A ONE DIMENSIONAL QUANTUM TRANSPORT MODEL WITH SMALL COHERENCE LENGTHS

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Abstract

A one dimensional stationary transport model accounting for both, quantum effects and smallness of coherence length is presented and analyzed. The physical system extension is an interval $[a, b]$ whose length is of the order of few to several times the coherence length of particles. An arbitrary decomposition of the domain into intervals of lengths comparable to the coherence length is chosen. On each interval, the particle density is given as the superposition of densities of scattering states of the Schrödinger equation. The statistics in the various intervals are solution of a linear system whose coefficients depend on the reflection and transmission coefficients. This system is shown to have a unique minimal solution. In the limit of very small coherence lengths, a collisionless kinetic equation is obtained.

Keywords : Schrödinger equation; Quantum transmitting boundary conditions; Hybrid models; Reflection-Transmission coefficients

1 Introduction

Nanostructures such as tunneling diodes, ultrashort channel transistors and split gate devices exhibit non linear features due to quantum effects [1, 2, 5, 15]. Quantum interference effects are present when the de Broglie wavelength of charge carriers is of the same order of magnitude as the device typical length; they tend to vanish in the semiclassical limit, when the wavelength is much smaller than the device lengthscale [10, 11, 12, 13]. This is true in ballistic devices for which collisions are negligible. One effect of collisions is the breaking of phase coherence. Electrons may loose their phase over distances, called coherence lengths, which might be smaller than the de Broglie wavelength. This results in a classical transport although the device length is of the same order of magnitude as the de Broglie wavelength.

In this paper we are interested in situations where the device length is of the order of magnitude of the de Broglie length and a few times bigger than the coherence length. Degond and Zhang [6] proposed a model for superlatticies which covers this situation. The domain is decomposed into small intervals with sizes of the order of the coherence length. In these intervals, the electrons are represented by uniform distribution functions coupled to each other through reflection and transmission coefficients. In the limit of small coherence lengths, a diffusion equation (SHE model) is obtained in [6]. The model that we propose is similar. It assumes that, in each interval, electrons are in a quantum mixed state, whose statistics are given by distribution functions. The distribution functions are coupled to each other in a similar manner to [6]. We prove the existence of solutions for the obtained sytem for a nonvanishing coherence length. We show then that in the limit of very small coherence lengths, the system "tends" to the Vlasov equation, while the limit equation in [6] is a diffusion equation.

Kinetic formulation. We start with a brief description of the Vlasov model. We consider a one dimensional device represented by the bounded interval $[a,b]$. Electrons are injected at $x=a$ and $x=b$ with the known distributions $f_a \in L^\infty(\mathbb{R}^+)$ resp. $f_b \in L^\infty(\mathbb{R}^-)$ and are exposed in $[a,b]$ to a given stationary electrostatic potential $V \in C^1([a,b])$. We suppose throughout this paper, that the transport is ballistic.
The evolution of the electrons through the device is described by the distribution function $f(x,p)$, which satisfies the linear stationary Vlasov equation

$$p\frac{\partial f}{\partial x} + \frac{dV}{dx}\frac{\partial f}{\partial p} = 0\,, \tag{1.1}$$

with the boundary conditions

$$f(a,p) = f_a(p)\,, \qquad \text{for } p > 0\,, \tag{1.2}$$

$$f(b,p) = f_b(p)\,, \qquad \text{for } p < 0\,. \tag{1.3}$$

The variable x denotes the position and p the momentum. The electron mass m and charge q are set to one for notational simplicity. The macroscopic quantities as the charge density n and the current density j are given in terms of f by the relations

$$n(x) = \int_{-\infty}^{\infty} f(x,p)dp \quad ; \quad j(x) = \int_{-\infty}^{\infty} pf(x,p)dp\,. \tag{1.4}$$

Quantum formulation. We recall here the quantum analogue of the above problem and refer the reader to [4, 3, 8, 9] for more details. We still assume that electrons are injected at the left boundary ($x=a$), with a statistics $f_a(p)$ and at the right boundary with the statistics $f_b(p)$. The charge density and current density are given by

$$n(x) = \int_{-\infty}^{\infty} f_{inc}(p)|\psi_p(x)|^2\, dp \quad ; \quad j(x) = \int_{-\infty}^{\infty} f_{inc}(p)\mathcal{I}m\left(\overline{\psi}_p \frac{d\psi_p}{dx}\right)\, dp\,, \tag{1.5}$$

where $f_{inc}(p) = f_a(p)$ for $p>0$ and $f_{inc}(p) = f_b(p)$ for $p<0$. We denoted by ψ_p the wave function corresponding to the electrons injected from the left for $p>0$ respectively from the right for $p<0$. These elementary wave functions are solutions of

$$-\frac{1}{2}\frac{d^2\psi_p}{dx^2} - V\psi_p = (\frac{p^2}{2} - V_a)\psi_p \quad ; \quad \text{for} \;\; p > 0 \tag{1.6}$$

$$\psi_p'(a) + \mathbf{i}p\psi_p(a) = 2\mathbf{i}p \quad ; \quad \psi_p'(b) = \mathbf{i}\sqrt{p^2 + 2(V_b - V_a)}\psi_p(b)\,, \tag{1.7}$$

respectively

$$-\frac{1}{2}\frac{d^2\psi_p}{dx^2} - V\psi_p = (\frac{p^2}{2} - V_b)\psi_p \quad ; \quad \text{for} \quad p < 0 \tag{1.8}$$

$$\psi_p'(a) = -\mathbf{i}\sqrt{p^2 + 2(V_a - V_b)}\psi_p(a) \quad ; \quad \psi_p'(b) + \mathbf{i}p\psi_p(b) = 2\mathbf{i}p\,. \tag{1.9}$$

The Planck constant $\hbar$ was set to one, as in the present analysis it is considered as a constant. The boundary conditions for the wave functions are derived in the following way. To fix the ideas, le us consider the $p > 0$ case. The electrostatic potential being considered constant outside the interval $[a, b]$, the solution of the Schrödinger equation (1.6) has an explicit formula for $x \leq a$:

$$\psi_p(x) = a_p e^{ip(x-a)} + r_p e^{-ip(x-a)}.$$

The coefficient a_p is the amplitude of the incoming wave and is set to 1, while the coefficient r_p of the reflected wave is an unknown and is eliminated to obtain the first boundary condition for ψ_p. This is done by linking the solution in the lead with that one inside the device via continuity conditions. The same job can be done for $x > b$, where we assume that only a transmitted wave is present.
As we can see from (1.5), the density of electrons is obtained by adding up the contribution of each single wave function. The interference effects which are implicitly taken into account in the wave function are present on the whole interval $[a, b]$. The reflection and transmission coefficients are defined from ψ_p by the following formulae

$$R(p) = |\psi_p(a) - 1|^2 \quad ; \quad T(p) = \frac{1}{p}\mathcal{R}e(\sqrt{p^2 + 2(V_b - V_a)})|\psi_p(b)|^2\,, \quad (p > 0) \tag{1.10}$$

$$R(p) = |1 - \psi_p(b)|^2 \quad ; \quad T(p) = \frac{-1}{p}\mathcal{R}e(\sqrt{p^2 + 2(V_a - V_b)})|\psi_p(a)|^2\,, \quad (p < 0). \tag{1.11}$$

The reflection coefficient $R(p)$ represents the part of the wave which is reflected back to the injection source, whereas the transmission coefficient $T(p)$ is the part which is transmitted from one side of the device to the other. We have the following identity

$$R(p) + T(p) = 1\,, \quad \forall p,$$

which follows immediately by multiplying the Schrödinger equation by $\overline{\psi_p}$, integrating over $[a, b]$ and taking the imaginary part [3].

2 A model for a moderately small coherence length

In the above example, the electron transport is ballistic and ondulatory effects take place in the whole interval $[a, b]$. Let us now assume that the coherence length is smaller than the device length. We divide then the interval $[a, b]$ into cells $I_i = [x_i, x_{i+1}]$ with $a = x_1 < x_2 < \cdots < x_{N+1} = b$, where we have assumed that $h_i = x_{i+1} - x_i$ is of the order of magnitude of the coherence length. In each interval I_i, a quantum mechanical model describes the electron evolution. The charge and current densities in the cell I_i are given by the formulae

$$n_i^N(x) = \int_{-\infty}^{\infty} f_i(p)|\psi_{i,p}(x)|^2 dp\,, \quad x \in I_i\,, \tag{2.1}$$

$$j_i^N(x) = \int_{-\infty}^{\infty} f_i(p)\mathcal{I}m(\overline{\psi}_{i,p}(x)\frac{d\psi_{i,p}}{dx}(x))dp\,, \quad x \in I_i\,, \tag{2.2}$$

where $f_i(p)$ are the statistics of particles entering in the interval I_i and $\psi_{i,p}$ are the corresponding elementary wave functions, solving

$$\begin{cases} -\dfrac{1}{2}\dfrac{d^2\psi_{i,p}}{dx^2} - V\psi_{i,p} = \left(\dfrac{p^2}{2} - V_i\right)\psi_{i,p}\,, \qquad (\text{if } p > 0) \\ \dfrac{d\psi_{i,p}}{dx}(x_i) + \mathbf{i}p\psi_{i,p}(x_i) = 2\mathbf{i}p \\ \dfrac{d\psi_{i,p}}{dx}(x_{i+1}) = \mathbf{i}\sqrt{p^2 + 2(V_{i+1} - V_i)}\psi_{i,p}(x_{i+1})\,, \end{cases} \tag{2.3}$$

or

$$\begin{cases} -\dfrac{1}{2}\dfrac{d^2\psi_{i,p}}{dx^2} - V\psi_{i,p} = \left(\dfrac{p^2}{2} - V_{i+1}\right)\psi_{i,p}\,, \qquad (\text{if } p < 0) \\ \dfrac{d\psi_{i,p}}{dx}(x_i) = -\mathbf{i}\sqrt{p^2 + 2(V_i - V_{i+1})}\psi_{i,p}(x_i) \\ \dfrac{d\psi_{i,p}}{dx}(x_{i+1}) + \mathbf{i}p\psi_{i,p}(x_{i+1}) = 2\mathbf{i}p\,. \end{cases} \tag{2.4}$$

In the above equations V_i denotes $V(x_i)$. We notice that the pure quantum problem is recovered by taking $N = 1$ and $f_1 = f_{inc}$. In each interval, we compute the reflection and transmission coefficients by

$$R_i(p) := |\psi_{i,p}(x_i) - 1|^2 \quad ; \quad T_i(p) := \frac{1}{p}\sqrt{(p^2 + 2(V_{i+1} - V_i))^+}|\psi_{i,p}(x_{i+1})|^2, \quad (p > 0) \tag{2.5}$$

and

$$R_i(p) := |\psi_{i,p}(x_{i+1}) - 1|^2 \quad ; \quad T_i(p) := \frac{1}{(-p)}\sqrt{(p^2 + 2(V_i - V_{i+1}))^+}|\psi_{i,p}(x_i)|^2, \quad (p < 0) \tag{2.6}$$

where for real ξ the notation ξ^+ denotes $\max\{\xi, 0\}$.
It is convenient from analytical purposes to extend the domain of definition of the statistics f_i to the whole space $\mathbb{C}$, by setting

$$f_i(p) = 0\,, \quad \forall p \in \mathbb{C}\backslash\mathbb{R}\,, \forall i\,,$$

and to introduce the transmission and reflection coefficients even for complex arguments as follows

$$R_i(p) := 1 \quad ; \quad T_i(p) := 0\,, \quad \forall p \in \mathbb{C}\backslash\mathbb{R}\,. \tag{2.7}$$

Of course

$$T_i(p) + R_i(p) = 1\,, \quad \forall i = 1, \ldots, N\,, \quad \forall p \in \mathbb{C}\,, \tag{2.8}$$

$$0 \le T_i(p), R_i(p) \le 1\,, \quad \forall i=1,\dots,N\,, \quad \forall p \in \mathbb{C}\,, \tag{2.9}$$

and we have the following reciprocity identities [3]

$$\begin{cases} T_i(p) = T_i\left(-\sqrt{p^2+2(V_{i+1}-V_i)}\right) & \forall i=1,\dots,N \quad \forall p>0 \\ T_i\left(\sqrt{p^2+2(V_i-V_{i+1})}\right) = T_i(p) & \forall i=1,\dots,N \quad \forall p<0\,. \end{cases} \tag{2.10}$$

The statistics of particles entering the interval I_i are connected to that ones of the intervals I_{i-1} resp. I_{i+1} through the following reflection-transmission formulae

$$\begin{cases} f_i\,(p) = R_{i-1}(-p)f_{i-1}(-p) + \\ \quad +T_{i-1}\left(\sqrt{p^2+2(V_{i-1}-V_i)}\right) f_{i-1}\left(\sqrt{p^2+2(V_{i-1}-V_i)}\right)\,, \quad \text{for } p>0\,, \\ f_i\,(p) = R_{i+1}(-p)f_{i+1}(-p) + \\ \quad +T_{i+1}\left(-\sqrt{p^2+2(V_{i+2}-V_{i+1})}\right) f_{i+1}\left(-\sqrt{p^2+2(V_{i+2}-V_{i+1})}\right)\,, \quad \text{for } p<0. \end{cases} \tag{2.11}$$

Using the notation

$$P_i(p) := \sqrt{p^2+2(V_i-V_1)}\,,$$

for the momentum of an electron at the position $x=x_i$ and which would possess at $x=x_1$ the momentum p, the system satisfied by the statistics $f_i(P_i(p))$ and $f_i(-P_{i+1}(p))$ is the following (see Figure 1):

$$\begin{aligned} f_1(-P_2(p)) &= T_2(-P_3(p))f_2(-P_3(p)) + R_2(P_2(p))f_2(P_2(p)) \\ f_2(P_2(p)) &= T_1(p)f_1(p) + R_1(-P_2(p))f_1(-P_2(p)) \\ f_2(-P_3(p)) &= T_3(-P_4(p))f_3(-P_4(p)) + R_3(P_3(p))f_3(P_3(p)) \\ f_3(P_3(p)) &= T_2(P_2(p))f_2(P_2(p)) + R_2(-P_3(p))f_2(-P_3(p)) \\ &\vdots \end{aligned} \tag{2.12}$$

This can be written as a linear system

$$Ax = B\,, \tag{2.13}$$

with

$$A = \begin{pmatrix} 1 & -R_2^+ & -T_2^- & 0 & 0 & & 0 & 0 & 0 \\ -R_1^- & 1 & 0 & 0 & 0 & & 0 & 0 & 0 \\ 0 & 0 & 1 & -R_3^+ & -T_3^- & & 0 & 0 & 0 \\ 0 & -T_2^+ & -R_2^- & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & & 0 & 0 & 0 \\ 0 & 0 & 0 & -T_3^+ & -R_3^- & & 0 & 0 & 0 \\ & & & \vdots & & \ddots & & & \\ 0 & 0 & 0 & 0 & 0 & & 0 & 1 & -R_N^+ \\ 0 & 0 & 0 & 0 & 0 & & -T_{N-1}^+ & -R_{N-1}^- & 1 \end{pmatrix}$$

and

$$x = \begin{pmatrix} f_1^- \\ f_2^+ \\ f_2^- \\ f_3^+ \\ f_3^- \\ f_4^+ \\ \vdots \\ f_{N-1}^- \\ f_N^+ \end{pmatrix} \quad ; \quad B = \begin{pmatrix} 0 \\ T_1^+ f_1^+ \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ T_N^- f_N^- \\ 0 \end{pmatrix}$$

In the above system, the arguments of f_i, R_i and T_i are omitted for notational simplicity. The notation f_i^+ stands for $f_i(P_i(p))$, f_i^- stands for $f_i(-P_{i+1}(p))$ and analogously for $R_i^\pm$ and $T_i^\pm$.

Remark 2.1 *If the momentum $P_i(p)$ is imaginary or equal 0, then the following holds, due to (2.7) and (2.10)*

$$T_i^+ = T_i^- = T_{i-1}^+ = T_{i-1}^- = 0\,.$$

Remark 2.2 *If* $\quad P_i(p) > 0 \quad$ *then* $\quad \psi_{i,P_i(p)}(x_{i+1}) \neq 0$ *and* $\psi_{i-1,-P_i(p)}(x_{i-1}) \neq 0$.

Indeed $\psi_{i,P_i(p)}(x_{i+1}) = 0$ implies $\psi'_{i,P_i(p)}(x_{i+1}) = 0$, thus leading to $\psi_{i,P_i(p)} \equiv 0$. Hence, $\psi'_{i,P_i(p)}(x_i) + \mathbf{i}P_i(p)\psi_{i,P_i(p)}(x_i) = 0 \neq 2\mathbf{i}P_i(p)$. The second statement can be obtained similarly.

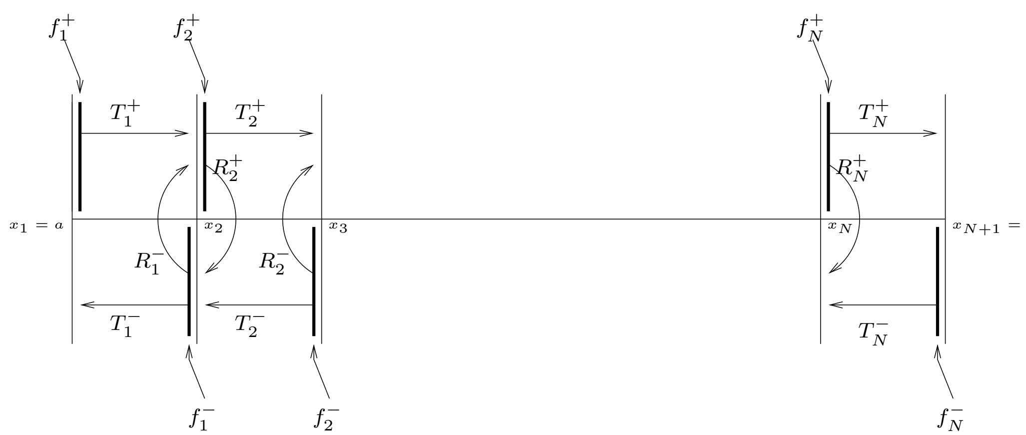

Figure 1: Representation of the statistics $f_i^\pm$ and the reflection-transmission coefficients.

Theorem 2.3 *The linear system (2.13) has a unique minimal, positive solution, if $f_1(p)$, $p > 0$ and $f_N(p)$, $p < 0$ are prescribed positive statistics.*

Remark 2.4 *A solution f of (2.13) is called minimal positive solution, if $f_i \geq 0$ $\forall i$ and if for any other positive solution h with $h_i \leq f_i$ $\forall i$, we have $h = f$.*

Proof: We start by constructing one solution of the linear system (2.13) and shall prove in the end, that this solution is the unique minimal, positive one.
If all $T_i^\pm$ are $\neq 0$, then the matrix of the system (2.13) is weakly diagonal dominant and irreducible, hence invertible. The linear system has, in this case, a unique solution.
Let otherwise $T_{i_0}^+$ be the first transmission coefficient equal zero. That means, that $P_{i_0+1}(p)$ is imaginary or equal 0, which follows immediately from Remark 2.2 and the definition of the transmission coefficients. We have thus with Remark 2.1

$$T_{i_0}^+ = T_{i_0}^- = T_{i_0+1}^+ = T_{i_0+1}^- = 0\,.$$

The matrix is then divided into (minimal) three blocs on the diagonal, as follows

$$\begin{pmatrix} A_{1,2i_0-2} & 0 & 0 \\ 0 & A_{2i_0-1,2i_0} & 0 \\ 0 & 0 & A_{2i_0+1,2N-2} \end{pmatrix}.$$

The first bloc $A_{1,2i_0-2}$ is a regular matrix. That means, that $f_1^-,\cdots,f_{i_0}^+$ are uniquely determinable. The second bloc has the form

$$A_{2i_0-1,2i_0} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

We can choose in this case $f_{i_0}^- = f_{i_0+1}^+ = 0$. The third bloc $A_{2i_0+1,2N-2}$ is either invertible, if the transmission coefficients are all $\neq 0$, or we can split it one more time. A further splitting would signify that there exist closed trajectories. Let for example the bloc have the dimensions $2s \times 2s$, with $s \geq 1$. Then due to the properties of the reflection and transmission coefficients, we can show that $f_{i_0+1}^- = f_{i_0+2}^\pm = \cdots = f_{i_0+s}^\pm = f_{i_0+s+1}^+$. As peviously we can set these statistics equal zero and continue in this manner.
The just constructed solution is positive. In fact, let $g := \min\{f_i^\pm / i = 1,\ldots,N\}$ and suppose that $g < 0$. The equation, in which g appears with the coefficient 1, for example let this be the equation

$$-T_i^+ f_i^+ - R_i^- f_i^- + g = 0\,,$$

can only be satisfied, if $f_i^+ = f_i^- = g$ (see (2.8), (2.9)). Recursively, we get either one of the relations

$$\begin{aligned} -R_1^- g + g &= T_1^+ f_1^+\,, \\ -R_N^+ g + g &= T_N^- f_N^-\,, \end{aligned}$$

which are, in view of

$$f_1^+ \geq 0 \quad ; \quad f_N^- \geq 0\,,$$

untrue, or we come to a contradiction by reaching an $f_i^\pm = 0$, which has to be equal to $g < 0$ by the previous arguments. Thus we have proven, that $g \geq 0$, which means that $f_i^\pm \geq 0 \quad \forall i$.
Finally it is obvious, by the construction of this solution, that this is the unique minimal positive solution of (2.13) and we have finished the proof.

∎

The next lemma shows the important property that the current is preserved at the interfaces x_i.

Lemma 2.5 (Current conservation)
Let $j^N(x)$ be defined on each I_i $(i = 1, \cdots, N)$ by the formula

$$j^N(x) = \int_{-\infty}^{\infty} f_i(p)\mathcal{I}m(\overline{\psi}_{i,p}(x)\frac{d\psi_{i,p}}{dx}(x))dp\,, \quad x \in I_i\,,$$

with $(f_i)_{i=1}^N$ solution of (2.13). Then j^N is constant all along the interval $[a, b]$ and in particular continuous at the interfaces x_i.

Proof: It is readily seen that $j^N(x)$ is independent on x within each interval I_i. Indeed

$$\frac{d}{dx}\mathcal{I}m(\overline{\psi_{i,p}}(x)\psi'_{i,p}(x)) = \mathcal{I}m(\overline{\psi'_{i,p}}(x)\psi'_{i,p}(x)) + \mathcal{I}m(\overline{\psi_{i,p}}(x)\psi''_{i,p}(x)) = 0\,.$$

Denoting by j_i^N the value of this current in I_i, let us prove that $j_i^N = j_{i+1}^N$. First, we notice that taking $\mathcal{I}m(\overline{\psi_{i,p}}(x)\psi'_{i,p}(x)) = \mathcal{I}m(\overline{\psi_{i,p}}(x_{i+1})\psi'_{i,p}(x_{i+1}))$ for $p > 0$ and similarly $\mathcal{I}m(\overline{\psi_{i,p}}(x)\psi'_{i,p}(x)) = \mathcal{I}m(\overline{\psi_{i,p}}(x_i)\psi'_{i,p}(x_i))$ for $p < 0$, we get

$$j_i^N = \int_{-\infty}^{\infty} pT_i(p)f_i(p)dp \quad \forall x \in I_i \quad \forall i = 1, \ldots, N\,.$$

Denoting

$$\begin{aligned} \mathcal{Q} &:= \{q > 0\} \cap \{q^2 > 2(V_i - V_{i+1})\} \\ \mathcal{P} &:= \{p > 0\} \\ \mathcal{R} &:= \{r > 0\} \cap \{r^2 > 2(V_{i+2} - V_{i+1})\}\,, \end{aligned}$$

we deduce

$$j_i^N = \int_{\mathcal{Q}} qT_i(q)f_i(q)dq - \int_{\mathcal{P}} pT_i(-p)f_i(-p)dp\,.$$

This last expression follows from the fact, that $T_i(q)$ is equal 0, if $q^2 + 2(V_{i+1} - V_i) < 0$. In the same way,

$$j_{i+1}^N = \int_{\mathcal{P}} pT_{i+1}(p)f_{i+1}(p)dp - \int_{\mathcal{R}} rT_{i+1}(-r)f_{i+1}(-r)dr\,.$$

In the sequel, the following change of variables will be used

$$q := \sqrt{p^2 + 2(V_i - V_{i+1})} \quad r := \sqrt{p^2 + 2(V_{i+2} - V_{i+1})}\,.$$

Notice that we have $qdq = rdr = pdp$. Using the relations (2.11), in particular

$$f_{i+1}(p) = T_i(q)f_i(q) + R_i(-p)f_i(-p) \quad ; \quad f_i(-p) = R_{i+1}(p)f_{i+1}(p) + T_{i+1}(-r)f_{i+1}(-r)\,,$$

we deduce

$$f_{i+1}(p)(1 - R_i(-p)R_{i+1}(p)) = T_i(q)f_i(q) + R_i(-p)T_{i+1}(-r)f_{i+1}(-r)\,,$$

and

$$f_i(-p)(1 - R_i(-p)R_{i+1}(p)) = R_{i+1}(p)T_i(q)f_i(q) + T_{i+1}(-r)f_{i+1}(-r)\,,$$

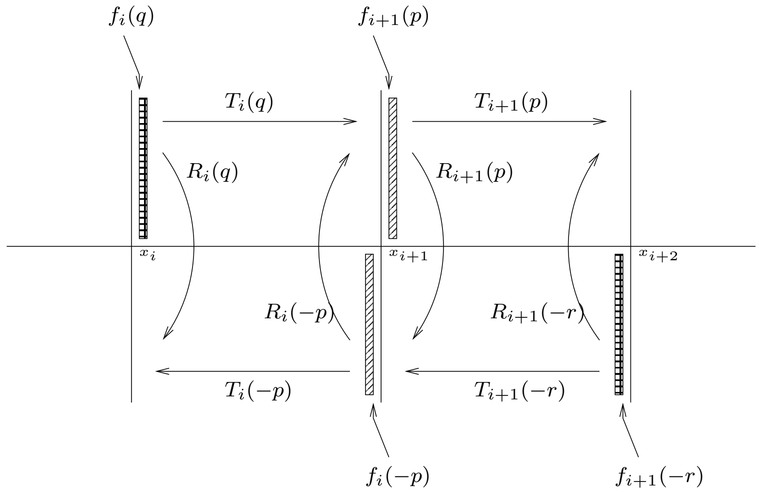

Figure 2: A detailed reflection-transmission picture at $x = x_i$.

leading to

$$j_i^N = \int_{\mathcal{Q}} qT_i(q)f_i(q)dq - \int_{\mathcal{P}} p\frac{T_i(-p)\{R_{i+1}(p)T_i(q)f_i(q) + T_{i+1}(-r)f_{i+1}(-r)\}}{1 - R_i(-p)R_{i+1}(p)}dp.$$

Therefore

$$\begin{aligned} j_i^N &= \int_{\mathcal{Q}} qT_i(q)f_i(q)\{1 - \frac{T_i(-p)R_{i+1}(p)}{1 - R_i(-p)R_{i+1}(p)}\}dq - \int_{\mathcal{R}} r\frac{T_i(-p)T_{i+1}(-r)}{1 - R_i(-p)R_{i+1}(p)}f_{i+1}(-r)dr \\ &= \int_{\mathcal{Q}} qT_i(q)f_i(q)\frac{T_{i+1}(p)}{1 - R_i(-p)R_{i+1}(p)}dq - \int_{\mathcal{R}} r\frac{T_i(-p)T_{i+1}(-r)}{1 - R_i(-p)R_{i+1}(p)}f_{i+1}(-r)dr\,. \end{aligned}$$

Analogously, it can be seen that

$$\begin{aligned} j_{i+1}^N &= -\int_{\mathcal{R}} rT_{i+1}(-r)f_{i+1}(-r)dr + \int_{\mathcal{P}} p\frac{T_{i+1}(p)\{T_i(q)f_i(q) + R_i(-p)T_{i+1}(-r)f_{i+1}(-r)\}}{1 - R_i(-p)R_{i+1}(p)}dp \\ &= -\int_{\mathcal{R}} rT_{i+1}(-r)f_{i+1}(-r)\left\{1 - \frac{R_i(-p)T_{i+1}(p)}{1 - R_i(-p)R_{i+1}(p)}\right\}dr + \int_{\mathcal{Q}} q\frac{T_{i+1}(p)\,T_i(q)f_i(q)}{1 - R_i(-p)R_{i+1}(p)}dq \\ &= -\int_{\mathcal{R}} rT_{i+1}(-r)f_{i+1}(-r)\frac{T_i(-p)}{1 - R_i(-p)R_{i+1}(p)}dr + \int_{\mathcal{Q}} q\frac{T_{i+1}(p)}{1 - R_i(-p)R_{i+1}(p)}T_i(q)f_i(q)dq\,. \end{aligned}$$

This shows that $j_i^N = j_{i+1}^N$ and concludes the proof. ∎

Analogy with the Vlasov equation. In general, the boundary value problem (1.1)-(1.3) is not uniquely solvable. The solutions are constant along the characteristics defined by Newton laws

$$\frac{dx}{dt} = p(t) \quad ; \quad \frac{dp}{dt} = \frac{dV}{dx}(x(t)).$$

These characteristics are the possible trajectories of the electrons. On open trajectories the value of f is uniquely given by the boundary condition. However on closed trajectories, the value of f can be arbitrarily chosen, which underlines the nonuniqueness of solutions of the Vlasov problem. If f is set to be zero on these trajectories, the so obtained solution is the minimal solution. A solution f of (1.1)-(1.3) is minimal, if for any solution g of (1.1)-(1.3) with $|g| \leq |f|$, we have $g = f$.
Mathematically, to avoid the nonuniqueness for the Vlasov problem an absorbtion term νf is added in the Vlasov equation, which writes then

$$p\frac{\partial f_\nu}{\partial x} + \frac{dV}{dx}\frac{\partial f_\nu}{\partial p} + \nu f_\nu = 0\,.$$

The new problem is uniquely solvable and the solutions f_ν converge, as ν tends to zero, to the minimal solution of the initial problem.
We point out furthermore two properties of the solutions of the Vlasov problem, which follow from the maximum principle. If f_a and f_b are nonnegative functions, then the solutions of (1.1)-(1.3) are positive and if this incident distributions satisfy the inequalities

$$f_a(p) \leq G\left(\frac{p^2}{2} - V_a\right) \text{ for } p > 0 \quad \text{and} \quad f_b(p) \leq G\left(\frac{p^2}{2} - V_b\right) \text{ for } p < 0\,,$$

with G a real valued function, then the minimal solution satisfies

$$f(x,p) \leq G\left(\frac{p^2}{2} - V(x)\right) \quad \text{f.a.a. } (x,p) \in [a,b] \times \mathbb{R}\,.$$

For more details about the stationary Vlasov equation we refer the reader to [14].

Analogously to the Vlasov equation, Theorem 2.3 can be proven by adding an absorbtion term in the Schrödinger equation, turning into

$$-\frac{1}{2}\psi''_{i,p}(x) - V(x)\psi_{i,p}(x) = \left(\frac{p^2}{2} - V_i + \mathbf{i}\frac{\nu}{2}\right)\psi_{i,p}(x)\,, \quad \text{for } p > 0\,,$$

respectively

$$-\frac{1}{2}\psi''_{i,p}(x) - V(x)\psi_{i,p}(x) = \left(\frac{p^2}{2} - V_{i+1} + \mathbf{i}\frac{\nu}{2}\right)\psi_{i,p}(x)\,, \quad \text{for } p < 0\,.$$

This procedure ensures, that the coefficients defined by (2.5) and (2.6) satisfy the strict inequality $T_i(p) + R_i(p) < 1 \quad \forall p$, implying that the matrix of the linear system (2.13) is regular. The passage to the limit leads then to the minimal, positive solution constructed in the above proof. Moreover, the so constructed solution satifies the following estimates

Theorem 2.6 *If the boundary statistics satisfy the inequalities*

$$f_1(p) \leq G\left(\frac{p^2}{2} - V_a\right)\,, \quad \textit{for } p > 0 \quad ; \quad f_N(p) \leq G\left(\frac{p^2}{2} - V_b\right)\,, \quad \textit{for } p < 0 \tag{2.14}$$

then we have for all solutions of the linear system (2.13), $\forall i = 1, \ldots, N$

$$f_i(p) \leq G\left(\frac{p^2}{2} - V_i\right)\,, \quad \textit{for } p > 0 \quad ; \quad f_i(p) \leq G\left(\frac{p^2}{2} - V_{i+1}\right)\,, \quad \textit{for } p < 0\,.$$

Proof: This theorem follows immediately from the maximum principle. ∎

3 The limit of an infinitely small coherence length

In this section, the limit of an infinitely small coherence length is considered. Defining $h = \max_{i=1,\cdots,N} h_i$ with $h_i = x_{i+1} - x_i$, we let N tend to $+\infty$ in such a way, that h tends to 0. The main result of this paper is the following

Theorem 3.1 (Limit of a small coherence length)
Let the charge and current densities n^N and j^N be defined by (2.1)-(2.2). Then up to a subsequence

$$n^N \to n(x) := \int_{-\infty}^{\infty} f(x,p)dp \quad \textit{weak * in} \quad L^\infty(a,b),$$
$$j^N \to j(x) := \int_{-\infty}^{\infty} pf(x,p)dp \quad \textit{weak * in} \quad L^\infty(a,b).$$

where f is a solution of the Vlasov equation

$$\begin{cases} p\dfrac{\partial f}{\partial x} + \dfrac{dV}{dx}\dfrac{\partial f}{\partial p} = 0 \\ f(a,p) = f_a(p) \qquad \textit{for } p > 0 \\ f(b,p) = f_b(p) \qquad \textit{for } p < 0\,. \end{cases} \tag{3.1}$$

We shall assume throughout this section that the prescribed statistics on the boundary of the device are nonnegative and satisfy the inequalities (2.14) with $G \in C_0^1(\mathbb{R})$.
As a first step we establish a lemma, which will be needed in the sequel.

Lemma 3.2 (Asymptotical behaviour)
Assume that $V \in C^1[a,b]$ and let $0 < \epsilon < M$ be fixed real numbers. Then, there exists a constant $C = C(M, \varepsilon, \|V\|_{C^1})$ such that $\forall i = 1, \ldots, N$

$$|T_i(p) - 1| \le Ch_i^2 \quad , \quad R_i(p) \le Ch_i^2\,, \quad \textit{for} \quad h \in (0,1), \quad \epsilon \le |p| \le M\,,$$

$$\sup_{x \in I_i} |\psi_{i,p}(x) - 1| + |\frac{d\psi_{i,p}}{dx} - \mathbf{i}p| \le Ch_i\,, \quad \textit{for} \quad h \in (0,1), \quad \epsilon \le |p| \le M\,,$$

where $h := \max_{i=0,\ldots,N} h_i$ and $h_i = |x_{i+1} - x_i|$.

Proof: We shall only treat the case $p > 0$. The $p < 0$ case follows by analogy. Let $A := \{p \in \mathbb{R}^+/\epsilon \le p \le M\}$. For h small enough

$$T_i(p) = \frac{1}{p}\sqrt{(p^2 + 2(V_{i+1} - V_i))}|\psi_{i,p}(x_{i+1})|^2 \quad \forall i = 1, \ldots, N \quad \forall p \in A\,.$$

It is readily seen that the function $\psi_{i,p}$ is given by

$$\psi_{i,p} = \frac{2\mathbf{i}p}{\theta'(x_i) + \mathbf{i}p\theta(x_i)}\theta\,, \tag{3.2}$$

where θ is the solution of the initial value problem

$$\begin{cases} -\frac{1}{2}\theta''(x) - V(x)\theta(x) = (\frac{p^2}{2} - V_i)\theta(x) \\ \theta(x_{i+1}) = 1 \\ \theta'(x_{i+1}) = \mathbf{i}\sqrt{p^2 + 2(V_{i+1} - V_i)}. \end{cases} \tag{3.3}$$

Straightforward computations lead to

$$\theta(x) = \frac{1}{2}[e^{-\mathbf{i}p(x_{i+1}-x)} + e^{\mathbf{i}p(x_{i+1}-x)}] + \frac{1}{2p}\sqrt{p^2 + 2(V_{i+1} - V_i)}[e^{-\mathbf{i}p(x_{i+1}-x)} - e^{\mathbf{i}p(x_{i+1}-x)}] + \\ + \frac{\mathbf{i}}{p}\int_x^{x_{i+1}} [e^{\mathbf{i}p(y-x)} - e^{-\mathbf{i}p(y-x)}](V(y) - V_i)\theta(y)dy\,, \tag{3.4}$$

$$\theta'(x) = \frac{\mathbf{i}p}{2}[e^{-\mathbf{i}p(x_{i+1}-x)} - e^{\mathbf{i}p(x_{i+1}-x)}] + \frac{\mathbf{i}}{2}\sqrt{p^2 + 2(V_{i+1} - V_i)}[e^{-\mathbf{i}p(x_{i+1}-x)} + e^{\mathbf{i}p(x_{i+1}-x)}] + \\ + \int_x^{x_{i+1}} [e^{\mathbf{i}p(y-x)} + e^{-\mathbf{i}p(y-x)}](V(y) - V_i)\theta(y)dy. \tag{3.5}$$

A Gronwall argument yields the uniform boundedness of θ and θ' in $L^\infty(I_i)$. The following identity

$$\theta'(x_i) + \mathbf{i}p\theta(x_i) = \mathbf{i}[p + \sqrt{p^2 + 2(V_{i+1} - V_i)}]e^{-\mathbf{i}ph} + 2\int_{x_i}^{x_{i+1}} e^{-\mathbf{i}p(y-x_i)}(V(y) - V_i)\theta(y)dy, \tag{3.6}$$

implies then for $\epsilon \le p \le M$

$$\left| |\theta'(x_i) + \mathbf{i}p\theta(x_i)|^2 - \left(p + \sqrt{p^2 + 2(V_{i+1} - V_i)}\right)^2 \right| \le Ch^2.$$

The asymptotic behaviour of $\psi_{i,p}$, $\psi'_{i,p}$ and $T_i(p)$ follows from the above estimates after lengthy but straightforward computations. ∎

Proof of Theorem 3.1 Let us define the functions

$$f^N(x,p) := f_i^N(p) \quad ; \quad T^N(x,p) := T_i(p)\,, \qquad \forall p \in \mathbb{R}, \quad \forall x \in (x_i, x_{i+1}) \quad \forall i = 1, \ldots, N\,,$$

$$\psi_p^N(x) := \psi_{i,p}(x) \quad \forall p \in \mathbb{R}, \quad \forall x \in (x_i, x_{i+1}) \quad \forall i = 1, \ldots, N.$$

Then the charge and current densities write

$$\begin{aligned} n^N(x) &= \int_{-\infty}^{\infty} f^N(x,p)|\psi_p^N(x)|^2 dp\,, \\ j^N(x) &= \int_{-\infty}^{\infty} f^N(x,p)\mathcal{I}m(\overline{\psi}_p^N(x)\frac{d}{dx}\psi_p^N(x))dp \\ &= \int_{-\infty}^{\infty} pT^N(x,p)f^N(x,p)dp\,. \end{aligned}$$

Moreover let us introduce

$$\tilde{n}^N(x) := \int_{-\infty}^{\infty} f^N(x,p)dp \quad ; \quad \tilde{j}^N(x) := \int_{-\infty}^{\infty} pf^N(x,p)dp\,.$$

A direct consequence of Theorem 2.6 and Lemma 3.2 is that n^N, $\tilde{n}^N$, j^N and $\tilde{j}^N$ are convergent in $L^\infty(a,b)$ weak * (up to the extraction of a subsequence) and that the L^∞-limit of $n^N - \tilde{n}^N$ and of $j^N - \tilde{j}^N$ is equal to zero. Moreover, the sequence (f^N) converges in $L^\infty((a,b)\times \mathbb{R})$ weak * towards a limit f. Since f^N is uniformly, compactly supported in the variable p, it is readily seen that the limits n, j of $\tilde{n}^N$ and $\tilde{j}^N$ are nothing but

$$n(x) = \int_{-\infty}^{\infty} f(x,p)dp \quad , \quad j(x) = \int_{-\infty}^{\infty} pf(x,p)dp.$$

It remains to prove that f is solution of the Vlasov equation (3.1). Since we do not know the behaviour of $T_i(p)$ for small p, we shall prove that f is a solution of the Vlasov equation (3.1) in two steps. By using test functions compactly supported in $[a,b)\times \mathbb{R}_*^+$ or in $(a,b]\times \mathbb{R}_*^-$, the limit f will be shown to solve the Vlasov equation on $[a,b]\times \mathbb{R}_*$ with the inflow boundary conditions $f_a(p)$ and $f_b(p)$. This will show that f satisfies

$$\begin{cases} p\dfrac{\partial f}{\partial x} + \dfrac{dV}{dx}\dfrac{\partial f}{\partial p} = S(x)\delta(p=0) \\ f(a,p) = f_a(p)\,, \qquad \text{for } p>0 \\ f(b,p) = f_b(p)\,, \qquad \text{for } p<0\,, \end{cases}$$

where $S(x) := [f(x,0+) - f(x,0-)]\frac{dV}{dx}(x)$ for $x \in (a,b)$. Then, we conclude the proof as $S = dj/dx$ and the current j is constant, being the limit of j^N.

Let us now prove that

$$p\frac{\partial f}{\partial x} + \frac{dV}{dx}\frac{\partial f}{\partial p} = 0\,, \quad \text{on} \quad (a,b)\times \mathbb{R}_*^+\,,$$

with the inflow boundary condition

$$f(a,p) = f_a(p) \text{ for } p > 0\,.$$

This means that $\mathcal{T}(\vartheta) = 0$, where

$$\mathcal{T}(\vartheta) = \int_a^b \int_0^\infty f(x,p)[p\partial_x\vartheta(x,p) + \frac{dV}{dx}(x)\partial_p\vartheta(x,p)]dpdx + \int_0^\infty pf_a(p)\vartheta(a,p)dp,$$

and ϑ is an arbitrary C^1 test function of (x,p) compactly supported in $[a,b)\times \mathbb{R}_*^+$. To this aim, it is enough to prove that $\lim_{N\to+\infty} \mathcal{T}^N(\vartheta) = 0$ where $\mathcal{T}^N(\vartheta)$ is given by

$$\mathcal{T}^N(\vartheta) = \int_a^b \int_0^\infty f^N(x,p)[p\partial_x\vartheta(x,p) + \frac{dV}{dx}(x)\partial_p\vartheta(x,p)]dpdx + \int_0^\infty pf_a(p)\vartheta(a,p)dp. \quad (3.7)$$

Since ϑ is compactly supported in $[a,b) \times \mathbb{R}_*^+$, there exist positive constants $M > \epsilon > 0$ such that

$$\begin{aligned}
\mathcal{T}^N(\vartheta) &= \int_a^b \int_\epsilon^M f^N(x,p)[p\partial_x\vartheta(x,p) + \frac{dV}{dx}(x)\partial_p\vartheta(x,p)]dpdx + \int_\epsilon^M pf_a(p)\vartheta(a,p)dp \\
&= \sum_{i=1}^N \int_{x_i}^{x_{i+1}} \int_\epsilon^M f_i^N(p)[p\partial_x\vartheta(x,p) + \frac{dV}{dx}(x)\partial_p\vartheta(x,p)]dpdx + \int_\epsilon^M pf_a(p)\vartheta(a,p)dp.
\end{aligned}$$

The first term of the right hand side can be evaluated as follows

$$\int_{x_i}^{x_{i+1}} \int_\epsilon^M f_i^N(p)p\partial_x\vartheta(x,p)dpdx = \int_\epsilon^M f_i^N(p)p[\vartheta(x_{i+1},p) - \vartheta(x_i,p)]dp\,.$$

Using the change of variables $q^2 = p^2 + 2(V_i - V_{i+1})$, we have

$$\begin{aligned}
\int_\epsilon^M pf_{i+1}^N(p)\vartheta(x_{i+1},p)dp &= \int_\epsilon^M [T_i(q)f_i^N(q) + R_i(-p)f_i^N(-p)]q\vartheta(x_{i+1}, \sqrt{q^2 + 2(V_{i+1} - V_i)})dq \\
&= \int_\epsilon^M qf_i^N(q)\vartheta(x_{i+1}, q + \frac{V_{i+1} - V_i}{q})dq + O(h_i^2) \\
&= \int_\epsilon^M qf_i^N(q)\{\vartheta(x_{i+1},q) + \left(\frac{V_{i+1} - V_i}{q}\right)\partial_q\vartheta(x_{i+1},q)\}dq + O(h_i^2) \\
&= \int_\epsilon^M qf_i^N(q)\vartheta(x_{i+1},q)dq + \int_{x_i}^{x_{i+1}} \int_\epsilon^M f_i^N(q)\frac{dV}{dx}\partial_q\vartheta(x_{i+1},q)dqdx + O(h_i^2) \\
&= \int_\epsilon^M qf_i^N(q)\vartheta(x_{i+1},q)dq + \int_{x_i}^{x_{i+1}} \int_\epsilon^M f_i^N(q)\frac{dV}{dx}\partial_q\vartheta(x,q)dqdx + O(h_i^2).
\end{aligned}$$

Consequently, we have

$$\begin{aligned}
\textstyle\int_{x_i}^{x_{i+1}} \int_\epsilon^M f_i^N(p)p\partial_x\vartheta(x,p)dpdx &= \int_\epsilon^M f_{i+1}^N(p)p\vartheta(x_{i+1},p)\,dp - \int_\epsilon^M pf_i^N(p)\vartheta(x_i,p)dp \\
&\quad - \int_{x_i}^{x_{i+1}} \int_\epsilon^M f_i^N(q)\frac{dV}{dx}\partial_q\vartheta(x,q)\,dqdx \,+\, O(h_i^2)\,,
\end{aligned}$$

which leads after a summation over the indices i

$$\int_a^b \int_\epsilon^M f^N \left[p\partial_x\vartheta + \frac{dV}{dx}\partial_p\vartheta\right] dpdx = -\int_\varepsilon^M f_a(p)p\vartheta(a,p)\,dp + \sum_{i=1}^N O(h_i^2).$$

This show that

$$|\mathcal{T}^N(\vartheta)| \le Ch\,,$$

where C is a constant depending on ϑ and not on h. ∎

4 Conclusion

The model proposed in this paper is an intermediate model between a fully quantum model and a fully classical one. It includes in a phenomenological way the phase breakdown for lengths exceeding the coherence length, and leads to a ballistic kinetic equation in the limit of very small coherence length. In [3] a hybrid model which models a device consisting in a quantum zone sandwiched between two classical kinetic zones is considered. This hybrid model can be obtained from the model developed in this paper by letting the coherence length tend to zero in the "kinetic" zones, while keeping it large in the quantum zone.

Contrary to the work of Degond and Zhang [6], the limit problem, obtained by letting the coherence length tend to zero, is a ballistic model while in the reference [6], the limiting equation is a diffusion equation (a SHE model). This is due to the fact, that the transmission coefficient tends to 1 in our case, while it has to stay away from zero and 1 in [6], and the system has to be rescaled to account for diffusion phenomena.

In this paper, the electrostatic potential is a given regular function. The self consistent case (coupling with the Poisson equation) can be treated without additional difficulty by taking advantage of the supersolution estimates. In particular, it is possible to pass to the limit of small coherence length in the selfconsistent case and to obtain the Vlasov-Poisson equation.

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