1}) - f_n f_{m,1}(1-\eta f'_r)(1-\eta f'_{s,1})]$$
$$[\ln(f'_r f'_{s,1}(1-\eta f_n)(1-\eta f_{m,1})) - \ln(f_n f_{m,1}(1-\eta f'_r)(1-\eta f'_{s,1}))] \, dv dv_1 dv' dv'_1 \,.$$

□

Let us now pass to the description of the kernel of the operator $Q_e + Q_0$.

Proposition 3.2 *The kernel of the operator $Q_e + Q_0$ is given by*

$$Ker(Q_e + Q_0) = \{ f(t,x,v) \;\; ; \;\exists\; \mu(t,x),\; T(t,x) \;\; \text{such that} \;\; f_n(t,x,v) = F_{\mu,T}(t,x,\mathbf{e}_n(v)) \} \,,$$

with the Fermi-Dirac distribution function

$$F_{\mu,T}(t,x,\varepsilon) := \frac{1}{\eta + exp \frac{\varepsilon - \mu(t,x)}{T(t,x)}} \,, \tag{3.10}$$

where μ is the associated chemical potential and $T > 0$ the electron temperature .

Proof In this proof we shall consider t and x as fixed parameters. To show the inclusion "$\subset$", let $f \in \ker(Q_e + Q_0)$ and $H(x) := \ln \frac{x}{1-\eta x}$. Then we have $\langle Q_0(f) + Q_e(f), H(f) \rangle = 0$, which implies in view of (2.6) and (3.8)

$$\langle Q_0(f), H(f) \rangle = 0 \quad ; \quad \langle Q_e(f), H(f) \rangle = 0 \,.$$

As in the case of the SHE model, we deduce from the first equality the existence of a function $F(t,x,\varepsilon)$, such that

$$f_n(t,x,v) = F(t,x,\epsilon_n + \frac{|v|^2}{2}) \,.$$

The second equation implies

$$\ln(f'_r f'_{s,1}(1-\eta f_n)(1-\eta f_{m,1})) = \ln(f_n f_{m,1}(1-\eta f'_r)(1-\eta f'_{s,1})) \,, \tag{3.11}$$

for all $(n,m,r,s) \in \mathbb{N}^4$ and $(v,v_1,v',v_1') \in (\mathbb{R}^2)^4$ with

$$\begin{cases} v + v_1 = v' + v_1' \,, \\ \epsilon_n + \frac{|v|^2}{2} + \epsilon_m + \frac{|v_1|^2}{2} = \epsilon_r + \frac{|v'|^2}{2} + \epsilon_s + \frac{|v_1'|^2}{2} \,. \end{cases}$$

Equation (3.11) can be rewritten in the form

$$\ln \frac{f_n}{1-\eta f_n} + \ln \frac{f_{m,1}}{1-\eta f_{m,1}} = \ln \frac{f_r'}{1-\eta f_r'} + \ln \frac{f_{s,1}'}{1-\eta f_{s,1}'} \,,$$

or simply

$$(H \circ F)(\epsilon_n + \frac{|v|^2}{2}) + (H \circ F)(\epsilon_m + \frac{|v_1|^2}{2}) = (H \circ F)(\epsilon_r + \frac{|v'|^2}{2}) + (H \circ F)(\epsilon_s + \frac{|v_1'|^2}{2}) \,.$$

Let us now fix for each energy $\varepsilon > \epsilon_1$ a subband n and a velocity $v \neq 0$, such that $\epsilon_n + \frac{|v|^2}{2} = \varepsilon$. Placing us in the n-th subband, we shall assume, that for each $\varepsilon > \epsilon_1$ there exists an $\alpha_\varepsilon > 0$, such that

$$[\varepsilon - \alpha_\varepsilon, \varepsilon + \alpha_\varepsilon] \quad \subset \quad \left\{ \mathbf{e}_n' \;\; / \;\; \mathbf{e}_n = \mathbf{e}_{n,1} = \varepsilon \;;\; v + v_1 = v' + v_1' \;;\; \mathbf{e}_n + \mathbf{e}_{n,1} = \mathbf{e}_n' + \mathbf{e}_{n,1}' \right\} \,,$$

$$[\varepsilon - \alpha_\varepsilon, \varepsilon + \alpha_\varepsilon] \quad \subset \quad \left\{ \mathbf{e}_{n,1}' \;\; / \;\; \mathbf{e}_n = \mathbf{e}_{n,1} = \varepsilon \;;\; v + v_1 = v' + v_1' \;;\; \mathbf{e}_n + \mathbf{e}_{n,1} = \mathbf{e}_n' + \mathbf{e}_{n,1}' \right\} \,.$$

In other words, the sets of outgoing electron energies $\mathbf{e}_n'$ and $\mathbf{e}_{n,1}'$ contain the set $[\varepsilon - \alpha_\varepsilon, \varepsilon + \alpha_\varepsilon]$, when the incoming energies are equal ε. This means that $\forall \varepsilon > \epsilon_1$ there exists an $\alpha_\varepsilon > 0$, such that

$$2(H \circ F)(\varepsilon) = (H \circ F)(\varepsilon - \alpha) + (H \circ F)(\varepsilon + \alpha) \qquad \forall \alpha \in [-\alpha_\varepsilon, \alpha_\varepsilon] \,.$$

Hence $H \circ F : (\epsilon_1, \infty) \to \mathbb{R}$ is an affine function, implying thus the existence of two functions μ and T with

$$F_{\mu,T}(\varepsilon) = \frac{1}{\eta + exp\frac{\varepsilon - \mu}{T}} \,,$$

and $T > 0$, ensuring the integrability of F.
The other inclusion $'' \supset ''$ is immediate.

□

Remark 3.3 *A consequence of Proposition 3.2 is that the solutions of (3.5) are given by a Fermi-Dirac distribution function*

$$f_n^0(t,x,v) = F_{\mu,T}(t,x,\epsilon_n + \frac{|v|^2}{2}) \,. \tag{3.12}$$

3.2 Properties of the operator $DQ_e(f^0)+Q_0$: formal approach

Before discussing the properties of the operator $DQ_e(f^0)+Q_0$, let us introduce the right functional framework. Straightforward computations lead to the following expression for the derivative of the electron-electron collision operator Q_e at F

$$\begin{aligned}[DQ_e(F)(f)]_n(v) &= \sum_{m,r,s}\int_{(\mathbb{R}^2)^3} \beta_{nmrs}\delta_{\mathbf{e}}\delta_v F'_r F'_{s,1}(1-\eta F_n)(1-\eta F_{m,1}) \\ &\qquad\qquad [h'_r + h'_{s,1} - h_n - h_{m,1}]\, dv_1 dv' dv'_1\,,\end{aligned} \tag{3.13}$$

with $F = F_{\mu,T}$ the Fermi-Dirac distribution function and

$$h_n(v) := \frac{f_n(v)}{F_n(v)(1-\eta F_n(v))}\,.$$

This leads to

$$\begin{aligned}\langle DQ_e(F)(f), g\rangle &= -\frac{1}{4}\sum_{n,m,r,s}\int_{(\mathbb{R}^2)^4} \beta_{nmrs}\delta_{\mathbf{e}}\delta_v F'_r F'_{s,1}(1-\eta F_n)(1-\eta F_{m,1}) \\ &\quad [h'_r + h'_{s,1} - h_n - h_{m,1}][g'_r + g'_{s,1} - g_n - g_{m,1}]\, dv dv_1 dv' dv'_1\,,\end{aligned} \tag{3.14}$$

Let us now define the Hilbert space

$$\mathbb{L}^2_F := \left\{ f = (f_n)_{n\in\mathbb{N}}, \quad \sum_{n=1}^{+\infty}\int_{\mathbb{R}^2} |f_n(v)|^2 \frac{1}{F_n(1-\eta F_n)}\, dv < +\infty \right\},$$

provided with the weighted scalar product

$$\langle f, g\rangle_F := \sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} f_n g_n \frac{1}{F_n(1-\eta F_n)}\, dv\,.$$

Moreover let us shortly denote by D_e the derivative operator $DQ_e(F)$ and let $\mathcal{Q} := Q_0 + D_e$. Then we have

Proposition 3.4 *Under Hypothesis 1 and 2, the operators Q_0 and D_e satisfy the following properties:*
(i) The operators Q_0 and D_e are bounded, symmetric, non-positive operators on $\mathbb{L}^2_F$.
(ii) The kernel of $\mathcal{Q}$ is given by

$$Ker(\mathcal{Q}) = \left\{ f \in \mathbb{L}^2_F \;;\; f_n(v) = G(\epsilon_n + \frac{|v|^2}{2}) \text{ with } G \in Span\{F(1-\eta F), F(1-\eta F)\epsilon\} \right\}$$

(iii) Let $\mathcal{P} : \mathbb{L}^2_F \to Ker(\mathcal{Q})$ be the orthogonal projection on $Ker(\mathcal{Q})$, then we have the coercivity inequality with a constant $C > 0$,

$$-\langle \mathcal{Q} f, f\rangle_F \geq C\|f - \mathcal{P} f\|^2_F\,, \quad \forall f \in \mathbb{L}^2_F\,.$$

(iv) The range of $\mathcal{Q}$ is closed and we have

$$R(\mathcal{Q}) = Ker(\mathcal{Q})^\perp = \left\{ f \in \mathbb{L}^2_F \;/\; \sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} f_n(v) \begin{pmatrix} 1 \\ \mathbf{e}_n \end{pmatrix} dv = 0 \right\}.$$

Proof Item (i) is immediate by using Hypothesis 1 and 2. To prove item (ii), let f belong to $Ker(\mathcal{Q})$. This implies $\langle (Q_0 + D_e)(f), f\rangle_F = 0$, and as Q_0 and D_e are non-positive operators, we obtain thus

$$\langle Q_0 f, f\rangle_F = 0 \quad ; \quad \langle D_e f, f\rangle_F = 0 \, .$$

From the first equality we deduce the existence of an energy dependent function $G(t, x, \varepsilon)$ such that

$$f_n(t,x,v) = G(t,x,\epsilon_n + \frac{|v|^2}{2}) \, .$$

From the second equality we deduce

$$\frac{G_n}{F_n(1-\eta F_n)} + \frac{G_{m,1}}{F_{m,1}(1-\eta F_{m,1})} = \frac{G'_r}{F'_r(1-\eta F'_r)} + \frac{G'_{s,1}}{F'_{s,1}(1-\eta F'_{s,1})} \, ,$$

for all $(n, m, r, s) \in \mathbb{N}^4$ and $(v, v_1, v', v'_1) \in (\mathbb{R}^2)^4$ with

$$\begin{cases} v + v_1 = v' + v'_1 \, , \\ \epsilon_n + \frac{|v|^2}{2} + \epsilon_m + \frac{|v_1|^2}{2} = \epsilon_r + \frac{|v'|^2}{2} + \epsilon_s + \frac{|v'_1|^2}{2} \, . \end{cases}$$

Similar arguments as in the proof of Proposition 3.2 imply that the function $\frac{G}{F(1-\eta F)}$ is an affine function of the energy variable ε, such that we can write with some functions $a(t, x)$ and $b(t, x)$

$$G(t,x,\varepsilon) = F(t,x,\varepsilon)(1-\eta F(t,x,\varepsilon))(a(t,x)\varepsilon + b(t,x)).$$

The proof of item (iii) is similar as in [3]. The operator D_e can be written in the form

$$(D_e f)_n(v) = -\nu_n f_n + \sum_i \int_{\mathbb{R}^2} K_{i,n}(u,v) \frac{f_i(u)}{F_i(u)(1-\eta F_i(u))} du = (\Upsilon f)_n(v) + (\mathcal{K} f)_n(v) \, ,$$

with

$$\nu_n(v) := \sum_{m,r,s} \int_{(\mathbb{R}^2)^3} \beta_{nmrs} \delta_{\mathbf{e}} \delta_v F'_r F'_{s,1} (1-\eta F_n)(1-\eta F_{m,1}) \frac{1}{F_n(1-\eta F_n)} \, dv_1 dv' dv'_1 \, ,$$

and

$$\begin{aligned} K_{i,n}(u,v) \;\; := \;\; & 2 \sum_{l,j} \int_{(\mathbb{R}^2)^2} \beta_{nlij} \delta(\mathbf{e}_n(v) + \mathbf{e}_l(v_1) - \mathbf{e}_i(u) - \mathbf{e}_j(v'_1)) \delta(v + v_1 - u - v'_1) \\ & \qquad F_i(u) F_j(v'_1)(1-\eta F_n(v))(1-\eta F_l(v_1)) \, dv_1 dv'_1 - \\ & - \sum_{l,j} \int_{(\mathbb{R}^2)^2} \beta_{nilj} \delta(\mathbf{e}_n(v) + \mathbf{e}_i(u) - \mathbf{e}_l(v') - \mathbf{e}_j(v'_1)) \delta(v + u - v' - v'_1) \\ & \qquad F_l(v') F_j(v'_1)(1-\eta F_n(v))(1-\eta F_i(u)) \, dv' dv'_1 \, . \end{aligned}$$

Using the boundedness property of the cross sections β_{nmrs}, it can be shown that $0 < \varrho_1 \leq \nu_n \leq \varrho_2$ with ϱ_1 and ϱ_2 independent on n, v, x and t, such that the spectrum of the self-adjoint operator $\Upsilon : \mathbb{L}^2_F \to \mathbb{L}^2_F$ satisfies

$$\sigma(\Upsilon) \subset [-\varrho_2, -\varrho_1] .$$

Moreover, the operator $\mathcal{K} : \mathbb{L}^2_F \to \mathbb{L}^2_F$ is shown to be a Hilbert-Schmidt operator and thus compact, implying with Weyl's theorem $\sigma_{ess}(D_e) = \sigma_{ess}(\Upsilon)$. Here we have denoted by σ_{ess} the essential spectrum of an operator. As furthermore D_e is self-adjoint and non-positive, we have $\sigma(D_e) \subset (-\infty, 0]$. Hence

$$\sigma(D_e) \subset]-\infty, -\varrho_3] \cup \{0\} \quad \text{with} \quad \varrho_3 > 0 .$$

Denoting by $\mathcal{P}_e : \mathbb{L}^2_F \to \ker D_e$ the orthogonal projection on $\ker D_e$, we have proven thus, that

$$-\langle D_e f, f\rangle_F \geq \varrho_3 ||f - \mathcal{P}_e f||^2_F \qquad \forall f \in \mathbb{L}^2_F .$$

The rest of the proof is identical to the proof in [3].

Finally, Item (iv) is a simple consequence of items (iii) and (ii). □

We can now pass to the resolution of the equation (3.6), which reads $\mathcal{Q}(f^1) = g$, with

$$g_n(v) := v \cdot \nabla_x f^0_n - \nabla_x \epsilon_n \cdot \nabla_v f^0_n .$$

According to (3.12), g can be rewritten as $g = v \cdot \nabla_x F$, where

$$\nabla_x F(t, x, \varepsilon) = -F(1 - \eta F) \left[\varepsilon \nabla_x \left(\frac{1}{T} \right) - \nabla_x \left(\frac{\mu}{T} \right) \right] .$$

The solvability condition $g \in Ker(\mathcal{Q})^\perp$ is obviously satisfied and we obtain

Proposition 3.5 *Equation (3.6) admits a unique solution $f^1 \in Ker(\mathcal{Q})^\perp$, which can be written in the form*

$$f^1 = -\nabla_x \left(\frac{\mu}{T} \right) \cdot \Psi^1 + \nabla_x \left(\frac{1}{T} \right) \cdot \Psi^2 , \tag{3.15}$$

with Ψ^1 and Ψ^2 unique solutions in $Ker(\mathcal{Q})^\perp$ of

$$\begin{aligned} (\mathcal{Q}(\Psi^1))_n(v) &= -v F_n (1 - \eta F_n) , \\ (\mathcal{Q}(\Psi^2))_n(v) &= -\mathbf{e}_n v F_n (1 - \eta F_n) . \end{aligned} \tag{3.16}$$

Finally we have to solve the last equation (3.7). The solvability condition reads

$$\sum_{n \in \mathbb{N}^*} \int_{\mathbb{R}^2} (\partial_t f^0_n + v \cdot \nabla_x f^1_n - \nabla_x \epsilon_n \cdot \nabla_v f^1_n) \begin{pmatrix} 1 \\ \mathbf{e}_n \end{pmatrix} dv = 0 , \tag{3.17}$$

where we have used the fact, that

$$\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} D^2Q_e(F)(f^1,f^1)_n \begin{pmatrix} 1 \\ \mathbf{e}_n \end{pmatrix} dv = 0\,. \tag{3.18}$$

Indeed, (3.9) is valid for all $f \in \mathbb{L}^2_F$, such that differentiating twice at F leads to (3.18). Let us now analyze (3.17) term by term. The first condition gives

- $$\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} \partial_t(F(t,x,\epsilon_n+\frac{|v|^2}{2}))dv = \partial_t\left(\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} F(t,x,\epsilon_n+\frac{|v|^2}{2})dv\right),$$

- $$\begin{aligned}\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} \nabla_x\cdot(vf^1_n)dv &= -\nabla_x\cdot\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} v\left[\nabla_x\left(\frac{\mu}{T}\right)\cdot\Psi^1_n - \nabla_x\left(\frac{1}{T}\right)\cdot\Psi^2_n\right]dv \\ &= -\nabla_x\cdot\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2}\left[(v\otimes\Psi^1_n)\cdot\nabla_x\left(\frac{\mu}{T}\right) - (v\otimes\Psi^2_n)\cdot\nabla_x\left(\frac{1}{T}\right)\right]dv \\ &= -\nabla_x\cdot\left\{\sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2} v\otimes\Psi^1_n dv\right)\cdot\nabla_x\left(\frac{\mu}{T}\right) - \sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2} v\otimes\Psi^2_n dv\right)\cdot\nabla_x\left(\frac{1}{T}\right)\right\},\end{aligned}$$

- $$\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} \nabla_v\cdot(f^1_n\nabla_x\epsilon_n)dv = 0\,.$$

For the second condition we get

- $$\begin{aligned}&\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} \partial_t(F(t,x,\epsilon_n+\frac{|v|^2}{2}))\mathbf{e}_n dv = \\ &\qquad = \partial_t\left(\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} F(t,x,\mathbf{e}_n)\mathbf{e}_n dv\right) - \sum_{n\in\mathbb{N}^*}\partial_t\epsilon_n\int_{\mathbb{R}^2} F(t,x,\mathbf{e}_n)\; dv\,,\end{aligned}$$

- $$\begin{aligned}&\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} \nabla_x\cdot(vf^1_n)\mathbf{e}_n dv = \nabla_x\cdot\sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2} vf^1_n\mathbf{e}_n dv\right) - \sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2} f^1_n v\cdot\nabla_x\epsilon_n dv\right) \\ &= -\nabla_x\cdot\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} v\left[\nabla_x\left(\frac{\mu}{T}\right)\cdot\Psi^1_n - \nabla_x\left(\frac{1}{T}\right)\cdot\Psi^2_n\right]\mathbf{e}_n dv - \sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2} f^1_n v\cdot\nabla_x\epsilon_n dv\right) \\ &= -\nabla_x\cdot\left\{\sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2}(v\otimes\Psi^1_n)\mathbf{e}_n dv\right)\cdot\nabla_x\left(\frac{\mu}{T}\right) - \sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2}(v\otimes\Psi^2_n)\mathbf{e}_n dv\right)\cdot\nabla_x\left(\frac{1}{T}\right)\right\} \\ &\qquad - \sum_{n\in\mathbb{N}^*}\left(\int_{\mathbb{R}^2} f^1_n v\cdot\nabla_x\epsilon_n dv\right),\end{aligned}$$

- $$\begin{aligned}-\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2}\nabla_x\epsilon_n\cdot\nabla_v f^1_n\mathbf{e}_n dv &= -\sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2}\nabla_v\cdot(\nabla_x\epsilon_n f^1_n\mathbf{e}_n)dv + \sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} f^1_n\nabla_x\epsilon_n\cdot v\,dv \\ &= \sum_{n\in\mathbb{N}^*}\int_{\mathbb{R}^2} f^1_n\nabla_x\epsilon_n\cdot v\,dv\,.\end{aligned}$$

Let us denote by ρ and $\rho\mathcal{E}$ the charge density respectively the energy associated to the Fermi-Dirac distribution function $F_{\mu,T}$

$$\rho(\mu,T) := \sum_{n\in\mathbb{N}^*} \int_{\mathbb{R}^2} F_{\mu,T}(t,x,\epsilon_n + \frac{|v|^2}{2})dv \quad ; \quad \rho\mathcal{E}(\mu,T) := \sum_{n\in\mathbb{N}^*} \int_{\mathbb{R}^2} F_{\mu,T}(t,x,\mathbf{e}_n)\mathbf{e}_n dv\,. \tag{3.19}$$

The diffusion matrices are given by

$$D_{1j} := \sum_{n\in\mathbb{N}^*} \left(\int_{\mathbb{R}^2} v \otimes \Psi_n^j dv \right) \quad ; \quad D_{2j} := \sum_{n\in\mathbb{N}^*} \left(\int_{\mathbb{R}^2} (v \otimes \Psi_n^j)\mathbf{e}_n dv \right)\,, \quad j=1,2\,, \tag{3.20}$$

where Ψ^1, Ψ^2 are solutions of (3.16). Then we can state the main theorem of this section

Theorem 3.6 (Formal diffusion limit)
The system of equations (3.5)-(3.7) is solvable if and only if f^0 and f^1 are determined by (3.12), respectively (3.15), and if moreover the functions $\mu(t,x)$ and $T(t,x)$, associated to the Fermi-Dirac distribution function $F_{\mu,T}$, which is given by

$$F_{\mu,T}(t,x,\varepsilon) := \frac{1}{\eta + exp\frac{\varepsilon-\mu(t,x)}{T(t,x)}}\,,$$

satisfy the following system

$$\partial_t \rho(\mu,T) + \nabla_x \cdot J_\rho = 0\,, \tag{3.21}$$

$$\partial_t(\rho\mathcal{E})(\mu,T) - \sum_{n\in\mathbb{N}^*} \partial_t \epsilon_n \int_{\mathbb{R}^2} F_{\mu,T}(t,x,\mathbf{e}_n)dv + \nabla_x \cdot J_{\mathcal{E}} = 0 \tag{3.22}$$

where the particle respectively energy currents J_ρ and $J_{\mathcal{E}}$ are defined as

$$\begin{aligned} J_\rho(\mu,T) &:= -D_{11}\cdot\nabla_x\left(\frac{\mu}{T}\right) + D_{12}\cdot\nabla_x\left(\frac{1}{T}\right) \\ J_{\mathcal{E}}(\mu,T) &:= -D_{21}\cdot\nabla_x\left(\frac{\mu}{T}\right) + D_{22}\cdot\nabla_x\left(\frac{1}{T}\right)\,, \end{aligned} \tag{3.23}$$

and where ρ, $\rho\mathcal{E}$ are given in (3.19)-(3.20).

The Energy-Transport model (3.21)-(3.23) is constituted of two continuity equations for the charge density and energy, completed by two relations for the charge and energy fluxes. The temperature of the particles is a variable of the problem, which is not the case for the Drift-Diffusion model, where the electron temperature coincides with that of the lattice. The parabolicity of the ET model is proven by the following

Lemma 3.7 *The composed diffusion matrix*

$$\mathcal{D} := \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix},$$

is a symmetric, positive definite matrix.

Proof The symmetry is an easy consequence of the self-adjointness of the operator $\mathcal{Q}$. Indeed

$$D_{ij}^{kl} = -\langle \mathcal{Q}\Psi_k^i, \Psi_l^j \rangle_F = -\langle \Psi_k^i, \mathcal{Q}\Psi_l^j \rangle_F = -\langle \mathcal{Q}\Psi_l^j, \Psi_k^i \rangle_F = D_{ji}^{lk}.$$

To prove, that $\mathcal{D}$ is positive definite, let $\xi = (\xi_1^1, \xi_1^2, \xi_2^1, \xi_2^2) \in \mathbb{R}^4$ be arbitrary chosen. Then, using the non-positivity of $\mathcal{Q}$, we get

$$\xi^t \mathcal{D} \xi = \sum_{l,j=1}^{2} \left[\sum_{i,k=1}^{2} \xi_i^k D_{ij}^{kl} \right] \xi_j^l = -\left\langle \mathcal{Q} \left(\sum_{i,k=1}^{2} \xi_i^k \Psi_k^i \right), \sum_{l,j=1}^{2} \xi_j^l \Psi_l^j \right\rangle_F \geq 0.$$

From (3.16) we remark that Ψ_l^j are linearly independent functions. Thus due to the coercivity of the operator $-\mathcal{Q}$ we have $\xi^t \mathcal{D} \xi = 0$ if and only if $\xi = 0$. Hence there exists even a constant $\gamma > 0$, such that

$$\xi^t \mathcal{D} \xi \geq \gamma |\xi|^2, \quad \forall \xi \neq 0.$$

□

To carry out the rigorous diffusion limit, we have to specify the right functional framework (see [4]) in order to introduce the notion of weak solution of the Boltzmann equation (3.1) and to state the properties of the operator $Q_e + Q_0$ correctly. Besides, an entropy dissipation estimate will be needed to prove the convergence of f^α towards a Fermi-Dirac distribution function $F_{\mu,T}$. This entropy estimate requires a bound for f^α ($\beta \leq f^\alpha \leq 1-\beta, \quad \beta > 0$), which is a very strong assumption. Possibilities to avoid this assumption have to be investigated. And finally, a compactness argument will permit to pass to the limit in the weak formulation of (3.1) in order to get the ET model, which was formally obtained in this paper. Due to its complexity, this rigorous diffusion limit is deferred to a future work.

4 Conclusion

In the present paper we have investigated two diffusion limits corresponding to different collision operators. Starting model was a coupled quantum/kinetic subband model, describing the electron evolution in the confinement direction by the Schrödinger equation and in the transport direction by the Boltzmann equation. In the limit of a vanishing scaling parameter $\alpha \to 0$, we obtained either the adiabatic Schrödinger/SHE model or the Schrödinger/ET model. By means of this diffusion approximation, we were able to derive expressions for the diffusion matrices, which are even explicitly computable in some simplified cases.

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