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A SCATTERING MATRIX MODEL OF SEMICONDUCTOR SUPERLATTICES IN MULTIDIMENSIONAL WAVE-VECTOR SPACE AND ITS DIFFUSION LIMIT***

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Abstract

The authors first establish a quantum microscopic scattering matrix model in multidimensional wave-vector space, which relates the phase space density of each superlattice cell with that of the neighbouring cells. Then, in the limit of a large number of cells, a SHE (Spherical Harmonics Expansion)-type model of diffusion equations for the particle number density in the position-energy space is obtained. The crucial features of diffusion constants on retaining the memory of the quantum scattering characteristics of the superlattice elementary cell (like e.g. transmission resonances) are shown in order. Two examples are treated with the analytically computation of the diffusion constants.

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§1. Introduction

Recently the mathematical modelling of semiconductor superlattices has attracted a lot of attention in the applied mathematics world. New related works have been made in [5, 15]. In fact, the so-called semiconductor superlattices are processed by growing periodic layers of two different semiconductor materials, like $GaAs$ and $GaAlAs$ (see [24, 25]). The establishment of a periodic electrostatic potential in the direction of the growth axis, which is discontinuous at the interfaces of the two materials, is carried out through the electronic properties of the two different materials. This periodic potential is always superimposed

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with a non periodic potential when the structure is biased with an external electric field. There are a lot of interesting applications of superlattices to optoelectronics[24] and other relevant problems, especially the example of the infrared radiation detector described in [33].

Ideally, Bloch's theory of bands[1,25] applies to the superlattice periodic potential, resulting in the establishment of superlattice energy bands. Bloch's theory of bands is a fully quantum mechanical theory which relies on the perfect phase coherence of the electron wave functions between the different potential periods. Then, electrons subject to a constant electric field in the direction of the growth axis undergo a periodic motion called 'Bloch oscillations'[24]. For transport to occur, collisions are necessary as they allow electrons to hop from one Bloch trajectory to another one. On this basis, Esaki and Tsu[18] established the first quantitative model of transport in a superlattice.

But collisions also have the effect of breaking the phase coherence of the electron waves between neighbouring superlattice cells and consequently destroying the quantum nature of transport. The typical distance beyond which phase coherence is broken is called the coherence length. If the coherence length is of the same order as the superlattice period, wave functions lose their correlations over too short distances for Bloch theory to apply. In particular, scattering by interface roughness (see [11] or Sibille's contribution in [24]) is one of the most important collision mechanism: because of imperfections in the growth process, the interfaces between the two different materials are not perfectly planar, but instead exhibit a random staircase-like structure. Particles crossing the interfaces may be strongly scattered by the resulting random potential.

The aim of the present paper is to present and derive a transport model aimed at the description of this situation. We suppose that the electron wave-functions lose their phase coherence over a distance comparable with the superlattice period (or possibly, a multiple of the period). Therefore, it is legitimate to speak of the classical phase space density $f_{n+\frac{1}{2}}(k,t)$ at the interface between the n-th and $(n+1)$-th superlattice period. This density is related to those of the neighbouring cells by means of the quantum scattering matrix of the superlattice potential. This gives rise to a discrete difference system in space and time, refered to in the literature as a 'scattering matrix model'[32]. It fully retains the quantum nature of transport over distances of the order of the phase coherence length, but deals with the evolution of a semiclassical quantity over larger distances.

In this paper, we investigate the limit of a large number of cells. After space and time rescaling, the resulting perturbation problem appears similar to a diffusion approximation problem in kinetic theory and gives rise to a diffusion equation for the electron number density in the position-energy space (or energy distribution function). The obtained equation is a class of Spherical Harmonics Expansion (SHE) equations, which have been turned out to be extremely useful in the context of standard semiconductor modelling. Besides [15], the present paper is the only another one (to our knowledge) to establish the SHE model in the framework of superlattices. A direct link between the quantum transport characteristics of the superlattice structure (the scattering coefficients and time delays) and the coefficients of the SHE model (the density-of-states, which gives the number of available states at a given energy[6], and the diffusivity) is furnished by the derivation of the model. This model can provide means of achieving fast and reliable simulations of electron transport in superlattices.

A related approach can be found in [5] where the superlattice is treated as a periodic array of planar interfaces. This is valid if one of the layers is much narrower than the other one and can be approximated by a zero-width interface. In that case, a more conventional kinetic model can be used and a complete mathematical theory of the large number-of-cells limit can be given. The model presented here is physically more relevant as much milder assumptions on the relative size of the layers is required but the mathematical theory is still at a formal level due to the time and space discreteness of the scattering model.

We should point out that the paper [15] is one dimensional in k where the scattering operator is far simpler (it does not involve any k- integral). However, in [15] the link with the Schrödinger equation in the elementary period is well developed (Section 3), and the action on the scaling on the scattering coefficients is derived in detail (Section 4). The coupling with the Possion equation is considered (Sections 4 and 5). The boundary conditions for the limit SHE model are given (Section 5). In the present paper, we focus on the multidimensional k- space and do not give so much detail on the link with the Schrödinger or the Poisson equation, the scaling of the scattering coefficients or the boundary conditions. On the other hand, the multidimensional k- space requires to introduce more elements of functional and operator analysis than in [15]. Also, the derivation of the final SHE model is fairly more complex. This is why we focus on these aspects here and refer to [15] for the other points.

Alternate macroscopic models for superlattices, of Drift-Diffusion type, have also been proposed. We refer the reader to e.g. [24], [7] for these phenomenological approaches.

As far as the diffusion approximation methodology of Hilbert, Chapman and Enskog ,and its application to bulk semiconductors as well as its modern mathematical view are concerned, we refer to [10, 29, 12, 2, 28, 23]. In addition, one can see [26, 31] for semiconductor modelling in more details. In a word, the diffusion approximation is a theoretical tool which links the evolution of macroscopic quantities like number or energy densities to the microscopic particle dynamics described by a kinetic equation. In particular, it provides a direct expression of the diffusion constants involved in the macroscopic model in terms of particle interactions with the surrounding medium.

A recently useful enough diffusion model- the 'SHE' model (Spherical Harmonics Expansion Model[34]) for the particle number density in the position-energy space[17,3,13] has been derived in terms of analyzing the various collision scales. Its application to semiconductor device modelling and plasma physics as well as gas discharge physics can be found in [14, 20, 21, 22] and [14]. An alternate derivation from careful inspection of individual particle transport is exposed in [9] (where it is referred to as the 'Fokker-Planck equation').

The outline of the paper is as follows: the microscopic scattering matrix model is exposed in Section 2. The properties of the quantum scattering coefficients and time delays of the structure are outlined in Section 3 and the diffusion limit, stated in Section 4. Examples and the conclusion of the entire paper are given in Section 5. Finally, intermediate steps in the derivation of the diffusion model are detailed in appendices A and B.

§2. The Microscopic Scattering-Matrix Model for Superlattices

In this section a semiconductor superlattice consisting of layers of two materials labeled A and B is taken into account, which is periodically arranged in the direction x and generates a permanent periodic potential of period ℓ in this direction. Generally electron motion through the structure of superlattice with very small period (10 to 100 nm) must be described in terms of quantum mechanics. However, we assume that various sources of scattering (e.g. interface roughness scattering due to some cristalline disorder at the A/B and B/A heterojunctions[24,11]) lead to a phase decoherence of the electron wave-functions over distances comparable with the superlattice period. In this context, quantum effects are limited within one superlattice period $\frac{1}{2}A/B/\frac{1}{2}A$ where $\frac{1}{2}A$ denotes a half A-layer, this layer being supposed to be significantly larger than the B-layer.

Let us denote the interval occupied by the n-th superlattice pattern $\frac{1}{2}A/B/\frac{1}{2}A$ by $[(n-\frac{1}{2}\ell),(n+\frac{1}{2}\ell)]$, where the points $(n+\frac{1}{2}\ell)$, $n\in\mathbb{Z}$ are the mid-points of the A layers. Our assumption is that the state of the electron gas in a given A layer can be described by $f_{n+\frac{1}{2}}(k,t)$ which represents the number of electrons at time t with momentum k at the mid-point of the $(n+\frac{1}{2})$-th A layer (that connecting the n-th and $(n+1)$-th pattern). Then,

finding the motion of an electron through the elementary pattern $\frac{1}{2}A/B/\frac{1}{2}A$ reduces to a standard quantum mechanical scattering problem. Such a problem is characterized by the reflection-transmission coefficients $\sigma^n(k',k)$ and by the time delays $\tau^n(k',k)$ (see [27, 30]).

For the convenience of readers, we first need to introduce some additional definitions. Here, although we restrict to a one dimensional spatial geometry along the periodicity axis x, we allow momenta of all directions, belonging to the Brillouin zone $\mathcal{B}$ of the A-layer material. We recall that the Brillouin zone is a fundamental domain of the torus $\mathbb{R}^3/L^*$, where L^* is the reciprocal lattice of material A. All functions of k will be considered as periodic with periodicity L^*. The electron kinetic energy in material A is a given smooth L^* periodic function of k denoted by $\varepsilon(k)$ (the so-called 'band diagram'), and the electron velocity associated with momentum k is

$$v(k) = \frac{1}{\hbar}\nabla_k \varepsilon(k)\,, \quad k \in \mathcal{B}\,,$$

where $\hbar$ is the reduced Planck constant. $v_x(k)$ is the x-component of v.

For momenta k', k such that the associated velocities satisfy $v_x(k') > 0$ and $v_x(k) < 0$ (respectively $v_x(k') < 0$ and $v_x(k) > 0$) , the scattering coefficient $\sigma^n(k',k)$ is the reflection coefficient of the n-th pattern for particles incoming from the left (resp. from the right) with momentum k' and thus reflected to the left (resp. to the right) with momentum k. On the other hand, for k', k such that $v_x(k') > 0$ and $v_x(k) > 0$ (respectively $v_x(k') < 0$ and $v_x(k) < 0$), $\sigma^n(k',k)$ is the transmission coefficient for particles incoming from the left (resp. from the right) with momentum k', transmitted through the structure and exiting on the right (resp. on the left) with momentum k. The index n indicates that a large scale variation of the characteristics of the elementary pattern can be superimposed to periodicity.

The time delays $\tau^n(k',k)$ are the times needed for a particle to achieve reflection or transmission. For instance, for k', k such that $v_x(k') > 0$ and $v_x(k) < 0$, $\tau^n(k',k)$ is the time needed for a particle starting at point $(n - \frac{1}{2}\ell)$ and velocity $v_x(k') > 0$ to be reflected back at the same point with velocity $v_x(k)$. The semi-classical time delays are obtained as the derivatives with respect to the energy of the phase of the reflection or transmission amplitude (whereas the reflection and transmission coefficients are the squared modules of the same amplitude, see [27] or Section 5). Scattering coefficients and time delays satisfy a number of relations that will be listed later on. In the present work, we shall consider that the scattering coefficients or time delays are known.

First of all, we establish the dynamics obeyed by the discrete distribution function $f_{n+\frac{1}{2}}(k,t)$ in the absence of an external electric field. Consider $f_{n+\frac{1}{2}}(k,t)$ for $v_x(k) > 0$, which corresponds to particles at point $(n + \frac{1}{2}\ell)$ moving to the right and let us trace back these particles at previous times. Some of them have been transmitted through the n-th pattern and come from point $(n - \frac{1}{2}\ell)$ with a momentum k' such that $v_x(k') > 0$. The number of these is $\sigma^n(k',k) f_{n-\frac{1}{2}}(k', t - \tau^n(k',k))\delta(\varepsilon(k') - \varepsilon(k))$, where the delta function reminds that scattering by a time-independent potential is an energy conservative process. The other contribution to $f_{n+\frac{1}{2}}(k,t)$ is made of particles reflected by the n-th pattern and coming from point $(n + \frac{1}{2}\ell)$ with a momentum k' such that $v_x(k') < 0$. The number of these is $\sigma^n(k',k) f_{n+\frac{1}{2}}(k', t - \tau^n(k',k))\delta(\varepsilon(k') - \varepsilon(k))$. To obtain the total number $f_{n+\frac{1}{2}}(k,t)$, we must integrate these two contributions with respect to all possible original momenta k'. For

$v_x(k) > 0$, this leads to

$$f_{n+\frac{1}{2}}(k,t) = \int_{v_x(k')>0} \sigma^n(k',k) f_{n-\frac{1}{2}}(k', t-\tau^n(k',k))\delta(\varepsilon(k')-\varepsilon(k))|v_x(k')|\,dk' + \int_{v_x(k')<0} \sigma^n(k',k) f_{n+\frac{1}{2}}(k', t-\tau^n(k',k))\delta(\varepsilon(k')-\varepsilon(k))|v_x(k')|\,dk'. \tag{2.1}$$

Symmetrically, we consider $f_{n-\frac{1}{2}}(k,t)$ for $v_x(k) < 0$ and find:

$$f_{n-\frac{1}{2}}(k,t) = \int_{v_x(k')<0} \sigma^n(k',k) f_{n+\frac{1}{2}}(k', t-\tau^n(k',k))\delta(\varepsilon(k')-\varepsilon(k))|v_x(k')|\,dk' + \int_{v_x(k')>0} \sigma^n(k',k) f_{n-\frac{1}{2}}(k', t-\tau^n(k',k))\delta(\varepsilon(k')-\varepsilon(k))|v_x(k')|\,dk'. \tag{2.2}$$

Here and in what follows, the symbol dk will refer to $dk = (4\pi^3)^{-1}d\tilde{k}$ where $d\tilde{k}$ is the usual volume element in momentum space. The factor $(4\pi^3)^{-1}$ is referred to in the literature as the momentum-density-of-states[6]. Now, we can give a physical interpretation of the reflection-transmission coefficients in terms of transition probabilities: $\sigma^n(k',k)\delta(\varepsilon(k')-\varepsilon(k))|v_x(k)|\,dk$ is the probability for an incident particle with momentum k' to be reflected or transmitted to a volume element dk about k in momentum space. It is notable that in [15], there are no k integrals and that the scattering operator is simpler.

In practical applications, superlattice structures are biased, i.e. related to an external circuit. The bias superimposes a non-periodic potential ϕ to the periodic potential originating from the superlattice. Let $E(x)$ be the electric-field associated with ϕ: $E = -\frac{d\phi}{dx}$. We decompose E into its average over the n-th elementary cell:

$$E^n = \frac{1}{\ell}\int_{(n-\frac{1}{2})\ell}^{(n+\frac{1}{2})\ell} E(x)dx, \tag{2.3}$$

and a rest of zero average. Since,

$$E^n\ell = \phi\Big(\Big(n-\frac{1}{2}\Big)\ell\Big) - \phi\Big(\Big(n+\frac{1}{2}\Big)\ell\Big),$$

the zero average contribution merely amounts to a large scale deformation of the superlattice pattern and is already accounted for in the dependence of the scattering coefficients and time delays upon the index n of the pattern. On the other hand, the constant contribution E^n results in a change of the kinetic energy of the particles when crossing a cell. Now, we shall denote by $\sigma^n(E^n,k',k)$, $\tau^n(E^n,k',k)$ the scattering portrait of the n-th cell biased by a constant electric field E^n (or equivalently by a linear potential in the interval $[(n-\frac{1}{2}\ell),(n+\frac{1}{2}\ell)]$). For $E^n = 0$, these quantities coincide with those previously defined.

Taking into account the shift in energy due to the presence of the electric field, the evolution dynamics is now given for $v_x(k) > 0$ by

$$f_{n+\frac{1}{2}}(k,t) = \int_{v_x(k')>0} \sigma^n(E^n,k',k) f_{n-\frac{1}{2}}(k', t-\tau^n)\delta(\varepsilon(k')-(\varepsilon(k)+\ell eE^n))|v_x(k')|\,dk' + \int_{v_x(k')<0} \sigma^n(E^n,k',k) f_{n+\frac{1}{2}}(k', t-\tau^n)\delta(\varepsilon(k')-\varepsilon(k))|v_x(k')|\,dk', \tag{2.4}$$

and for $v_x(k) < 0$, by

$$f_{n-\frac{1}{2}}(k,t) = \int_{v_x(k')<0} \sigma^n(E^n,k',k) f_{n+\frac{1}{2}}(k',t-\tau^n)\delta(\varepsilon(k') - (\varepsilon(k) - \ell e E^n))|v_x(k')|\,dk' + \int_{v_x(k')>0} \sigma^n(E^n,k',k) f_{n-\frac{1}{2}}(k',t-\tau^n)\delta(\varepsilon(k') - \varepsilon(k))|v_x(k')|\,dk', \tag{2.5}$$

where e denotes the elementary positive charge and where the dependences of the time delays upon the field and momenta have been omitted for brevity. System (2.4), (2.5) belongs to the class of scattering matrix models which are sometimes used in the literature[32]. Here, the scattering matrix is nothing else than the quantum scattering matrix of the potential structure.

That the external electric field should be time-independent is related to the energy conservation relation expressed by the delta functions in (2.4), (2.5). Time-dependent electric fields could however be considered if they varied over large time scales compared with the time delays or, in other words, if they evolved adiabatically. In the present work, we shall restrict to time-independent fields to avoid technicalities related to the fact that time delays may be infinite for certain energies (those corresponding to maxima of the potential).

To preserve causality, we require of system (2.4), (2.5) to be a backwards difference system in time. Therefore, we assume that the time delays are positive. This can be viewed as a regularity assumption for the potential because negative time delays can occur for certain singular potentials (like delta function potentials[30]). We consider that (2.4), (2.5) describes the evolution of the system for $t > 0$, starting from known states for all $t \le 0$. A typical situation is a system at equilibrium, which is suddenly driven into a non-equilibrium state by some external action (for instance a change in the boundary conditions or in the applied potential). Therefore, we prescribe the distribution functions for all negative times:

$$f_{n-\frac{1}{2}}(k,t) = (f_I)_{n-\frac{1}{2}}(k,t) = \text{ given}\,, \quad \forall t \le 0\,, \quad \forall n \in \mathbb{Z}\,, \quad \forall k \in \mathcal{B}, \tag{2.6}$$

and we additionally suppose that f_I is continuous at time $t = 0$.

We note that ℓ does not need to coincide with a superlattice period, but can also be an integer multiple of the period. Indeed, if the phase-coherence length of the particles is larger than the superlattice period, it is necessary to identify ℓ with the smallest integer multiple of the superlattice period larger than the coherence length.

In order to give a precise meaning to the integrals involving a delta function in the formulae above, we recall the co-area formula in geometric measure theory. Denote by $\mathcal{S}_\varepsilon$ the manifold in k-space $\mathcal{S}_\varepsilon = \{k \in \mathcal{B}, \varepsilon(k) = \varepsilon\}$. Let $dS_\varepsilon(k)$ be the Euclidean surface element (divided by $(4\pi)^3$) on $\mathcal{S}_\varepsilon$ and $\mathcal{R}$ the closure of the numerical range of $\varepsilon(k)$. We also denote by $dN_\varepsilon(k)$ the co-area and by $N(\varepsilon)$ the energy-density-of-states (or shortly 'density-of-states'[6]):

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

By Sard's theorem and the implicit function theorem, these objects are defined for all $\varepsilon \in \mathcal{R} \setminus \mathcal{R}_0$ where $\mathcal{R}_0$ is a set of measure zero. We also assume that $N(\varepsilon) \in L^\infty(\mathcal{R})$. With this hypothesis, the coarea formula applies[19]: for any continuous function $\psi(k)$ defined on B, we have

$$\int_{\mathcal{B}} \psi(k)dk = \int_{\mathcal{R}} \int_{\mathcal{S}_\varepsilon} \psi(k) \frac{dS_\varepsilon(k)}{|\nabla_k \varepsilon(k)|}. \tag{2.8}$$

With the coarea formula (2.8), the meaning of the integrals written above is defined by

duality:

$$\int_{\mathcal{B}} f(k)\delta(\varepsilon(k)-\varepsilon)\,dk = \int_{\mathcal{S}_\varepsilon} f(k)dN_\varepsilon(k)\,. \tag{2.9}$$

Therefore, formulae (2.4), (2.5) are also written for $v_x(k) > 0$,

$$\begin{aligned} f_{n+\frac12}(k,t) = &\int_{\S^+_{\varepsilon(k)+\ell eE^n}} \sigma^n(E^n,k',k) f_{n-\frac12}(k',t-\tau^n)|v_x(k')|\,dN_{\varepsilon(k)+\ell eE^n}(k') \\ &+ \int_{\S^-_{\varepsilon(k)}} \sigma^n(E^n,k',k) f_{n+\frac12}(k',t-\tau^n)|v_x(k')|\,dN_{\varepsilon(k)}(k'), \end{aligned} \tag{2.10}$$

and for $v_x(k) < 0$,

$$\begin{aligned} f_{n-\frac12}(k,t) = &\int_{\S^-_{\varepsilon(k)-\ell eE^n}} \sigma^n(E^n,k',k) f_{n+\frac12}(k',t-\tau^n)|v_x(k')|\,dN_{\varepsilon(k)-\ell eE^n}(k') \\ &+ \int_{\S^+_{\varepsilon(k)}} \sigma^n(E^n,k',k) f_{n-\frac12}(k',t-\tau^n)|v_x(k')|\,dN_{\varepsilon(k)}(k'), \end{aligned} \tag{2.11}$$

where $\mathcal{S}_\varepsilon{}^\pm = \{k \in \mathcal{S}_\varepsilon,\ \pm v_x(k) > 0\}$. From now on, we shall write $dN(k')$ for $dN_{\varepsilon(k)}(k')$, $dN_{\varepsilon(k)+\ell eE^n}(k')$, etc., and v_x, v_x' instead of $v_x(k)$, $v_x(k')$, when the context will be clear.

It is helpful to interpolate the discrete quantities into piecewise continuous functions of the position variable x. We define

$$\begin{aligned} &f(x,k,t) = f_{n+\frac12}(k,t)\,, \quad f_I(x,k,t) = (f_I)_{n+\frac12}(k,t)\,, \quad x \in [n\ell,(n+1)\ell), \\ &\overline{E}(x) = E^n\,, \quad \sigma(x,E,k',k) = \sigma^n(E,k',k)\,, \quad \tau(x,E,k',k) = \tau^n(E,k',k)\,, \\ &\qquad x \in \Big[\Big(n-\frac12\Big)\ell, \Big(n+\frac12\Big)\ell\Big)\,. \end{aligned}$$

From these definitions, system (2.10), (2.11), (2.6) becomes the following equivalent system

$$\begin{aligned} f\Big(x+\frac{\ell}{2},k,t\Big) = &\int_{\S^+_{\varepsilon(k)+\ell e\overline{E}(x)}} \sigma(x,\overline{E}(x),k',k) f\Big(x-\frac{\ell}{2},k',t-\tau\Big)|v_x'|\,dN(k') \\ &+ \int_{\S^-_{\varepsilon(k)}} \sigma(x,\overline{E}(x),k',k) f\Big(x+\frac{\ell}{2},k',t-\tau\Big)|v_x'|\,dN(k'), \end{aligned} \tag{2.12}$$

for $v_x > 0$ and

$$\begin{aligned} f\Big(x-\frac{\ell}{2},k,t\Big) = &\int_{\S^-_{\varepsilon(k)-\ell e\overline{E}(x)}} \sigma(x,\overline{E}(x),k',k) f\Big(x+\frac{\ell}{2},k',t-\tau\Big)|v_x'|\,dN(k') \\ &+ \int_{\S^+_{\varepsilon(k)}} \sigma(x,\overline{E}(x),k',k) f\Big(x-\frac{\ell}{2},k',t-\tau\Big)|v_x'|\,dN(k'), \end{aligned} \tag{2.13}$$

for $v_x < 0$, with the initial condition

$$f(x,k,t) = f_I(x,k,t)\,, \quad \forall t \le 0\,, \quad \forall (x,k) \in \mathbb{R} \times \mathcal{B}\,. \tag{2.14}$$

We now introduce new position and time coordinates according to

$$\tilde{x} = \alpha x\,, \quad \tilde{t} = \alpha^2 t\,, \tag{2.15}$$

where $\alpha \langle 1$ is a small parameter. $\tilde{x}$ and $\tilde{t}$ are the macroscopic position and time coordinates. Indeed, if one moves along the x-axis a distance such that $\tilde{x}$ varies of an order 1 quantity, a large number (of order α^{-1}) of superlattice cells (of size α) are crossed. Analogously, the

use of the time coordinate $\tilde{t}$ focuses on the long time dynamics of the system, of diffusion type.

Now, we would like to express that the scattering parameters σ, τ depend on the macroscopic position variable only. However, this cannot be entirely true since, by definition, they must be constant within each superlattice period. However, we shall suppose that, apart from this unavoidable discrepancy, they are functions of the macroscopic variable only. This assumption can be expressed through the change of coordinates (2.15) as follows:

$$\sigma(x,E,k',k)=\tilde{\sigma}^{\alpha}(\tilde{x},E,k',k)\,,\quad \tau(x,E,k',k)=\tilde{\tau}^{\alpha}(\tilde{x},E,k',k)\,, \tag{2.16}$$

where $\tilde{\sigma}^{\alpha}$, $\tilde{\tau}^{\alpha}$ are defined by means of functions $\tilde{\sigma}$, $\tilde{\tau}$, independent of α through

$$\tilde{\sigma}^{\alpha},\,\tilde{\tau}^{\alpha}\,(\tilde{x},E,k',k)=\tilde{\sigma},\,\tilde{\tau}\,\Big(\alpha\ell\Big[\frac{\tilde{x}}{\alpha\ell}+\frac{1}{2}\Big],E,k',k\Big)\,, \tag{2.17}$$

with $[y]$ denoting the integer part of the real number y, i.e. the largest integer number smaller than or equal to y.

In a similar fashion, we suppose that the external potential ϕ only depends on the macroscopic variable, i.e. there exists a function $\tilde{\phi}$, independent of α, such that $\phi(x)=\tilde{\phi}(\tilde{x})$. Defining the macroscopic electric field by $\tilde{E}(\tilde{x})=-\frac{d\tilde{\phi}}{d\tilde{x}}(\tilde{x})$, we have $E(x)=\alpha\tilde{E}(\tilde{x})$ and

$$\overline{E}(x)=\alpha\tilde{E}^{\alpha}(\tilde{x})\,,$$

with $\tilde{E}^{\alpha}$ defined by

$$\tilde{E}^{\alpha}(\tilde{x})=\frac{1}{\alpha\ell}\int_{(n-\frac{1}{2})\alpha\ell}^{(n+\frac{1}{2})\alpha\ell}\tilde{E}(\tilde{y})\,d\tilde{y}\,,\quad \tilde{x}\in\Big[\Big(n-\frac{1}{2}\Big)\alpha\ell,\Big(n+\frac{1}{2}\Big)\alpha\ell\Big)\,, \tag{2.18}$$

i.e. $\tilde{E}^{\alpha}$ is the mean value of the macroscopic electric field over a superlattice period.

We refer to [15] for a justification of the scaling of the scattering coefficient and that of the electric field.

Finally, a similar assumption is made for f_I:

$$f_I(x,k,t)=\tilde{f}_I^{\alpha}(\tilde{x},k,\tilde{t})\,,\quad \tilde{f}_I^{\alpha}(\tilde{x},k,\tilde{t})=\tilde{f}_I\Big(\alpha\ell\Big[\frac{\tilde{x}}{\alpha\ell}\Big],k,\tilde{t}\Big)\,. \tag{2.19}$$

Additionally, to avoid initial layers in dealing with the limit $\alpha\to 0$, we suppose that $\tilde{f}_I$ is a function of the energy only :

$$\tilde{f}_I(\tilde{x},k,\tilde{t})=\tilde{F}_I(\tilde{x},\varepsilon(k),\tilde{t})\,. \tag{2.20}$$

This is quite natural since initial conditions are usually equilibrium states which are functions of the total (kinetic and potential) energy.

These scaling assumptions are valid when, on the scale of the superlattice period, the externally applied potential has only small variations and the discrepancy to perfect periodicity of the superlattice is also small. These hypotheses are satisfied in practice as soon as the number of superlattice periods is large (of the order of 10 or more) between the biasing contacts. In this case, the applied bias is shared in almost equal amounts by each superlattice period and the potential jump through one period is small as well as the deformation of the superlattice potential by the (zero period-average part of the) external electric field.

For future use, we note that relations (2.17), (2.19) and (2.18) can also be written

$$\tilde{\sigma}^{\alpha},\,\tilde{\tau}^{\alpha}\,(\tilde{x},E,k',k)=\tilde{\sigma},\,\tilde{\tau}\,(\tilde{x}+\alpha\ell\Delta(\alpha,\ell,\tilde{x}),E,k',k)\,, \tag{2.21}$$

$$\tilde{f}_I^{\alpha}(\tilde{x},k,\tilde{t})=\tilde{F}_I(\tilde{x}+\alpha\ell\delta(\alpha,\ell,\tilde{x}),\varepsilon(k),\tilde{t}):=\tilde{F}_I^{\alpha}(\tilde{x},\varepsilon(k),\tilde{t})\,, \tag{2.22}$$

and

$$\tilde{E}^{\alpha}(\tilde{x})=\frac{1}{\alpha\ell}\int_{\tilde{x}+\alpha\ell(\Delta(\alpha,\ell,\tilde{x})-\frac{1}{2})}^{\tilde{x}+\alpha\ell(\Delta(\alpha,\ell,\tilde{x})+\frac{1}{2})}\tilde{E}(\tilde{y})\,d\tilde{y}\,, \tag{2.23}$$

where

$$\Delta(\alpha,\ell,\tilde{x}) = \frac{1}{2} - \left\{ \frac{\tilde{x}}{\alpha\ell} + \frac{1}{2} \right\}, \quad \delta(\alpha,\ell,\tilde{x}) = \frac{1}{2} - \left\{ \frac{\tilde{x}}{\alpha\ell} \right\}, \tag{2.24}$$

and $\{y\} = y - [y]$ denotes the fractional part of the real number y. In particular, since $|\Delta|, |\delta| \leq 1$, we have

$$\tilde{\sigma}^\alpha,\ \tilde{\tau}^\alpha = \tilde{\sigma},\ \tilde{\tau} + O(\alpha)\,, \quad \tilde{F}_I^\alpha = \tilde{F}_I + O(\alpha)\,, \quad \tilde{E}^\alpha = \tilde{E} + O(\alpha)\,. \tag{2.25}$$

Now, introducing the scaled distribution function f^α according to

$$\tilde{f}^\alpha(\tilde{x},k,\tilde{t}) = f(x,k,t)\,,$$

the change of scales (2.15) in equations (2.12), (2.13), (2.14) yields (omitting the tildes for clarity):

$$\begin{aligned} f^\alpha\Big(x+\frac{\alpha\ell}{2},k,t\Big) = &\int_{\S^+_{\varepsilon(k)+\alpha\ell e E^\alpha(x)}} \sigma^\alpha(x,\alpha E^\alpha(x),k',k) f^\alpha\Big(x-\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)|v'_x|\,dN(k') \\ &+ \int_{\S^-_{\varepsilon(k)}} \sigma^\alpha(x,\alpha E^\alpha(x),k',k) f^\alpha\Big(x+\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)|v'_x|\,dN(k'), \end{aligned} \tag{2.26}$$

for $v_x > 0$ and

$$\begin{aligned} f^\alpha\Big(x-\frac{\alpha\ell}{2},k,t\Big) = &\int_{\S^-_{\varepsilon(k)-\alpha\ell e E^\alpha(x)}} \sigma^\alpha(x,\alpha E^\alpha(x),k',k) f^\alpha\Big(x+\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)|v'_x|\,dN(k') \\ &+ \int_{\S^+_{\varepsilon(k)}} \sigma^\alpha(x,\alpha E^\alpha(x),k',k) f^\alpha\Big(x-\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)|v'_x|\,dN(k'), \end{aligned} \tag{2.27}$$

for $v_x < 0$, with the initial condition

$$f^\alpha(x,k,t) = F_I^\alpha(x,\varepsilon(k),t)\,, \quad \forall t<0\,, \quad \forall (x,k) \in \mathbb{R}\times\mathcal{B}\,. \tag{2.28}$$

In this paper what we want is to find the formal limit of model (2.26), (2.27), (2.28) when α tends to zero. To reach this aim, we have to state the main properties of the reflection-transmission coefficients in the next section.

§3. The Reflection-Transmission Coefficients

First, we suppose that the flux of particles of given energy ε through the elementary superlattice structure is conserved. This reads as follows:

$$\begin{aligned} 1 = &\int_{\S^+_{\varepsilon(k')-\alpha\ell e E}} \sigma^\alpha(x,E,k',k)|v_x|\,dN(k) + \int_{\S^-_{\varepsilon(k')}} \sigma^\alpha(x,E,k',k)|v_x|\,dN(k), \\ &\forall k'\in\mathcal{B}\,,\ v_x(k')>0\,, \quad \forall x\in\mathbb{R}\,, \quad \forall E\in\mathbb{R}\,, \end{aligned} \tag{3.1}$$

$$\begin{aligned} 1 = &\int_{\S^-_{\varepsilon(k')+\alpha\ell e E}} \sigma^\alpha(x,E,k',k)|v_x|\,dN(k) + \int_{\S^+_{\varepsilon(k')}} \sigma^\alpha(x,E,k',k)|v_x|\,dN(k). \\ &\forall k'\in\mathcal{B}\,,\ v_x(k')<0\,, \quad \forall x\in\mathbb{R}\,, \quad \forall E\in\mathbb{R}. \end{aligned} \tag{3.2}$$

This assumption supposes that generation-recombination of electrons is negligible and that transmission or reflection through the superlattice elementary pattern occurs elastically. In particular, interactions with phonons or photons, which produce a change of the electron energy by absorption or emission and which can induce trapping on (or excitation from) the potential bound states, must be neglected. These phenomena, which are important in practical applications (see e.g. [33] for applications to lasers or infrared radiation detetection), could be introduced but would add unnecessary technical complexity for the present introductory exposition. They will be dealt with in details in future work.

Second, we suppose that the reflection-transmission coefficients and time delays satisfy the following reciprocity relations, which is a translation of the time-reversibility of the underlying quantum dynamics:

$$\sigma^\alpha(x,E,k',k)=\sigma^\alpha(x,E,-k,-k')\,, \tag{3.2}$$

$$\tau^\alpha(x,E,k',k)=\tau^\alpha(x,E,-k,-k')\,, \tag{3.4}$$

for all admissible values of (x,E,k',k). We note that the reflection-transmission coefficients and time delays are only defined on certain submanifolds of $\mathcal{B}\times\mathcal{B}$. For instance, for $v_x(k')>0$ and $v_x(k)>0$, $\sigma^\alpha(x,E,k',k)$ is defined on $\{(k',k)\in\mathcal{B}\times\mathcal{B},\ \varepsilon(k')=\varepsilon(k)+\alpha\ell eE\}$. We assume that these coefficients are strictly positive on their manifold of definition:

$$\sigma^\alpha,\,\tau^\alpha\,>0\,. \tag{3.5}$$

As a direct consequence of the flux conservation and reciprocity relations (3.1)–(3.2), we get the following 'normalization' identities

$$1=\int_{\S^+_{\varepsilon(k)+\alpha\ell eE}}\sigma^\alpha(x,E,k',k)|v'_x|\,dN(k')+\int_{\S^-_{\varepsilon(k)}}\sigma^\alpha(x,E,k',k)|v'_x|\,dN(k'),$$
$$\forall k\in\mathcal{B}\,,\ v_x(k)>0\,,\quad \forall x\in\mathbb{R}\,,\quad \forall E\in\mathbb{R}\,. \tag{3.6}$$

$$1=\int_{\S^-_{\varepsilon(k)-\alpha\ell eE}}\sigma^\alpha(x,E,k',k)|v'_x|\,dN(k')+\int_{\S^+_{\varepsilon(k)}}\sigma^\alpha(x,E,k',k)|v'_x|\,dN(k').$$
$$\forall k\in\mathcal{B}\,,\ v_x(k)<0\,,\quad \forall x\in\mathbb{R}\,,\quad \forall E\in\mathbb{R}\,. \tag{3.7}$$

We now introduce the following operator which will occupy a central position in the forthcoming theory: for $\varphi:\ k\in\mathcal{S}_\varepsilon\to\varphi(k)\in\mathbb{R}$, the operator $K(x,\varepsilon)$ operates according to

$$(K(x,\varepsilon)\varphi)(k)=\int_{\S_\varepsilon}\sigma(x,k',k)\varphi(k')|v'_x|dN_\varepsilon(k'), \tag{3.8}$$

where we recall that $\sigma(x,k',k)\equiv\sigma(x,E=0,k',k)$. $K(x,\varepsilon)$ depends on the position and energy variables as parameters. We denote by $L^2(S_\varepsilon)$ the space of square integrable functions on $\mathcal{S}_\varepsilon$ with respect to the measure $|v_x(k)|dN_\varepsilon(k)$, and by $(f,g)_\varepsilon$ and $|f|_\varepsilon$, the associated scalar product and norm. From now on, we assume:

Hypothesis 3.1. *$K(x,\varepsilon)$ is a compact operator on $L^2(\mathcal{S}_\varepsilon)$ for all $(x,\varepsilon)\in\mathbb{R}\times\mathcal{R}$.*

This assumption can be viewed as a regularity hypothesis for the scattering matrix $\sigma(x,k',k)$ which is always satisfied in practice. The formal adjoint of $K(x,\varepsilon)$ is obviously given by

$$(K^*(x,\varepsilon)\varphi)(k')=\int_{\mathcal{S}_\varepsilon}\sigma(x,k',k)\varphi(k)|v_x(k)|dN_\varepsilon(k)\,, \tag{3.9}$$

and is also a compact operator. First, we notice that relations (3.1)–(3.7) translate in

$$1=\int_{\S_{\varepsilon(k')}}\sigma(x,k',k)|v_x|\,dN(k)\,,\quad \forall k'\in\mathcal{B}\,,\quad \forall x\in\mathbb{R}\,, \tag{3.10}$$

$$1=\int_{\S_{\varepsilon(k)}}\sigma(x,k',k)|v'_x|\,dN(k')\,,\quad \forall k\in\mathcal{B}\,,\quad \forall x\in\mathbb{R}\,, \tag{3.11}$$

$$\sigma(x,k',k)=\sigma(x,-k,-k')\,,\quad \forall k,k'\in\mathcal{B}\,,\quad \forall x\in\mathbb{R}\,, \tag{3.12}$$

$$\sigma(x,k',k)>0\,,\quad \forall k,k'\in\mathcal{S}_\varepsilon\,,\quad \forall\varepsilon\in\mathcal{R}\,,\quad \forall x\in\mathbb{R}\,. \tag{3.13}$$

Equivalently, (3.10), (3.11) and (3.13) can be respectively rephrased as

$$K(x,\varepsilon)1=1\,,\quad K^*(x,\varepsilon)1=1\,,\quad \forall(x,\varepsilon)\in\mathbb{R}\times\mathcal{R}\,, \tag{3.14}$$

$$\varphi\geq 0\implies K(x,\varepsilon)\varphi>0\,,\quad K^*(x,\varepsilon)\varphi>0\,. \tag{3.15}$$

The following result is an easy consequence of the compactness hypothesis, of (3.14)–(3.15), of Krein-Rutman's theorem and of Fredholm's theory[8]. Its proof is omitted as it can be easily adapted from that of [5].

Lemma 3.1. (i) *The null spaces $N(I-K(x,\varepsilon))$ and $N(I-K^*(x,\varepsilon))$ are spanned by the constant functions in $L^2(S_\varepsilon)$.*

(ii) *$K(x,\varepsilon)$ is of norm 1, i.e. $|K(x,\varepsilon)\varphi|_\varepsilon \le |\varphi|_\varepsilon$, for all $\varphi \in L^2(\mathcal{S}_\varepsilon)$. Furthermore, there exists a constant $0 \le C(x,\varepsilon) < 1$ such that for all $\varphi \in N(I-K(x,\varepsilon))^\perp$ (i.e. such that*

$$\int_{\mathcal{S}_\varepsilon} \varphi(k)|v_x(k)|dN_\varepsilon(k) = 0\,,\Big)$$

then, $|K(x,\varepsilon)\varphi|_\varepsilon \le C(x,\varepsilon)|\varphi|_\varepsilon$. Similar properties are true of $K^*(x,\varepsilon)$.

(iii) *The ranges $R(I-K(x,\varepsilon))$ and $R(I-K^*(x,\varepsilon))$ satisfy*

$$R(I-K(x,\varepsilon)) = N(I-K^*(x,\varepsilon))^\perp\,, \quad R(I-K^*(x,\varepsilon)) = N(I-K(x,\varepsilon))^\perp\,. \tag{3.16}$$

In particular, for any given $\psi \in L^2(\mathcal{S}_\varepsilon)$, there exists a solution $\varphi \in L^2(\mathcal{S}_\varepsilon)$ of equation

$$(I-K^*(x,\varepsilon))\varphi = \psi\,, \tag{3.17}$$

if and only if ψ satisfies

$$\int_{\mathcal{S}_\varepsilon} \psi(k)|v_x(k)|dN_\varepsilon(k) = 0\,. \tag{3.18}$$

Furthermore, φ is unique among functions satisfying(3.18).

Property (ii) is reminiscent of Darrozes-Guiraud inequality for accomodation boundary conditions in gas dynamics[10]. It tells that $K(x,\varepsilon)$ has a 'good' diffusion behaviour which can be measured in terms of the distance of the constant C to 1. This will be important for the well-posedness of the limit diffusion model (see Lemma 4.1).

Let $\mathrm{sgn}(v_x)$ denote the sign of $v_x(k)$. As an application of Lemma 3.1, we note that there exists a unique solution $\lambda(x,k) \in L^2(\mathcal{S}_\varepsilon)$ to the problem

$$-(\mathrm{I}-K^*(x,\varepsilon))\lambda = \mathrm{sgn}(v_x)\,, \tag{3.19}$$

satisfying the orthogonality condition (3.18). Indeed, a solution of (3.19) exists because

$$\int_{\mathcal{S}_\varepsilon} \mathrm{sgn}(v_x)\,|v_x|dN_\varepsilon(k) = \frac{1}{\hbar}\int_{\mathcal{B}} \frac{\partial\varepsilon}{\partial k_x}(k)\delta(\varepsilon(k)-\varepsilon)\,dk = \frac{1}{\hbar}\int_{\mathcal{B}} \frac{\partial}{\partial k_x}H(\varepsilon(k)-\varepsilon)\,dk = 0\,,$$

where $H(u)$ is the Heaviside function ($H(u)=1$ for $u>0$ and $H(u)=0$ for $u<0$) and the last integral is zero because it is the integral of the derivative of an L^* periodic function over one lattice period $\mathcal{B}$.

In addition, we note that Lemma 3.1 becomes trivial in the case of a one dimensional model in k like in [15].

§4. The Diffusion Model

The main goal of this paper is to show that in the limit $\alpha \to 0$, the distribution function $f^\alpha(x,k,t)$ converges, at least formally, to a function $F(x,\varepsilon(k),t)$ which only depends on k through the energy $\varepsilon(k)$ and such that $F(x,\varepsilon,t)$ satisfies the following diffusion equation (SHE model):

$$M(x,\varepsilon)\frac{\partial F}{\partial t} + \Big(\frac{\partial}{\partial x} - eE\frac{\partial}{\partial\varepsilon}\Big)J = 0\,, \tag{4.1}$$

$$J(x,\varepsilon,t) = -D(x,\varepsilon)\Big(\frac{\partial}{\partial x} - eE\frac{\partial}{\partial\varepsilon}\Big)F\,, \tag{4.2}$$

$$F(x,\varepsilon,t=0) = F_I(x,\varepsilon,0)\,, \tag{4.3}$$

where $M(x,\varepsilon)$ and $D(x,\varepsilon)$ are defined by

$$M(x,\varepsilon)=\frac{1}{\ell}\int\int_{k,k'\in\S_\varepsilon}\sigma(x,k',k)\tau(x,k',k)\,|v_x(k)|\,|v_x(k')|\,dN_\varepsilon(k)\,dN_\varepsilon(k')\,, \tag{4.4}$$

$$D(x,\varepsilon)=\ell\left(-\int\int_{k,k'\in\S_\varepsilon^+}+\int\int_{k,k'\in\S_\varepsilon^-}\right)\sigma(x,k',k)\,\lambda(k) \times|v_x(k)|\,|v_x(k')|\,dN_\varepsilon(k)\,dN_\varepsilon(k')\,, \tag{4.5}$$

and λ is the unique solution of (3.9) satisfying (3.18). M and D are respectively referred to as the 'density-of-states' and the 'diffusivity'. Note that M is the density-of-states of neither material A nor B (that of material A being defined by (2.7)). The SHE model derived in [15] has the same form, but the expressions of M and D are fully explicit due to the simple form of the scattering operator. In particular, in [15], it is obvious that D is positive, while in the present context, we shall need to prove it (Proposition 4.1).

Next we provide a (formal) justification of the limit $\alpha\to 0$ and prove that the diffusion model (4.1), (4.2) is well-posed, i.e. that the diffusivity is positive.

The investigation of the limit $\alpha\to 0$ consists of three steps. The first one is to show that f^α formally converges to a function of $(x,\varepsilon(k),t)$ only. The second and third ones correspond to the derivations of the continuity and current Equations (4.1), (4.2). To reach these aims, two methods can be employed: the Hilbert expansion method[2,13] and the moment method[23]. It is better for us to choose the latter due to its involving more straightforward computations. In the present case, the establishment of the continuity equation is more difficult than in the usual case[23] due to the time-discreteness of the scattering model (2.26), (2.27). The derivation of the current equation is the most delicate point. We multiply (2.26), (2.27) by the 'auxiliary function' λ (the solution of (3.19)), integrate the result with respect to k (hence justifying the terminology 'moment method') and need to process some tedious algebra. Roughly speaking, λ gives the typical response of the microscopic system to gradients of the macroscopic variables.

In this section, we only prove that f^α formally converges to $F(x,\varepsilon(k),t)$. The proof of the continuity and the current equations (4.1), (4.2) are deferred to Appendices A and B for the reader's convenience. In what follows, we shall take the existence of solutions for the original discrete model (2.26), (2.27) as well as the convergence of f^α to some function f in appropriate functional spaces for granted and we shall solely focus on the establishment of the limit model. We stress that the derivation of the model is 'exact' in the sense that it does not involve any approximation (other than the fact that $\alpha\to 0$).

The fact that $\lim f^\alpha$ is a function of the energy only is an easy consequence of Lemma 3.1. Indeed, suppose that $f^\alpha(x,k,t)$, $\alpha>0$ is a sequence of solution to problem (2.26), (2.27) which converges in a sufficiently smooth way to a function $f(x,k,t)$ as α tends to zero. Then formally, $f(x,k,t)$ satisfies for all time $t\ge 0$,

$$f(x,k,t)=\int_{\S_{\varepsilon(k)}}\sigma(x,k',k)f(x,k',t)|v_x'|\,dN(k')\,,\quad\forall k\in\mathcal{B}\,. \tag{4.6}$$

This is no longer a dynamical equation for f, but a state equation which can be put in the form

$$(\mathrm{I}-K(x,\varepsilon))f(x,\cdot,t)=0\,,\quad\forall(x,\varepsilon)\in\mathbb{R}\times\mathcal{R}\,, \tag{4.7}$$

where I is the identity and the operator $K(x,\varepsilon)$ is defined by (3.8). Now, in view of (4.7) and Lemma 3.1(i), f is a constant function on each energy surface $\mathcal{S}_\varepsilon$. Therefore, it is a function of the energy only. Thus, we have

$$f^\alpha(x,k,t)\to f(x,k,t)=F(x,\varepsilon(k),t)\,,\quad\text{as}\quad\alpha\to 0\,. \tag{4.8}$$

We refer to Appendices A and B for the derivation of (4.1), (4.2).

The well-posedness of model (4.1), (4.2) relies on the positivity of the coefficients M and D. The positivity of M is guaranteed by the positivity assumption on the scattering coefficients and time delays. The following proposition relates the positivity of D to the dissipative character of the scattering operator $K(x,\varepsilon)$.

Proposition 4.1. *The diffusion coefficient $D(x,\varepsilon)$ given by* (4.5) *is positive for all x and ε :*

$$D(x,\varepsilon) > 0\,. \tag{4.9}$$

Proof. We first compute, denoting $K(x,\varepsilon)$, $K^*(x,\varepsilon)$ by K, K^* and using $d\nu = |v_x||v_x'|\, dN(k)dN(k')$ for short:

$$\begin{aligned}(\mathrm{sgn}(v_x), K^*\lambda)_\varepsilon &= \int\!\!\int_{k,k'\in\mathcal{S}_\varepsilon} \mathrm{sgn}(v_x')\sigma(k',k)\lambda(k)d\nu \\ &= \Big(\int_{k\in\S_\varepsilon^+}\int_{k'\in\S_\varepsilon^+} - \int_{k\in\S_\varepsilon^-}\int_{k'\in\S_\varepsilon^-} + \int_{k\in\S_\varepsilon^-}\int_{k'\in\S_\varepsilon^+} - \int_{k\in\S_\varepsilon^+}\int_{k'\in\S_\varepsilon^-}\Big)\sigma(k',k)\lambda(k)d\nu\,.\end{aligned} \tag{4.10}$$

Now we transform the last two terms using (3.6), (3.7) and get

$$\begin{aligned}&\Big(\int_{k\in\S_\varepsilon^-}\int_{k'\in\S_\varepsilon^+} - \int_{k\in\S_\varepsilon^+}\int_{k'\in\S_\varepsilon^-}\Big)\sigma(k',k)\lambda(k)d\nu \\ &= \Big(\int_{k\in\S_\varepsilon^-} - \int_{k\in\S_\varepsilon^+}\Big)\lambda(k)|v_x|dN(k) - \Big(\int_{k\in\S_\varepsilon^-}\int_{k'\in\S_\varepsilon^-} - \int_{k\in\S_\varepsilon^+}\int_{k'\in\S_\varepsilon^+}\Big)\sigma(k',k)\lambda(k)d\nu\,.\end{aligned} \tag{4.11}$$

Then, inserting (4.11) into (4.10) and using the definition (4.5) of D, we obtain

$$(\mathrm{sgn}(v_x), K^*\lambda)_\varepsilon = -2\ell^{-1}D - (\mathrm{sgn}(v_x), \lambda)_\varepsilon\ .$$

Therefore, using the definition (3.19), we get

$$\begin{aligned}\ell^{-1}D &= -\frac{1}{2}\,(\mathrm{sgn}(v_x), (\mathrm{I} + K^*)\lambda)_\varepsilon = \frac{1}{2}\,((\mathrm{I} - K^*)\lambda, (\mathrm{I} + K^*)\lambda)_\varepsilon \\ &= \frac{1}{2}\left[|\lambda|_\varepsilon^2 - |K^*\lambda|_\varepsilon^2\right] \geq \left(1 - C(x,\varepsilon)^2\right)|\lambda|_\varepsilon^2 > 0\,.\end{aligned} \tag{4.12}$$

The last inequality follows from Lemma 3.1(ii) and the orthogonality condition (3.18) for λ.

In view of (4.12), we notice that the diffusion coefficient D is the same as in [5]. On the other hand, the density-of-states in [5] is the standard one (2.7), so that the obtained SHE models are not fully identical.

In the remainder of the present section, we give a few comments on the physical relevance of the obtained model . The 'SHE' model (4.1), (4.2) can provide information about the electron energy distribution function at a much lower cost than a Monte-Carlo simulation of the Boltzmann equation[21,22]. Therefore it is of great practical interest for semiconductor device simulations. For instance, the model has proved very useful in the modelling of impact ionization (which requires the knowledge of the 'tail' of the energy distribution function above the ionization energy)[20].

To our knowledge, the derivation of the 'SHE' model in the framework of superlattices is a very new feature in the context of the modelling of semiconductor devices. If collisions with impurities or phonons are included, the continuity equation (4.1) takes the form

$$M(x,\varepsilon)\frac{\partial F}{\partial t} + \left(\frac{\partial}{\partial x} - eE\frac{\partial}{\partial \varepsilon}\right) J = Q(F)\,, \tag{4.13}$$

where the operator $Q(F)$ models the rate of change of F due to collisions. We shall defer the derivation of adequate expressions of $Q(F)$ to future work.

This model has another interesting property that it gives rise to a hierarchy of moment models[3,13], including the usual Drift-Diffusion model[26,31] and the so-called Energy-Transport model, which is an extension of the Drift-Diffusion model with an additional energy balance equation (see [4] and references therein). In the present case, the unusual form of the density-of-states M makes it interesting to develop this hierarchy in more details. Integrating (4.13) with respect to the energy ε, we obtain conservation equations for the particle and energy densities:

$$\frac{\partial n}{\partial t}+\frac{\partial j_n}{\partial x}=q_n\,,\quad \frac{\partial \mathcal{E}}{\partial t}+\frac{\partial j_{\mathcal{E}}}{\partial x}+eEj_n=q_{\mathcal{E}}\,, \tag{4.14}$$

where the particle density $n\,(x,\,t)$, the energy density $\mathcal{E}\,(x,\,t)$, the particle current $j_n\,(x,\,t)$ and the energy current $j_{\mathcal{E}}\,(x,\,t)$ are given by

$$\begin{pmatrix} n \\ \mathcal{E} \end{pmatrix}=\int_{\mathcal{R}} F\,(x,\varepsilon,\,t)\begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} M(x,\varepsilon)\,d\varepsilon\ \ , \tag{4.15}$$

$$\begin{pmatrix} j_n \\ j_{\mathcal{E}} \end{pmatrix}=\int_{\mathcal{R}} J\,(x,\varepsilon,\,t)\begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} d\varepsilon\ \ , \tag{4.16}$$

while q_n, $q_{\mathcal{E}}$ are the particle and energy creation rates due to collisions:

$$\begin{pmatrix} q_n \\ q_{\mathcal{E}} \end{pmatrix}=\int_{\mathcal{R}} Q(F)\,(x,\varepsilon,\,t)\begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} d\varepsilon\ \ . \tag{4.17}$$

In order to close system (4.14) we assume that the superlattice structure is near thermodynamical equilibrium (which is valid as long as the applied potential bias is not too large), and therefore, that F can be approximated by a Fermi-Dirac distribution (which is the quantum thermodynamical equilibrium distribution function of electrons[6]):

$$F_{\mu,T}(\varepsilon)=\frac{1}{\exp\left(\frac{\varepsilon-\mu}{k_BT}\right)+1}\,, \tag{4.18}$$

where $\mu=\mu(x,t)$ and $T=T(x,t)$ are the chemical potential and temperature, and k_B is the Boltzmann constant. With (4.18), Equation (4.15) furnishes a local relationship between the pairs $(n,\mathcal{E})$ and (μ,T), through the particular superlattice density-of-states M. Similarly, (4.17) gives the rates of change $(q_n,q_{\mathcal{E}})$ as functions of (μ,T). Instead, inserting (4.18) into (4.16) and using (4.2), we obtain the currents as combinations of the field and of gradients of μ and T (see [3, 13]):

$$\begin{pmatrix} j_n \\ j_{\mathcal{E}} \end{pmatrix}=-\mathcal{D}\begin{pmatrix} \frac{\partial}{\partial x}\left(\frac{\mu}{k_BT}\right)+\frac{eE}{k_BT} \\ \frac{\partial}{\partial x}\left(\frac{-1}{k_BT}\right) \end{pmatrix}, \tag{4.19}$$

where $\mathcal{D}$ is a diffusion matrix $\mathcal{D}=(\mathcal{D}_{ij})_{i,j=1,2}$ given by

$$\mathcal{D}(x,\mu,T)=\begin{pmatrix} \mathcal{D}_{11} & \mathcal{D}_{12} \\ \mathcal{D}_{21} & \mathcal{D}_{22} \end{pmatrix}=\int_{\mathcal{R}} D(x,\varepsilon)F_{\mu,T}(1-F_{\mu,T})\begin{pmatrix} 1 & \varepsilon \\ \varepsilon & \varepsilon^2 \end{pmatrix} d\varepsilon. \tag{4.20}$$

The model (4.14), supplemented with the constitutive relation (4.19) is the Energy-Transport model[4]. If only the first Equation (4.14) and the first line of (4.19) are retained, with $T=$ constant, the model reduces to the so-called Drift-Diffusion model[26]. The Drift-Diffusion model has been used for decades in semiconductor engineering[31] but it tends to be replaced by the Energy-Transport model (see [3, 4] and references therein) which provides a significant improvement in physical accuracy with little additional complexity. We remark that $\mathcal{D}$ is a symmetric positive-definite matrix. The symmetry expresses Onsager's reciprocity relation[16]. The positive-definiteness makes the Energy-Transport model consistent with entropy requirements[13].

Now, we discuss the particular form of the density-of-states M which makes the definitions of the particle and energy densities (4.15) slightly different than in bulk semiconductor materials. M can be viewed as an 'averaged density-of-states' over the superlattice elementary period. To see this, we first show that M reduces to the usual density-of-states $N(\varepsilon)$ (2.7) if the potential is constant in the elementary cell. Indeed, in this case, there is no scattering at all and the scattering coefficients express that the outgoing wave-vector of the particle exiting the elementary period is identical to its incoming one :

$$\sigma(k',k)\delta(\varepsilon(k')-\varepsilon(k))|v'_x| = \delta(k'-k)\,. \tag{4.21}$$

Similarly, the time delay is easily found as

$$\tau(k',k) = \frac{\ell}{|v_x|}\,. \tag{4.22}$$

Therefore, inserting (4.21), (4.22) in (4.4) we find

$$M(\varepsilon) = \frac{1}{\ell}\int\int_{k,k'\in\mathcal{B}} \delta(k'-k)\frac{\ell}{|v_x|}\delta(\varepsilon(k)-\varepsilon)\,|v_x|\,dk\,dk' = \int_{\mathcal{B}}\delta(\varepsilon(k)-\varepsilon)\,dk = N(\varepsilon)\,.$$

The superlattice density-of-states M is proportional to the product of the time delays τ by the scattering probability σ and by the reciprocal of the period length ℓ. This can be understood as follows: a density is a particle flux divided by a velocity. Here the velocity can be estimated by the period length ℓ divided by the time delay τ (i.e. the time spent to cross the elementary period). Now, the flux is proportional to the scattering probability σ. The result is clearly proportional to the factor $\tau\sigma/\ell$. For a given energy, this quantity must be integrated over all possible incoming and outgoing wave-vectors, hence giving rise to (4.4).

Because of this particular form of M, the relationship between $(n,\mathcal{E})$ and (μ,T) in the superlattice can significantly depart from that of bulk materials. In particular, at resonant energies (see below the example of square potentials), the time delays are significantly longer than the time delays given by classical mechanics. Symmetrically, at energies away from resonances, they can be shorter. Therefore, in (4.15), M weights more strongly the resonant energies and less strongly the non resonant ones. The relation $(\mu,T)\to(n,\mathcal{E})$ keeps the memory of these effects.

Next we discuss the value of the electron mobility in the superlattice, given by

$$\mu_{\rm SL} = \frac{e\,\mathcal{D}_{11}}{n\,k_BT}\,. \tag{4.23}$$

We recall that the mobility is the coefficient of Ohm's law

$$j_n = \mu_{\rm SL}\,nE\,,$$

which is an expression of the first line of (4.19) when the chemical potential μ and the temperature T are constant in space. The mobility is one of the most important transport parameters in semiconductors as it is easily accessible to measurements and characterizes the ability of electrons to react to an external electric field. In the present case, the mobility of the electrons induced solely by their scattering by the superlattice potential pattern is given, according to (4.20), by

$$\mu_{\rm SL} = \frac{e}{n\,k_BT}\int_{\mathcal{R}} D(x,\varepsilon)F_{\mu,T}(1-F_{\mu,T})d\varepsilon\,. \tag{4.24}$$

At low electron densities, i.e. when $(\varepsilon-\mu)/k_BT$ is large, the Fermi-Dirac distribution function can be approximated by the Maxwellian

$$F_{\mu,T}(\varepsilon) \approx M_{\mu,T}(\varepsilon) = \exp\Big(-\frac{\varepsilon-\mu}{T}\Big)\,, \tag{4.25}$$

and (4.24) yields

$$\mu_{\rm SL} = \frac{e}{n\, k_B T} e^{\mu/T} \int_{\mathcal{R}} D(x,\varepsilon) e^{-\varepsilon/T} d\varepsilon\,. \tag{4.26}$$

This quite simple expression provides a mean to evaluate the influence of the superlattice pattern on the overall electron mobility. A realistic expression of the mobility must also include the influence of 'bulk interactions' like phonon or impurity interactions. As already pointed out, this is not done yet in full rigour in the present work, but a rough estimate of the total mobility $\mu_{\rm tot}$ can be obtained by

$$\frac{1}{\mu_{\rm tot}} = \frac{1}{\mu_{\rm bulk}} + \frac{1}{\mu_{\rm SL}}, \tag{4.27}$$

where $\mu_{\rm bulk}$ is the mobility under the influence of bulk collisions alone (for instance, one can take the harmonic average of the bulk mobilities of materials A and B weighted by their relative width in the period). Formula (4.27) can be understood by a circuit analogy in which the resistances (proportional to the reciprocal of the mobility) of the bulk and of the superlattice add up in series. It provides a first answer to the problem of determining the electron mobility in the superlattice. This question was left open for instance in [33], where by default, the superlattice mobility was assumed to be equal to that of the bulk.

§5. Examples and Conclusion

In this section, we first deal with two limiting cases corresponding to extremely rough and perfectly clean interfaces. In the former case, the scattering matrix is isotropic while in the last case, it preserves the parallel momentum to the interface. In these two cases, the potential profile in the direction transverse to the interfaces is still arbitrary. Then we give a simple summary of results in this paper.

Since the coefficients M and D of the SHE model only depend on the scattering matrix at zero electric field, we shall only specify them in this case.

5.1. Rough Interfaces

The one-dimensional scattering matrix model is actually an averaged description over the direction parallel to the interfaces. If the interface is rough, a particle of given momentum is scattered towards very different directions according to the point at which it hits the material interface. Therefore, it is reasonable to think that the 'averaged' scattering matrix is isotropic in the outgoing wave-vector. Using then the reciprocity and conservation relations (3.10)–(3.12), we easily deduce that the scattering matrix must take the form (omitting the x-dependence for simplicity):

$$\sigma(k',k) = \frac{1}{\mathcal{V}(\varepsilon)} \begin{cases} T(\varepsilon), & \text{if } (v_x(k') \geq 0 \text{ and } v_x(k) \geq 0) \\ & \text{or } (v_x(k') \leq 0 \text{ and } v_x(k) \leq 0), \\ 1 - T(\varepsilon), & \text{if } (v_x(k') \geq 0 \text{ and } v_x(k) \leq 0) \\ & \text{or } (v_x(k') \leq 0 \text{ and } v_x(k) \geq 0), \end{cases} \tag{5.1}$$

where $T(\varepsilon) \in [0,1]$ is the transmission probability of particles of energy ε through the potential structure, $1 - T(\varepsilon)$ is the reflection probability and $\mathcal{V}(\varepsilon)$ is the normalizing factor:

$$\mathcal{V}(\varepsilon) = \int_{\mathcal{S}_\varepsilon{}^+} |v_x| dN = \int_{\mathcal{S}_\varepsilon{}^-} |v_x| dN\,.$$

We have implicitly assumed that the energy function $\varepsilon(k)$ is even in k. In this case, the operator K is self-adjoint and easy computations lead to

$$\lambda = -\frac{1}{2(1-T(\varepsilon))}\, \mathrm{sgn}(v_x)\,, \quad D(\varepsilon) = \ell\, \mathcal{V}(\varepsilon)\, \frac{T(\varepsilon)}{1-T(\varepsilon)}\,. \tag{5.2}$$

We notice that the diffusion vanishes when the transmission T vanishes, which is physically consistent, because the particles are indefinitely trapped between two neighbouring potential patterns. When the reflection $1-T$ vanishes, the diffusion goes to infinity because the potential structure does not slow down the particles enough. We note that the connection between the diffusion constant and the scattering properties of the potential pattern is particularly tight. In particular, the transmission lineshape of the potential pattern as a function of the energy of the particles translates directly into a corresponding lineshape of the diffusion constant. If transmission resonances occur near certain energies, they result in a peak of the diffusion constant. The macroscopic model is therefore adequate to capture a certain number of resonant features of superlattices.

However, we note that the time delays and therefore, the 'modified' density-of-states M are not easily accessible.

5.2. Clean Interface

This case is opposite to the preceding one. We suppose that the material interfaces are perfectly clean, so that momentum in the direction parallel to the interfaces is preserved. This is the most interesting regime physically, where the filtering capabilities of superlattices are the most efficient. In this case, only the one-dimensional x-component of momentum is considered. We suppose that the directional energy $\varepsilon_x(k_x)$ in the x-direction can be defined. This is possible in the case of a parabolic band structure, i.e. when the energy is a quadratic function of momentum, but is only an approximation in the general case. The x-component of the velocity is then written:

$$v_x = \frac{1}{\hbar}\frac{\partial \varepsilon_x}{\partial k_x}(k_x)\,.$$

We also suppose that ε_x is a strictly monotonous even function of $k_x \in \mathcal{B}_x$ where the interval $\mathcal{B}_x = [-K_x, K_x]$ is the cut of the Brillouin zone $\mathcal{B}$ by the k_x axis. The monotony assumption simplifies the computations below but can be relaxed easily. The equation $\varepsilon(k_x) = \varepsilon$, which defines the manifold $\mathcal{S}_\varepsilon$, has only 2 solutions $\pm k_x(\varepsilon)$ where $k_x(\varepsilon)$ is the positive one. The coarea measure and the density of states are given by

$$\int_{\mathcal{S}_\varepsilon} \varphi(k_x)|v_x| dN_\varepsilon(k_x) = \frac{1}{\hbar\pi}(\varphi(k_x(\varepsilon)) + \varphi(-k_x(\varepsilon)))\,, \quad \forall \varphi(k_x)\,, \tag{5.3}$$

$$N(\varepsilon) = \frac{2}{\hbar\pi|v_x|}\,, \tag{5.4}$$

where the factor π^{-1} comes from the one-dimensional momentum-density-of-states.

Using the reciprocity and conservation relations (3.10)–(3.12), we deduce that the scattering matrix model gives rise to an operator K given by

$$K\varphi(k_x) = T(\varepsilon_x(k_x))\,\varphi(k_x) \,+\, (1 - T(\varepsilon_x(k_x)))\,\varphi(-k_x)\,, \tag{5.5}$$

where $T(\varepsilon_x)$ and $1 - T(\varepsilon_x)$ are the transmission and reflection probabilities of particles of x-directional energy ε_x through the potential structure.

After some easy computations using (5.3), we find:

$$\lambda(k_x) = -\frac{1}{2(1 - T(\varepsilon_x(k_x)))}\,\mathrm{sgn}(v_x)\,,$$

$$D(\varepsilon) = \frac{\ell}{\hbar\pi}\,\frac{T(\varepsilon)}{1 - T(\varepsilon)}\,, \quad M(\varepsilon) = \frac{1}{\hbar\pi\ell}\,[2T\tau_t + (1-T)(\tau_r + \tau_l)]\,, \tag{5.6}$$

where $\tau_t = \tau_t(\varepsilon)$ is the transmission time delay of particles of energy ε, while τ_r and τ_l are the reflection time delays for particles reflected on the right and on the left of the structure respectively. The two reflection time delays may not be equal if the structure has no reflection symmetry. The same remarks as in the isotropic case can be made about

the connection between the scattering coefficients and the value of the diffusivity. Finally, in [15], this example is further restricted to one-dimensional wave-vectors and square wells or barriers. Explicit expressions for M and D can be obtained. The relation between the singularities of D and the transmission resonances becomes even more transparent.

5.3. Conclusion

In this paper, we have presented a scattering matrix model describing electron transport in semiconductor superlattices when the electron phase coherence length is of the order of the superlattice period. Then, we have investigated the limit of a large number of superlatice cells. We have shown that , at the diffusion time scale, the scattering matrix model formally converges to a diffusion model in the position-energy space, the so-called 'SHE' model and explained how it can improve our knowledge of electron transport in superlattices. Analytical examples have been given to support the theory.

Appendix A: The Continuity Equation

We introduce the current of particles of given energy ε:

$$J^\alpha(x,\varepsilon,t)=\frac{1}{\alpha}\int_{\mathcal{S}_\varepsilon} f^\alpha(x,k,t)v_x(k)dN_\varepsilon(k)\,. \tag{A.1}$$

In view of (4.8), J^α is the ratio of two quantities tending to zero. We shall see in the next section that (at least formally) the limit $J^\alpha\to J$ exists and is finite. In this appendix, assuming that

$$J^\alpha(x,\varepsilon,t)=J(x,\varepsilon,t)+o(1)\quad\text{as}\quad\alpha\to 0, \tag{A.2}$$

we prove the continuity equation (4.1).

We consider the difference

$$I^\alpha=\frac{1}{\alpha\ell}\Big[J^\alpha\Big(x+\frac{\alpha\ell}{2},\varepsilon,t\Big)-J^\alpha\Big(x-\frac{\alpha\ell}{2},\varepsilon+\alpha\ell eE^\alpha(x),t\Big)\Big]\,. \tag{A.3}$$

Formally, in view of (A.2) and of the fact that $E^\alpha=E+o(1)$ as $\alpha\to 0$ (see (2.23)), we have

$$I^\alpha=\frac{\partial J}{\partial x}-eE\frac{\partial J}{\partial\varepsilon}+o(1)\qquad\text{as }\alpha\to 0. \tag{A.4}$$

On the other hand, using (A.1) and (2.26), (2.27), we have (noting $d\nu=|v_x||v_x'|\,dN(k)dN(k')$)

$$\begin{aligned}
I^\alpha=\frac{1}{\alpha^2\ell}\Big\{&\int_{k\in\S_\varepsilon^+}\int_{k'\in\S_\varepsilon^-}\sigma^\alpha(x,\alpha E^\alpha(x),k',k)f^\alpha\Big(x+\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)\,d\nu\\
&+\int_{k\in\S_\varepsilon^+}\int_{k'\in\S^+_{\varepsilon+\alpha\ell eE^\alpha(x)}}\sigma^\alpha(x,\alpha E^\alpha(x),k',k)f^\alpha\Big(x-\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)\,d\nu\\
&-\int_{k\in\S_\varepsilon^-}f^\alpha\Big(x+\frac{\alpha\ell}{2},k,t\Big)\,|v_x|\,dN(k)\\
&+\int_{k\in\S^-_{\varepsilon+\alpha\ell eE^\alpha(x)}}\int_{k'\in\S^+_{\varepsilon+\alpha\ell eE^\alpha(x)}}\sigma^\alpha(x,\alpha E^\alpha(x),k',k)f^\alpha\Big(x-\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)\,d\nu\\
&+\int_{k\in\S^-_{\varepsilon+\alpha\ell eE^\alpha(x)}}\int_{k'\in\S_\varepsilon^-}\sigma^\alpha(x,\alpha E^\alpha(x),k',k)f^\alpha\Big(x+\frac{\alpha\ell}{2},k',t-\alpha^2\tau^\alpha\Big)\,d\nu\\
&-\int_{k\in\S^+_{\varepsilon+\alpha\ell eE^\alpha(x)}}f^\alpha\Big(x-\frac{\alpha\ell}{2},k,t\Big)\,|v_x|dN(k)\Big\}.
\end{aligned} \tag{A.5}$$

Inserting the Taylor expansion

$$f^\alpha\Big(x \pm \frac{\alpha\ell}{2}, k', t - \alpha^2\tau\Big) = f^\alpha\Big(x \pm \frac{\alpha\ell}{2}, k', t\Big) - \alpha^2\tau\frac{\partial f^\alpha}{\partial t}(x, k', t) + o(\alpha^2)\,,$$

we can write

$$I^\alpha = I_1^\alpha + I_2^\alpha + o(1) \quad \text{as} \quad \alpha \to 0, \tag{A.6}$$

where

$$\begin{aligned} I_1^\alpha = \frac{1}{\alpha^2\ell}\Big\{ & \int_{k\in\S_\varepsilon^+}\int_{k'\in\S_\varepsilon^-} \sigma^\alpha(x, \alpha E^\alpha(x), k', k) f^\alpha\Big(x + \frac{\alpha\ell}{2}, k', t\Big)\, d\nu \\ & + \int_{k\in\S_\varepsilon^+}\int_{k'\in\S^+_{\varepsilon+\alpha\ell e E^\alpha(x)}} \sigma^\alpha(x, \alpha E^\alpha(x), k', k) f^\alpha\Big(x - \frac{\alpha\ell}{2}, k', t\Big)\, d\nu \\ & - \int_{k\in\S_\varepsilon^-} f^\alpha\Big(x + \frac{\alpha\ell}{2}, k, t\Big)\,|v_x|\, dN(k) \\ & + \int_{k\in\S^-_{\varepsilon+\alpha\ell e E^\alpha(x)}}\int_{k'\in\S^+_{\varepsilon+\alpha\ell e E^\alpha(x)}} \sigma^\alpha(x, \alpha E^\alpha(x), k', k) f^\alpha\Big(x - \frac{\alpha\ell}{2}, k', t\Big)\, d\nu \\ & + \int_{k\in\S^-_{\varepsilon+\alpha\ell e E^\alpha(x)}}\int_{k'\in\S_\varepsilon^-} \sigma^\alpha(x, \alpha E^\alpha(x), k', k) f^\alpha\Big(x + \frac{\alpha\ell}{2}, k', t\Big)\, d\nu \\ & - \int_{k\in\S^+_{\varepsilon+\alpha\ell e E^\alpha(x)}} f^\alpha\Big(x - \frac{\alpha\ell}{2}, k, t\Big)\,|v_x| dN(k)\Big\}\,, \end{aligned} \tag{A.7}$$

$$-I_2^\alpha = \frac{1}{\ell}\int_{k\in\S_\varepsilon}\int_{k'\in\S_\varepsilon} \sigma(x, k', k)\tau(x, k', k)\frac{\partial f^\alpha}{\partial t}(x, k', t)\, d\nu\,. \tag{A.8}$$

Now, the flux conservation relations (3.1), (3.2) imply

$$I_1^\alpha = 0\,. \tag{A.9}$$

In the limit $\alpha \to 0$, by (4.8), we also deduce that

$$I_2^\alpha \to -M(x, \varepsilon)\frac{\partial F}{\partial t}\,, \quad \text{as } \alpha \to 0\,, \tag{A.10}$$

where M is given by (4.4). Finally, collecting (A.4), (A.6), (A.9), (A.10), we deduce that the continuity Equation (4.4) is satisfied with M given by (4.4). This concludes the present appendix.

Appendix B: The Current Equation

The goal of this appendix is to give a formal derivation of (4.2). First, let us rewrite (2.26), (2.27) in the following form

$$\begin{aligned} f^\alpha(x, k, t) = & \int_{\S^-_{\varepsilon(k)}} \sigma^\alpha\Big(x - \frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x - \frac{\alpha\ell}{2}\Big), k', k\Big) f^\alpha(x, k', t - \alpha^2\tau^\alpha)|v'_x|\, dN(k') \\ & + \int_{\S^+_{\varepsilon(k)+\alpha\ell e E^\alpha\left(x - \frac{\alpha\ell}{2}\right)}} \sigma^\alpha\Big(x - \frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x - \frac{\alpha\ell}{2}\Big), k', k\Big) \\ & \times f^\alpha(x - \alpha\ell, k', t - \alpha^2\tau^\alpha)|v'_x|\, dN(k') \end{aligned} \tag{B.1}$$

for $v_x > 0$ and

$$f^\alpha(x,k,t) = \int_{\S^+_{\varepsilon(k)}} \sigma^\alpha\Big(x, \alpha E^\alpha\Big(x+\frac{\alpha\ell}{2}\Big), k', k\Big) f^\alpha(x,k',t-\alpha^2\tau^\alpha)|v'_x|\, dN(k')$$
$$+ \int_{\S^-_{\varepsilon(k)-\alpha\ell e E^\alpha\left(x+\frac{\alpha\ell}{2}\right)}} \sigma^\alpha\Big(x, \alpha E^\alpha\Big(x+\frac{\alpha\ell}{2}\Big), k', k\Big)$$
$$\times f^\alpha(x+\alpha\ell, k', t-\alpha^2\tau^\alpha)|v'_x|\, dN(k'), \tag{B.2}$$

for $v_x < 0$. Equations (B.1) and (B.2) can be written

$$\frac{1}{\alpha}\left(\mathrm{I} - K(x,\varepsilon)\right) f^\alpha(\cdot,\cdot,t) = g^\alpha\,, \tag{B.3}$$

where

$$g^\alpha(x,k,t) = \frac{1}{\alpha}\Big\{\Big[\int_{\S^-_{\varepsilon(k)}} \sigma^\alpha\Big(x-\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x-\frac{\alpha\ell}{2}\Big), k', k\Big) f^\alpha(x,k',t)|v'_x| dN(k')$$
$$- \int_{\S^-_{\varepsilon(k)}} \sigma(x,k',k) f^\alpha(x,k',t)|v'_x| dN(k')\Big]$$
$$+ \Big[\int_{\S^+_{\varepsilon(k)+\alpha\ell e E^\alpha\left(x-\frac{\alpha\ell}{2}\right)}} \sigma^\alpha\Big(x-\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x-\frac{\alpha\ell}{2}\Big), k', k\Big)$$
$$\times f^\alpha(x-\alpha\ell, k', t)|v'_x| dN(k')$$
$$- \int_{\S^+_{\varepsilon(k)}} \sigma(x,k',k) f^\alpha(x,k',t)|v'_x| dN(k')\Big]\Big\} + o(1)\,, \quad v_x > 0\,, \tag{B.4}$$

$$g^\alpha(x,k,t) = \frac{1}{\alpha}\Big\{\Big[\int_{\S^+_{\varepsilon(k)}} \sigma^\alpha\Big(x+\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x+\frac{\alpha\ell}{2}\Big), k', k\Big) f^\alpha(x,k',t)|v'_x| dN(k')$$
$$- \int_{\S^+_{\varepsilon(k)}} \sigma(x,k',k) f^\alpha(x,k',t)|v'_x| dN(k')\Big]$$
$$+ \Big[\int_{\S^-_{\varepsilon(k)-\alpha\ell e E^\alpha\left(x+\frac{\alpha\ell}{2}\right)}} \sigma^\alpha\Big(x+\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x+\frac{\alpha\ell}{2}\Big), k', k\Big)$$
$$\times f^\alpha(x+\alpha\ell, k', t)|v'_x| dN(k')$$
$$- \int_{\S^-_{\varepsilon(k)}+} \sigma(x,k',k) f^\alpha(x,k',t)|v'_x| dN(k')\Big]\Big\} + o(1)\,, \quad v_x < 0\,. \tag{B.5}$$

Now we take the scalar product of (B.3) by λ in $L^2(\mathcal{S}_\varepsilon)$:

$$\frac{1}{\alpha}\left((\ \mathrm{I}\ - K(x,\varepsilon)) f^\alpha, \lambda\right)_\varepsilon = \left(g^\alpha, \lambda\right)_\varepsilon\,. \tag{B.6}$$

But

$$\frac{1}{\alpha}\left((\ \mathrm{I}\ - K(x,\varepsilon)) f^\alpha, \lambda\right)_\varepsilon = \frac{1}{\alpha}\left(f^\alpha, (\ \mathrm{I}\ - K^*(x,\varepsilon))\lambda\right)_\varepsilon$$
$$= -\frac{1}{\alpha}\left(f^\alpha, \mathrm{sgn}(v_x)\right)_\varepsilon = -\frac{1}{\alpha}\int_{\mathcal{S}_\varepsilon} f^\alpha v_x(k) dN_\varepsilon(k) = -J^\alpha(x,\varepsilon,t)\,. \tag{B.7}$$

Now, we compute the right-hand side of (B.6). Using (B.5), (B.4), we obtain

$$-J^\alpha(x,\varepsilon,t) = I^1_\alpha + I^2_\alpha + I^3_\alpha + I^4_\alpha + o(1) \quad \text{as } \alpha \to 0\,, \tag{B.8}$$

where (still noting $d\nu = |v_x||v'_x|dN(k)dN(k')$)

$$\begin{aligned}
\alpha\, I^1_\alpha &= \int_{k\in\S^+_\varepsilon}\int_{k'\in\S^-_\varepsilon} \sigma^\alpha\Big(x-\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x-\frac{\alpha\ell}{2}\Big), k', k\Big)\lambda(k) f^\alpha(x,k',t)d\nu \\
&\quad - \int_{k\in\S^+_\varepsilon}\int_{k'\in\S^-_\varepsilon} \sigma(x,k',k)\lambda(k) f^\alpha(x,k',t)d\nu\,, \qquad \text{(B.9)}\\
\alpha\, I^2_\alpha &= \int_{k\in\S^+_\varepsilon}\int_{k'\in\S^+_{\varepsilon+\alpha\ell e E^\alpha\left(x-\frac{\alpha\ell}{2}\right)}} \sigma^\alpha\Big(x-\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x-\frac{\alpha\ell}{2}\Big), k', k\Big) \\
&\quad \times \lambda(k) f^\alpha(x-\alpha\ell, k', t)d\nu \\
&\quad - \int_{k\in\S^+_\varepsilon}\int_{k'\in\S^+_\varepsilon} \sigma(x,k',k)\lambda(k) f^\alpha(x,k',t)d\nu\,, \qquad \text{(B.10)}\\
\alpha\, I^3_\alpha &= \int_{k\in\S^-_\varepsilon}\int_{k'\in\S^+_\varepsilon} \sigma^\alpha\Big(x+\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x+\frac{\alpha\ell}{2}\Big), k', k\Big)\lambda(k) f^\alpha(x,k',t)d\nu \\
&\quad - \int_{k\in\S^-_\varepsilon}\int_{k'\in\S^+_\varepsilon} \sigma(x,k',k)\lambda(k) f^\alpha(x,k',t)d\nu\,, \qquad \text{(B.11)}\\
\alpha\, I^4_\alpha &= \int_{k\in\S^-_\varepsilon}\int_{k'\in\S^-_{\varepsilon-\alpha\ell e E^\alpha\left(x+\frac{\alpha\ell}{2}\right)}} \sigma^\alpha\big(x+\frac{\alpha\ell}{2}, \alpha E^\alpha\Big(x+\frac{\alpha\ell}{2}\Big), k', k\Big) \\
&\quad \times \lambda(k) f^\alpha(x+\alpha\ell, k', t)d\nu \\
&\quad - \int_{k\in\S^-_\varepsilon}\int_{k'\in\S^-_\varepsilon} \sigma(x,k',k)\lambda(k) f^\alpha(x,k',t)d\nu\,. \qquad \text{(B.12)}
\end{aligned}$$

Now, in view of (2.17), we write

$$\sigma^\alpha\Big(x-\frac{\alpha\ell}{2}, E, k', k\Big) = \sigma\Big(\alpha\ell\Big[\frac{x}{\alpha\ell}\Big], E, k', k\Big) = \sigma(x-\alpha X^\alpha(x), E, k', k)\,, \qquad \text{(B.13)}$$

$$\begin{aligned}
\sigma^\alpha\Big(x+\frac{\alpha\ell}{2}, E, k', k\Big) &= \sigma\Big(\alpha\ell\Big(\Big[\frac{x}{\alpha\ell}\Big]+1\Big), E, k', k\Big) \\
&= \sigma(x+\alpha(\ell - X^\alpha(x)), E, k', k)\,, \qquad \text{(B.14)}
\end{aligned}$$

where $X^\alpha(x) = \ell\Big\{\frac{x}{\alpha\ell}\Big\}$, and $\{y\}$ denotes the decimal part like in Section 2. Again, we notice that $X^\alpha(x) = O(1)$.

Now, we obtain, using (4.8)

$$\begin{aligned}
I^1_\alpha &= -X^\alpha(x)F(x,\varepsilon,t)\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^-_\varepsilon}\frac{\partial\sigma}{\partial x}(x,k',k)\lambda(k)d\nu \\
&\quad + E(x)\,F(x,\varepsilon,t)\,\frac{\partial}{\partial E}\Big(\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^-_\varepsilon}\sigma(x,E,k',k)\lambda(k)d\nu\Big)_{E=0} + o(1)\,, \qquad \text{(B.15)}
\end{aligned}$$

and similarly

$$\begin{aligned}
I^3_\alpha &= (\ell - X^\alpha(x))F(x,\varepsilon,t)\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^+_\varepsilon}\frac{\partial\sigma}{\partial x}(x,k',k)\lambda(k)d\nu \\
&\quad + E(x)\,F(x,\varepsilon,t)\frac{\partial}{\partial E}\Big(\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^+_\varepsilon}\sigma(x,E,k',k)\lambda(k)d\nu\Big)_{E=0} + o(1)\,. \qquad \text{(B.16)}
\end{aligned}$$

In a similar fashion:

$$I^2_\alpha = -X^\alpha(x)F(x,\varepsilon,t)\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^+_\varepsilon}\frac{\partial\sigma}{\partial x}(x,k',k)\lambda(k)d\nu$$
$$+E(x)\,\frac{\partial}{\partial E}\Big(F(x,\varepsilon+\ell eE,t)\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^+_{\varepsilon+\ell eE}}\sigma(x,E,k',k)\lambda(k)d\nu\Big)_{E=0}$$
$$-\ell\frac{\partial F}{\partial x}(x,\varepsilon,t)\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^+_\varepsilon}\sigma(x,k',k)\lambda(k)d\nu+o(1)\,, \tag{B.17}$$

$$I^4_\alpha = (\ell-X^\alpha(x))F(x,\varepsilon,t)\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^-_\varepsilon}\frac{\partial\sigma}{\partial x}(x,k',k)\lambda(k)d\nu$$
$$+E(x)\,\frac{\partial}{\partial E}\Big(F(x,\varepsilon-\ell eE,t)\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^-_{\varepsilon-\ell eE}}\sigma(x,E,k',k)\lambda(k)d\nu\Big)_{E=0}$$
$$+\ell\frac{\partial F}{\partial x}(x,\varepsilon,t)\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^-_\varepsilon}\sigma(x,k',k)\lambda(k)d\nu+o(1)\,. \tag{B.18}$$

Now, differentiating identities (3.6), (3.7) (for $E=0$) with respect to x, we obtain:

$$0=\Big(\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^-_\varepsilon}+\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^+_\varepsilon}\Big)\frac{\partial\sigma}{\partial x}(x,k',k)\lambda(k)\,d\nu, \tag{B.19}$$

$$0=\Big(\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^+_\varepsilon}+\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^-_\varepsilon}\Big)\frac{\partial\sigma}{\partial x}(x,k',k)\lambda(k)\,d\nu, \tag{B.20}$$

Similarly, differentiating identities (3.6), (3.7) with respect to E and summing up yields

$$\frac{\partial}{\partial E}\Big(\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^-_\varepsilon}+\int_{k\in\S^+_\varepsilon}\int_{k'\in\S^+_{\varepsilon+\ell eE}}$$
$$+\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^+_\varepsilon}+\int_{k\in\S^-_\varepsilon}\int_{k'\in\S^-_{\varepsilon-\ell eE}}\sigma(x,E,k',k)\,\lambda(k)\,d\nu\Big)$$
$$=\frac{\partial}{\partial E}\Big(\int_{k\in\S^+_\varepsilon}+\int_{k\in\S^-_\varepsilon}\lambda(k)|v_x|dN(k)\Big)$$
$$=\frac{\partial}{\partial E}\Big(\int_{k\in\S_\varepsilon}\lambda(k)|v_x(k)|dN_\varepsilon(k)\Big)=0\,, \tag{B.21}$$

because λ satisfies the normalization condition (B.15). Therefore, summing up (B.15) to (B.18) and using (B.19), (B.20), we obtain

$$J^\alpha(x,\varepsilon,t)=J(x,\varepsilon,t)+o(1)\quad\text{as}\quad\alpha\to0\,, \tag{B.22}$$

with J given by (4.2). This ends the appendix.

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