Macroscopic models for semiconductor heterostructures

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Abstract

The semiconductor Boltzmann equation is considered within a material with a space-dependent band characteristic. Its fluid limit under strong elastic collisions leads to the so-called Spherical Harmonics Expansion (SHE) model. For this model, the influence of smoothly space-dependent or abruptly discontinuous band characteristics is analyzed. For the latter case which occurs at heterojunction interfaces, kinetic boundary layers are analyzed and higher order transmission conditions are derived. In a further step, transmission conditions through heterojunctions for the energy-transport and drift-diffusion models (which are obtained as moments of the SHE model) are constructed.

Key words: Semiconductor Boltzmann Equation, Spherical Harmonics Expansion, Energy Transport model, Drift-Diffusion model, Space dependent band characteristics, Heterojunctions, Kinetic boundary layers.

AMS Subject classification : 35Q20, 76P05, 82A70, 78A35

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1 Introduction

The drift-diffusion (DD) model of semiconductors is, by far, the most simple and widely used macroscopic semiconductor model [23], [14]. Its derivation from the more fundamental kinetic model, the semiconductor Boltzmann equation, has been made mathematically rigorous in [12], [19].

However, the search for more accurate descriptions of carrier transport in semiconductors has been motivated by the recent developments of the microelectronics technology. Several models have been proposed to improve the DD model, including the hydrodynamic (HD) model [1] the energy-transport (ET) model [24], and the spherical Harmonic Expansion (SHE) model [8], [10]. Among these, the SHE and ET models have been proved to derive from a diffusion approximation of the Boltzmann Transport Equation [3], [4], [8], [17], while this question still remains open for the HD model. The diffusion approximation naturally provides consistent closure relations to the SHE and ET models while phenomenological arguments must be invoked to close the HD model. For this reason, in the present paper, we shall concentrate on the SHE and ET models, and on the DD model which stands as a submodel of the ET model.

The available derivations of the SHE and ET models concern materials with homogeneous crystalline structure [8], [4], [3]. The goal of the present paper is to extend them to materials with smoothly space-dependent band diagrams and to abrupt heterojunctions. Smoothly space dependent band diagrams appear in materials with graded stoechiometry (like $Al_x\, Ga_x\, As_{1-x}$) which are used in certain microelectronics components. Heterojunctions are now widely used in various applications. The DD model has been extended to smoothly space-dependent band diagrams in [15] and to heterojunctions in [20].

In section 2, we show that the SHE model for smoothly space-dependent band diagrams is structurally identical as for space independent band diagrams, provided that an adequate set of variables and unknowns are used. Similar conclusions are drawn for the ET and DD models in section 6.

For abrupt heterojunctions, the problem is more complicated. We start with the interface problem at the level of the Boltzmann equation. Interface conditions at the band discontinuity are set up in terms of reflexion-transmission matrices which take into account carrier scattering by the irregularities of the potential at the interface. Various properties of these interface conditions are reviewed in section 3, together with a few practical examples.

In section 4, we proceed to the diffusion approximation of the Boltzmann equation complemented with the interface conditions at the heterojunction. Transmission conditions for the SHE model are naturally derived from this procedure. As usual, the order of accuracy of the diffusion approximation is measured in terms of the dimensionless mean free path, ratio of the mean free path (associated with elastic collisions) to the typical size of the device. If the first order of accuracy is retained, two natural continuity relations are derived, one relating the values of the SHE-distribution function on each side, the other one relating its fluxes on each side. At the second order of accuracy, the continuity condition on the SHE distribution function is replaced by a condition which links its jump at the interface to the common value of its fluxes on each side of the interface. The coefficient in this combination is similar to the "extrapolation length" originating from the presence of kinetic boundary layers [2], [11] and introduced in the semiconductor context in [7], [27]. It is obtained as the equilibrium limit of two half space stationary kinetic problems connected with the interface conditions, which will later be referred to as a "two-sided Milne problem", in reference to the Milne problem of kinetic theory [2]. In section 5, it is shown that the two-sided Milne problem is sovable under reasonable assumptions on the solution of one-sided Milne problems with inflow boundary conditions. For special cases these assumptions can be verified. An approximation procedure in the spirit of, e.g., [11] is carried out leading (for rotationally invariant models) to explicit formulas for the above mentioned coefficient in the second order transmission condition.

Transmission conditions at heterojunction interfaces are then derived for the ET and the DD models by a moment expansion of the corresponding transmission conditions for the SHE model (section 6). This procedure supposes that there is no boundary layer in the ET or DD limit of the SHE model, or at least, that the influence of this boundary layer is negligible. This point will be discussed in detail in future work. The obtained first order transmission condition for the DD model reduces to the classical one [20]. For the DD model, transmission conditions of the form of the second order conditions have been derived in [26]. They correspond to a very rough approximation of the solution of the two-sided Milne problem.

We believe that the use of these second order transmission conditions will significantly improve the accuracy of the numerical treatment of heterojunction interfaces. Future work will be devoted to the numerical implementation of these conditions and their validation against experimental and numerical data.

2 The Spherical Harmonic Expansion (SHE) model

The SHE model is derived from the semiconductor Boltzmann equation through a diffusion approximation procedure using elastic collisions as dominant scattering mechanism. We refer to [3] for a discussion of the validity of the elastic approximation of the phonon collision operator. Here, our starting point will be the following Boltzmann equation

$$\frac{\partial f^\alpha}{\partial t} + \frac{1}{\alpha}\left(\nabla_k \varepsilon . \nabla_x f^\alpha - \nabla_x \varepsilon . \nabla_k f^\alpha\right) = \frac{1}{\alpha^2} Q(f^\alpha) + S(f^\alpha) , \tag{2.1}$$

where $f^\alpha = f^\alpha(x, k, t)$ is the electron distribution function depending on the position $x \in \mathbb{R}^3$, the momentum $k \in B$ and the time $t > 0$. The Brillouin zone B is the elementary cell of the dual lattice L^* and is identified with the torus $B = \mathbb{R}^3/L^*$. We suppose that B does not depend on x, which means that the interatomic distances remain the same as the material changes. This hypothesis is reasonable because abrupt heterojunctions or materials with graded stoechiometry are based on materials which share almost the same lattice characteristics.

The function $\varepsilon = \varepsilon(x, k, t)$ is the total particle energy of an electron in the lattice. It can be decomposed in the following way :

$$\varepsilon(x, k, t) = e(x, k) - V(x, t) = e(x, k) - \chi(x) - \phi(x, t)\,, \tag{2.2}$$

with $e(x, 0) = 0$. The function $e(x, k)$ is the kinetic energy measured from the bottom of the conduction band, while $-V(x, t)$ is the energy of the bottom of the conduction band measured from an arbitrary fixed origin [25]. The potential $V(x, t)$ can itself be decomposed into the Coulomb potential $\phi(x, t)$ arising from the electron space-charge, the doping and the applied bias, which is smooth and may depend upon t, and the electron affinity $\chi(x)$, which only depends on the material and is therefore independent of t. In the present section, we shall first suppose that $\chi(x)$ and $e(x, k)$ are smooth. The space-dependent kinetic energy $e(x, k)$ takes into account the variations of the band diagram as the material smoothly changes. A typical form of $e(x, k)$ is that of a parabolic band diagram with a space-dependent effective mass :

$$e(x, k) = \frac{k^2}{2m_*(x)}\,. \tag{2.3}$$

However, in the remainder of this section, any smooth C^1 function $e : (x, k) \in \mathbb{R}^3 \times B \longrightarrow \mathbb{R}$ will be admissible. We denote by $v(x, k) = \nabla_k \varepsilon(x, k, t) = \nabla_k e(x, k)$ the particle velocity.

The collision operator $Q(f)$ takes into account both impurity scattering and phonon scattering in its elastic limit [3], [8]. It is written :

$$Q(f)(k) = \int_B \Phi(x, k, k')\delta\left(\varepsilon(k') - \varepsilon(k)\right)\left(f(k') - f(k)\right) dk'\,, \tag{2.4}$$

where the (x, t) dependence of ε, f and $Q(f)$ has been omitted for brevity. The δ function in (2.4) expresses the elastic character of the interaction. $\Phi(x, k, k')$ is the transition matrix associated with the considered interactions. We shall not specify it (see [21]), assuming only its positivity and invariance under exchange of k and k'.

The collision operator $S(f)$ takes into account all the other interactions, these being considered as weaker than the elastic interaction: the inelastic correction to the phonon collisions, the electron-electron collisions, and possibly, other interaction mechanisms. Their exact expression will not be needed here and we refer to [3] for more details.

The equation (2.1) is already written in scaled form. The scaling is detailed in [3]. Let us just recall that the energy scale is that of the applied bias, and not that of the thermal energy associated with the lattice temperature, and consequently, to some extent, high field effects are included. The parameter α represents the scaled mean free path, i.e., the ratio of the mean free path for elastic interactions to the typical size of the phenomena under consideration. It is supposed small ($\alpha \ll 1$).

The SHE model is obtained as the formal limit of (2.1) when α tends to zero [3], [8], [22], by means of the Hilbert expansion:

$$f^\alpha = f^0 + \alpha f^1 + \alpha^2 f^2 + \dots . \tag{2.5}$$

After inserting the Ansatz (2.5) in (2.1), terms of equal powers of α at the left and right hand sides of (2.1) are identified. This formal expansion procedure will be carried out in the following, and a rigorous justification is left as the subject for future work. This means in particular that the occurring functions will be assumed sufficiently smooth such that the computations are justified.

Before proceeding, we recall the coarea formula [9]

$$\int_B \psi(k) dk = \int_{-\infty}^{\infty} \int_{\mathcal{S}_{(x,\varepsilon,t)}} \psi(k) \frac{dS_{(x,\varepsilon,t)}(k)}{|\nabla_k \varepsilon(x,k,t)|} d\varepsilon \, , \tag{2.6}$$

where $\mathcal{S}_{(x,\varepsilon,t)}$ is the ((x,t) dependent) manifold

$$\mathcal{S}_{(x,\varepsilon,t)} = \{k \in B, \, \varepsilon(x,k,t) = \varepsilon\} \, ,$$

in k-space and $dS_{(x,\varepsilon,t)}(k)$ is the Euclidean surface element on $\mathcal{S}_{(x,\varepsilon,t)}$. We denote by $dN_{(x,\varepsilon,t)}(k)$ the coarea and by $N(x,\varepsilon,t)$ the energy-density of states:

$$dN_{(x,\varepsilon,t)}(k) = \frac{dS_{(x,\varepsilon,t)}(k)}{|\nabla_k \varepsilon(x,k,t)|} \, , \quad N(x,\varepsilon,t) = \int_{\mathcal{S}_{(x,\varepsilon,t)}} dN_{(x,\varepsilon,t)}(k) \, . \tag{2.7}$$

The coarea formula (2.6) is valid for every $\psi \in C(\overline{B})$, if

$$N(x,\varepsilon,t) < \infty \quad \forall \, (x,\varepsilon,t) \in \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}^+ \tag{2.8}$$

holds. This is an assumption on the set where $\nabla_k \varepsilon$ vanishes and on its behaviour close to this set.

The collisions modelled by the operator Q do not change the energy of a particle. Therefore, we can consider Q as an operator acting on $L^2(\mathcal{S}_{(\S,\varepsilon,\sqcup)}, \lceil \mathcal{N}_{(\S,\varepsilon,\sqcup)})$ for every fixed (x,ε,t). From [3], we have

Lemma 2.1 *(i) The null space of Q consists of the constants only.*
(ii) The equation $Q(f) = g$ is solvable if and only if

$$\int_{\mathcal{S}_{(x,\varepsilon,t)}} g(k) \, dN_{(x,\varepsilon,t)}(k) = 0 \, , \tag{2.9}$$

and its solution f is unique provided that

$$\int_{\mathcal{S}_{(x,\varepsilon,t)}} f(k)\, dN_{(x,\varepsilon,t)}(k) = 0\,. \tag{2.10}$$

(iii) Q is a non-positive self-adjoint operator, i.e.,

$$\int_{\mathcal{S}_{(x,\varepsilon,t)}} Q(f)\, g\, d\, N_{(x,\varepsilon,t)} = \int_{\mathcal{S}_{(x,\varepsilon,t)}} f Q(g) dN_{(x,\varepsilon,t)}\,,$$
$$\int_{\mathcal{S}_{(x,\varepsilon,t)}} Q(f)\, f\, d\, N_{(x,\varepsilon,t)} \leq 0\,,$$

with equality implying that f is in the null space of Q.

A more precise functional setting and additional properties of Q can be found in [3] or [22]. A consequence of point (i) is that if $Q(f) = 0$ holds for a function $f(x,k,t)$, then $f(x,k,t) = F(x, \varepsilon(x,k,t), t)$ for a function F of position, energy and time.

The Hilbert procedure leads to the following sequence of equations for f^i, $i = 0,1,2$:

$$Q(f^0) = 0\,, \tag{2.11}$$
$$Q(f^1) = \nabla_k\varepsilon.\nabla_x f^0 - \nabla_x\varepsilon.\nabla_k f^0\,, \tag{2.12}$$
$$Q(f^2) = \nabla_k\varepsilon.\nabla_x f^1 - \nabla_x\varepsilon.\nabla_k f^1 + \frac{\partial f^0}{\partial t} - S(f^0)\,. \tag{2.13}$$

From (2.11) and Lemma 2.1 (i), it follows that there exists $F = F(x, \varepsilon, t)$, such that

$$f^0(x,k,t) = F(x, \varepsilon(x,k,t), t)\,. \tag{2.14}$$

The function $F(x,\varepsilon,t)$ cannot be specified further by using equation (2.11) alone. To derive the equation for F that we are looking for, we must solve the next order equations (2.12), (2.13). Equation (2.12) reduces to

$$Q(f^1) = \nabla_k\varepsilon.\nabla_x F\,.$$

Since $\nabla_x F$ only depends on the energy, f^1 can be written as

$$f^1 = -\lambda(x,k,t)\,.\nabla_x F + F^1(x, \varepsilon(x,k,t), t)\,, \tag{2.15}$$

where F^1 is arbitrary and λ is the solution of

$$-Q(\lambda) = \nabla_k\varepsilon\,, \quad \int_{\mathcal{S}_{(x,\varepsilon,t)}} \lambda\, dN_{(x,\varepsilon,t)} = 0\,. \tag{2.16}$$

Existence and uniqueness of solutions of (2.16) are guaranteed by Lemma 2.1 (ii), since $\int_{\mathcal{S}} \nabla_k\varepsilon\, dN = 0$. Note that (2.16) must be understood componentwise. Then we have the

Theorem 2.2 *Let f^0 and f^1 be given by (2.14) and (2.15). Then, a solution f^2 of (2.13) exists if and only if $F(x,\varepsilon,t)$ satisfies*

$$N(x,\varepsilon,t)\left(\frac{\partial F}{\partial t}-\frac{\partial\phi}{\partial t}\frac{\partial F}{\partial\varepsilon}\right)-\nabla_x.\left(D(x,\varepsilon,t)\nabla_x F\right)=\bar{S}(F)\,, \tag{2.17}$$

with the diffusion matrix $D(x,\varepsilon,t)$ given by

$$D(x,\varepsilon,t)=\int_{\mathcal{S}_{(x,\varepsilon,t)}}\nabla_k\varepsilon\otimes\lambda\,dN_{(x,\varepsilon,t)}\,, \tag{2.18}$$

where $\otimes$ denotes the tensor product, and

$$\bar{S}(F)=\int_{\mathcal{S}_{(x,\varepsilon,t)}}S(F)\,dN_{(x,\varepsilon,t)}\,.$$

Proof : With (2.15), (2.13) is written as

$$\begin{aligned} Q(f^2) &= \nabla_k\varepsilon\cdot\nabla_x F^1-\nabla_x\cdot\left(\nabla_k\varepsilon\,(\lambda\cdot\nabla_x F)\right)\\ &\quad+\nabla_k\cdot\left(\nabla_x\varepsilon\,(\lambda\cdot\nabla_x F)\right)+\frac{\partial F}{\partial t}+\frac{\partial F}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial t}-S(F)\,. \end{aligned}$$

Then, the solvability condition (2.9), together with the identities (valid for any smooth function $u(x,k,t)$, denoting, for short, $\mathcal{S}_\varepsilon:=\mathcal{S}_{(x,\varepsilon,t)}$, $dN_\varepsilon:=dN_{(x,\varepsilon,t)}$):

$$\begin{aligned} \nabla_x\left(\int_{\mathcal{S}_\varepsilon}u\,dN_\varepsilon\right) &= \int_{\mathcal{S}_\varepsilon}\nabla_x u\,dN_\varepsilon-\frac{\partial}{\partial\varepsilon}\left(\int_{\mathcal{S}_\varepsilon}u\,\nabla_x\varepsilon dN_\varepsilon\right)\,,\\ \int_{\mathcal{S}_\varepsilon}\nabla_k u\,dN_\varepsilon &= \frac{\partial}{\partial\varepsilon}\int_{\mathcal{S}_\varepsilon}\nabla_k\varepsilon\,u\,dN_\varepsilon\,, \end{aligned}$$

leads to the result. Here, we have used (2.2) to ensure that $\frac{\partial\varepsilon}{\partial t}=-\frac{\partial\phi}{\partial t}$ is independent of k. ∎

Remark 2.3 The SHE model (2.17) with an x-dependent band diagram is identical to the standard SHE model expressed in terms of the total energy variable (compare to [3], equs. (III.23), (III.24)). The only difference lies in the position-dependent density of states N and diffusivity D. We also note that, following [3], the diffusivity is a symmetric non negative matrix, which satisfies

$$D\geq\frac{C}{N}\int_{\mathcal{S}_\varepsilon}\nabla_k\varepsilon\otimes\nabla_k\varepsilon\,dN_\varepsilon\,,$$

where $C>0$ is a constant related to the coercivity constant of Q and $(\nabla_k\varepsilon\ \nabla_k\varepsilon)$ is the tensor square of $\nabla_k\varepsilon$. We shall not detail this point here. ∎

Remark 2.4 $F(x,\varepsilon,t)$ is defined on the (time-dependent) domain (see figure 1)

$$\mathcal{O}_t = \{(x,\varepsilon) \in \Omega \times \mathrm{I\!R} \mid N(x,\varepsilon,t) > 0\} = \{(x,\varepsilon) \in \Omega \times \mathrm{I\!R} \mid \varepsilon \in \mathcal{R}\varepsilon(x,.,t)\}\,, \quad (2.19)$$

where Ω is the device domain in x-space and $\mathcal{R}\varepsilon(x,.,t)$ is the numerical range of the energy function $k \in B \to \varepsilon(x,k,t)$. Therefore, boundary conditions must be prescribed for $x \in \partial\Omega$ or $\varepsilon \in \partial\mathcal{R}\varepsilon(x,.,t)$. For $x \in \partial\Omega$, we refer to [7] where this question is addressed in detail. For $\varepsilon \in \partial\mathcal{R}\varepsilon(x,.,t)$, it is enough to note that the diffusion constant D (see (2.18)) vanishes, because the density of states vanishes. Thus, the parabolic problem (2.17) degenerates (see [3] for details) and no boundary condition needs to be prescribed. ∎

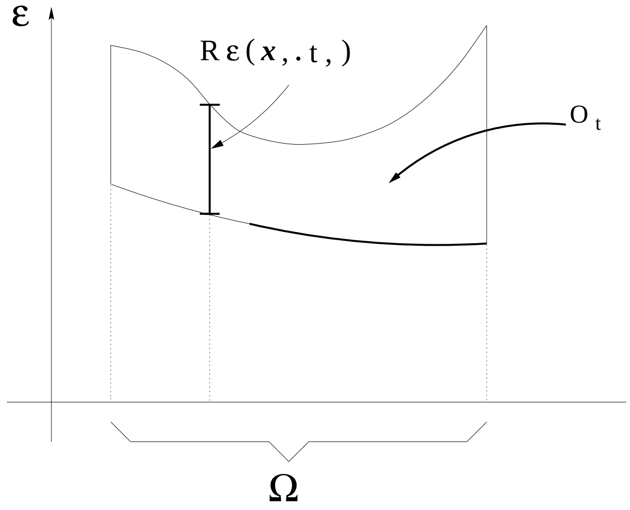

Figure 1: *Domain of definition of F: Case of a smooth band diagram*

Now, instead of a smoothly x-dependent band diagram, we consider a heterojunction, modeled as an abrupt interface Σ separating two media Ω_1 and Ω_2 which have different band diagram characteristics. Let us denote by $e_i(k)$ and χ_i , $i = 1,2$, the kinetic energy and the affinity of each material. For simplicity, we now assume that e_i and χ_i do not vary within Ω_i. Therefore

$$\varepsilon(x,k,t) = e_i(k) - \chi_i - \phi(x,t)\,, \quad x \in \Omega_i\,,\ k \in B\,,\ t > 0\,.$$

For $x \in \Sigma$, let

$$\varepsilon_i(x,k,t) = \lim_{y \to x,\, y \in \Omega_i} \varepsilon(y,k,t)\,,$$

The jump discontinuity of the band diagram characteristics across Σ results in similar jump discontinuities of the coefficients $N(x,\varepsilon,t)$ and $D(x,\varepsilon,t)$ (see formulas (2.7) and (2.18)). In a weak formulation of (2.17) this does not cause any problem, and the resulting interface conditions are continuity of F and of the normal flux $\nu^T D \nabla_x F$ across Σ:

$$F_1 = F_2 \quad , \quad \nu^T D_1 \nabla_x F_1 = \nu^T D_2 \nabla_x F_2 \, , \quad x \in \Sigma \, . \tag{2.20}$$

Here, $\nu(x)$ denotes the normal vector to Σ at a given point x oriented say from 1 to 2, ν^T, the transpose of ν and:

$$\nu^T D \nabla_x F = \sum_{i,j} \nu_i D_{ij} \frac{\partial F}{\partial x_j} \, .$$

Remark 2.5 For $x \in \Sigma$, conditions (2.20) are only valid for the values of ε such that $(x, \varepsilon) \notin \partial \mathcal{O}_t$, where $\mathcal{O}_t$ is the domain of definition of F (2.19). When $(x, \varepsilon) \in \partial \mathcal{O}_t$, for instance, if $\min \varepsilon_1(x, ., t) < \varepsilon < \min \varepsilon_2(x, ., t)$, a boundary condition must be assigned to F_1 instead (see figure 2). But since electrons of energy ε are totally reflected by the potential barrier, there is no net flux across the heterojunction, and the boundary condition is naturally the zero flux condition:

$$\nu^T D_1 \nabla_x F_1(x, \varepsilon, t) = 0 \tag{2.21}$$

At variance with Remark 2.3, D_1 is not necessarily degenerate because ε is not an extremal value of $\varepsilon_1(x, ., t)$. A similar condition must of course be assigned to F_2 when (x, ε) is an end point of the domain of definition of F_2. ∎

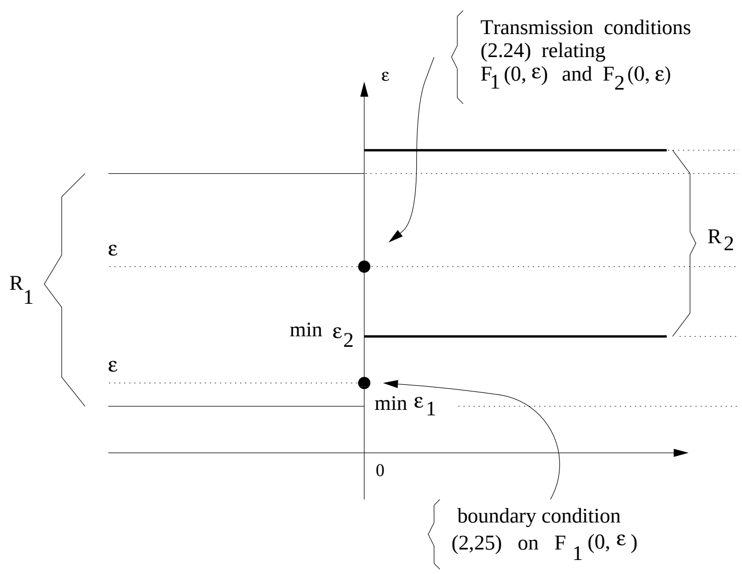

Figure 2: *Domain of definition of F: Case of an abrupt heterojunction at Σ*

Transmission conditions (2.20), (2.21) may be justified by successively performing a diffusion limit of the Boltzmann equation for a smoothed band diagram and then letting the smoothing parameter go to zero. A natural question is whether these two procedures commute, or equivalently, does the diffusion limit of a kinetic model with discontinuous band diagram lead to transmission conditions (2.20), (2.21)? In the next section, we set up the heterojunction transmission problem at the kinetic level. Then, in section 4, we show that conditions (2.20), (2.21) are deduced from a first order diffusion approximation of this problem. We then derive more accurate conditions from a second order diffusion approximation.

3 The kinetic transmission problem at a heterojunction

We focus on a transmission problem which describes a one-dimensional heterojunction. We let $\Omega_1 = (-\infty, 0)$, $\Omega_2 = (0, \infty)$ and we denote by $f_i^\alpha(x, k, t)$, $x \in \Omega_i$, $k \in B$, $t \geq 0$, the distribution function in Ω_i, which solves (with obvious notations)

$$\frac{\partial f_i^\alpha}{\partial t} + \frac{1}{\alpha}\left(v_{i,x}\frac{\partial f_i^\alpha}{\partial x} + \frac{\partial \phi}{\partial x}\frac{\partial f_i^\alpha}{\partial k_x}\right) = \frac{1}{\alpha^2}Q_i(f_i^\alpha) + S_i(f_i^\alpha)\,, \tag{3.1}$$

where $e_i(k)$, $i = 1, 2$, is the kinetic energy in each domain Ω_i and $v_{i,x}(k) = (\partial e_i/\partial k_x)(k)$ is the associated velocity in the x-direction. We recall that the affinity χ_i is constant over Ω_i and that the total energy is given by

$$\varepsilon(x, k, t) = e_i(k) - \chi_i - \phi(x, t)\,, \qquad x \in \Omega_i\,.$$

For simplicity, we set $\phi(0, t) = 0$ and we denote by $\varepsilon_i(k)$ the right and left limits of ε at 0:

$$\varepsilon_i(k) = e_i(k) - \chi_i \tag{3.2}$$

The numerical range of ε_i is denoted by $\mathcal{R}_i$.

In the following, we shall assume (which is satisfied in practice [21]) a reflection symmetry of the model. As a consequence, the functions $e_i(k)$, $i = 1, 2$ are even and the collision operators are even in the sense that for any arbitrary smooth function $f(k)$, we have:

$$Q_i(f(-k)) = Q_i(f)(-k)\,, \quad S_i(f(-k)) = S_i(f)(-k) \tag{3.3}$$

We now set up boundary conditions for f_i at $x = 0$. Particle scattering by the interface is due to the localized potential which sits at the heterojunction because of the change in crystalline structure. It may be described at the kinetic level by scattering operators mutually relating the incoming and outgoing parts (relative to Ω_i) of the two distribution functions f_i, $i = 1, 2$ at the interface. The spirit is similar to gas-surface interaction operators [5]. However, here we assume the scattering to be of purely elastic nature and the theory of [5] must be slightly adapted.

We respectively denote by f_i^+ and f_i^- the outgoing and incoming parts of the distribution function f_i at $x = 0$:

$$f_i^{\pm} = f_i|_{\{k \in B\,,\, \pm\sigma_i\, v_{i,x}(k) > 0\}} \quad \text{with} \quad \sigma_1 = +1 \quad \text{and} \quad \sigma_2 = -1\,. \tag{3.4}$$

The reflexion-transmission problem for f_i at $x = 0$ is written as

$$f_i^- = \mathcal{T}_i(f_1^+, f_2^+)\,, \quad i = 1, 2\,, \tag{3.5}$$

with, for $k \in B$ such that $\sigma_i v_{i,x}(k) < 0$:

$$\begin{aligned} \mathcal{T}_i(f_1^+, f_2^+)(k) = &\int_{\{k' \in B,\ \sigma_i v_{i,x}\,(k') > 0\}} R_i(k' \to k)\, \delta(\varepsilon_i(k) - \varepsilon_i(k'))\, f_i(k')\, dk' \\ &+ \int_{\{k' \in B,\ \sigma_j v_{j,x}(k') > 0\}} T_{j \to i}(k' \to k)\, \delta(\varepsilon_i(k) - \varepsilon_j(k'))\, f_j(k')\, dk'\,. \end{aligned} \tag{3.6}$$

In (3.6), the first integral accounts for the reflexion of particles of Ω_i by the interface, while the second one describes their transmission from Ω_j into Ω_i. The delta functions express that reflexion as well as transmission occur with conservation of total particle energy. The coefficients $R_i(k' \to k)$ and $T_{i \to j}(k' \to k)$ are nonnegative measures derived from the scattering operator of the underlying microscopic dynamics [18].

For $\varepsilon \in \mathbb{R}$, we introduce

$$\mathcal{S}_\varepsilon^i = \{k \in B\,,\, \varepsilon_i(k) = \varepsilon\}\,, \quad dN_\varepsilon^i(k) = \frac{dS_\varepsilon^i(k)}{|\nabla_k \varepsilon_i(k)|}\,, \tag{3.7}$$

$dS_\varepsilon^i(k)$ being the Euclidean surface element on $\mathcal{S}_\varepsilon^i$. Also, we introduce

$$\mathcal{S}_\varepsilon^{i,\pm} = \{k \in \mathcal{S}_\varepsilon^i, \quad \pm\, \sigma_i\, v_{i,x}\,(k) > 0\}$$

and σ_i given by (3.4). Then, using the coarea formula (2.6), relation (3.6) can be rewritten for $k \in B$ such that $\sigma_i v_{i,x}(k) < 0$:

$$\begin{aligned} \mathcal{T}_i(f_1^+, f_2^+)(k) \;\; &= \;\; \int_{\mathcal{S}^{i,+}_{\varepsilon_i(k)}} R_i(k' \to k)\, f_i(k')\, dN^i_{\varepsilon_i(k)}(k') \\ &+ \;\; \int_{\mathcal{S}^{j,+}_{\varepsilon_i(k)}} T_{j \to i}(k' \to k)\, f_j(k')\, dN^j_{\varepsilon_i(k)}(k')\,, \end{aligned} \tag{3.8}$$

with the convention that $j \neq i$ in (3.8). In particular, we note that, if $\varepsilon_i(k) \notin \mathcal{R}_j$ (where we recall that $\mathcal{R}_i$ denotes the numerical range of $\varepsilon_i(k)$), the second integral in (3.8) is identically zero (because $\mathcal{S}^j_{\varepsilon_i(k)} = \emptyset$). Thus, for such particle energies, only reflexion occurs, as expressed by the first integral in (3.8).

We now set up conditions for the reflexion-transmission operators $\mathcal{T}_i$ to provide a physically sound description of electron scattering by the interface.

Hypothesis 1: Current conservation.

$$\begin{aligned}|v_{i,x}(k)| &= \int_{\mathcal{S}^{i,-}_{\varepsilon_i(k)}} |v_{i,x}(k')|\, R_i(k \to k')\, dN^i_{\varepsilon_i(k)}(k') \\ &\quad + \int_{\mathcal{S}^{j,-}_{\varepsilon_i(k)}} |v_{j,x}(k')|\, T_{i\to j}(k \to k')\, dN^j_{\varepsilon_i(k)}(k')\,, \end{aligned} \tag{3.9}$$

holds for all $k \in B$ such that $\sigma_i\, v_{i,x}(k) > 0$, with again $j \neq i$ in (3.9).

With property (3.9), the flux of particles of given energy ε is continuous through the interface, as asserted by the following Lemma, the proof of which is a simple computation:

Lemma 3.1 *Let $f_i(k)$, $i = 1, 2$, be connected through relation (3.5) with R_i and $T_{i\to j}$ satisfying Hypothesis 1. Then, we have,*

$$\int_{\mathcal{S}^1_\varepsilon} v_{1,x}\, f_1\, dN^1_\varepsilon = \int_{\mathcal{S}^2_\varepsilon} v_{2,x}\, f_2\, dN^2_\varepsilon\,, \quad \forall \varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2\,, \tag{3.10}$$

$$\int_{\mathcal{S}^i_\varepsilon} v_{i,x}\, f_i\, dN^i_\varepsilon = 0\,, \quad \forall \varepsilon \in \mathcal{R}_i \setminus \mathcal{R}_j\,. \tag{3.11}$$

Conversely, for (3.10) and (3.11) to be satisfied for any pair (f_1, f_2) connected by (3.5), R_i and $T_{i\to j}$ must satisfy (3.9).

Hypothesis 2: Reciprocity. For all k, k' in B such that $\varepsilon_i(k) = \varepsilon_i(k')$ and $\sigma_i v_{i,x}(k) > 0$, $\sigma_i v_{i,x}(k') < 0$, we assume

$$|v_{i,x}(k')|\, R_i(k \to k') = |v_{i,x}(-k)|\, R_i(-k' \to -k)\,, \tag{3.12}$$

Similarly, for all k, k' in B such that $\varepsilon_i(k) = \varepsilon_j(k')$ and $\sigma_i v_{i,x}(k) > 0$, $\sigma_j v_{j,x}(k') < 0$, we assume

$$|v_{j,x}(k')|\, T_{i\to j}(k \to k') = |v_{i,x}(-k)|\, T_{j\to i}(-k' \to -k)\,, \tag{3.13}$$

where σ_i is given by (3.4).

Relations (3.12), (3.13) result from the time reversibility (and thus, the unitarity of the scattering matrix) of the microscopic particle dynamics at the interface (see e.g. [18]). The validity of the reciprocity relation is discussed in [5] for gas-surface interaction.

Combining (3.9) with (3.12) and (3.13), and using the evenness of $e_i(k)$, we obtain:

$$1 = \int_{\mathcal{S}^{i,+}_{\varepsilon_i(k)}} R_i(k' \to k)\, dN^i_{\varepsilon_i(k)}(k') + \int_{\mathcal{S}^{j,+}_{\varepsilon_i(k)}} T_{j\to i}(k' \to k)\, dN^j_{\varepsilon_i(k)}(k')\,, \tag{3.14}$$

for all k such that $\sigma_i v_{i,x}(k) < 0$. It follows that the constant function equal to 1 is a particular solution of the interface condition (3.5).

Hypothesis 3: Transmittivity. Some transmission occurs whenever it is energetically possible:

$$\overline{T}_{j\to i}(k,\varepsilon) := \int_{\mathcal{S}_\varepsilon^{j,+}} T_{j\to i}(k'\to k)dN_\varepsilon^j(k') > 0 \tag{3.15}$$

for every $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$ and for k in a subset of $\mathcal{S}_\varepsilon^{i,-}$ with positive measure.

Note that by the reciprocity relation (3.13), (3.15) holds for both $T_{1\to2}$ and $T_{2\to1}$, even if it is only required for one of them. As mentioned above, only reflexion occurs for particle energies not in the common range of ε_1 and ε_2:

$$\overline{T}_{j\to i}(\cdot,\varepsilon) = 0\,, \qquad \varepsilon \in \mathcal{R}_i \setminus \mathcal{R}_j\,. \tag{3.16}$$

Lemma 3.2 *Let R_i and $T_{i\to j}$ satisfy Hypotheses 1–3. Assume, in addition, that the functions $e_i(k)$ are even. Then, two functions $F_1(\varepsilon_1(k))$ and $F_2(\varepsilon_2(k))$ of the energy satisfy the transmission condition (3.5) if and only if*

$$F_1(\varepsilon) = F_2(\varepsilon) \qquad \forall\, \varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2\,. \tag{3.17}$$

Proof : Using (3.14), the transmission conditions for F_1 and F_2 can be written as

$$\overline{T}_{j\to i}(k,\varepsilon)(F_1(\varepsilon) - F_2(\varepsilon)) = 0\,. \tag{3.18}$$

The result follows immediately from (3.15) and (3.16). ∎

With (3.14), relation (3.8) expresses that f_i^- is a convex combination of f_1^+ and f_2^+. We deduce the following version of the Darrozes-Guiraud inequality [5] for our particular transmission process:

Lemma 3.3 *Let f_i satisfy the transmission condition (3.5), with reflexion-transmission matrices satisfying Hypotheses 1 and 2 and with even functions $e_i(k)$. Then, we have (with σ_i given by (3.4)):*

$$\int_{\mathcal{S}_\varepsilon^2} v_{2,x}\,|f_2|^2\,dN_\varepsilon^2 \le \int_{\mathcal{S}_\varepsilon^1} v_{1,x}\,|f_1|^2\,dN_\varepsilon^1, \quad \forall \varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2, \tag{3.19}$$

$$\sigma_i \int_{\mathcal{S}_\varepsilon^i} v_{i,x}\,|f_i|^2\,dN_\varepsilon^i \ge 0\,, \quad \forall \varepsilon \in \mathcal{R}_i \setminus \mathcal{R}_j\,, \tag{3.20}$$

Proof : Using Jensen's inequality on (3.8), assuming $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$, and $\varepsilon_i(k) = \varepsilon$, we get

$$\begin{aligned} |f_i^-(k)|^2 \;&\le\; \int_{\mathcal{S}_\varepsilon^{i,+}} R_i(k'\to k)\,|f_i(k')|^2\,dN_\varepsilon^i(k') \\ &+\; \int_{\mathcal{S}_\varepsilon^{j,+}} T_{j\to i}(k'\to k)\,|f_j(k')|^2\,dN_\varepsilon^j(k')\,. \end{aligned} \tag{3.21}$$

Then, multiplying (3.21) by $v_{i,x}(k)$, integrating over $\mathcal{S}_\varepsilon^{i,-}$, summing up the contributions of f_1 and f_2 and using (3.9) we obtain (3.19). The inequality (3.20) can be proven in a similar way. ∎

We now give two examples of transmission operators $\mathcal{T}_i$ which satisfy the above Hypotheses 1–3.

Example 1: semi-classical transmission of particles between media with spherically symmetric band diagrams accross a perfectly plane interface. From Hamiltonian mechanics, we know that the transmission of a particle accross a perfectly plane interface occurs with conservation of parallel momentum and total energy. We assume that transmission of a particle with momentum k from side i to side j produces a particle with momentum k'. Denoting by y and z the coordinates parallel to the heterojunction, the transmission process can be written as:

$$k'_y = k_y, \quad k'_z = k_z, \quad \varepsilon_j(k') = \varepsilon_i(k) \tag{3.22}$$

with ε_i given by (3.2). We suppose that e_i is spherically symmetric: $e_i(k) = \overline{e}_i(|k|)$, with a strictly monotone $\overline{e}_i$ (parabolic band diagrams (2.3) being obviously covered by this assumption). Relation $\varepsilon = \overline{e}_i(|k|) - \chi_i$ can be inverted and we denote by $|k| = \kappa_i(\varepsilon)$ the inverse relation. From the first two relations in (3.22), we deduce that

$$|k'|^2 - k_x'^2 = |k|^2 - k_x^2\,,$$

and, with the last relation (3.22) and the definition of κ_i, we obtain that the transverse momentum is transmitted according to

$$k'_x = \sigma_i \psi_i(k)^{1/2}\,, \quad \psi_i(k) = k_x^2 - |k|^2 + \kappa_j(\varepsilon_i(k))^2\,, \tag{3.23}$$

if $\psi_i(k) > 0$, the particle being reflected (with $k'_x = -k_x$) otherwise.

Now, we define the reflexion-transmission operator $\mathcal{T}_i$ according to:

$$\mathcal{T}_i(f_1^+, f_2^+)(k) = (1 - \overline{T}_{j\to i}(k)) f_i^+(rk) + \overline{T}_{j\to i}(k) f_j^+(t_{j\to i}k)\,, \tag{3.24}$$

with $i = 1, 2$, $j \neq i$, $k \in B$, such that $\sigma_i k_x \leq 0$ and with $\overline{T}_{j\to i}(k)$ being the transmission probability of the semiclassical transmission process, satisfying:

$$0 \leq \overline{T}_{j\to i}(k) \leq 1\,, \qquad \overline{T}_{j\to i}(k) = 0 \quad \text{if } \psi_i(k) < 0\,. \tag{3.25}$$

The case of a purely classical transmission is covered with $\overline{T}_{j\to i}(k) = 1$ when $\psi_i(k) > 0$ and $\overline{T}_{j\to i}(k) = 0$ otherwise.

In (3.24), r and $t_{j\to i}$ are particle reflexion and transmission operators defined by inverting (3.23):

$$t_{j\to i}\,k = (-\sigma_i \psi_i(k)^{1/2},\, k_y, k_z) \quad \text{if} \quad \psi_i(k) > 0\,, \tag{3.26}$$

$$rk = (-k_x, k_y, k_z)\,, \tag{3.27}$$

for $k \in B$, such that $\sigma_i k_x \le 0$.

The reflexion and transmission matrices associated with (3.24) can be determined from:

$$T_{j\to i}(k' \to k)\, \delta(\varepsilon_i(k) - \varepsilon_j(k')) = \overline{T}_{j\to i}(k)\, \delta(k' - t_{j\to i} k)\,, \qquad (3.28)$$

$$R_i(k' \to k)\, \delta(\varepsilon_i(k) - \varepsilon_i(k')) = (1 - \overline{T}_{j\to i}(k))\, \delta(k' - rk)\,. \qquad (3.29)$$

We easily deduce that Hypotheses 1 and 2 hold if and only if $\overline{T}_{j\to i}$ satisfy the following properties:

$$\overline{T}_{j\to i}(k_x, -k_y, -k_z) = \overline{T}_{j\to i}(k_x, k_y, k_z)\,, \quad \overline{T}_{j\to i}(k) = \overline{T}_{i\to j}(r t_{j\to i} k)\,. \qquad (3.30)$$

The last property is the usual quantum-mechanical reciprocity relation [16]. A simple computation using (3.28) shows that the notation $\overline{T}_{j\to i}$ for the transmission probabilities is compatible with its definition in (3.15). Thus, the assumption

$$\overline{T}_{j\to i}(k) > 0 \qquad \text{for } \psi_i(k) > 0\,,$$

is sufficient for Hypothesis 3 to be satisfied.

Semi-classical transmission probabilities $\overline{T}_{j\to i}$ can be deduced from a scattering analysis of a one-dimensional Schrödinger model of the heterojunction. A simple example is the formula [26]

$$\overline{T}_{j\to i}(k) = \frac{4k_x (t_{j\to i}k)_x m_i m_j}{(k_x m_j + (t_{j\to i}k)_x m_i)^2}$$

for the case of a step barrier and parabolic bands $e_i(k) = k^2/(2m_i)$ on both sides. ∎

Example 2: Purely isotropic reflexion-transmission operators: Here we assume that the reflexion-transmission coefficients are such that the incoming distributions f_i^- only depend on $\varepsilon_i(k)$. This implies that $R_i(k \to k')$ and $T_{i\to j}(k \to k')$ only depend on k. Then, Hypothesis 2 implies that R_i and $T_{i\to j}$ are of the form

$$R_i(k \to k') = \hat{R}_i(\varepsilon_i(k))|v_{i,x}(k)|\,, \qquad T_{i\to j}(k \to k') = \hat{T}(\varepsilon_i(k))|v_{i,x}(k)|\,.$$

Moreover, by Hypothesis 1, we deduce that $\hat{R}_i$ and $\hat{T}$ must satisfy the relations

$$1 = \alpha_i(\varepsilon)\hat{R}_i(\varepsilon) + \alpha_j(\varepsilon)\hat{T}(\varepsilon)\,, \qquad i \ne j\,,$$

for $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$ with

$$\alpha_i(\varepsilon) = \int_{\mathcal{S}_\varepsilon^{i,-}} |v_{i,x}|\, dN_\varepsilon^i\,. \qquad (3.31)$$

Therefore, R_i and $T_{i\to j}$ are given in terms of the single arbitrary function $\hat{T}(\varepsilon)$:

$$R_i(k \to k') = |v_{i,x}(k)| \frac{1 - \alpha_j \hat{T}}{\alpha_i}(\varepsilon_i(k))\,, \quad T_{i\to j}(k \to k') = |v_{i,x}(k)|\hat{T}(\varepsilon_i(k))\,, \quad (3.32)$$

with $0 \le \hat{T}(\varepsilon) \le \min(1/\alpha_1(\varepsilon), 1/\alpha_2(\varepsilon))$ for $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$ and $\hat{T}(\varepsilon) = 0$ otherwise. By $\overline{T}_{i\to j} = \alpha_i \hat{T}$, the assumption $\hat{T}(\varepsilon) > 0$ for $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$ is sufficient for Hypothesis 3 to be satisfied. ∎

4 Diffusion approximation of the heterojunction model

In this section we assume that the transmission operator is given by (3.6) and satisfies Hypotheses 1–3. We start with the definition of an order k approximate solution:

Definition 4.1 *f_i^α is an order k approximate solution of the Boltzmann transmission problem (3.1), (3.5) if*
(i) f_i^α solves the Boltzmann equation (3.1) up to order α^k terms in each domain Ω_i:

$$\frac{\partial f_i^\alpha}{\partial t} + \frac{1}{\alpha}\left(v_{i,x}\,\frac{\partial f_i^\alpha}{\partial x} + \frac{\partial \phi}{\partial x}\,\frac{\partial f_i^\alpha}{\partial k_x}\right) - \frac{1}{\alpha^2}\,Q_i(f_i^\alpha) - S_i(f_i^\alpha) = \mathcal{O}(\alpha^k)\,, \tag{4.1}$$

(ii) f_i^α satisfies the transmission condition (3.5) up to order α^k terms:

$$f_i^\alpha(0,.,t)^- = \mathcal{T}_i\left(f_1^\alpha(0,.,t)^+,\, f_2^\alpha(0,.,t)^+\right) + \mathcal{O}(\alpha^k)\,, \tag{4.2}$$

(iii) The flux of particles of given energy ε given by

$$J_i^\alpha(x,\varepsilon,t) = \frac{1}{\alpha}\int_{\mathcal{S}_{(x,\varepsilon,t)}} v_{i,x}(k)\, f_i^\alpha(x,k,t)\, dN_{(x,\varepsilon,t)}(k)\,,$$

is continuous through the interface up to order α^k terms, i.e.

$$J_1^\alpha(0,\varepsilon,t) - J_2^\alpha(0,\varepsilon,t) = \mathcal{O}(\alpha^k)\,, \quad \forall \varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2\,, \tag{4.3}$$

$$J_i^\alpha(0,\varepsilon,t) = \mathcal{O}(\alpha^k)\,, \quad \forall \varepsilon \in \mathcal{R}_i \setminus \mathcal{R}_j\,. \tag{4.4}$$

Condition (iii) needs some explanation: On a first glance it seems superfluous, since flux conservation is already included in the transmission conditions. However, the analysis below shows that (iii) is needed both to completely specify an order k approximate solution and to enable the construction of an order $k+1$ approximation.

In this section, we are concerned with the derivation of interface conditions for the SHE distribution function $F(x,\varepsilon,t)$ accross the heterojunction at $x = 0$. We shall successively derive first and second order transmission conditions, by respectively constructing order 1 and order 2 approximate solutions of the Boltzmann transmission problem (3.1), (3.5). We start with the first order transmission conditions. Following section 2, the Hilbert expansion (2.5) of f_i^α in each domain Ω_i leads to an approximate solution of the form

$$\begin{aligned} f_i^\alpha(x,k,t) &= F_i^0(x,\varepsilon(x,k,t),t) \\ &+\alpha\left(F_i^1(x,\varepsilon(x,k,t),t) - \lambda_{i,x}(x,k,t)\frac{\partial F_i^0}{\partial x}(x,\varepsilon(x,k,t),t)\right) + \alpha^2 f_i^2(x,k,t) \end{aligned} \tag{4.5}$$

where F_i^0 is a solution of the SHE equation in Ω_i:

$$N_i(x,\varepsilon,t)\left(\frac{\partial F_i^0}{\partial t}-\frac{\partial \phi}{\partial t}\frac{\partial F_i^0}{\partial \varepsilon}\right)-\frac{\partial}{\partial x}\left(D_i(x,\varepsilon,t)\frac{\partial F_i^0}{\partial x}\right)=\overline{S}_i(F_i^0)\,. \tag{4.6}$$

Here, $N_i(x,\varepsilon,t)$ is the density of states (2.7) in each domain Ω_i, and $D_i(x,\varepsilon,t)$ is the scalar which corresponds to the x-x entry of the diffusion matrix (2.18) in Ω_i:

$$D_i(x,\varepsilon,t)=\int_{\mathcal{S}_{(x,\varepsilon,t)}}\lambda_{i,x}(x,k,t)\,v_{i,x}(k)\,dN_{(x,\varepsilon,t)}(k)\,. \tag{4.7}$$

The following theorem states that the first order interface conditions coincide with those established in section 2.

Theorem 4.2 *Let f_i^α be defined by (4.5) with F_i^0 solving (4.6). Then, f_i^α is an order 1 approximate solution of the Boltzmann transmission problem (3.1), (3.5) if and only if F_i^0 verifies the following continuity relations:*

$$F_1^0(0,\varepsilon,t)=F_2^0(0,\varepsilon,t)\,,\quad \forall\varepsilon\in\mathcal{R}_1\cap\mathcal{R}_2\,, \tag{4.8}$$

$$D_1\frac{\partial F_1^0}{\partial x}(0,\varepsilon,t)=D_2\frac{\partial F_2^0}{\partial x}(0,\varepsilon,t)\,,\quad \forall\varepsilon\in\mathcal{R}_1\cap\mathcal{R}_2\,, \tag{4.9}$$

$$D_i\frac{\partial F_i^0}{\partial x}(0,\varepsilon,t)=0\,,\quad \forall\varepsilon\in\mathcal{R}_i\setminus\mathcal{R}_j\,. \tag{4.10}$$

Proof : By construction, f_i^α is an order 1 approximate solution of the Boltzmann equation (3.1) inside each Ω_i. Now, inserting Ansatz (4.5) into the transmission condition (3.5), we get

$$(f_i^\alpha)^- - \mathcal{T}_i\left((f_1^\alpha)^+,\,(f_2^\alpha)^+\right)=[F_i^{0-}-\mathcal{T}_i\,(F_1^{0+},\,F_2^{0+})]+\mathcal{O}(\alpha)\,.$$

By Lemma 3.2, imposing (4.8) is necessary and sufficient to guarantee that

$$F_i^{0-}-\mathcal{T}_i(F_1^{0+},\,F_2^{0+})=0\,,$$

and thus to ensure (4.2) with $k=1$. Finally, the flux of particles of energy ε associated with (4.5) is given at $x=0$ by

$$J_i^\alpha(0,\varepsilon,t)=-\left(D_i\frac{\partial F_i^0}{\partial x}\right)(0,\varepsilon,t)\;+\;\mathcal{O}(\alpha)\,.$$

Therefore condition (4.3) requires (4.9) while (4.4) requires (4.10). ∎

We now proceed to the derivation of second order transmission conditions. The forthcoming procedure is inspired from the now classical method of [2], already applied to semiconductors in [7], [13], to derive higher order boundary conditions and kinetic-fluid coupling algorithms. We start again with the Hilbert expansion (away from the heterojunction), like in (2.5), but retaining an additional term:

$$f_i^\alpha = F_i^0 + \alpha \left(F_i^1 - \lambda_{i,x} \frac{\partial F_i^0}{\partial x} \right) + \alpha^2 f_i^2 + \alpha^3 f_i^3 \tag{4.11}$$

Inserting Anzatz (4.11) in (4.1) and identifying terms of equal powers of α yields the equations (2.13) for the determination of f_i^2 and

$$Q_i(f_i^3) = \frac{\partial \varepsilon}{\partial k_x} \frac{\partial f_i^2}{\partial x} - \frac{\partial \varepsilon}{\partial x} \frac{\partial f_i^2}{\partial k_x} + \frac{\partial f_i^1}{\partial t} - S_i(f_i^1)\,. \tag{4.12}$$

Here, we suppose that S_i is linear (a nonlinear S_i would just result in slightly more complicated calculations). The first step of the procedure is to look for conditions which ensure the solvability of system (2.11)-(2.13), (4.12), and thus, the existence of the terms involved in expansion (4.11). This guarantees that Ansatz (4.11) satisfies (4.1) with $k = 2$.

Recall that the solution of (2.11), (2.12) is given by:

$$f_i^0(x,k,t) = F_i^0(x, \varepsilon_i(k), t)\,, \tag{4.13}$$

$$f_i^1(x,k,t) = -\lambda_{i,x}(k) \frac{\partial F_i^0}{\partial x}(x, \varepsilon_i(k), t) + F_i^1(x, \varepsilon_i(k), t)\,, \tag{4.14}$$

Proposition 4.3 *Let f_i^0 and f_i^1 be respectively given by (4.13) and (4.14). Then, there exist f_i^2 and f_i^3, respectively solutions of (2.13), (4.12), if and only if F_i^0 and F_i^1 both satisfy the SHE equation (4.6).*

Proof : That the SHE-equation for F_i^0 is necessary for the existence of f_i^2, has already been verified in section 2.

To find the solvability condition for (4.12), we need an explicit expression of f_i^2. For that purpose, let h_i^2 be the unique solution of (2.13) in which F_i^1 is set to zero, and satisfying (2.10). With hypothesis (3.3) and the uniqueness statement of lemma 2.1 (ii), we deduce that h_i^2 is an even function with respect to k. Then, the most general solution f_i^2 of (2.13) is

$$f_i^2 = h_i^2 - \lambda_{i,x} \frac{\partial F_i^1}{\partial x} + F_i^2 \tag{4.15}$$

where $F_i^2 = F_i^2(x, \varepsilon, t)$ is arbitrary. Inserting (4.15) in (4.12) yields

$$Q_i^0(f_i^3) = \left(\frac{\partial \varepsilon}{\partial k_x} \frac{\partial}{\partial x} - \frac{\partial \varepsilon}{\partial x} \frac{\partial}{\partial k_x} \right) (-\lambda_{i,x} \frac{\partial (F_i^1)}{\partial x}) + \frac{\partial (F_i^1)}{\partial t} - S_i(F_i^1)$$
$$+ \left(\frac{\partial \varepsilon}{\partial k_x} \frac{\partial}{\partial x} - \frac{\partial \varepsilon}{\partial x} \frac{\partial}{\partial k_x} \right) (h_i^2 + (F_i^2)) + \frac{\partial}{\partial t} (-\lambda_{ix} \frac{\partial (F_i^0)}{\partial x}) - S_i(-\lambda_{i,x} \frac{\partial (F_i^0)}{\partial x})\,.$$

Here the notation (F_i^m), $m = 0, 1$ is a shorthand for $F_i^m(x, \varepsilon_i(x, k, t), t)$.

The last line consists of odd terms in k which vanish after integration over $\mathcal{S}_{(x,\varepsilon,t)}$. Therefore, the solvability condition (2.9) reduces to the integration of the first line, which obviously yields the SHE equation (4.6) for F_i^1. ∎

With proposition 4.3, Ansatz (4.11) satisfies condition (4.1) with $k = 2$. We must now find transmission conditions on F_i^0 and F_i^1 which guarantee that (4.11) is also of order 2 at the interface, i.e. satisfies (4.2), (4.3), (4.4) with $k = 2$. Conditions (4.8)-(4.10) must be imposed on F_i^0 because they are necessary to guarantee the order 1 approximation (theorem 4.2). However, whatever transmission conditions are prescribed to F_i^1, it is impossible to make Ansatz (4.11) an order 2 approximate solution at the interface. Indeed, if this were the case, the first order term f_i^1 given by (4.14) would have to satisfy the transmission condition (3.5). But f_i^1 involves $\lambda_{i,x}(k)$, which is not a function of the energy only and which cannot be cancelled at the interface by just a suitable choice of F_i^1. Therefore, we need to modify Ansatz (4.11) by introducing a transmission layer term, which is exponentially small inside each domain Ω_i, but which cancels the first order term f_i^1 at the interface. The definition of this transmission layer term is the second step of the procedure.

To derive the transmission layer term, we start from the kinetic problem (3.1) and we stretch the position variable in the direction normal to the boundary. Letting

$$E(x,t) = \frac{\partial \phi}{\partial x}(x,t)\,, \quad \theta_i^\alpha(\xi,k,t) = f_i^\alpha(\alpha\xi,k,t)\,,$$

we get:

$$\frac{\partial \theta_i^\alpha}{\partial t} + \frac{1}{\alpha^2} v_{i,x} \frac{\partial \theta_i^\alpha}{\partial \xi} - \frac{1}{\alpha} E(\alpha x,t) \frac{\partial \theta_i^\alpha}{\partial k_x} = \frac{1}{\alpha^2} Q_i(\theta_i^\alpha) + S_i(\theta_i^\alpha)\,, \tag{4.16}$$

We suppose that $E(\alpha x,t) = \mathcal{O}(1)$ as $\alpha \to 0$, which implies that there exists no sharp transition layer in the electrostatic potential. Keeping only the leading order terms of (4.16), we obtain the following kinetic layer equation with unknown $\theta_i(\xi,k)$, $\sigma_i\xi < 0$, $k \in B$, $i = 1, 2$:

$$v_{i,x}(k) \frac{\partial \theta_i}{\partial \xi} = Q_i(\theta_i)\,. \tag{4.17}$$

Since the transmission layer term θ_i must cancel the first order term f_i^1 at the interface, we need to consider inhomogeneous transmission conditions at the interface. Namely, given two functions $\ell_i(k)$, $i = 1, 2$, for $k \in B$, we impose

$$(\theta_i(0,.) - \ell_i)^- = \mathcal{T}_i\left((\theta_1(0,.) - \ell_1)^+,\, (\theta_2(0,.) - \ell_2)^+\right). \tag{4.18}$$

Layer terms need to have limits as $|\xi| \to \infty$. At least, we look for bounded solutions of problem (4.17), (4.18). Integrating (4.17) over $\mathcal{S}_\varepsilon^i$ (see (3.7) for the definition of $\mathcal{S}_\varepsilon^i$), we get

$$\frac{\partial}{\partial \xi} J_i(\xi,\varepsilon) = 0\,, \quad J_i(\xi,\varepsilon) = \int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,\theta_i(\xi,k)\,dN_\varepsilon^i(k)\,.$$

Therefore, $J_i(\xi,\varepsilon) = J_i(\varepsilon)$ is constant with respect to ξ. Then, we multiply (4.17) by $\lambda_{i,x}(k)$, integrate over $\mathcal{S}^i_\varepsilon$, use the self-adjointness of Q_i (property (iii) of Lemma 2.1) and get:

$$\frac{\partial}{\partial \xi} K_i(\xi,\varepsilon) + J_i(\varepsilon) = 0\,, \quad K_i(\xi,\varepsilon) = \int_{\mathcal{S}^i_\varepsilon} v_{i,x}(k)\,\lambda_{i,x}(k)\,\theta_i(\xi,k)\,dN^i_\varepsilon(k)\,, \tag{4.19}$$

or

$$K_i(\xi,\varepsilon) = -J_i(\varepsilon)\xi + K_i(0,\varepsilon)\,. \tag{4.20}$$

Bounded solutions θ_i (leading to bounded K_i) therefore satisfy the zero flux condition:

$$J_i(\varepsilon) = \int_{\mathcal{S}^i_\varepsilon} v_{i,x}(k)\,\theta_i(\xi,k)\,dN^i_\varepsilon(k) = 0\,, \quad \varepsilon \in \mathcal{R}_i\,. \tag{4.21}$$

The transmission condition (4.18) and Lemma 3.1 imply that the flux produced by $\theta_1(0,.) - \ell_1$ is equal to the flux produced by $\theta_2(0,.) - \ell_2$. Since by (4.21) the fluxes produced by the $\theta_i(0,.)$ vanish, a necessary condition for the existence of a bounded solution of (4.17), (4.18) is given by the flux continuity condition

$$\int_{\mathcal{S}^1_\varepsilon} v_{1,x}\,\ell_1\,dN^1_\varepsilon = \int_{\mathcal{S}^2_\varepsilon} v_{2,x}\,\ell_2\,dN^2_\varepsilon\,, \quad \forall\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2\,, \tag{4.22}$$

$$\int_{\mathcal{S}^i_\varepsilon} v_{i,x}\,\ell_i\,dN^i_\varepsilon = 0\,, \quad \forall\varepsilon \in \mathcal{R}_i \setminus \mathcal{R}_j\,. \tag{4.23}$$

For the homogeneous version of (4.17), (4.18) ($\ell_1 = \ell_2 = 0$) an easy computation shows that bounded solutions are given by

$$\theta_i(\xi,k) = \Theta(\varepsilon_i(k))\,, \quad i = 1,2 \tag{4.24}$$

where Θ is an arbitrary bounded function of ε.

Problem (4.17), (4.18) belongs to the class of Milne problems, which are widely used in many areas of kinetic theory [2], [6], [7], [11], [27]. In the present paper is the first occurrence (to our knowledge) of a "two-sided" Milne problem. In section 5 an existence theorem will be proved under strong assumptions on the solutions of the corresponding one-sided Milne problems for $\xi > 0$ and $\xi < 0$ with inflow boundary conditions. For rotationally symmetric band diagrams $e_i(k)$ and collision operators Q_i these assumptions can be verified (see section 5). For more general band diagrams, they are conjectures which will be dealt with in future work.

In the rest of this section, we shall assume the results of the existence theorem: Under conditions (4.22), (4.23), problem (4.17), (4.18) has a bounded solution, which is unique up to the addition of a function of the type (4.24) with arbitrary Θ. For $|\xi| \to \infty$, $\theta_i(\xi,k)$ converges exponentially to an element $\theta_i^\infty(\varepsilon_i(k))$ of the kernel of Q_i.

Finally, a simple computation shows that when θ_i is a bounded solution corresponding to the inhomogeneities ℓ_i, then $A(\varepsilon_i(k))\theta_i(\xi,k)$ is a bounded solution corresponding to the inhomogeneities $A(\varepsilon_i(k))\ell_i(k)$ for arbitrary functions $A(\varepsilon)$.

Once the transmission layer problem is set up, the third step of the procedure is to find a modified Ansatz (4.11) which provides a true order 2 approximate solution of the Boltzmann transmission problem (3.1), (3.5). We introduce the following modified Hilbert expansion:

$$\begin{aligned} f_i^\alpha &= F_i^0(x,\varepsilon,t) + \alpha\Big[-\lambda_{i,x}(k)\frac{\partial F_i^0}{\partial x}(x,\varepsilon,t) + F_i^1(x,\varepsilon,t) \\ &\quad + \Big(\theta_i(\frac{x}{\alpha},k) - \theta_i^\infty(\varepsilon_i(k))\Big)\; J_{int}^0(\varepsilon_i(k),t)\Big] + \alpha^2\, f_i^2 + \alpha^3 f_i^3 \end{aligned} \tag{4.25}$$

We recall that F_i^0 and F_i^1 satisfy the SHE-equation and that F_i^0 satisfies the first order transmission conditions (4.8), (4.9), (4.10). We denote by $J_{int}^0(\varepsilon,t)$, the common value in the expression (4.9), i.e.

$$J_{int}^0(\varepsilon,t) = \left(D_i\,\frac{\partial F_i^0}{\partial x}\right)(0,\varepsilon,t)\,, \quad \varepsilon\in\mathcal{R}_1\cap\mathcal{R}_2\,. \tag{4.26}$$

J_{int}^0 is the (leading order) flux of particles of energy ε at the interface. The transmission layer corrector term θ_i is a solution of the two-sided Milne problem (4.17), (4.18) with $\ell_i(k)$ given by

$$\ell_i(k) = D_i^{-1}(0,\varepsilon_i(k))\,\lambda_{i,x}(k)\,,$$

if $\varepsilon_i(k)$ belongs to $\mathcal{R}_1\cap\mathcal{R}_2$ and $\ell_i(k)=0$ otherwise. From the definition (4.7) of D_i, we have for $\varepsilon\in\mathcal{R}_1\cap\mathcal{R}_2$:

$$\int_{\mathcal{S}_\varepsilon^i} v_{i,x}\,\ell_i\,dN_\varepsilon^i = D_i(0,\varepsilon,t)^{-1}\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,\lambda_{i,x}(k)\,dN_\varepsilon^i(k) = 1\,,$$

so that the flux continuity conditions (4.22),(4.23) are satisfied. With our assumptions on the two-sided Milne problem, the layer term θ_i exists and the difference

$$\theta(\varepsilon) = \theta_2^\infty(\varepsilon) - \theta_1^\infty(\varepsilon) \tag{4.27}$$

of its asymptotic values when $|\xi|\to\infty$ is determined uniquely. The next theorem provides interface conditions on F_i^1, necessary for an ansatz of the form (4.25) to be an order 2 approximate solution of the Boltzmann transmission problem.

Theorem 4.4 *Let $F_i^0(x,\varepsilon,t)$ and $F_i^1(x,\varepsilon,t)$ satisfy the SHE equation (4.6), and let F_i^0 satisfy the transmission conditions (4.8), (4.9), (4.10). Then, for f_i^α given by Ansatz (4.25) to be an order 2 approximate solution of the Boltzmann transmission problem (3.1), (3.5), it is necessary that F_i^1 satisfies:*

$$F_2^1(0,\varepsilon,t) - F_1^1(0,\varepsilon,t) = \theta(\varepsilon)J_{int}^0(\varepsilon,t)\,, \quad \forall\varepsilon\in\mathcal{R}_1\cap\mathcal{R}_2\,, \tag{4.28}$$

together with the current relations (4.9), (4.10).

Proof : Inserting Ansatz (4.25) into the transmission condition (3.5), we get, at $x = 0$:

$$(f_i^\alpha)^- - \mathcal{T}_i\left((f_1^\alpha)^+, (f_2^\alpha)^+\right) = (F_i^0(\varepsilon_i)^- - \mathcal{T}_i\left(F_1^0(\varepsilon_1)^+,\ F_2^0(\varepsilon_2)^+\right)$$
$$+\alpha\left[\left(\theta_i J_{int}^0 - \lambda_{i,x}\frac{\partial F_i^0}{\partial x}\right)^- - \mathcal{T}_i\left(\left(\theta_1 J_{int}^0 - \lambda_{1,x}\frac{\partial F_1^0}{\partial x}\right)^+, \left(\theta_2 J_{int}^0 - \lambda_{2,x}\frac{\partial F_2^0}{\partial x}\right)^+\right)\right]$$
$$+\alpha\left[\left(F_i^1 - \theta_i^\infty J_{int}^0\right)^- - \mathcal{T}_i\left((F_1^1 - \theta_1^\infty J_{int}^0)^+, (F_2^1 - \theta_2^\infty J_{int}^0)^+\right)\right] + \mathcal{O}(\alpha^2)\,. \quad (4.29)$$

The order α^0 term at the right-hand side of (4.29) is zero because F_i^0 satisfies (4.8) and because of Lemma 3.2. The second one of the order α terms is also zero by a similar application of Lemma 3.2 as soon as transmission condition (4.28) is imposed to F_i^1. For the first one of the order α terms, we use the fact that $\theta_i\, J_{int}^0(\varepsilon_i)$ is a solution of the two-sided Milne problem (4.17), (4.18), (4.21) associated with

$$\ell_i(k) = D_i(\varepsilon_i)^{-1}\lambda_{i,x}(k)\, J_{int}^0(\varepsilon_i) = \lambda_{i,x}(k)\,\frac{\partial F_i^0}{\partial x}\,(\varepsilon_i)\,.$$

Therefore $\theta_i\, J_{int}^0(\varepsilon_i) - \lambda_{i,x}\partial F_i^0/\partial x(\varepsilon_i)$ satisfies the interface condition (3.5), which shows that the first one of the order α terms in (4.29) also vanishes. We deduce that Ansatz (4.25) satisfies the transmission condition (3.5) up to order α^2 terms.

Finally, we turn to the flux condition (4.3). Inserting Ansatz (4.25) into (4.3) and recalling that fluxes of functions of ε only vanish, that the flux of θ_i is zero by definition (condition (4.21)), and that condition (4.9) holds for F_i^0, we get for $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$:

$$J_1^\alpha(0,\varepsilon,t) - J_2^\alpha(0,\varepsilon,t) = \alpha\left[\int_{\mathcal{S}_\varepsilon^1} v_{1,x}(k)\, f_1^2\,(0,k,t)\, dN_\varepsilon^1(k)\right.$$
$$\left. - \int_{\mathcal{S}_\varepsilon^2} v_{2,x}(k)\, f_2^2\,(0,k,t)\, dN_\varepsilon^2(k)\right] + \mathcal{O}(\alpha^2)\,. \quad (4.30)$$

But, with (4.15), given that F_i^2 is a function of ε only and that h_i^2 is an even function of k, the order α term in (4.30) reduces to

$$-\left(\int_{\mathcal{S}_\varepsilon^1} v_{1,x}(k)\,\lambda_{1,x}(k)\, dN_\varepsilon^1(k)\right)\frac{\partial F_1^1}{\partial x}\,(\varepsilon) + \left(\int_{\mathcal{S}_\varepsilon^2} v_{2,x}(k)\,\lambda_{2,x}(k)\, dN_\varepsilon^2(k)\right)\frac{\partial F_2^1}{\partial x}\,(\varepsilon)\,.$$

The integral terms in the above expressions are nothing else than $D_i(\varepsilon)(= D_i(0,\varepsilon,t))$ according to (4.7). Thus, condition (4.9) for F_i^1 ensures that the order α term in (4.30) is identically zero and that relation (4.3) holds with $k = 2$. The same arguments can be used to derive relation (4.4) with $k = 2$, which completes the proof of theorem 4.4 ∎

The construction of a complete $O(\alpha^2)$-approximation would require $O(\alpha^2)$ and $O(\alpha^3)$ layer terms. Let instead f_i^2 and f_i^3 be outer approximations given by Proposition 4.3. Inserting Ansatz (4.25) into the Boltzmann equation (3.1) and using the proof of Proposition 4.3, we obtain:

$$\partial_t f_i^\alpha + \frac{1}{\alpha}\left(v_{i,x}\,\frac{\partial f_i^\alpha}{\partial x} + \frac{\partial \phi}{\partial x}\,\frac{\partial f_i^\alpha}{\partial k_x}\right) - \frac{1}{\alpha^2}\,Q_i(f_i^\alpha) - S_i(f_i^\alpha)$$
$$= \alpha^2\left[\partial_t f_i^2 + \alpha\partial_t f_i^3 - S_i(f_i^2) - \alpha S_i(f_i^3) + \left(v_{i,x}\,\frac{\partial}{\partial x} + \frac{\partial \phi}{\partial x}\,\frac{\partial}{\partial k_x}\right) f_i^3\right]$$
$$+\left(\alpha\partial_t + \frac{\partial \phi}{\partial x}\,\frac{\partial}{\partial k_x} - \alpha S_i\right)\left(\left(\theta_i(\frac{x}{\alpha}, k) - \theta_i^\infty(\varepsilon_i(k))\right)\, J_0^{int}(\varepsilon_i(k), t)\right)\,. \quad (4.31)$$

The first line of the right-hand side of (4.31) is $O(\alpha^2)$ while the last line of (4.31) is exponentially small away from $x = 0$. Therefore, f_i^α is a formal approximate solution of order 2 to the Boltzmann equation (3.1), in domains of the form $\{|x| \geq x_0\}$.

The last step of the procedure is to combine F_i^0 and F_i^1 into a single SHE distribution function:

$$F_i^\alpha = F_i^0 + \alpha F_i^1\,,$$

which satisfies the SHE equation (4.6) in each Ω_i, the flux conditions (4.9) and (4.10) and the jump relation (deduced from (4.8) for F_i^0 and from (4.28) for F_i^1):

$$F_2^\alpha(0, \varepsilon, t) - F_1^\alpha(0, \varepsilon, t) = \alpha\theta(\varepsilon) J_{int}^0(\varepsilon, t) \quad (4.32)$$

However, in (4.32), J_{int}^0 is the flux of F_i^0 and not that of F_i^α. It would thus be desirable to replace it by J_{int}^α, (with J_{int}^α being defined by (4.26) with F_i^0 replaced by F_i^α), in order to obtain a self-contained transmission problem for F_i^α. But first, we must check if this problem would be well-posed.

Lemma 4.5 *We have*

$$\theta(\varepsilon) \geq 0\,, \quad \forall \varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2 \quad (4.33)$$

Proof : We apply the Darrozes-Guiraud inequality (3.19) to the transmission condition

$$\left(\theta_i - D_i^{-1}\,\lambda_{i,x}\right)^- = \mathcal{T}_i\left((\theta_1 - D_1^{-1}\,\lambda_{1,x})^+,\, (\theta_2 - D_2^{-}\,\lambda_{2,x})^+\right)\,,$$

and obtain for $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$

$$\int_{\mathcal{S}_\varepsilon^2} v_{2,x}(k)\,|\theta_2(0, k) - \lambda_{2,x}(k)\,D_2(\varepsilon)^{-1}|^2\,dN_\varepsilon^2(k)$$
$$\leq \int_{\mathcal{S}_\varepsilon^1} v_{1,x}(k)\,|\theta_1(0, k) - \lambda_{1,x}(k)\,D_1(\varepsilon)^{-1}|^2\,dN_\varepsilon^1(k)\,. \quad (4.34)$$

We develop:

$$\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,|\theta_i(0, k) - \lambda_{i,x}(k)\,D_i(\varepsilon)^{-1}|^2\,dN_\varepsilon^i(k) =$$
$$\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,|\theta_i(0, k)|^2\,dN_\varepsilon^i(k) + \left(\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,|\lambda_{i,x}(k)|^2\,dN_\varepsilon^i(k)\right)\,D_i(\varepsilon)^{-2}$$
$$-2\left(\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,\lambda_{i,x}(k)\,\theta_i(0, k)\,dN_\varepsilon^i(k)\right)\,D_i(\varepsilon)^{-1}\,. \quad (4.35)$$

Multiplying equation (4.17) by $\theta_i(\xi,k)$, integrating over k, and using property (iii) of Lemma 2.1, we get

$$\frac{1}{2}\frac{\partial}{\partial\xi}\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,|\theta_i(\xi,k)|^2\,dN_\varepsilon^i(k) = \int_{\mathcal{S}_\varepsilon^i} Q_i(\theta_i)\theta_i\,dN_\varepsilon^i(k) \le 0\,.$$

Moreover, since $\lim_{|\xi|\to\infty}\theta_i(\xi,k) = \theta_i^\infty(\varepsilon_i(k))$ is an even function of k, we have

$$\lim_{|\xi|\to\infty}\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,|\theta_i(\xi,k)|^2\,dN_\varepsilon^i(k) = 0\,.$$

We deduce

$$\sigma_i\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,|\theta_i(0,k)|^2\,dN_\varepsilon^i(k) \le 0, \quad \sigma_1 = 1,\, \sigma_2 = -1\,. \tag{4.36}$$

Then, using that $\lambda_{i,x}(k)$ is an odd function of k, we obtain:

$$\int_{\mathcal{S}_\varepsilon^i} v_{i,x}\,|\lambda_{i,x}|^2\,dN_\varepsilon^i = 0\,. \tag{4.37}$$

Finally, we have

$$\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\,\lambda_{i,x}(k)\,\theta_i(0,k)\,dN_\varepsilon^i(k) = K_i(0,\varepsilon)\,,$$

where the K-integral $K_i(\xi,\varepsilon)$ has been defined at (4.19) and is constant with respect to ξ (because of (4.20) and because $J_i = 0$). Thus, using (4.7):

$$K_i(0,\varepsilon) = \lim_{|\xi|\to\infty} K_i(\xi,\varepsilon) = D_i(\varepsilon)\,\theta_i^\infty(\varepsilon)\,. \tag{4.38}$$

Inserting (4.35), (4.36), (4.37) and (4.38) into (4.34) leads to the result. ∎

We may now introduce $\tilde F_i^\alpha$, a solution of the SHE equation (4.6) in each domain Ω_i, with the flux relations (4.9) and (4.10) at $x=0$ and the jump relation

$$\tilde F_2^\alpha - \tilde F_1^\alpha - \alpha\,\theta\,\tilde J_\alpha^{int} = 0, \quad \forall\varepsilon\in\mathcal{R}_1\cap\mathcal{R}_2\,, \tag{4.39}$$

where $\tilde J_\alpha^{int}$ is the common value of the current at the interface (formula (4.26) with F_i^0 replaced by $\tilde F_i^\alpha$). Relation (4.39) is the final form of the order 2 transmission condition for the SHE distribution, that we are looking for. We note that $\theta \ge 0$ is a sufficient condition for the SHE equation with transmission conditions (4.9), (4.10) and (4.39) to be well-posed. As a matter of example, we look at the following model problem

Lemma 4.6 *The stationary one-dimensional transmission problem for $F(x)$, $x \in (-1,1)$ given by*

$$-(DF')' + F = S, \quad x\in(-1,1) \tag{4.40}$$

$$F(-1) = F(1) = 0 \tag{4.41}$$

$$D_1\,F_1' = D_2 F_2' := J^{int}, \quad F_1' = \lim_{x\to 0^-} F'(x), \quad F_2' = \lim_{x\to 0^+} F(x) \tag{4.42}$$

$$F_2 - F_1 - \theta\,J^{int} = 0 \quad F_1 = \lim_{x\to 0^-} F(x), \quad F_2 = \lim_{x\to 0^+} F(x) \tag{4.43}$$

with $D(x) = D_1$ for $x\in(-1,0)$, $D(x) = D_2$ for $x \in (0,1)$, is well-posed for $\theta \ge 0$.

Proof : Multiplying (4.40) by F, integrating by parts and using (4.41), (4.42), (4.43), leads to the following variational formulation:

$$\int_{-1}^{1} D|F'|^2\,dx + \int_{-1}^{1} |F|^2\,dx + \theta^{-1}|F_2 - F_1|^2 = \int_{-1}^{1} F\,S\,dx \qquad (4.44)$$

If $\theta = 0$, the term $\theta^{-1}|F_2 - F_1|^2$ must be replaced by 0. From (4.44), it is easy to prove existence of solution by Lax-Milgram theory. ∎

The difference $F_i^\alpha - \tilde{F}_i^\alpha$ satisfies the same SHE problem (4.6), (4.9), (4.10), but with an inhomogeneous transmission condition (4.39) where the right hand side is of order α^2, (use (4.32)). A stability theory derived from the existence theory of Lemma 4.6 then shows that $\tilde{F}_i^\alpha - F_i^\alpha$ is of order α^2. By virtue of (4.25) and of evenness considerations, we have, away from $x = 0$:

$$\frac{1}{N_i(x,\varepsilon,t)} \int_{\mathcal{S}_{(x,\varepsilon,t)}} f_i^\alpha(k)\,dN_\varepsilon^i(k) \;=\; F_i^\alpha(x,\varepsilon,t) + \mathcal{O}(\alpha^2)\,.$$

Therefore, as a final theorem we can state:

Theorem 4.7 *Let $\tilde{F}_i^\alpha$ be the solution of the transmission problem for the SHE equation (4.6) with transmission conditions (4.9), (4.10), (4.39). Then $\tilde{F}_i^\alpha(\varepsilon)$ is formally an order 2 approximation of the energy-shell average of f_i^α, away from the interface.*

5 The kinetic transmission layer problem

In this section, we are concerned with the existence and uniqueness theory of the transmission layer problem (4.17), (4.18). In particular, rotationally symmetric models will be treated in detail. We shall start, however, dealing with the general case.

Our analysis will be based on assumptions on the one-sided Milne problems

$$v_{i,x}\frac{\partial\theta_i}{\partial\xi} = Q_i(\theta_i)\,, \qquad \xi \in I_i = \sigma_i(-\infty, 0]\,, \quad k \in \mathcal{S}_\varepsilon^i\,, \qquad (5.1)$$

$$\theta_i^- \text{ given on } \mathcal{S}_\varepsilon^{i,-}\,, \qquad (5.2)$$

for $\varepsilon \in \mathcal{R}_i$, where the abbreviation $\theta_i^\pm = \theta_i(0,.)^\pm$ is used. Note that we use the fact that the Milne problem is decoupled in the energy direction.

Hypothesis 4: For $i = 1$ or 2, $\varepsilon \in \mathcal{R}_i$ and arbitrary $\theta_i^- \in L^2(\mathcal{S}_\varepsilon^{i,-}, dN_\varepsilon^i)$ the problem (5.1), (5.2) has a unique solution in $L^\infty(I_i, L^2(\mathcal{S}_\varepsilon^i, dN_\varepsilon^i))$ such that the Albedo operator $\mathcal{A}_i$, determined from $\theta_i^+ = \mathcal{A}_i\theta_i^-$ is compact from $L^2(\mathcal{S}_\varepsilon^{i,-}, dN_\varepsilon^i)$ to $L^2(\mathcal{S}_\varepsilon^{i,+}, dN_\varepsilon^i)$. Furthermore, as $|\xi| \to \infty$, θ_i converges exponentially to a constant.

It will be shown below that this assumption can be verified for rotationally symmetric models. Its verification for more general cases remains the subject of future work.

Theorem 5.1 *Assume the hypotheses 1–4. Then the two-sided Milne problem (4.17), (4.18) has a bounded solution iff ℓ_1 and ℓ_2 satisfy the solvability conditions (4.22), (4.23). In this case, the solution is unique up to the addition of a solution of the form (4.24) of the homogeneous problem.*

Proof : With the help of the Albedo operators, the transmission conditions (4.18) can be written as

$$\theta_i^- - \mathcal{T}_i(\mathcal{A}_1\theta_1^-, \mathcal{A}_2\theta_2^-) = \ell_i^- - \mathcal{T}_i(\ell_1^+, \ell_2^+)\,,$$

reducing the problem to a fixed point problem for the θ_i^-:

$$\begin{pmatrix} \theta_1^- \\ \theta_2^- \end{pmatrix} - K \begin{pmatrix} \theta_1^- \\ \theta_2^- \end{pmatrix} = \begin{pmatrix} \ell_1^- \\ \ell_2^- \end{pmatrix} - \begin{pmatrix} \mathcal{T}_1(\ell_1^+, \ell_2^+) \\ \mathcal{T}_2(\ell_1^+, \ell_2^+) \end{pmatrix}, \tag{5.3}$$

with

$$K \begin{pmatrix} \theta_1^- \\ \theta_2^- \end{pmatrix} = \begin{pmatrix} \mathcal{T}_1(\mathcal{A}_1\theta_1^-, \mathcal{A}_2\theta_2^-) \\ \mathcal{T}_2(\mathcal{A}_1\theta_1^-, \mathcal{A}_2\theta_2^-) \end{pmatrix}. \tag{5.4}$$

An application of Jensen's inequality as in the proof of Lemma 3.3 and an integration with respect to k shows that $\mathcal{T}_i$ is a continuous operator from $L^2(\mathcal{S}_\varepsilon^{1,+}, dN_\varepsilon^1) \times L^2(\mathcal{S}_\varepsilon^{2,+}, dN_\varepsilon^2)$ to $L^2(\mathcal{S}_\varepsilon^{i,-}, dN_\varepsilon^i)$. Therefore, by hypothesis 4, K is a compact operator on $L^2(\mathcal{S}_\varepsilon^{1,-}, dN_\varepsilon^1) \times L^2(\mathcal{S}_\varepsilon^{2,-}, dN_\varepsilon^2)$.

Let now $\ell_i = 0$, $i = 1, 2$. Multiplying (4.17) by θ_i, integrating it with respect to k and using Lemma 2.1 (iii) yields

$$\frac{1}{2}\frac{\partial}{\partial \xi}\int_{\mathcal{S}_\varepsilon^i} v_{i,x}\theta_i^2 dN_\varepsilon^i = \int_{\mathcal{S}_\varepsilon^i} Q_i(\theta_i)\theta_i dN_\varepsilon^i \le 0\,. \tag{5.5}$$

By hypothesis 4, θ_i tends to a constant independent of $k \in \mathcal{S}_\varepsilon^i$ as $|\xi|$ tends to infinity. Therefore, integrating (5.5) with respect to ξ over I_i and using the oddness of $v_{i,x}$ leads to

$$\int_{\mathcal{S}_\varepsilon^1} v_{1,x}(k)\theta_1(0,k)^2 dN_\varepsilon^1(k) \le 0 \le \int_{\mathcal{S}_\varepsilon^2} v_{2,x}(k)\theta_2(0,k)^2 dN_\varepsilon^2(k)\,.$$

Combined with the Darrozes-Guiraud inequality (Lemma 3.3), this implies that

$$\int_{\mathcal{S}_\varepsilon^i} v_{i,x}(k)\theta_i(0,k)^2 dN_\varepsilon^i(k) = 0\,, \qquad i = 1, 2.$$

Therefore, we have:

$$\int_{I_i}\int_{\mathcal{S}_\varepsilon^i} Q_i(\theta_i)\theta_i dN_\varepsilon^i d\xi = 0\,,$$

which implies, with Lemma 2.1 (iii) that θ_i is constant on $\mathcal{S}_\varepsilon^i$: $\theta_i = \theta_i(\xi, \varepsilon)$. Then using equation (4.17), we see that θ_i is also independent of ξ: $\theta_i = \theta_i(\varepsilon)$. Finally, Lemma 3.2 implies

$$\theta_1(\varepsilon) = \theta_2(\varepsilon)\,,$$

completing the proof for the homogeneous case.

We now turn to the inhomogeneous case. It has already been observed in section 4 that (4.22), (4.23) are necessary solvability conditions. Since $I - K$ (where I is the identity operator) is a Fredholm operator on $L^2(\mathcal{S}_\varepsilon^{1,-}, dN_\varepsilon^1) \times L^2(\mathcal{S}_\varepsilon^{2,-}, dN_\varepsilon^2)$ whose kernel is the one-dimensional vector space spanned by the constants, its range is closed and of codimension 1, and (4.22), (4.23) are thus also sufficient for the existence of a solution. ∎

We now specialize to a spherically symmetric model and, thus, consider a spherically symmetric band diagram

$$e_i(k) = \overline{e}_i(|k|) \tag{5.6}$$

with a strictly monotone $\overline{e}_i$, and rotationally symmetric collision and transmission operators. The parabolic band diagram (2.3) is a particular case of (5.6).

Because of the monotonicity hypothesis on $\overline{e}_i$, there exists a one-to-one correspondence between $|k|$ and $\varepsilon = \varepsilon_i(k) = \overline{e}_i(|k|) - \chi_i$. We denote the inverse relation by $|k| = \kappa_i(\varepsilon)$. It will be convenient to introduce a new set of variables $\varepsilon \in \mathcal{R}_i$, $\mu \in [-1, 1]$, $\varphi \in [0, 2\pi)$ such that

$$k = \kappa_i(\varepsilon)(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi)\,. \tag{5.7}$$

The measure $dN_\varepsilon^i(k)$ is given in these coordinates by

$$dN_\varepsilon^i(k) = \overline{v}_i(\varepsilon)^{-1}\,\kappa_i^2(\varepsilon)\,d\mu d\varphi\,, \quad \text{with} \quad \overline{v}_i(\varepsilon) = \frac{\partial \overline{e}_i}{\partial |k|}(\kappa_i(\varepsilon))\,. \tag{5.8}$$

The hypothesis of rotational symmetry for Q_i implies that the matrix element $\Phi_i(k, k')$ (see (2.4)) is invariant under all orthogonal transformations of $\mathbb{R}^3$, i.e. $\Phi_i(Rk, Rk') = \Phi(k, k')$, for all R in the orthogonal group $O_3(\mathbb{R})$. Therefore, Φ_i is of the form

$$\Phi_i(k, k') = \tilde{\Phi}_i\left(\varepsilon, \frac{k}{|k|}\cdot\frac{k'}{|k'|}\right)\,, \tag{5.9}$$

(since Φ_i needs to be defined only when $\varepsilon_i(k) = \varepsilon_i(k') = \varepsilon$). A special case is the relaxation time model

$$\Phi_i = \Phi_i(\varepsilon) = \frac{\overline{v}_i(\varepsilon)}{4\pi\kappa_i(\varepsilon)^2\tau_i(\varepsilon)}\,, \tag{5.10}$$

where the collision operator takes the form

$$Q_i(f) = \frac{1}{\tau_i(\varepsilon)}\left(\frac{1}{4\pi}\int_{-1}^{1}\int_0^{2\pi} f(\varepsilon, \mu', \varphi')d\varphi' d\mu' - f(\varepsilon, \mu, \varphi)\right)\,. \tag{5.11}$$

The hypothesis of rotational symmetry for the transmission operator $\mathcal{T}_i$ is that R_i and $T_{i\to j}$ are invariant under all the orthogonal transformations that leave the interface Σ globally invariant. Therefore, $R_i(k \to k')$ for $\varepsilon_i(k) = \varepsilon_i(k') = \varepsilon \in \mathcal{R}_i$ and $T_{i\to j}(k \to k')$ for $\varepsilon_i(k) = \varepsilon_j(k') = \varepsilon$ are of the form:

$$
\begin{aligned}
R_i(k \to k') &= \tilde{R}_i\left(\varepsilon, \frac{k_y k'_y + k_z k'_z}{\sqrt{k_y^2+k_z^2}\sqrt{k_y'^2+k_z'^2}}; \frac{k_x}{|k_x|} \to \frac{k'_x}{|k'_x|}\right), \\
T_{i\to j}(k \to k') &= \tilde{T}_{i\to j}\left(\varepsilon, \frac{k_y k'_y + k_z k'_z}{\sqrt{k_y^2+k_z^2}\sqrt{k_y'^2+k_z'^2}}; \frac{k_x}{|k_x|} \to \frac{k'_x}{|k'_x|}\right). \qquad (5.12)
\end{aligned}
$$

With the spherical symmetry assumption and the relaxation time model for the collision operator, hypothesis 4 can be verified:

Lemma 5.2 *Assume (5.6) and (5.10). Then Hypothesis 4 holds.*

Proof : We have to analyze the one-sided Milne problem

$$
\begin{aligned}
&\overline{v}_i \mu \frac{\partial \theta_i}{\partial \xi} = Q_i(\theta_i)\,, \qquad \xi \in I_i\,, \quad \mu \in [-1,1]\,, \quad \varphi \in [0, 2\pi)\,, \qquad (5.13) \\
&\theta_i(0,\mu,\varphi) = \theta_B(\mu,\varphi)\,, \qquad \sigma_i\mu < 0\,, \qquad (5.14)
\end{aligned}
$$

where Q_i is given by (5.11). Here and in the following we skip the dependencies on ε since it is only a parameter. For the solution we make the ansatz

$$
\theta_i(\xi,\mu,\varphi) = \overline{\theta}_i(\xi,\mu) + \begin{cases} e^{-\xi/|\mu|}(\theta_B(\mu,\varphi) - \overline{\theta}_B(\mu))\,, & \sigma_i\mu < 0\,, \\ 0\,, & \sigma_i\mu > 0\,, \end{cases} \qquad (5.15)
$$

where $\overline{\theta}_B$ is the average with respect to φ of θ_B:

$$
\overline{\theta}_B(\mu) = \frac{1}{2\pi}\int_0^{2\pi} \theta_B(\mu,\varphi)d\varphi\,.
$$

It is easily checked that (5.15) is a solution of (5.13), (5.14) if $\overline{\theta}_i$ satisfies the φ-averaged problem

$$
\begin{aligned}
&\overline{v}_i \mu \frac{\partial \overline{\theta}_i}{\partial \xi} = \frac{1}{\tau_i}\left(\frac{1}{2}\int_{-1}^{1} \overline{\theta}_i(\xi,\mu')d\mu' - \overline{\theta}_i(\xi,\mu)\right), \qquad \xi \in I_i\,, \quad \mu \in [-1,1]\,, \qquad (5.16) \\
&\overline{\theta}_i(0,\mu) = \overline{\theta}_B(\mu)\,, \qquad \sigma_i\mu < 0\,, \qquad (5.17)
\end{aligned}
$$

Now the proof can be completed by references to the literature. The φ-averaged problem is a version of the Milne problem of neutron transport. Results on existence, uniqueness and exponential decay to an equilibrium state can be found in [2]. This provides existence for the full problem (5.13), (5.14). Uniqueness can be shown analogously to the correspoding result for (5.16), (5.17) in [2]. By (5.15), the Albedo operator for the full problem is the composition of the φ-average and the Albedo operator for the averaged problem. The compactness of the latter follows from its representation in terms of the Chandrasekhar H-function [6]. Compactness of the full Albedo operator is then obvious. ∎

We now return to the general problem without symmetry assumptions and investigate a scheme which, in the spirit of those reviewed in [11], approximately solves the two-sided Milne problem and provides approximate values of the parameter θ (4.27). In the following, a fixed value of $\varepsilon \in \mathcal{R}_1 \cap \mathcal{R}_2$ is considered. We start by applying the Albedo operators to the rows of (5.3) and obtaining a fixed point problem for the θ_i^+:

$$\theta_i^+ = \mathcal{A}_i(\mathcal{T}_i(\theta_1^+, \theta_2^+) + \varphi_i^-)\,, \qquad i = 1, 2. \tag{5.18}$$

Now the Albedo operators are approximated by $\tilde{\mathcal{A}}_i$, $i = 1, 2$, defined by the requirements that a constant function is returned and that the vanishing flux property of the full problem is preserved:

$$f^+ = \tilde{\mathcal{A}}_i f^- \qquad \Longleftrightarrow \qquad f^+ = f^+(\varepsilon) \quad \text{and} \quad \int_{\mathcal{S}_\varepsilon^i} v_{i,x} f \, dN_\varepsilon^i = 0\,.$$

The approximating Albedo operators are explicitly given by

$$\tilde{\mathcal{A}}_i f^- = \frac{1}{\alpha_i} \int_{\mathcal{S}_\varepsilon^{i,-}} |v_{i,x}| f^- \, dN_\varepsilon^i\,,$$

with α_i defined in (3.31). When (5.18) is approximated by

$$\theta_i^+ = \tilde{\mathcal{A}}_i(\mathcal{T}_i(\theta_1^+, \theta_2^+) + \varphi_i^-)\,, \qquad i = 1, 2. \tag{5.19}$$

the θ_i^+ are constant on $\mathcal{S}_\varepsilon^{i,+}$. Application of the transmission operator to constant data gives

$$\mathcal{T}_i(\theta_1^+, \theta_2^+) = \theta_i^+ + (\theta_j^+ - \theta_i^+)\overline{T}_{j\to i}\,, \tag{5.20}$$

where $\overline{T}_{j\to i}$ has been defined in (3.15) and (3.14) has been used. Substitution in (5.19) gives

$$\theta_i^+ - \theta_j^+ = \frac{\tilde{\mathcal{A}}_i \varphi_i^-}{\tilde{\mathcal{A}}_i \overline{T}_{j\to i}}\,, \tag{5.21}$$

where we have used that constant factors can be taken out of $\tilde{\mathcal{A}}_i$ and that $\tilde{\mathcal{A}}_i$ reduces to the identity when applied to constants. The positivity of the denominator in the right hand side of (5.21) is a consequence of the transmittivity hypothesis 3.

Of course, the question arises if the result for $\theta_1^+ - \theta_2^+$ is the same for the two formulas ($i = 1$, $j = 2$ and $i = 2$, $j = 1$) contained in (5.21). With the help of the reciprocity relation (3.13) it is easy to show that

$$\alpha_1 \tilde{\mathcal{A}}_1 \overline{T}_{2\to 1} = \alpha_2 \tilde{\mathcal{A}}_2 \overline{T}_{1\to 2}$$

holds. On the other hand, a straightforward computation using the flux conservation property of the transmission operator (Lemma 3.1) shows that

$$\alpha_1 \tilde{\mathcal{A}}_1 \varphi_1^- = -\alpha_2 \tilde{\mathcal{A}}_2 \varphi_2^-$$

holds iff the ℓ_i satisfy the solvability condition (4.22). The approximating problem requires the same solvability condition as the original one.

The K-integral (4.19)

$$K_i = \int_{\mathcal{S}_\varepsilon^i} v_{i,x}\lambda_{i,x}\theta_i dN_\varepsilon^i$$

is constant in each Ω_i. Evaluation at $|\xi| = \infty$ gives

$$K_i = D_i\theta_i^\infty .$$

With the transmission conditions (4.18) and with (5.20), $\theta_i(\xi = 0)$ can be expressed in terms of the θ_i^+:

$$K_i = \int_{\mathcal{S}_\varepsilon^{i,-}} v_{i,x}\lambda_{i,x}\varphi_i^- dN_\varepsilon^i + D_i(\theta_i^+ + \beta_i(\theta_j^+ - \theta_i^+)) ,$$

with

$$\beta_i = \frac{1}{D_i}\int_{\mathcal{S}_\varepsilon^{i,-}} v_{i,x}\lambda_{i,x}\overline{T}_{j\to i} dN_\varepsilon^i .$$

Note that $\overline{T}_{j\to i} \le 1$ (3.14) and the oddness of $v_{i,x}$ and $\lambda_{i,x}$ imply

$$\beta_i \le \frac{1}{2} .$$

By elimination of K_i, θ_i^∞ can be computed. Taking the difference gives

$$\begin{aligned} \theta = \theta_2^\infty - \theta_1^\infty &= (1 - \beta_1 - \beta_2)(\theta_2^+ - \theta_1^+) \\ &\quad + \frac{1}{D_2}\int_{\mathcal{S}_\varepsilon^{2,-}} v_{2,x}\lambda_{2,x}\varphi_2^- dN_\varepsilon^2 - \frac{1}{D_1}\int_{\mathcal{S}_\varepsilon^{1,-}} v_{1,x}\lambda_{1,x}\varphi_1^- dN_\varepsilon^1 . \qquad (5.22) \end{aligned}$$

The formulation of the second order transmission conditions for the SHE-model requires the value of θ for the choice $\ell_i = \lambda_{i,x}/D_i$ of the inhomogeneities. In this case, our result can be simplified.

Lemma 5.3 *Assume $\ell_i = \lambda_{i,x}/D_i$. Then*

$$\alpha_i\tilde{\mathcal{A}}_i\varphi_i^- = \sigma_i(1 - \beta_1 - \beta_2) .$$

Proof : With

$$\varphi_i^- = \frac{\lambda_{i,x}}{D_i} - \mathcal{T}_i\left(\frac{\lambda_{1,x}^+}{D_1}, \frac{\lambda_{2,x}^+}{D_2}\right)$$

we obtain $\alpha_i\tilde{\mathcal{A}}_i\varphi_i^- = A + B + C$ with

$$A = \frac{1}{D_i}\int_{S_\varepsilon^{i,-}} |v_{i,x}|\lambda_{i,x} dN_\varepsilon^i = \frac{\sigma_i}{2} ,$$

as well as

$$\begin{aligned} B &= -\frac{1}{D_i}\int_{S_\varepsilon^{i,-}}\int_{S_\varepsilon^{i,+}} R_i(k' \to k)|v_{i,x}(k)|\lambda_{i,x}(k')dN_\varepsilon^i(k')dN_\varepsilon^i(k) \\ &= \sigma_i\left(\frac{1}{2} - \beta_i\right) \qquad (5.23) \end{aligned}$$

by the reciprocity relation (3.12) and by (3.14). Similarly we show

$$\begin{aligned} C &= -\frac{1}{D_j}\int_{S_\varepsilon^{i,-}}\int_{S_\varepsilon^{j,+}} T_{j\to i}(k'\to k)|v_{i,x}(k)|\lambda_{j,x}(k')dN_\varepsilon^j(k')dN_\varepsilon^i(k) \\ &= \sigma_j\beta_j\,, \end{aligned} \tag{5.24}$$

completing the proof. ∎

After substitution of (5.21), (5.22) becomes

$$\theta = \frac{(1-\beta_1-\beta_2)^2}{\alpha_i\tilde{\mathcal{A}}_i\overline{T}_{j\to i}} - \sum_{i=1}^{2}\frac{\sigma_i}{D_i}\int_{\mathcal{S}_\varepsilon^{i,-}} v_{i,x}\lambda_{i,x}\varphi_i^- dN_\varepsilon^i\,, \tag{5.25}$$

which is explicit up to the computation of $\lambda_{i,x}$.

A simplification can be achieved by returning to the assumptions (5.6), (5.10), (5.12) of spherical symmetry and the relaxation time model for the collision operator. In this case, $\lambda_{i,x}$ can be computed explicitly:

$$\lambda_{i,x} = \tau_i v_{i,x} = \tau_i\overline{v}_i\mu\,.$$

The quantities needed in (5.25) are

$$\begin{aligned} \beta_i &= \frac{3}{2}\int_{\sigma_i\mu<0}\mu^2\overline{T}_{j\to i}(\varepsilon,\mu)d\mu\,, \\ \alpha_i\tilde{\mathcal{A}}_i\overline{T}_{j\to i} &= 2\pi\kappa_i^2\int_{\sigma_i\mu<0}|\mu|\overline{T}_{j\to i}(\varepsilon,\mu)d\mu\,, \end{aligned}$$

with

$$\overline{T}_{j\to i}(\varepsilon,\mu) = \frac{\kappa_j^2}{\overline{v}_j}\int_{\sigma_j\mu'>0}\int_0^{2\pi}\tilde{T}_{j\to i}(\varepsilon,\cos\varphi;\mu'\to\mu)d\varphi d\mu'\,,$$

as well as

$$\frac{1}{D_i}\int_{\mathcal{S}_\varepsilon^{i,-}} v_{i,x}\lambda_{i,x}\varphi_i^- dN_\varepsilon^i = \frac{3}{2}\int_{\sigma_i\mu<0}\mu^2\varphi_i^-(\varepsilon,\mu)d\mu\,,$$

with

$$\begin{aligned} \varphi_i^-(\varepsilon,\mu) &= \frac{3\mu}{4\pi\kappa_i^2} - \frac{3}{4\pi\overline{v}_i}\int_{\sigma_i\mu'>0}\int_0^{2\pi}\mu'\tilde{R}_i(\varepsilon,\cos\varphi;\mu'\to\mu)d\varphi d\mu' \\ &\quad - \frac{3}{4\pi\overline{v}_j}\int_{\sigma_j\mu'>0}\int_0^{2\pi}\mu'\tilde{T}_{j\to i}(\varepsilon,\cos\varphi;\mu'\to\mu)d\varphi d\mu'\,. \end{aligned}$$

We conclude this section by applying our results to the examples of transmission operators from section 3.

Example 1: semi-classical transmission conditions (3.24). Let k_1, k_2 be such that $k_2 = t_{2\to 1}k_1$ or $k_1 = t_{1\to 2}k_2$ (see (3.26)). Relation (3.23) translates to the (ε,μ) geometry into $\varepsilon_1 = \varepsilon_2 = \varepsilon$ and:

$$\kappa_1^2(\varepsilon)\left(1-\mu_1^2\right) = \kappa_2^2(\varepsilon)\left(1-\mu_2^2\right)\,. \tag{5.26}$$

We now suppose, without loss of generality, that $\kappa_1^2(\varepsilon)/\kappa_2^2(\varepsilon) > 1$ and define $\mu_0 \in (0,1)$ by $\kappa_2^2(\varepsilon) = (1-\mu_0^2)\kappa_1^2(\varepsilon)$. Equ. (5.26) is then written

$$1-\mu_1^2 = (1-\mu_0^2)(1-\mu_2^2)\,. \tag{5.27}$$

It allows us to define the particle transmission process $t_{j\to i}$ in the (ε,μ) system of coordinates by $\mu_j = t_{j\to i}\,\mu_i$ with, for all $\mu_2 > 0$ and $\mu_1 < -\mu_0$:

$$t_{1\to 2}\,\mu_2 = \sqrt{1-(1-\mu_0^2)(1-\mu_2^2)}\,, \quad t_{2\to 1}\,\mu_1 = -\sqrt{1-\frac{1-\mu_1^2}{1-\mu_0^2}}\,. \tag{5.28}$$

If $-\mu_0 < \mu_1 < 0$, $t_{2\to 1}\,\mu_1$ is not defined. The reflexion operator r is simply defined by $r\mu_i = -\mu_i$. Rotational symmetry for R_i and $T_{i\to j}$ respectively given by (3.28) and (3.29) simply means that the transmission probability $\overline{T}_{j\to i}$ satisfies: $\overline{T}_{j\to i} = \overline{T}_{j\to i}(\varepsilon_i,\mu_i)$ for all $\sigma_i\mu_i < 0$, $i=1,2$, and with $0 \le \overline{T}_{j\to i} \le 1$. The reciprocity relation (3.30) gives:

$$\overline{T}_{2\to 1}(\varepsilon,\mu) = \begin{cases} \overline{T}_{1\to 2}(\varepsilon, r t_{2\to 1}\mu)\,, & \mu < -\mu_0\,, \\ 0\,, & \text{else.} \end{cases} \tag{5.29}$$

The transmission and reflection rates (5.12) are now given by

$$\begin{aligned} \tilde{R}_i(\varepsilon;\mu\to\mu') &= \frac{\overline{v}_i}{2\pi\kappa_i^2}(1-\overline{T}_{j\to i}(\varepsilon,\mu'))\delta(\mu+\mu')\,, \\ \tilde{T}_{i\to j}(\varepsilon;\mu\to\mu') &= \frac{\overline{v}_i}{2\pi\kappa_i^2}\overline{T}_{j\to i}(\varepsilon,\mu')\delta(\mu - t_{i\to j}\mu')\,. \end{aligned}$$

Of course, purely classical transmission is described within this framework with $\overline{T}_{1\to 2}(\mu) = 1$, for $\mu \in [0,1]$. Now we substitute into the above formulas for the spherically symmetric case and compute

$$\begin{aligned} \beta_1+\beta_2 &= \frac{3\kappa_2^2}{2}\int_0^1 \mu\left(\frac{t_{1\to 2}\mu}{\kappa_1^2}+\frac{\mu}{\kappa_2^2}\right)\overline{T}_{1\to 2}(\varepsilon,\mu)d\mu\,, \\ \alpha_i\tilde{\mathcal{A}}_i\overline{T}_{j\to i} &= 2\pi\kappa_2^2\int_0^1 \mu\overline{T}_{1\to 2}(\varepsilon,\mu)d\mu\,, \\ -\sum_{i=1}^2\frac{\sigma_i}{D_i}\int_{\mathcal{S}_\varepsilon^{i,-}} v_{i,x}\lambda_{i,x}\varphi_i^- dN_\varepsilon^i &= \frac{9}{16\pi}\left[\frac{1}{\kappa_1^2}+\frac{1}{\kappa_2^2}\right. \\ &\qquad \left. -2\kappa_2^2\int_0^1 \mu\left(\frac{t_{1\to 2}\mu}{\kappa_1^2}+\frac{\mu}{\kappa_2^2}\right)^2\overline{T}_{1\to 2}(\varepsilon,\mu)d\mu\right]. \end{aligned}$$

Note that these results apply to the case $\kappa_2^2/\kappa_1^2 < 1$. In the converse situation $\kappa_2^2/\kappa_1^2 > 1$, the roles of 1 and 2 must be exchanged. The above formulas cannot be simplified further without specifying the values of the transmission coefficients.

In the case of purely classical transmission ($\overline{T}_{1\to 2} = 1$) we substitue in (5.25) and obtain

$$\theta = \frac{9}{32\pi\kappa_1^2}\,\mu_0^4\left[1 + \frac{8}{9}\,\frac{\mu_0^2}{1-\mu_0^2} + \frac{1}{2(1-\mu_0^2)^{3/2}}\,\ln\left(\frac{1+\sqrt{1-\mu_0^2}}{1-\sqrt{1-\mu_0^2}}\right)\right], \tag{5.30}$$

We note that $\theta = 0$ when $\kappa_1 = \kappa_2$ ($\mu_0^2 = 1 - \kappa_2^2/\kappa_1^2 = 0$), i.e. when there is no heterojunction at all. On the other hand, $\theta \to \infty$ when $\kappa_2 \to 0$, i.e. when ε tends to the boundary of the region $\mathcal{R}_1 \cap \mathcal{R}_2$. Thanks to that, when ε crosses the boundary between $\mathcal{R}_1 \cap \mathcal{R}_2$ and $\mathcal{R}_1 \setminus \mathcal{R}_2$, there is a continuous shift from the transmission conditions (4.39), (4.9), to the Neumann condition (4.10). ∎

Example 2: Isotropic reflexion-transmission conditions. We consider the reflexion-transmission rates (3.32). Clearly, the corresponding transmission operator is rotationally symmetric and the reflection and transmission rates (5.12) are

$$\begin{aligned}\tilde{R}_i(\varepsilon;\mu\to\mu') &= \frac{\overline{v}_i(\varepsilon)}{\pi\kappa_i(\varepsilon)^2}(1-\pi\kappa_j(\varepsilon)^2\hat{T}(\varepsilon))|\mu|\,,\\ \tilde{T}_{i\to j}(\varepsilon;\mu\to\mu') &= \overline{v}_i(\varepsilon)\hat{T}(\varepsilon)|\mu|\,.\end{aligned}$$

with $\hat{T}$ being the transmission coefficient from (3.32), satisfying $0 \le \hat{T}\pi\kappa_i^2 \le 1$, $i = 1,2$. If, in addition, relaxation time collision operators are considered, the above formulas yield, after some easy computations:

$$\theta = \frac{1}{\pi^2\kappa_1^2\kappa_2^2}\left(\frac{1}{\hat{T}} - \frac{15\pi}{32}(\kappa_1^2+\kappa_2^2)\right) \ge 0\,.$$

∎

6 Application to the energy-transport and drift-diffusion models.

The energy-transport (ET) and drift-diffusion (DD) models are usually directly derived from the semi conductor Boltzmann equation (2.1) by a diffusion approximation using appropriate assumptions on the dominant scattering (see [4], [12]). However, using the knowledge that the equilibrium distribution of electrons is a Fermi-Dirac distribution, they can also be derived from the SHE model by the moment method, using a Fermi-Dirac Ansatz to compute the fluxes. We shall use this method to derive the ET and DD models for an x-dependent band diagram, and their associated transmission conditions at a heterojunction interface.

We first consider a band diagram which depends smoothly on x and define the macroscopic density n, total energy $\mathcal{E}_{tot}$, particle current j_n and total energy current $j_{\mathcal{E}_{tot}}$ according to

$$\begin{pmatrix} n \\ n\mathcal{E}_{tot} \end{pmatrix} = \int_{\mathbb{R}} F \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} N \, d\varepsilon \,, \quad \begin{pmatrix} j_n \\ j_{\mathcal{E}_{tot}} \end{pmatrix} = - \int_{\mathbb{R}} D \nabla_x F \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} d\varepsilon \,, \tag{6.1}$$

where F is a solution of the SHE equation (2.17). We also let q_n and $q_{\mathcal{E}_{tot}}$ the particle and total energy gain rates due to the collisions modeled by $S(F)$:

$$\begin{pmatrix} q_n \\ q_{\mathcal{E}_{tot}} \end{pmatrix} = \int_{\mathbb{R}} S(F) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} d\varepsilon$$

Then, multiplying (2.17) by 1 and ε and integrating over ε leads to the particle and total energy conservation equations:

$$\frac{\partial n}{\partial t} + \nabla_x \cdot j_n = q_n \tag{6.2}$$

$$\frac{\partial}{\partial t}(n\mathcal{E}_{tot}) + n\frac{\partial \phi}{\partial t} + \nabla_x \cdot j_{\mathcal{E}_{tot}} = q_{\mathcal{E}_{tot}} \tag{6.3}$$

The ET model is obtained by closing these equations assuming that F is a Fermi-Dirac distribution:

$$F(x,\varepsilon,t) = \mathcal{F}_{\varepsilon_F,T}(\varepsilon) := \frac{1}{\exp\left(\frac{\varepsilon-\varepsilon_F}{T}\right) + 1} \tag{6.4}$$

where $\varepsilon_F = \varepsilon_F(x,t)$ and $T = T(x,t)$ are respectively the scaled Fermi energy and temperature. We define the functions $n(\varepsilon_F, T; x, t)$ and $n\mathcal{E}_{tot}(\varepsilon_F, T; x, t)$ by:

$$\begin{pmatrix} n \\ n\mathcal{E}_{tot} \end{pmatrix} (\varepsilon_F, T; x, t) = \int_{\mathbb{R}} \mathcal{F}_{\varepsilon_F,T}(\varepsilon) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} N(x,\varepsilon,t) \, d\varepsilon \tag{6.5}$$

where the (x,t) dependence of n and $n\mathcal{E}_{tot}$ comes from the dependence of the band diagram characteristics upon (x,t). We also define the diffusion matrices $D_{ij} = D_{ij}(\varepsilon_F, T; x, t)$, $i = 1, 2$, $j = 1, 2$, by

$$D_{ij}(\varepsilon_F, T; x, t) = \int_{\mathbb{R}} \mathcal{F}_{\varepsilon_F,T}(\varepsilon) \left(1 - \mathcal{F}_{\varepsilon_F,T}(\varepsilon)\right) D(x,\varepsilon,t) \varepsilon^{i+j-2} \, d\varepsilon \tag{6.6}$$

We note that each D_{ij} is a nonnegative symmetric 3×3 matrix, that $D_{12} = D_{21}$, and that under weak geometric assumptions on $e(x,k)$, the 6×6 matrix

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

is symmetric positive definite (see [3] for details). With these definitions, inserting (6.4) in (6.1) leads to

$$j_n = -D_{11}\nabla_x\left(\frac{\varepsilon_F}{T}\right) - D_{12}\nabla_x\left(-\frac{1}{T}\right) \tag{6.7}$$

$$j_{\mathcal{E}_{tot}} = -D_{21}\nabla_x\left(\frac{\varepsilon_F}{T}\right) - D_{22}\nabla_x\left(-\frac{1}{T}\right) \tag{6.8}$$

The ET model written in terms of the Fermi energy-temperature variables consists in equations (6.2) , (6.3), (6.7), (6.8) together with the closure relation (6.5). The DD model is just the ET model in which the temperature is kept constant equal to the lattice temperature. If the lattice temperature is uniform, its formulation in terms of the Fermi-energy variable consists of (6.2) and (6.7) in which $\nabla_x(-1/T) = 0$. The ET and DD models are sometimes more conveniently expressed in terms of the chemical potential $\varepsilon_F + V$ rather than in terms of the Fermi energy ε_F [4].

Now, we turn towards discontinuous band diagrams. We shall use the results of sections 4 and 5 to derive appropriate transmission conditions for the ET and DD models. We begin with the first order transmission conditions (4.8), (4.9), (4.10). First, inserting the Fermi-Dirac Ansatz (6.4) into relation (4.8) leads to the continuity of the temperatures and of the Fermi levels, i.e. with obvious notations:

$$\varepsilon_{F_1} = \varepsilon_{F_2}\,, \quad T_1 = T_2\,. \tag{6.9}$$

Then, inserting the Fermi-Dirac Ansatz (6.4) and taking the first two moments (in ε) of relations (4.9), (4.10) leads to:

$$\left[\int_{\mathcal{R}_1\cap\mathcal{R}_2} D_i(\varepsilon)(\mathcal{F}_i(1-\mathcal{F}_i))(\varepsilon)\left(\nabla\left(\frac{\varepsilon_{F_i}}{T_i}\right)+\varepsilon\nabla\left(-\frac{1}{T_i}\right)\right)\begin{pmatrix}1\\ \varepsilon\end{pmatrix}d\varepsilon\right] = 0\,, \tag{6.10}$$

$$\int_{\mathcal{R}_i\setminus\mathcal{R}_j} D_i(\varepsilon)\,(\mathcal{F}_i(1-\mathcal{F}_i))(\varepsilon)\left(\nabla\left(\frac{\varepsilon_{F_i}}{T_i}\right)+\varepsilon\nabla\left(-\frac{1}{T_i}\right)\right)\begin{pmatrix}1\\ \varepsilon\end{pmatrix}d\varepsilon = 0,\ i=1,2\,, \tag{6.11}$$

where $\mathcal{F}_i := \mathcal{F}_{\varepsilon_{F_i},T_i}$ and where, for a quantity A, we denote by $[A]$ its jump across the heterojunction: $[A_i] = A_2 - A_1$. But (6.11) can be added to the corresponding term of (6.10) to give the flux continuity condition (using (6.6)-(6.8)):

$$j_{n_1} = j_{n_2} := j_n^{int} \quad , \quad (j_{\mathcal{E}_{tot}})_1 = (j_{\mathcal{E}_{tot}})_2 := j_{\mathcal{E}_{tot}}^{int} \tag{6.12}$$

The first order transmission conditions for the ET model at a heterojunction interface thus consist in (6.9), (6.12). Only the continuity of ε_F and j_n needs to be retained for the DD model. These conditions are classical for the DD model, and are derived or used by many authors (see, e.g. [20]).

We now turn towards the second order transmission condition (4.39). Of course, the continuity of the fluxes (6.12) remains unchanged in the second order conditions. Now, taking the moments of (4.39), we get:

$$\int_{\mathcal{R}_1\cap\mathcal{R}_2}\frac{1}{\theta(\varepsilon)}\left(F_2^\alpha - F_1^\alpha\right)\begin{pmatrix}1\\ \varepsilon\end{pmatrix}d\varepsilon = \alpha\int_{\mathcal{R}_1\cap\mathcal{R}_2} J_\alpha^{int}\begin{pmatrix}1\\ \varepsilon\end{pmatrix}d\varepsilon\,. \tag{6.13}$$

Inserting the Fermi-Dirac Ansatz (6.4) in the right-hand-side of (6.13) and using (6.10)-(6.12), we obtain:

$$\int_{\mathcal{R}_1 \cap \mathcal{R}_2} J_\alpha^{int} \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} d\varepsilon = \begin{pmatrix} j_n^{int} \\ j_{\mathcal{E}_{tot}}^{int} \end{pmatrix} . \tag{6.14}$$

Now, the Fermi-Dirac Ansatz (6.4) and Taylor's formula lead to:

$$F_2^\alpha - F_1^\alpha = \mathcal{F}_{\varepsilon_{F2}, T_2} - \mathcal{F}_{\varepsilon_{F1}, T_1} = \mathcal{G}(\varepsilon) \left(\left[\frac{\varepsilon_F}{T} \right] + \varepsilon \left[-\frac{1}{T} \right] \right) , \tag{6.15}$$

with

$$\begin{aligned} &\mathcal{G}(\varepsilon) = \int_0^1 \mathcal{F}_s(\varepsilon) \left(1 - \mathcal{F}_s(\varepsilon) \right) ds = \mathcal{G}(\varepsilon; \varepsilon_{F1}, T_1, \varepsilon_{F2}, T_2) \\ &\mathcal{F}_s(\varepsilon) = \left(\exp \left((1-s) \frac{\varepsilon - \varepsilon_{F1}}{T_1} + s \frac{\varepsilon - \varepsilon_{F2}}{T_2} \right) + 1 \right)^{-1} , \\ &\left[\frac{\varepsilon_F}{T} \right] = \frac{\varepsilon_{F_2}}{T_2} - \frac{\varepsilon_{F_1}}{T_1} \quad , \quad \left[-\frac{1}{T} \right] = - \left(\frac{1}{T_2} - \frac{1}{T_1} \right) . \end{aligned}$$

Inserting (6.15) into the left-hand-side of (6.13), we are led to

$$\int_{\mathcal{R}_1 \cap \mathcal{R}_2} \frac{1}{\theta(\varepsilon)} \left(F_2^\alpha - F_1^\alpha \right) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} d\varepsilon = \Lambda \begin{pmatrix} \left[\frac{\varepsilon_F}{T} \right] \\ \left[-\frac{1}{T} \right] \end{pmatrix} , \tag{6.16}$$

where $\Lambda = (\Lambda_{ij})_{i=1,2;\, j=1,2} = \Lambda(\varepsilon_{F1}, T_1, \varepsilon_{F2}, T_2)$ is the 2×2 matrix given by:

$$\Lambda_{k\ell} = \int_{\mathcal{R}_1 \cap \mathcal{R}_2} \frac{1}{\theta(\varepsilon)} \mathcal{G}(\varepsilon) \, \varepsilon^{k+\ell-2} \, d\varepsilon \, , \quad k = 1,2;\ \ell = 1,2 \, . \tag{6.17}$$

Following (6.13), equating (6.16) and (6.14) leads to the following transmission condition for the ET model

$$\Lambda(\varepsilon_{F_1}, T_1, \varepsilon_{F_2}, T_2) \begin{pmatrix} \left[\frac{\varepsilon_F}{T} \right] \\ \left[-\frac{1}{T} \right] \end{pmatrix} = \alpha \begin{pmatrix} j_n^{int} \\ j_{\mathcal{E}_{tot}}^{int} \end{pmatrix} . \tag{6.18}$$

For Λ to be finite, we need $1/\theta(\varepsilon)$ to be integrable. This is an additional requirement to be imposed on the reflexion-transmission operators R_i, $T_{i \to j}$. This requirement is satisfied for classical reflexion-transmission accross a plane interface (5.30), see the last discussion of example 1, section 5. When θ^{-1} is integrable, it is an easy matter to check that Λ is a symmetric positive-definite matrix.

Therefore, second order transmission conditions for the ET model consist of the flux continuity conditions (6.12), and the jump conditions (6.18). The symmetry and positive-definiteness of Λ is a sufficient condition for formal well-posedness of the problem, as can be viewed from an easy extension of Lemma 4.6 to vector valued functions (left to the reader). Second order transmission conditions for the DD model are simply obtained by taking the first condition (6.12) and the first component of (6.18), (with $\left[-\frac{1}{T}\right] = 0$). At the level of the DD model, interface conditions of this form have been considered in [26]. There the computation of Λ_{11} corresponds to using the crude approximation $\theta_2^+ - \theta_1^+$ from (5.21) for the value of θ.

Clearly, at equilibrium, when the currents j_n^{int} and $j_{\mathcal{E}_{tot}}^{int}$ are zero, condition (6.18) reduces to the continuity of the Fermi energy and temperature (6.9). In spite of their apparent complexity, the second order transmission conditions can easily be implemented in the framework of finite element codes or box method codes by means of weak formulations. This point will be developed in future work.

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