

SMALL COHERENCE LENGTH LIMIT FOR A TWO DIMENSIONAL QUANTUM TRANSPORT MODEL

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Abstract

In a previous work [N. Ben Abdallah, C. Negulescu, *A one-dimensional transport model with small coherence lengths*, *Transp. Theory and Stat. Phys.* **31**, no. 4-6 (2002), 559-578] a one dimensional transport model accounting for both, quantum phenomena and smallness of coherence lengths, has been analyzed. In the limit of infinitely small coherence lengths, this model leads to the classical Vlasov equation. In this paper the two dimensional situation is considered by adding to the one dimensional transport direction a transversal confined one. The transport direction is splitted into several regions of a size comparable to the coherence length. A quantum model, based on the 2D Schrödinger equation, describes the electron transport within each cell, while on larger distances, statistics defined on the interfaces of the cells, determine the electron motion. Reflection and transmission coefficients, deduced from the wavefunctions, solutions of the Schrödinger equation, relate neighbouring statistics with one another. In the limit of small coherence lengths, we obtain a collisionless subband model, which is classical in the transport direction and keeps quantum features in the confined one.

Keywords : Schrödinger-Poisson equation; Open boundary conditions; Reflection-Transmission-coefficients; Quantum/classical subband model

1 Introduction

The electron motion in ultrasmall electron systems, like tunneling diodes, ultrashort channel transistors, split gate devices, obeys quantum mechanics [1, 2, 10, 20]. This is caused by quantum interference effects, which are present when the de Broglie wavelength of the charge carriers is of the same order of magnitude as the device typical length and is true in the absence of collisions (ballistic devices). It relies on the perfect phase coherence of the electron wave functions. 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.

The aim of the present paper is to introduce and analyze a model describing this situation. Starting from a device whose dimensions are of the order of the de Broglie wavelength, we decompose it into several cells of a size comparable to the coherence length. Within each cell, the electron motion is completely determined by a quantum model, here

the Schrödinger equation with open boundary conditions. Discrete distribution functions, defined on the interfaces of the cells, describe the electron evolution over longer distances. The neighbouring statistics are related with each other through transmission-reflection coefficients, which are computed via the wave functions of the different cells. In this manner, the discrete distribution functions account for the quantum properties of the electron transport within each cell. In the limit of a large number of cells, these statistics are shown to converge towards a solution of a kinetic equation, namely the Vlasov equation.

Similar models for superlattices have been proposed in [11], [12] in a discrete setting and in [7], [5] in a continuous one. We shall call these references shortly the “discrete superlattice model” respectively the “continuous superlattice model”.

The continuous superlattice model starts from a kinetic description (Boltzmann equation) of the electron evolution within the superlattice cells. At the superlattice interfaces, the electrons are reflected or transmitted with a given rate. Under the assumption, that the reflection coefficient is strictly positive, space and time rescaling leads in the limit to a diffusion equation in the position-energy variables (the SHE model). For the discrete superlattice model, the reflection and transmission coefficients are computed from a quantum model. The charge density in the cells is given as the sum over scattering states and retains the quantum nature of transport. A similar asymptotics as in the continuous superlattice case, leads to the SHE model. The starting point of our model is identical to the discrete superlattice model in the stationary regime, with the important difference, that the limiting transmission is equal to one or to zero. This is less singular and leads to a kinetic equation (Vlasov equation). We prove rigorous existence and convergence results in the self-consistent one-dimensional case as well as in the non-self-consistent two-dimensional case, where the potential is assumed to be a given regular function.

The linear 1D case of the present model was treated in [9]. In Section 2, we extend these results to the self-consistent case. The principal result is Theorem 2.7, which states that the statistics converge, as the cell size tends to zero, towards a solution of the Vlasov-Poisson system. The key argument necessary to pass to the limit is an a priori estimate on the self-consistent potential, independent on the cell lengths (Lemma 2.4).

Section 3 is dedicated to the 2D model. We only consider here the linear case (no coupling with Poisson). An artificial, strictly positive absorption term $\nu > 0$ is introduced in order to guarantee the uniqueness of the solution of the linear 2D Schrödinger equation, as well as the existence of uniform bounds. Both directions, the transversal one (confined direction: z) and the longitudinal one (transport direction: x) have a length scale of the order of the de Broglie wave length. Electrons are supposed to be subject of collisions in the transport direction, fact which destroys the quantum nature of transport. Thus a domain decomposition of this transport direction is performed and following the same ideas as in the 1D case, we construct a model taking into consideration quantum effects as well as breaking of phase coherence. In the limit, our model is shown to tend towards a subband model, which is quantum in the confined direction and classical in the transport direction. This result is stated in the principal theorem of this paper: Theorem 3.7.

The proof of this theorem mainly relies on the asymptotic behaviour of the transmission and reflection coefficients, stated in Corollary 3.10. In the classical context, the transmission (respectively the reflection) is either equal to one or to zero. In the quantum

framework, these coefficients can take also intermediate values. Except for those energies corresponding to turning points, we are able to estimate these coefficients in terms of the cell lengths. Their limiting values are shown to be zero or one. Turning points have to be treated apart. In the 1D case they correspond to $E = V(x)$, while in the 2D case we have to consider all threshold energies $E = E_m(x)$, with E_m the energy subbands. To pass to the limit, one has to show the non occurrence of concentration around these energies. This is done thanks to the conservation of the current (Proposition 3.6). Some of the more technical proofs are postponed to the Appendix.

2 The one dimensional case

2.1 Description of the model and properties

We consider a 1D device represented by the bounded interval $[a, b]$ and of a size comparable to the de Broglie wave length. Electrons are injected at $x = a$ and $x = b$ with the known distributions $f_a^+ \in L^\infty(\mathbb{R})$, $f_b^- \in L^\infty(\mathbb{R})$. The electrostatic potential V , which governs the electron transport, is assumed to be constant outside the device. In the pure quantum mechanical framework, the electron transport is ballistic and interference effects take place in the whole interval $[a, b]$. We shall take here collisions into consideration, which destroy the quantum feature of the electron transport. The distance over which the electrons are in phase coherence, namely the coherence length, is assumed to be smaller than the device length. Thus we decompose the device into intervals $I_i = (x_i, x_{i+1})$ with $a = x_1 < x_2 < \dots < x_{N+1} = b$ and where $h_i = x_{i+1} - x_i$ is of the order of the coherence length. In each interval I_i , the transport of the electrons is described via a quantum model with open boundary conditions (QTBM [15]), which permit the electron flow through the interfaces $x = x_i$. In the following, $\psi_{i,E}^+$ (resp. $\psi_{i,E}^-$) will denote the elementary wave functions in I_i , describing the particles entering this interval at x_i with the energy $E > V_i$ (resp. at x_{i+1} with $E > V_{i+1}$) and where V_i stands for $V(x_i)$. We denote by $f_i^\pm(E)$ the corresponding statistics of the entering electrons, statistics which are related with each other by means of reflection and transmission coefficients and which describe the electron transport over longer distances than the coherence length. The electron mass m , the elementary charge q and the Planck constant \hbar were set to one in the present work. The correspondance between the momentum p_i and the total energy E at the position x_i reads

$$p_i(E) = \sqrt{2(E - V_i)} \quad ; \quad E(i, p) = \frac{p^2}{2} + V_i,$$

where we use the usual complex square root (with nonnegative imaginary part).

Let us now write down the model. The charge and current densities are given in each interval I_i as a superposition of the densities corresponding to the quantum states $\psi_{i,E}^\pm$

$$n_i(x) = \int_0^\infty f_i^+(E(i, p)) |\psi_{i,E}^+(x)|^2 dp + \int_0^\infty f_i^-(E(i+1, p)) |\psi_{i,E}^-(x)|^2 dp, \quad x \in I_i, \quad (2.1)$$

$$j_i(x) = \int_0^\infty f_i^+(E(i, p)) \mathcal{I}m(\bar{\psi}_{i,E}^+(x) \frac{d\psi_{i,E}^+(x)}{dx}) dp + \int_0^\infty f_i^-(E(i+1, p)) \mathcal{I}m(\bar{\psi}_{i,E}^-(x) \frac{d\psi_{i,E}^-(x)}{dx}) dp. \quad (2.2)$$

The elementary wave functions $\psi_{i,E}^\pm$ are solutions of the Schrödinger equation

$$\begin{cases} -\frac{1}{2} \frac{d^2 \psi_{i,E}^+}{dx^2} + V \psi_{i,E}^+ = \left(E + \mathbf{i} \frac{\nu}{2}\right) \psi_{i,E}^+, & (\text{if } E > V_i) \\ \frac{d\psi_{i,E}^+}{dx}(x_i) + \mathbf{i} p_i(E) \psi_{i,E}^+(x_i) = 2\mathbf{i} p_i(E) \\ \frac{d\psi_{i,E}^+}{dx}(x_{i+1}) = \mathbf{i} p_{i+1}(E) \psi_{i,E}^+(x_{i+1}), \end{cases} \quad (2.3)$$

respectively

$$\begin{cases} -\frac{1}{2} \frac{d^2 \psi_{i,E}^-}{dx^2} + V \psi_{i,E}^- = \left(E + \mathbf{i} \frac{\nu}{2}\right) \psi_{i,E}^-, & (\text{if } E > V_{i+1}) \\ \frac{d\psi_{i,E}^-}{dx}(x_i) = -\mathbf{i} p_i(E) \psi_{i,E}^-(x_i) \\ \frac{d\psi_{i,E}^-}{dx}(x_{i+1}) - \mathbf{i} p_{i+1}(E) \psi_{i,E}^-(x_{i+1}) = -2\mathbf{i} p_{i+1}(E). \end{cases} \quad (2.4)$$

In these equations, an artificial absorption term $\mathbf{i} \frac{\nu}{2} \psi_{i,E}^\pm$ ($\nu > 0$) is added in order to prove the existence of solutions for the nonlinear Schrödinger-Poisson system. This absorption term is not needed for the 1D linear Schrödinger equation (see [9]).

The statistics of particles entering the interval I_i are related to that ones of the intervals I_{i-1} and I_{i+1} through the following reflection-transmission formulae, which are schematically represented in Figure 1

$$\begin{aligned} f_i^+(E) &= R_{i-1}^-(E) f_{i-1}^-(E) + T_{i-1}^+(E) f_{i-1}^+(E), \\ f_i^-(E) &= R_{i+1}^+(E) f_{i+1}^+(E) + T_{i+1}^-(E) f_{i+1}^-(E). \end{aligned} \quad (2.5)$$

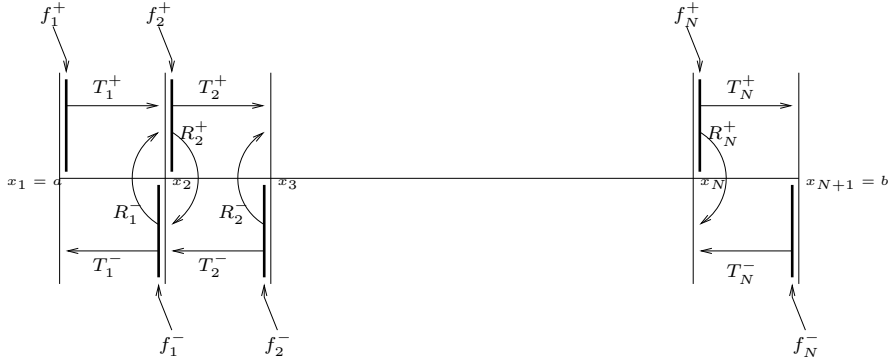


Figure 1: The statistics f_i^\pm and the reflection-transmission procedure in the 1D device.

Notice, that $f_1^+ = f_a^+$ and $f_N^- = f_b^-$ are the given incident statistics. Moreover recall that the reflection and transmission coefficients are obtained by

$$\begin{cases} R_i^+(E) := |\psi_{i,E}^+(x_i) - 1|^2, & (E > V_i) \\ R_i^+(E) := 0, & (E \leq V_i) \end{cases} ; \quad \begin{cases} T_i^+(E) := \frac{p_{i+1}(E)}{p_i(E)} |\psi_{i,E}^+(x_{i+1})|^2, & (E > V_{i,i+1}) \\ T_i^+(E) := 0, & (E \leq V_{i,i+1}) \end{cases} \quad (2.6)$$

and

$$\begin{cases} R_i^-(E) := |\psi_{i,E}^-(x_{i+1}) - 1|^2, & (E > V_{i+1}) \\ R_i^-(E) := 0, & (E \leq V_{i+1}) \end{cases} ; \begin{cases} T_i^-(E) := \frac{p_i(E)}{p_{i+1}(E)} |\psi_{i,E}^-(x_i)|^2, & (E > V_{i,i+1}) \\ T_i^-(E) := 0, & (E \leq V_{i,i+1}) \end{cases} \quad (2.7)$$

with $V_{i,i+1}$ denoting the maximum of V_i and V_{i+1} . All these equations are coupled, in the selfconsistent case, with the Poisson equation

$$\begin{cases} -\frac{d^2 V_s}{dx^2} = n, & \text{in } (a, b) \\ V_s(a) = V_s(b) = 0, \end{cases} \quad (2.8)$$

the electrostatic potential V being the sum of an exterior potential $V_e \in C^1(\mathbb{R})$ and the selfconsistent one V_s . Notice that the pure quantum problem, studied in [6], is recovered by taking $N = 1$ and $f_1 = f_{inc}$. Remark furthermore, that (2.5) implies $f_i^+(E) = 0$ for $E \leq V_i$ and $f_i^-(E) = 0$ for $E \leq V_{i+1}$, which is expected from a physical point of view. There is no difficulty to prove the following properties of the reflection and transmission coefficients [3, 9]

Lemma 2.1 *For $i \in \{1, \dots, N\}$ we have the relations*

$$T_i^\pm(E) + R_i^\pm(E) + \frac{\nu}{p_*(E)} \int_{x_i}^{x_{i+1}} |\psi_{i,E}^\pm(x)|^2 dx = 1, \quad \text{for } E > V_*, \quad (2.9)$$

where the star $*$ stands for i in the case of the sign $''+''$ and $* = i + 1$ for $''-''$. Besides

$$0 \leq T_i^\pm(E), R_i^\pm(E) \leq 1, \quad \forall E \in \mathbb{R}, \quad (2.10)$$

and we have the reciprocity identity

$$T_i^+(E) = T_i^-(E), \quad \forall E \in \mathbb{R}. \quad (2.11)$$

Note finally that the system (2.5) can be written in a simpler form as follows

$$A\mathcal{F} = \mathcal{S}, \quad (2.12)$$

with

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

and with the interface statistic vector \mathcal{F} and the source vector \mathcal{S} given by

$$\mathcal{F} = \left(f_1^- \ f_2^+ \ f_2^- \ f_3^+ \ \dots \ f_{N-1}^- \ f_N^+ \right)^t ; \quad \mathcal{S} = \left(0 \ T_1^+ f_1^+ \ 0 \ 0 \ \dots \ T_N^- f_N^- \ 0 \right)^t$$

Our main concern is now the existence of solutions for the selfconsistent problem (2.1)-(2.8). This is a rather classical result, which is based on the Schauder fixed point theorem. Therefore we shall not detail the proof and refer to [6].

Let us suppose in the rest of this paper that the entering data satisfy

Hypothesis A Let $G \in C_0(\mathbb{R})$. We assume that the incident statistics satisfy

$$0 \leq f_1^+(E) \leq G(E) \quad ; \quad 0 \leq f_N^-(E) \leq G(E), \quad \forall E \in \mathbb{R}.$$

The following analysis can be carried out in a similar way by supposing $G \in C(\mathbb{R})$ with $\lim_{|x| \rightarrow \infty} G(x) = 0$. However to avoid additional technical difficulties, we assumed G compactly supported. It was proven in [9], that for $V \in C([a, b])$, the linear system (2.12) has then a unique minimal, positive solution, satisfying $\forall i = 1, \dots, N$

$$0 \leq f_i^+(E) \leq G(E) \quad ; \quad 0 \leq f_i^-(E) \leq G(E), \quad \forall E \in \mathbb{R}. \quad (2.13)$$

Remark 2.2 A solution \mathcal{F} of (2.12) is minimal, if for any other solution \mathcal{H} with $|\mathcal{H}_l| \leq |\mathcal{F}_l| \forall l$, we have $\mathcal{H} = \mathcal{F}$.

Denoting by $\mathcal{E}_i^+ := \{E \in \mathbb{R} ; E > V_i\}$ resp. $\mathcal{E}_i^- := \{E \in \mathbb{R} ; E > V_{i+1}\}$ the sets of possible injection energies, we have

Proposition 2.3 [6] **(Existence result)**

Let $N \in \mathbb{N}$ and $\nu > 0$ be fixed numbers. Then the Schrödinger-Poisson problem (2.1)-(2.8) has a solution $(V_s, (\psi_{i,E}^\pm)_{i=1, \dots, N; E \in \mathcal{E}_i^\pm}, (f_i^\pm)_{i=1, \dots, N})$ with

$$V_s \in W^{2,\infty}(a, b); \quad \psi_{i,E}^\pm \in W^{4,\infty}(I_i); \quad f_i^\pm \in L^\infty(\mathbb{R}).$$

For the limit of infinitely small coherence lengths, we need in the selfconsistent case the following important *a priori* estimate for the potential.

Lemma 2.4 (A priori estimate)

There exists a constant $C_{pot} > 0$ independent of N and $\nu > 0$, such that

$$\|V_s^{N,\nu}\|_{W^{2,\infty}(a,b)} \leq C_{pot}. \quad (2.14)$$

Proof: The idea of the proof is to show that the density n_i , given by (2.1), is bounded in $L^\infty(I_i)$ independently on N , ν and on i . Since $V_s^{N,\nu}$ is solution of the Poisson equation (2.8), regularity results imply then immediately the boundedness of the potential. To simplify the notations, we will omit within this proof the indices N and ν . Multiplying the Schrödinger equation (2.3) by $\overline{\psi_{i,E}^+}$ (resp. (2.4) by $\overline{\psi_{i,E}^-}$), integrating over (x_i, x_{i+1}) and taking the real and imaginary parts, leads to the equation

$$\begin{aligned} \frac{1}{2} \int_{x_i}^{x_{i+1}} |\psi_{i,E}^+(x)|^2 dx + \int_{x_i}^{x_{i+1}} (V(x) - E) |\psi_{i,E}^+(x)|^2 dx = \\ -\frac{1}{2} \mathcal{I}m(p_{i+1}(E)) |\psi_{i,E}^+(x_{i+1})|^2 - p_i(E) \mathcal{I}m(\psi_{i,E}^+(x_i)). \end{aligned} \quad (2.15)$$

$$\begin{aligned} 0 = \frac{\nu}{2} \int_{x_i}^{x_{i+1}} |\psi_{i,E}^+(x)|^2 dx + \frac{1}{2} \mathcal{R}e(p_{i+1}(E)) |\psi_{i,E}^+(x_{i+1})|^2 - \\ - p_i(E) \mathcal{R}e(\psi_{i,E}^+(x_i)) + \frac{1}{2} p_i(E) |\psi_{i,E}^+(x_i)|^2. \end{aligned} \quad (2.16)$$

The same procedure for the electrons incident from the right in I_i with $E > V_{i+1}$, yields similar expressions. Equation (2.16) and the corresponding one, associated to $\psi_{i,E}^-$, permit to establish the estimates $|\psi_{i,E}^+(x_i)| \leq 2$ for $E > V_i$ (resp. $|\psi_{i,E}^-(x_{i+1})| \leq 2$ for $E > V_{i+1}$). Furthermore, equation (2.15) and that one associated to $\psi_{i,E}^-$, lead to

$$\begin{aligned} & \frac{1}{2} \int_0^\infty \int_{x_i}^{x_{i+1}} f_i^+(E) |\psi_{i,E}^{+\prime}(x)|^2 dx dp + \frac{1}{2} \int_0^\infty \int_{x_i}^{x_{i+1}} f_i^-(E) |\psi_{i,E}^{-\prime}(x)|^2 dx dp + \int_{x_i}^{x_{i+1}} V(x) n_i(x) dx \\ & \leq \int_0^\infty \int_{x_i}^{x_{i+1}} f_i^+(E) E(i, p) |\psi_{i,E}^+(x)|^2 dx dp + 2 \int_0^\infty p f_i^+(E) dp + \\ & \quad + \int_0^\infty \int_{x_i}^{x_{i+1}} f_i^-(E) E(i+1, p) |\psi_{i,E}^-(x)|^2 dx dp + 2 \int_0^\infty p f_i^-(E) dp. \end{aligned}$$

Recalling Hypothesis A and due to the fact that $V_s \geq 0$ (maximum principle), we obtain

$$\begin{aligned} & \frac{1}{2} \int_0^\infty \int_{x_i}^{x_{i+1}} f_i^+(E) |\psi_{i,E}^{+\prime}(x)|^2 dx dp + \frac{1}{2} \int_0^\infty \int_{x_i}^{x_{i+1}} f_i^-(E) |\psi_{i,E}^{-\prime}(x)|^2 dx dp \\ & \leq c_1 + c_1 \int_0^\infty f_i^+(E) \int_{x_i}^{x_{i+1}} |\psi_{i,E}^+(x)|^2 dx dp + c_1 \int_0^\infty f_i^-(E) \int_{x_i}^{x_{i+1}} |\psi_{i,E}^-(x)|^2 dx dp, \end{aligned} \quad (2.17)$$

with a constant $c_1 > 0$ independent of N, ν, i . Using the relation

$$\psi_{i,E}^+(x) = \psi_{i,E}^+(x_i) + \int_{x_i}^x \psi_{i,E}^{+\prime}(t) dt, \quad (2.18)$$

we get, for h_i small enough, the estimate

$$\int_{x_i}^{x_{i+1}} |\psi_{i,E}^+(x)|^2 dx \leq 8h_i + 2h_i^2 \int_{x_i}^{x_{i+1}} |\psi_{i,E}^{+\prime}(x)|^2 dx \leq c + \frac{1}{4c_1} \int_{x_i}^{x_{i+1}} |\psi_{i,E}^{+\prime}(x)|^2 dx.$$

and similarly for $\psi_{i,E}^-$, such that relation (2.17) turns finally to

$$\int_0^\infty \int_{x_i}^{x_{i+1}} f_i^+(E) |\psi_{i,E}^{+\prime}(x)|^2 dx dp + \int_0^\infty \int_{x_i}^{x_{i+1}} f_i^-(E) |\psi_{i,E}^{-\prime}(x)|^2 dx dp \leq c, \quad (2.19)$$

where $c > 0$ does not depend on N, ν and on i . We use now (2.18) and (2.19) as well as Hypothesis A to prove that n_i is bounded in I_i independently on N, ν and on i . \blacksquare

The estimate (2.14) enables moreover to pass to the limit $\nu \rightarrow 0$ in the Schrödinger-Poisson problem and to obtain thus the analogue of Proposition 2.3 for $\nu = 0$.

Corollary 2.5 *Let $N \in \mathbb{N}$ be a fixed number and let the solutions of the Schrödinger-Poisson problem (2.1)-(2.8) for $\nu > 0$ be $(V_s^\nu, (\psi_{i,E}^{\pm,\nu})_{i=1,\dots,N; E \in \mathcal{E}_i^{\pm,\nu}}, (f_i^{\pm,\nu})_{i=1,\dots,N})$. The corresponding charge and current densities are denoted by n^ν and j^ν .*

Then there exists a set of functions $(V_s, (\psi_{i,E}^\pm)_{i=1,\dots,N; E \in \mathcal{E}_i^\pm}, (f_i^\pm)_{i=1,\dots,N})$ with

$$V_s \in W^{2,\infty}(a, b); \quad \psi_{i,E}^\pm \in W^{4,\infty}(I_i); \quad f_i^\pm \in L^\infty(\mathbb{R}),$$

and $n, j \in L^\infty(a, b)$ such that we have for $\nu \rightarrow 0$

$$\begin{aligned} & V_s^\nu \rightarrow V_s \quad \text{in } C^1([a, b]) \quad ; \quad n^\nu \rightarrow n \quad \text{and} \quad j^\nu \rightarrow j \quad \text{in } L^\infty(a, b), \\ & \psi_{i,E}^{\pm,\nu} \rightarrow \psi_{i,E}^\pm \quad \text{in } C^1(I_i) \quad ; \quad f_i^{\pm,\nu} \rightarrow f_i^\pm \quad \text{weak } * \text{ in } L^\infty(\mathbb{R}). \end{aligned}$$

Moreover the limit $(V_s, (\psi_{i,E}^\pm)_{i=1,\dots,N; E \in \mathcal{E}_i^\pm}, (f_i^\pm)_{i=1,\dots,N})$ is shown to be a solution of the system (2.1)-(2.8) for $\nu = 0$ and n, j are the corresponding charge and current densities.

The next proposition shows the important property, that the current is conserved across the interfaces of the intervals I_i .

Proposition 2.6 [9] (Current conservation)

The current is continuous at the interfaces x_i between I_{i-1} and I_i , and we have

$$\frac{d}{dx} j_i(x) = -\nu n_i(x) \quad \text{for } x \in I_i. \quad (2.20)$$

2.2 The limit of an infinitely small coherence length

In this section, the limit of an infinitely small coherence length is considered. The problem treated in this paper is the extension to the selfconsistent case investigated in [9]. Defining $h = \max_{i=1,\dots,N} h_i$ with $h_i = x_{i+1} - x_i$, we let N tend to $+\infty$ in such a way, that h tends to 0. Throughout this limit procedure, we will keep the absorption coefficient $\nu \geq 0$ constant. To facilitate the following calculus, we express the functions in terms of the momentum p and not of the energy, as done in the previous sections. Let therefore

$$f_i^N(p) := \begin{cases} f_i^{+,N}(E(i,p)) & (p > 0) \\ f_i^{-,N}(E(i+1,p)) & (p < 0) \end{cases} \quad ; \quad \psi_{i,p}^N(x) := \begin{cases} \psi_{i,E(i,p)}^{+,N}(x) & (p > 0) \\ \psi_{i,E(i+1,p)}^{-,N}(x) & (p < 0) \end{cases}$$

and idem for the reflection and transmission coefficients. Let us furthermore interpolate the discrete quantities f_i^N and T_i^N to piecewise continuous ones and define ψ_p^N by

$$f^N(x,p) := f_i^N(p); \quad T^N(x,p) := T_i^N(p); \quad \psi_p^N(x) := \psi_{i,p}^N(x), \quad \forall (x,p) \in I_i \times \mathbb{R}, \quad \forall i.$$

Then

$$n^N(x) = \int_{-\infty}^{\infty} f^N(x,p) |\psi_p^N(x)|^2 dp \quad ; \quad j^N(x) = \int_{-\infty}^{\infty} f^N(x,p) \mathcal{I}m(\overline{\psi_p^N(x)} \frac{d}{dx} \psi_p^N(x)) dp.$$

The main result of the selfconsistent 1D case is the following

Theorem 2.7 (Small coherence length limit)

Let $\nu \geq 0$ be fixed. Under Hypothesis A, there exists a distribution function $f \in L^\infty((a,b) \times \mathbb{R})$ and a potential $V \in C^1([a,b])$ such that, up to a subsequence, we get for $N \rightarrow \infty$

$$\begin{aligned} f^N &\rightharpoonup f \quad \text{weak * in } L^\infty((a,b) \times \mathbb{R}) \quad ; \quad n^N \rightharpoonup n \quad \text{weak * in } L^\infty(a,b), \\ V^N &\rightarrow V \quad \text{strong in } C^1([a,b]) \quad ; \quad j^N \rightharpoonup j \quad \text{weak * in } L^\infty(a,b), \end{aligned}$$

with

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

Besides, the limit (f, V) is solution of the Vlasov-Poisson system

$$\begin{cases} p \frac{\partial f}{\partial x} - \frac{dV}{dx} \frac{\partial f}{\partial p} + \nu f = 0 & \text{in } (a,b) \times \mathbb{R} \\ f(a,p) = f_a(p), \quad \text{for } p > 0; \quad f(b,p) = f_b(p), \quad \text{for } p < 0, \end{cases} \quad (2.21)$$

$$\begin{cases} -\frac{d^2 V_s}{dx^2}(x) = n(x), & \text{in } (a, b) \\ V_s(a) = V_s(b) = 0, \end{cases} \quad (2.22)$$

where the total electrostatic potential is given by $V = V_e + V_s$.

For the proof of this theorem, we establish first the asymptotic behaviour of T_i^N , R_i^N and $\psi_{i,p}^N$, for a large number of cells N and far from a turning point $p = 0$. Due to the estimate (2.14), the proof of the next lemma is an easy extension of the linear case, treated in [9].

Lemma 2.8 [9] (Asymptotic behaviour)

Let $0 < \epsilon < K$ and $0 \leq \nu \leq 1$ be fixed real numbers. Then, there exists a constant $C = C(K, \epsilon, C_{pot}) > 0$ such that $\forall i = 1, \dots, N$

$$|T_i^N(p) - 1 + \frac{\nu h_i}{|p|}| \leq Ch_i^2 \quad , \quad R_i^N(p) \leq Ch_i^2; \quad \text{for } h \in (0, 1), \quad \epsilon \leq |p| \leq K,$$

$$\sup_{x \in I_i} |\psi_{i,p}^N(x) - 1| \leq Ch_i; \quad \text{for } h \in (0, 1), \quad \epsilon \leq |p| \leq K,$$

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

This lemma enables now to prove the main theorem :

Proof of Theorem 2.7

The proof was detailed in the case of a fixed potential $V \in C^1([a, b])$ in the previous paper [9]. The selfconsistent case can be easily adapted. We only recall here the main steps. Let

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

Using the previous lemma, we can show, that the L^∞ - limit of $n^N - \tilde{n}^N$ and $j^N - \tilde{j}^N$ are 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 (resp. j) of \tilde{n}^N (resp. \tilde{j}^N) are nothing but

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

Using Proposition 2.6, we deduce for these limit functions the analogue of relation (2.20)

$$\frac{dj}{dx}(x) + \nu n(x) = 0 \quad \text{in } [a, b]. \quad (2.23)$$

Furthermore, Lemma 2.4 implies the existence of a subsequence V_s^N converging in $C^1([a, b])$ towards a limit potential V , yielding thus (2.22). It remains to prove that f is a solution of the Vlasov equation (2.21). Since we do not know the behaviour of $T_i(p)$ for small p , we shall proceed in two steps. Using test functions compactly supported in $[a, b] \times \mathbb{R}_*^+$ or in $(a, b] \times \mathbb{R}_*^-$, the limit function f is shown to solve

$$\begin{cases} p \frac{\partial f}{\partial x} - \frac{dV}{dx} \frac{\partial f}{\partial p} + \nu f = S(x) \delta(p = 0) \\ f(a, p) = f_a(p), \quad \text{for } p > 0; \quad f(b, p) = f_b(p), \quad \text{for } p < 0, \end{cases} \quad (2.24)$$

for some L^∞ function S . Integrating the differential equation (2.24) with respect to p , we notice that $S(x) = \frac{dj}{dx} + \nu n$, yielding in view of (2.23) the identity $S \equiv 0$. \blacksquare

3 The two dimensional case

3.1 The subband model

We expose here briefly a model describing the collisionless transport process of particles in a partially confined 2D device, which behaves quantum mechanically in one direction and classically in the other one. This subband model will be the limiting transport model for small coherence lengths in the 2D case. The mathematical analysis is studied in [8].

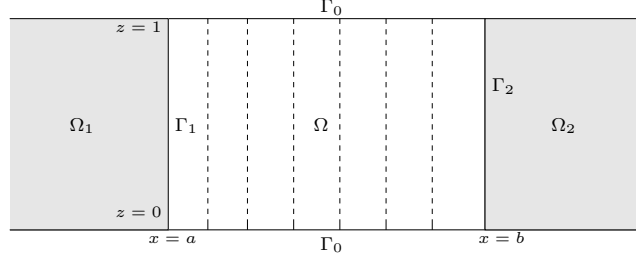


Figure 2: The two dimensional device.

The two dimensional device, illustrated in Figure 2, is represented by the bounded domain $\Omega := [a, b] \times [0, 1]$. We assume, that its width is of the order of the electron de Broglie wavelength, so that quantum models (Schrödinger equation) have to be used to account for the quantum effects occurring in this direction. This confined or transversal direction will be denoted in the sequel by $z \in [0, 1]$. The length of the device is assumed to be several times bigger than the width, such that the transport is well described by means of kinetic models (Vlasov equation). The transport or longitudinal direction is denoted by $x \in [a, b]$. A given stationary potential $V \in C^1(\mathbb{R}^2)$ governs the electron transport in the device. Outside the device, in the two electron leads $\Omega_1 := (-\infty, a] \times [0, 1]$ and $\Omega_2 := [b, \infty) \times [0, 1]$, the potential depends only on the variable z . Electrons are injected in the device by the two lateral leads with the known distributions $f_{a,m} \in L^\infty(\mathbb{R}^+)$ and $f_{b,m} \in L^\infty(\mathbb{R}^-)$. The index or transversal mode $m \in \mathbb{N}$ indicates the different subbands. Let us present the model. The electron and current densities are given at $(x, z) \in \Omega$ by

$$\begin{pmatrix} n \\ j \end{pmatrix} (x, z) := \sum_{m=1}^{\infty} \left\{ \int_{-\infty}^{\infty} \begin{pmatrix} 1 \\ p \end{pmatrix} f_m(x, p) dp \right\} |\chi_m(x, z)|^2 \quad (3.1)$$

The functions f_m represent the distribution functions of the electrons belonging to the m^{th} subband and are solutions of the Vlasov equation in the transport direction x

$$\begin{cases} p \frac{\partial f_m}{\partial x} - \frac{dE_m}{dx} \frac{\partial f_m}{\partial p} = 0 & \text{in } (a, b) \times \mathbb{R} \\ f_m(a, p) = f_{a,m}(p), \quad \text{for } p > 0; \quad f_m(b, p) = f_{b,m}(p), \quad \text{for } p < 0, \end{cases} \quad (3.2)$$

with E_m the potential energy of these electrons. Moreover χ_m represent the corresponding transversal wave functions, solutions of the Schrödinger equation in the confined direction

$$\begin{cases} -\frac{1}{2} \frac{\partial^2 \chi_m}{\partial z^2}(x, \cdot) + V(x, \cdot) \chi_m(x, \cdot) = E_m(x) \chi_m(x, \cdot) & \text{in } (0, 1) \\ \chi_m(x, \cdot) \in H_0^1(0, 1); \quad \int_0^1 \chi_m(x, z) \chi_{m'}(x, z) dz = \delta_{mm'}. \end{cases} \quad (3.3)$$

Notice that the problem is classical in the x direction and quantum in the z direction.

3.2 A model for a moderately small coherence length

We introduce now the 2D model taking into consideration small coherence lengths. Contrary to the 1D case, we shall not consider here the coupling with the Poisson equation, the electrostatic potential being thus given. As in the one-dimensional case, we will assume, that the coherence length is smaller than the device length and we split the device $[a, b] \times [0, 1]$ into domains $I_i = [x_i, x_{i+1}] \times [0, 1]$ with $a = x_1 < x_2 < \dots < x_{N+1} = b$, where $h_i = x_{i+1} - x_i$ is of the order of the coherence length (see Figure 2). Let $\Upsilon_i := [x_i, x_{i+1}]$. We denote by $\psi_{i,E,m}^+$ (resp. $\psi_{i,E,m}^-$) the wave functions in the strip I_i representing the electrons entering at x_i in the m^{th} transversal mode and with the total energy E (resp. the electrons entering at x_{i+1} in the m^{th} mode, with the total energy E). The corresponding statistics are $f_{i,m}^\pm(E)$ with $f_{1,m}^+ = f_{a,m}^+$ and $f_{N,m}^- = f_{b,m}^-$ the given incident ones. The functions provided with the sign "+" (resp. "-") correspond to the wave function coming from the left (resp. right). To simplify the notations let $\mathcal{I} := (i, E, m)$. Then, the charge and current densities in I_i write

$$n_i(x, z) = \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^+(E(i, m, k)) |\psi_{\mathcal{I}}^+(x, z)|^2 dk + \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^-(E(i+1, m, k)) |\psi_{\mathcal{I}}^-(x, z)|^2 dk, \quad (3.4)$$

$$\begin{aligned} j_i(x, z) &= \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^+(E(i, m, k)) \mathcal{I}m \left(\bar{\psi}_{\mathcal{I}}^+(x, z) \nabla \psi_{\mathcal{I}}^+(x, z) \right) dk + \\ &+ \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^-(E(i+1, m, k)) \mathcal{I}m \left(\bar{\psi}_{\mathcal{I}}^-(x, z) \nabla \psi_{\mathcal{I}}^-(x, z) \right) dk, \end{aligned} \quad (3.5)$$

where the energy-wavevector relations are given by the expressions

$$k_l^i(E) := \sqrt{2|E - E_l^i|}; \quad E(i, l, k) := \frac{k^2}{2} + E_l^i,$$

and E_l^i are the eigenvalues of the transversal Schrödinger operator (3.3) at the interfaces $x = x_i$, the corresponding eigenfunctions being χ_l^i . The wave functions $\psi_{\mathcal{I}}^\pm$ describe the electron evolution within each strip and are solutions of the Schrödinger equation with open boundary conditions [4, 15, 18]

$$\left\{ \begin{array}{ll} -\frac{1}{2}\Delta\psi_{\mathcal{I}}^+ + V\psi_{\mathcal{I}}^+ = \left(E + \mathbf{i}\frac{\nu}{2}\right)\psi_{\mathcal{I}}^+, & \text{for } (x, z) \in I_i \\ \psi_{\mathcal{I}}^+(x, 0) = \psi_{\mathcal{I}}^+(x, 1) = 0, & \text{for } x \in \Upsilon_i \\ \frac{\partial\psi_{\mathcal{I}}^+}{\partial x}(x_i, z) = 2\mathbf{i}k_m^i(E)\chi_m^i(z) - \Lambda_i^E(z; \Psi_{\mathcal{I}}^+) & \\ \frac{\partial\psi_{\mathcal{I}}^+}{\partial x}(x_{i+1}, z) = \Lambda_{i+1}^E(z; \Psi_{\mathcal{I}}^+), & \end{array} \right. \quad (3.6)$$

respectively

$$\left\{ \begin{array}{l} -\frac{1}{2}\Delta\psi_{\mathcal{I}}^- + V\psi_{\mathcal{I}}^- = \left(E + \mathbf{i}\frac{\nu}{2}\right)\psi_{\mathcal{I}}^-, \quad \text{for } (x, z) \in I_i \\ \psi_{\mathcal{I}}^-(x, 0) = \psi_{\mathcal{I}}^-(x, 1) = 0, \quad \text{for } x \in \Upsilon_i \\ \frac{\partial\psi_{\mathcal{I}}^-}{\partial x}(x_i, z) = -\Lambda_i^E(z; \Psi_{\mathcal{I}}^-) \\ \frac{\partial\psi_{\mathcal{I}}^-}{\partial x}(x_{i+1}, z) = -2\mathbf{i}k_m^{i+1}(E)\chi_m^{i+1}(z) + \Lambda_{i+1}^E(z; \Psi_{\mathcal{I}}^-), \end{array} \right. \quad (3.7)$$

where we used the following operator

$$\Lambda_j^E(z; \Theta) := \sum_{l=1}^{M^j(E)} \mathbf{i}k_l^j(E) \Theta_l^j \chi_l^j(z) - \sum_{l=M^j(E)+1}^{\infty} k_l^j(E) \Theta_l^j \chi_l^j(z),$$

with

$$M^j(E) := \sup\{l \in \mathbb{N}/E > E_l^j\} \quad ; \quad (\Psi_{\mathcal{I}}^{\pm})_l^j := \int_0^1 \psi_{\mathcal{I}}^{\pm}(x_j, z) \chi_l^j(z) dz.$$

We add an absorption term ($\nu > 0$) in the Schrödinger equation in order to overcome the nonuniqueness problem for the linear 2D equation. The value $M^j(E)$ is the number of propagating modes and $(\Psi_{\mathcal{I}}^{\pm})_l^j$ is the amplitude of that part of the incident wave $\psi_{\mathcal{I}}^{\pm}$, which belongs to the l^{th} mode at the position x_j . Denoting by β^{\pm} the amplitudes of the reflected, transmitted or vanishing part of the corresponding wave, we have

$$(\Psi^+)_l^j = (\beta^+)_l^j + \delta_{j=i, l=m} \quad ; \quad (\Psi^-)_l^j = (\beta^-)_l^j + \delta_{j=i+1, l=m}, \quad (3.8)$$

with $\delta_{j=i, l=m}$ the usual Kronecker symbol. The different strips I_i are related by means of the statistics $f_{i,m}^{\pm}(E)$ through the following reflection-transmission formulae

$$\left\{ \begin{array}{l} f_{i,m}^+(E) = \sum_{l \leq M^{i-1}(E)} T_{i-1, l \rightarrow m}^+(E) f_{i-1, l}^+(E) + \sum_{l \leq M^i(E)} R_{i-1, l \rightarrow m}^-(E) f_{i-1, l}^-(E) \\ f_{i,m}^-(E) = \sum_{l \leq M^{i+2}(E)} T_{i+1, l \rightarrow m}^-(E) f_{i+1, l}^-(E) + \sum_{l \leq M^{i+1}(E)} R_{i+1, l \rightarrow m}^+(E) f_{i+1, l}^+(E). \end{array} \right. \quad (3.9)$$

The transmission and reflection procedure is schematically represented in Figure 3.

In each strip we compute the reflection and transmission coefficients by

$$\left\{ \begin{array}{l} T_{i, m \rightarrow l}^+(E) := \frac{k_l^{i+1}(E)}{k_m^i(E)} |(\beta^+)_{l}^{i+1}|^2, \quad 1 \leq m \leq M^i(E), 1 \leq l \leq M^{i+1}(E) \\ T_{i, m \rightarrow l}^+(E) := 0, \quad m > M^i(E) \quad \text{or} \quad l > M^{i+1}(E), \end{array} \right. \quad (3.10)$$

$$\left\{ \begin{array}{l} R_{i, m \rightarrow l}^+(E) := \frac{k_l^i(E)}{k_m^i(E)} |(\beta^+)_{l}^i|^2, \quad 1 \leq m, l \leq M^i(E) \\ R_{i, m \rightarrow l}^+(E) := 0, \quad m > M^i(E) \quad \text{or} \quad l > M^i(E), \end{array} \right. \quad (3.11)$$

Notice that $f_{i,m}^+(E) = 0$ for $m > M^i(E)$ and $f_{i,m}^-(E) = 0$ for $m > M^{i+1}(E)$, which follows directly from (3.9). As in the 1D case, the system (3.9) can be written as a linear system

$$A\mathcal{F} = \mathcal{S}, \quad (3.19)$$

where A , \mathcal{F} and \mathcal{S} are given analogously to (2.12), with the difference that the entries are replaced by the following bloc matrices

$$\begin{aligned} \mathcal{R}_i^+ &:= \begin{pmatrix} R_{i,1 \rightarrow 1}^+ & \cdots & R_{i,M^i \rightarrow 1}^+ \\ \vdots & \ddots & \vdots \\ R_{i,1 \rightarrow M^i}^+ & \cdots & R_{i,M^i \rightarrow M^i}^+ \end{pmatrix}, & \mathcal{R}_i^- &:= \begin{pmatrix} R_{i,1 \rightarrow 1}^- & \cdots & R_{i,M^{i+1} \rightarrow 1}^- \\ \vdots & \ddots & \vdots \\ R_{i,1 \rightarrow M^{i+1}}^- & \cdots & R_{i,M^{i+1} \rightarrow M^{i+1}}^- \end{pmatrix} \\ \mathcal{T}_i^+ &:= \begin{pmatrix} T_{i,1 \rightarrow 1}^+ & \cdots & T_{i,M^i \rightarrow 1}^+ \\ \vdots & \ddots & \vdots \\ T_{i,1 \rightarrow M^{i+1}}^+ & \cdots & T_{i,M^i \rightarrow M^{i+1}}^+ \end{pmatrix}, & \mathcal{T}_i^- &:= \begin{pmatrix} T_{i,1 \rightarrow 1}^- & \cdots & T_{i,M^{i+1} \rightarrow 1}^- \\ \vdots & \ddots & \vdots \\ T_{i,1 \rightarrow M^i}^- & \cdots & T_{i,M^{i+1} \rightarrow M^i}^- \end{pmatrix} \\ \vec{f}_i^+ &:= \left(f_{i,1}^+ \quad \cdots \quad f_{i,M^i}^+ \right)^t, & \vec{f}_i^- &:= \left(f_{i,1}^- \quad \cdots \quad f_{i,M^{i+1}}^- \right)^t. \end{aligned}$$

3.3 Mathematical analysis of the model

For the sake of completeness, we recall here the main results concerning the existence of solutions of the problem (3.4)-(3.13). Let us first introduce the notion of solution of (3.6) (resp. (3.7)) for a fixed potential $V \in L^\infty(\Omega)$. For this we define the Hilbert space

$$H := \left\{ \psi \in H^1(I_i) / \psi(\cdot, 0) \equiv \psi(\cdot, 1) \equiv 0, \sum_{l=1}^{\infty} k_l^i(E) |\Psi_l^i|^2 + \sum_{l=1}^{\infty} k_l^{i+1}(E) |\Psi_l^{i+1}|^2 < \infty \right\},$$

with the scalar product

$$\langle \psi, \varphi \rangle_H := \int_{I_i} \nabla \psi \nabla \bar{\varphi} \, dx dz + \sum_{l=1}^{\infty} k_l^i(E) \Psi_l^i \bar{\Phi}_l^i + \sum_{l=1}^{\infty} k_l^{i+1}(E) \Psi_l^{i+1} \bar{\Phi}_l^{i+1}.$$

Remark 3.2 *It is proven in [4] that H is a separable Hilbert space, which does not depend on the energy E .*

The variational formulation of problem (3.6) respectively (3.7) is the following: Find $\psi_{\mathcal{I}}^\pm \in H$, such that $\forall \varphi \in H$

$$\begin{aligned} & \frac{1}{2} \int_{I_i} \nabla \psi_{\mathcal{I}}^+ \nabla \bar{\varphi} \, dx dz + \int_{I_i} \left(V - E - \mathbf{i} \frac{\nu}{2} \right) \psi_{\mathcal{I}}^+ \bar{\varphi} \, dx dz = \\ & \frac{1}{2} \left\{ -2\mathbf{i} k_m^i(E) \bar{\Phi}_m^i + \sum_{l=1}^{M^i(E)} \mathbf{i} k_l^i(E) (\Psi^+)_l \bar{\Phi}_l^i - \sum_{l=M^i(E)+1}^{\infty} k_l^i(E) (\Psi^+)_l \bar{\Phi}_l^i \right. \\ & \left. + \sum_{l=1}^{M^{i+1}(E)} \mathbf{i} k_l^{i+1}(E) (\Psi^+)_l \bar{\Phi}_l^{i+1} - \sum_{l=M^{i+1}(E)+1}^{\infty} k_l^{i+1}(E) (\Psi^+)_l \bar{\Phi}_l^{i+1} \right\}, \end{aligned} \quad (3.20)$$

respectively

$$\begin{aligned}
& \frac{1}{2} \int_{I_i} \nabla \psi_{\mathcal{I}}^- \nabla \bar{\varphi} dx dz + \int_{I_i} \left(V - E - \mathbf{i} \frac{\nu}{2} \right) \psi_{\mathcal{I}}^- \bar{\varphi} dx dz = \\
& \frac{1}{2} \left\{ \sum_{l=1}^{M^i(E)} \mathbf{i} k_l^i(E) (\Psi^-)_l^i \bar{\Phi}_l^i - \sum_{l=M^i(E)+1}^{\infty} k_l^i(E) (\Psi^-)_l^i \bar{\Phi}_l^i - 2 \mathbf{i} k_m^{i+1}(E) \bar{\Phi}_m^{i+1} \right. \\
& \left. + \sum_{l=1}^{M^{i+1}(E)} \mathbf{i} k_l^{i+1}(E) (\Psi^-)_l^{i+1} \bar{\Phi}_l^{i+1} - \sum_{l=M^{i+1}(E)+1}^{\infty} k_l^{i+1}(E) (\Psi^-)_l^{i+1} \bar{\Phi}_l^{i+1} \right\}. \tag{3.21}
\end{aligned}$$

Let us suppose in the 2D case, that the entering data satisfy:

Hypothesis B Let $G \in C_0(\mathbb{R})$. We assume that

$$0 \leq f_{1,m}^+(E) \leq G(E) \quad ; \quad 0 \leq f_{N,m}^-(E) \leq G(E), \quad \forall m, \forall E.$$

The existence of solutions is given by

Proposition 3.3 [4] (**Existence result**)

Let $V \in L^\infty(\Omega)$. Then the problem (3.20) (resp. (3.21)) admits a unique solution $\psi_{\mathcal{I}}^+ \in H$ (resp. $\psi_{\mathcal{I}}^- \in H$), for $\nu > 0$ and $\forall \mathcal{I}$ with $E > E_m^i$ (resp. $E > E_m^{i+1}$). Moreover, assuming Hypothesis B, the linear system (3.19) has a unique solution, satisfying $\forall i = 1, \dots, N$,

$$0 \leq f_{i,m}^\pm(E) \leq G(E), \quad \forall m, \forall E. \tag{3.22}$$

The proof of the second part of this proposition proceeds analogously to the 1D case and is left to the reader [9].

Remark 3.4 Note that in contrast to the 1D case, the condition $\nu > 0$ is here necessary. For $\nu = 0$, we have uniqueness of the solutions $\psi_{\mathcal{I}}^\pm$ only for almost every $E > E_m^i$ (resp. $E > E_m^{i+1}$). In particular, there exists a nondecreasing sequence of energies $\{E_j(V)\}_{j \in \mathbb{N}}$ tending to ∞ , such that problem (3.20) admits a unique solution $\psi_{\mathcal{I}}^+ \in H$, $\forall \mathcal{I}$ with $E > E_m^i$ and $E \neq E_j(V) \forall j$ (see [4] for more details).

Remark 3.5 Let E_0 be the energy threshold value, such that $G(E) = 0, \forall |E| \geq E_0$. Considering positive potentials $V \geq 0$ and using the properties of the nondecreasing sequence of eigenvalues $\{E_m\}_{m \in \mathbb{N}}$ [8, 14, 17, 19], we can prove the existence of $m_0 \in \mathbb{N}$ and $k_0 \in \mathbb{R}^+$ independent on V , such that $E(i, m, k) \geq E_0$ for $m \geq m_0$ or $k \geq k_0$ and $\forall i$. Thus we have $f_{i,m}^+(E(i, m, k)) = 0$ resp. $f_{i,m}^-(E(i+1, m, k)) = 0$ for $m \geq m_0$ or $k \geq k_0$ and $\forall i$.

The continuity of the current flux across the interfaces is given by the next proposition. Compare with Proposition 2.6 of the 1D case. With j_i given by (3.5), the current fluxes crossing the interface $x = x_i$ are denoted by

$$J_{i \rightarrow i+1} := \int_0^1 j_i(x_{i+1}, z) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} dz \quad ; \quad J_{i+1 \rightarrow i} := \int_0^1 j_{i+1}(x_{i+1}, z) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} dz, \tag{3.23}$$

Proposition 3.6 (Current conservation)

The following identities hold

$$\begin{aligned} J_{i \rightarrow i+1} &= J_{i+1 \rightarrow i}, \quad i = 2, \dots, N; \\ \nabla \cdot j_i(x, z) &= -\nu n_i(x, z) \quad \text{for } (x, z) \in I_i. \end{aligned} \quad (3.24)$$

Proof: With (3.5) we rewrite the current fluxes as follows

$$J_{i \rightarrow i+1} := \mathcal{A}^+ + \mathcal{A}^- \quad ; \quad J_{i+1 \rightarrow i} := \mathcal{B}^+ + \mathcal{B}^-,$$

with

$$\begin{aligned} \mathcal{A}^\pm &:= \int_0^1 \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^\pm(E) \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^\pm}(x_{i+1}, z) \frac{\partial}{\partial x} \psi_{\mathcal{I}}^\pm(x_{i+1}, z) \right) dk dz, \\ \mathcal{B}^\pm &:= \int_0^1 \sum_{m=1}^{\infty} \int_0^{\infty} f_{i+1,m}^\pm(E) \mathcal{I}m \left(\overline{\psi_{\mathcal{I}'}^\pm}(x_{i+1}, z) \frac{\partial}{\partial x} \psi_{\mathcal{I}'}^\pm(x_{i+1}, z) \right) dk dz, \end{aligned}$$

and the indices $\mathcal{I} = (i, E, m)$ and $\mathcal{I}' = (i+1, E, m)$. We have to show, that $\mathcal{A}^+ + \mathcal{A}^- = \mathcal{B}^+ + \mathcal{B}^-$. To this end, let us consider

$$\begin{aligned} \nabla \cdot \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^\pm}(x, z) \nabla \psi_{\mathcal{I}}^\pm(x, z) \right) &= \mathcal{I}m \left(|\nabla \psi_{\mathcal{I}}^\pm(x, z)|^2 \right) + \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^\pm}(x, z) \Delta \psi_{\mathcal{I}}^\pm(x, z) \right) \\ &= \mathcal{I}m \left\{ \overline{\psi_{\mathcal{I}}^\pm}(x, z) \left[2 \left(V - E - \mathbf{i} \frac{\nu}{2} \right) \psi_{\mathcal{I}}^\pm(x, z) \right] \right\} \\ &= -\nu |\psi_{\mathcal{I}}^\pm(x, z)|^2. \end{aligned} \quad (3.25)$$

This implies

$$\begin{aligned} \nabla \cdot \left\{ \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^+(E) \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^+} \nabla \psi_{\mathcal{I}}^+(x, z) \right) dk + \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^-(E) \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^-} \nabla \psi_{\mathcal{I}}^-(x, z) \right) dk \right\} \\ = -\nu \left\{ \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^+(E) |\psi_{\mathcal{I}}^+(x, z)|^2 dk + \sum_{m=1}^{\infty} \int_0^{\infty} f_{i,m}^-(E) |\psi_{\mathcal{I}}^-(x, z)|^2 dk \right\}, \end{aligned}$$

which is nothing but (3.24). We deduce moreover from (3.25), that

$$\begin{aligned} -\nu \int_{I_i} |\psi_{\mathcal{I}}^\pm(x, z)|^2 dx dz &= - \int_0^1 \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^\pm}(x_i, z) \frac{\partial}{\partial x} \psi_{\mathcal{I}}^\pm(x_i, z) \right) dz + \\ &+ \int_0^1 \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^\pm}(x_{i+1}, z) \frac{\partial}{\partial x} \psi_{\mathcal{I}}^\pm(x_{i+1}, z) \right) dz. \end{aligned}$$

Using this identity, we deduce after some straightforward calculations

$$\begin{aligned} \mathcal{A}^+ &= \int \sum_{m \leq M^i(E)} f_{i,m}^+(E) T_{i,m}^+(E) dE; & \mathcal{A}^- &= \int \sum_{m \leq M^{i+1}(E)} f_{i,m}^-(E) (R_{i,m}^-(E) - 1) dE, \\ \mathcal{B}^+ &= \int \sum_{m \leq M^{i+1}(E)} f_{i+1,m}^+(E) (1 - R_{i+1,m}^+(E)) dE; & \mathcal{B}^- &= - \int \sum_{m \leq M^{i+2}(E)} f_{i+1,m}^-(E) T_{i+1,m}^-(E) dE. \end{aligned}$$

Using finally the identities (3.9) we get the desired equality $\mathcal{A}^+ + \mathcal{A}^- = \mathcal{B}^+ + \mathcal{B}^-$. \blacksquare

3.4 The limit of an infinitely small coherence length

We shall present in this section the results concerning the limit of infinitely small coherence lengths. We consider the potential $V \in W^{2,3}(\Omega)$ to be given and a fixed absorption coefficient $\nu > 0$. Let us interpolate the discrete functions $f_{i,m}^{\pm,N}$ and define $\psi_{m,p}^N$ by

$$f_m^N(x, p) := \begin{cases} f_{i,m}^{+,N}(E(i, m, p)), & \text{for } \forall(x, p) \in \Upsilon_i \times \mathbb{R}^+ \\ f_{i,m}^{-,N}(E(i+1, m, -p)), & \text{for } \forall(x, p) \in \Upsilon_i \times \mathbb{R}^-, \end{cases} \quad (3.26)$$

$$\psi_{m,p}^N(x, z)|_{I_i} := \begin{cases} \psi_{i,E,m}^{+,N}(x, z), & \text{for } p > 0 \\ \psi_{i,E,m}^{-,N}(x, z), & \text{for } p < 0, \end{cases} \quad (3.27)$$

where E stands for $E(i, m, p)$ in the case $p > 0$ (resp. $E(i+1, m, -p)$ for $p < 0$). Besides let us denote for $(x, z) \in I_i$ and $i = 1, \dots, N$ the x -coordinate of the current density by

$$J_i^N(x, z) := j_i^N(x, z) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Then

$$\begin{aligned} n^N(x, z) &= \sum_{m=1}^{\infty} \int_{-\infty}^{\infty} f_m^N(x, p) |\psi_{m,p}^N(x, z)|^2 dp, \\ J^N(x, z) &= \sum_{m=1}^{\infty} \int_{-\infty}^{\infty} f_m^N(x, p) \mathcal{I}m \left(\overline{\psi_{m,p}^N}(x, z) \partial_x \psi_{m,p}^N(x, z) \right) dp. \end{aligned}$$

The main result of the two dimensional case is then the following

Theorem 3.7 (Limit of a small coherence length)

Let $\nu > 0$ and $V \in W^{2,3}(\Omega)$ be fixed. Under Hypothesis B, there exist distribution functions $f_m \in L^\infty((a, b) \times \mathbb{R})$, $m \geq 0$, such that, up to a subsequence, we have for $N \rightarrow \infty$

$$\begin{aligned} f_m^N &\rightarrow f_m, & \forall m \geq 0, & \text{ weak } * \text{ in } L^\infty((a, b) \times \mathbb{R}), \\ n^N &\rightarrow n(x, z) := \sum_{m=1}^{\infty} \left(\int_{-\infty}^{\infty} f_m(x, p) dp \right) |\chi_m(x, z)|^2, & \text{ weak } * \text{ in } L^\infty(\Omega), \\ J^N &\rightarrow j(x, z) := \sum_{m=1}^{\infty} \left(\int_{-\infty}^{\infty} p f_m(x, p) dp \right) |\chi_m(x, z)|^2, & \text{ weak } * \text{ in } L^\infty(\Omega). \end{aligned}$$

The limit functions f_m are solutions of the Vlasov equation

$$\begin{cases} p \frac{\partial f_m}{\partial x} - \frac{dE_m}{dx} \frac{\partial f_m}{\partial p} + \nu f_m = 0 & \text{in } (a, b) \times \mathbb{R} \\ f_m(a, p) = f_{a,m}(p), \quad \text{for } p > 0; \quad f_m(b, p) = f_{b,m}(p), \quad \text{for } p < 0, \end{cases}$$

and the transversal wave functions χ_m are solutions of the Schrödinger equation (3.3).

Remark 3.8 Considering Remark 3.5, we can set immediately for $m > m_0$ the distribution functions $f_m \equiv 0$.

3.5 Asymptotic behaviour of the transmission and reflection coefficients

The proof of Theorem 3.7 is based on the following two important results. Let us consider wavefunctions incident from the left in I_i , in the configuration $\mathcal{I} = (i, E, m)$, and their decomposition in terms of the $L^2(0, 1)$ -orthonormal basis χ_l , solution of (3.3),

$$\psi_{\mathcal{I}}^+(x, z) = \sum_{l=1}^{\infty} \zeta_l(x) \chi_l(x, z). \quad (3.28)$$

The case of the injection from the right can be treated similarly. The longitudinal wavefunctions ζ_l depend on \mathcal{I} , N and on the injection direction “+” or “-”, but we will omit these indices to simplify the notations. The following lemma provides us with some important estimates for the functions ζ_l and ζ'_l (see Appendix A for the proof).

Lemma 3.9 *There exists a constant $C > 0$, dependent only on α , M , ν and $V \in W^{2,3}(\Omega)$, such that we have $\forall \mathcal{I}$*

* for $E \in \mathcal{A}^m(x_i, \alpha)$

$$\max_{x \in [x_i, x_{i+1}]} \sum_l |\zeta_l(x)|^2 \leq C \quad ; \quad \max_{x \in [x_i, x_{i+1}]} \sum_{l \neq m} |\zeta_l(x)|^2 \leq Ch_i, \quad (3.29)$$

$$\int_{x_i}^{x_{i+1}} \sum_l |\zeta'_l(x)|^2 dx \leq Ch_i \quad ; \quad \int_{x_i}^{x_{i+1}} \sum_{l \neq m} |\mathcal{I}m(\zeta'_l(x))|^2 dx \leq Ch_i \sqrt{h_i}, \quad (3.30)$$

* for $E \in \mathcal{C}_r^m(x_i, \alpha)$, $r \neq m$

$$\max_{x \in [x_i, x_{i+1}]} \sum_l |\zeta_l(x)|^2 + \frac{1}{h_i} \int_{x_i}^{x_{i+1}} \sum_l |\zeta'_l(x)|^2 dx \leq C \frac{1}{k_r^i(E)}, \quad (3.31)$$

* for $E \in \mathcal{C}_m^m(x_i, \alpha)$

$$\max_{x \in [x_i, x_{i+1}]} \sum_l |\zeta_l(x)|^2 + \frac{1}{h_i} \int_{x_i}^{x_{i+1}} \sum_l |\zeta'_l(x)|^2 dx \leq C. \quad (3.32)$$

The asymptotic behaviour of the transmission and reflection coefficients in the limit of a large number of cells N is a consequence of the just stated *a priori* estimates and is proven in Appendix B.

Lemma 3.10 (Asymptotic behaviour)

Let $0 < \alpha < M$ and $0 < \nu \leq 1$ be fixed real numbers and $V \in W^{2,3}(\Omega)$. Then, there exists a constant $C = C(M, \alpha) > 0$ such that $\forall i = 1, \dots, N$ and $\forall m$ we have for energies far from turning points, $E \in \{|E| < M / E > E_m^i, |E - E_r^i| \geq \alpha \quad \forall r\} =: \mathcal{A}^m(x_i, \alpha)$

$$|T_{i,m \rightarrow m}^{\pm, N}(E) - 1 + \frac{\nu h_i}{k_m^i(E)}| \leq Ch_i^{5/4} \quad ; \quad |T_{i,m \rightarrow l}^{\pm, N}(E)| \leq Ch_i^2, \quad \forall l \neq m,$$

$$|R_{i,m \rightarrow l}^{\pm, N}(E)| \leq Ch_i^{5/4}, \quad \forall l,$$

For energies close to a turning point, $E \in \{|E| < M / E > E_m^i, |E - E_r^i| < \alpha\} =: \mathcal{C}_r^m(x_i, \alpha)$, $r > m$ we have the asymptotic behaviour

$$|T_{i,m \rightarrow m}^{\pm, N}(E) - 1| \leq C \frac{1}{k_r^i(E)} h_i \quad ; \quad |T_{i,m \rightarrow l}^{\pm, N}(E)| \leq C \frac{1}{k_r^i(E)} h_i, \quad \forall l \neq m,$$

$$|R_{i,m \rightarrow l}^{\pm, N}(E)| \leq C \frac{1}{k_r^i(E)} h_i, \quad \forall l.$$

The turning points and the decomposition of the injection energy interval into regions around the threshold energy values and far from them, are illustrated in Figures 4 and 5.

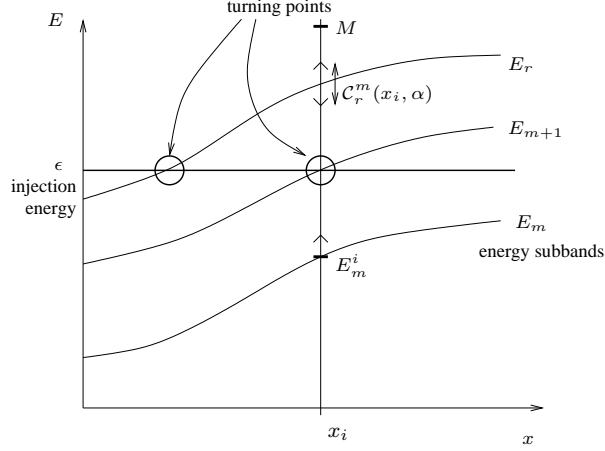


Figure 4: Representation of the turning points. ϵ is the electron injection energy, E_r are the energy subbands and the turning points are the positions where $\epsilon = E_r(x)$.

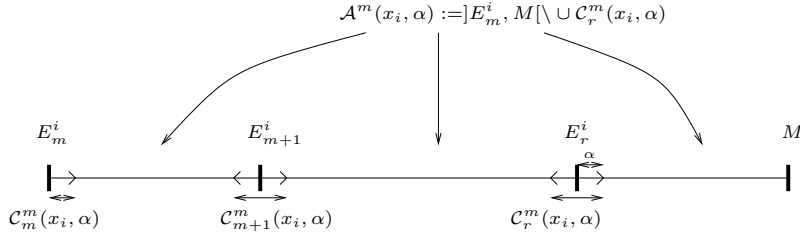


Figure 5: Decomposition of the injection energy interval at the position $x = x_i$ in regions $\mathcal{A}^m(x_i, \alpha)$ far from turning points and zones $\mathcal{C}_r^m(x_i, \alpha)$ around these points.

3.6 Proof of Theorem 3.7

We come now to the proof of the main theorem, whose fundamental features are similar to the one-dimensional case. The proof is decomposed into three steps.

Step 1: Limit of the charge and current densities.

Let us introduce the auxiliary functions

$$\begin{pmatrix} \tilde{n}^N \\ \tilde{J}^N \end{pmatrix} (x, z) := \sum_{m=1}^{\infty} \left\{ \int_{\mathbb{R}} \begin{pmatrix} 1 \\ p \end{pmatrix} f_m^N(x, p) dp \right\} |\chi_m(x, z)|^2.$$

We shall show, that the sequences $\tilde{n}^N - n^N$ and $\tilde{J}^N - J^N$ are convergent in $L^1(\Omega)$ towards zero. Reminding then, that f_m^N are bounded in $L^\infty((a, b) \times \mathbb{R})$, $\forall m$ and thus convergent

(up to a subsequence) in $L^\infty((a, b) \times \mathbb{R})$ weak * towards some limit functions f_m , we get

$$\begin{pmatrix} \tilde{n}^N \\ \tilde{j}^N \end{pmatrix} \rightarrow \sum_{m=1}^{\infty} \left\{ \int_{\mathbb{R}} \begin{pmatrix} 1 \\ p \end{pmatrix} f_m(x, p) dp \right\} |\chi_m(x, z)|^2, \quad \text{weak * in } (L^\infty(\Omega))^2,$$

and we conclude the first step of the proof. Let us thus show, that $\|J^N - \tilde{J}^N\|_{L^1(\Omega)} \rightarrow 0$:

$$\begin{aligned} \|J^N - \tilde{J}^N\|_{L^1(\Omega)} &\leq \sum_{i=1}^N \int_{x_i}^{x_{i+1}} \sum_{m=1}^{m_0} \left[\int_0^{k_0} f_{i,m}^{+,N}(E) \int_0^1 |\mathcal{I}m(\bar{\psi}_{\mathcal{I}}^+ \partial_x \psi_{\mathcal{I}}^+) - k|\chi_m(x, z)|^2| dz dk \right. \\ &\quad \left. + \int_0^{k_0} f_{i,m}^{-,N}(E) \int_0^1 |\mathcal{I}m(\bar{\psi}_{\mathcal{I}}^- \partial_x \psi_{\mathcal{I}}^-) + k|\chi_m(x, z)|^2| dz dk \right] dx. \end{aligned}$$

But

$$\begin{aligned} \mathcal{I}m(\bar{\psi}_{\mathcal{I}}^+ \partial_x \psi_{\mathcal{I}}^+) &= \mathcal{I}m \left\{ \sum_{l \neq m} \sum_{l'} \overline{\zeta_l(x)} \zeta_{l'}'(x) \chi_l \chi_{l'} + \sum_{l' \neq m} \overline{\zeta_m(x)} \zeta_{l'}'(x) \chi_m \chi_{l'} \right. \\ &\quad + \sum_{l \neq m} \sum_{l'} \overline{\zeta_l(x)} \zeta_{l'}(x) \chi_l \partial_x \chi_{l'} + \sum_{l' \neq m} \overline{\zeta_m(x)} \zeta_{l'}(x) \chi_m \partial_x \chi_{l'} \\ &\quad \left. + \overline{\zeta_m(x)} \zeta_m'(x) |\chi_m(x, z)|^2 + \underbrace{|\zeta_m(x)|^2 \chi_m(x, z) \partial_x \chi_m(x, z)}_{\in \mathbb{R}} \right\}, \end{aligned}$$

thus leading to

$$\begin{aligned} \int_0^1 |\mathcal{I}m(\bar{\psi}_{\mathcal{I}}^+ \partial_x \psi_{\mathcal{I}}^+) - k|\chi_m(x, z)|^2| dz &\leq \\ &\leq |\mathcal{I}m(\bar{\zeta}_m(x) \zeta_m'(x)) - k| + c_0 \left(\sum_{l' \neq m} |\zeta_{l'}(x)|^2 \right)^{1/2} |\zeta_m(x)| + \\ &+ \left(\sum_{l \neq m} |\zeta_l(x)|^2 \right)^{1/2} \left(\sum_{l'} |\zeta_{l'}'(x)|^2 \right)^{1/2} + \left(\sum_{l' \neq m} |\zeta_{l'}'(x)|^2 \right)^{1/2} |\mathcal{I}m(\bar{\zeta}_m(x))| + \\ &+ \left(\sum_{l' \neq m} |\mathcal{I}m(\zeta_{l'}'(x))|^2 \right)^{1/2} |\zeta_m(x)| + c_0 \left(\sum_{l \neq m} |\zeta_l(x)|^2 \right)^{1/2} \left(\sum_{l'} |\zeta_{l'}(x)|^2 \right)^{1/2}, \end{aligned} \tag{3.33}$$

with

$$c_0 = \left(\sum_{l'} \int_0^1 |\partial_x \chi_{l'}(x, z)|^2 dz \right)^{1/2} \leq \left(c \sum_{l'} \frac{1}{(l')^2} \right)^{1/2} < \infty.$$

Besides we will decompose the integral $\int_0^{k_0}$ into

$$\int_0^{k_0} = \int_0^\epsilon + \sum_{r=m}^{m_0} \int_{k_{m,r}^{\epsilon}}^{k_{m,r+1}^{\epsilon}} + \sum_{r=m+1}^{m_0} \int_{k_{m,r}^{\epsilon}}^{k_{m,r}^{\epsilon}} = I_A + \sum_{r=m}^{m_0} I_{B_r} + \sum_{r=m+1}^{m_0} I_{C_r},$$

where $k_{m,r}^{\epsilon} = k_{m,r}(x_i)$ is defined by

$$\frac{k_{m,r}^2(x_i)}{2} + E_m(x_i) = E_r(x_i), \quad \text{for } r \geq m,$$

and $\epsilon > 0$ is a little real number satisfying $\epsilon < \frac{\alpha}{k_0}$, such that we get for $k \in (k_{m,r}^i - \epsilon, k_{m,r}^i + \epsilon)$ the inequality $|E - E_r^i| \leq \epsilon k_0 < \alpha$. Let N and ϵ be fixed numbers for the beginning. We first analyze the integrals I_{B_r} :

In view of (A.5) and $k_m^i(E) = \sqrt{2|E - E_m^i|}$, where $E = \frac{k^2}{2} + E_m^i$, we have for the first term of (3.33)

$$\begin{aligned} \left| \mathcal{I}m(\bar{\zeta}_m(x)\zeta_m'(x)) - k \right| &= \left| \mathcal{I}m(\bar{\zeta}_m(x)\mathcal{R}e(\zeta_m'(x)) + \mathcal{R}e(\bar{\zeta}_m(x))\mathcal{I}m(\zeta_m'(x)) - k \right| \\ &\leq \left| \mathcal{I}m(\zeta_m'(x)) - k \right| + ch_i \leq c\sqrt{h_i}. \end{aligned}$$

Using Lemma 3.9 and analyzing each term of (3.33), we get with $c > 0$ dependent on ϵ

$$\sum_{i=1}^N \int_{x_i}^{x_{i+1}} \int_{k_{m,r}^i - \epsilon}^{k_{m,r}^i + \epsilon} f_{i,m}^{+,N}(E) \int_0^1 \left| \mathcal{I}m(\bar{\psi}_{\mathcal{I}}^+ \partial_x \psi_{\mathcal{I}}^+) - k |\chi_m(x, z)|^2 \right| dz dk dx \leq ch_i^{1/4}.$$

We come now to the integrals I_{C_r} . For this we will make use of the fact, that

$$\int_{\rho - \epsilon}^{\rho + \epsilon} \frac{1}{\sqrt{|k^2 - \rho^2|}} dk = \frac{\pi}{2} - \arcsin\left(1 - \frac{\epsilon}{\rho}\right) + \operatorname{arcosh}\left(1 + \frac{\epsilon}{\rho}\right) = g\left(\frac{\epsilon}{\rho}\right) < \infty, \quad \epsilon > 0,$$

where g is a continuous, monotonly increasing function with $g(\xi) \rightarrow 0$ as $\xi \rightarrow 0$. In our case we have $\rho = k_{m,r}(x_i) \geq \rho_0 = \sqrt{2E_{min}}$, with $E_{min} = \min_{l,x}(E_{l+1}(x) - E_l(x))$.

The first term can thus be estimated as follows:

$$\begin{aligned} \int_{x_i}^{x_{i+1}} \int_{k_{m,r}^i - \epsilon}^{k_{m,r}^i + \epsilon} \left| \mathcal{I}m(\bar{\zeta}_m \zeta_m') - k \right| dk dx &\leq \\ &\leq \int_{x_i}^{x_{i+1}} \int_{k_{m,r}^i - \epsilon}^{k_{m,r}^i + \epsilon} \left(\sum_l |\zeta_l(x)|^2 \right)^{1/2} \left(\sum_l |\zeta_l'(x)|^2 \right)^{1/2} dk dx + \int_{x_i}^{x_{i+1}} \int_{k_{m,r}^i - \epsilon}^{k_{m,r}^i + \epsilon} k dk dx \\ &\leq ch_i \left(g\left(\frac{\epsilon}{k_{m,r}^i}\right) + \epsilon \right) \leq ch_i \left(g\left(\frac{\epsilon}{\rho_0}\right) + \epsilon \right). \end{aligned}$$

Continuing in this manner and using Lemma 3.9 yields

$$\sum_{i=1}^N \int_{x_i}^{x_{i+1}} \int_{k_{m,r}^i - \epsilon}^{k_{m,r}^i + \epsilon} f_{i,m}^{+,N}(E) \int_0^1 \left| \mathcal{I}m(\bar{\psi}_{\mathcal{I}}^+ \partial_x \psi_{\mathcal{I}}^+) - k |\chi_m(x, z)|^2 \right| dz dk dx \leq c \left(g\left(\frac{\epsilon}{\rho_0}\right) + \epsilon \right),$$

with a constant $c > 0$ not depending on ϵ , but on α and where α is a fixed number.

Finally the integral I_A is analyzed similarly. With $c > 0$, not depending on ϵ , we have

$$\sum_{i=1}^N \int_{x_i}^{x_{i+1}} \int_0^\epsilon f_{i,m}^{+,N}(E) \int_0^1 \left| \mathcal{I}m(\bar{\psi}_{\mathcal{I}}^+ \partial_x \psi_{\mathcal{I}}^+) - k |\chi_m(x, z)|^2 \right| dz dk dx \leq c\epsilon.$$

Letting first $N \rightarrow \infty$ (that means $h_i \rightarrow 0$) and then $\epsilon \rightarrow 0$ and proceeding analogously for the integrals corresponding to the wave functions incident from right, we deduce the desired convergence $\|J^N - \tilde{J}^N\|_{L^1(\Omega)} \rightarrow 0$. Similar arguments yield $\|n^N - \tilde{n}^N\|_{L^1(\Omega)} \rightarrow 0$.

Step 2: Limit of the Schrödinger equation towards the Vlasov equation in the upper and lower half-plane.

Let $m \leq m_0$ be fixed. We will prove first of all, that

$$\begin{cases} p \frac{\partial f_m}{\partial x} - \frac{dE_m}{dx} \frac{\partial f_m}{\partial p} + \nu f_m = 0, & \text{on } (a, b) \times \mathbb{R}_*^+ \\ f_m(a, p) = f_{a,m}(p), & \text{for } p > 0, \end{cases}$$

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

$$\mathcal{T}_m(\vartheta) = \int_a^b \int_0^\infty f_m(x, k) [k \partial_x \vartheta(x, k) - \frac{dE_m}{dx}(x) \partial_k \vartheta(x, k) - \nu \vartheta] dk dx + \int_0^\infty k f_{a,m}(k) \vartheta(a, k) dk,$$

and ϑ is an arbitrary C^1 test function of (x, k) compactly supported in $[a, b) \times \mathbb{R}_*^+$. There exist thus $0 < \epsilon < K$, such that $\text{supp } \vartheta \subset [a, b) \times (2\epsilon, K - \epsilon)$. It is enough to prove that $\lim_{N \rightarrow +\infty} \mathcal{T}_m^N(\vartheta) = 0$ where $\mathcal{T}_m^N(\vartheta)$ is given by

$$\begin{aligned} \mathcal{T}_m^N(\vartheta) &= \sum_{i=1}^N \int_{x_i}^{x_{i+1}} \int_\epsilon^K f_{i,m}^{+,N}(E(i, m, k)) [k \partial_x \vartheta(x, k) - \frac{dE_m}{dx}(x) \partial_k \vartheta(x, k) - \nu \vartheta] dk dx + \\ &+ \int_\epsilon^K k f_{a,m}^{+,N}(E(1, m, k)) \vartheta(a, k) dk. \end{aligned} \tag{3.34}$$

With the notation $\vartheta_i := \vartheta(x_i, k)$, we evaluate the first term on the right hand side as

$$\begin{aligned} \int_{x_i}^{x_{i+1}} \int_\epsilon^K f_{i,m}^{+,N}(E(i, m, k)) k \partial_x \vartheta(x, k) dk dx &= \int_\epsilon^K f_{i,m}^{+,N}(E(i, m, k)) k [\vartheta(x_{i+1}, k) - \vartheta(x_i, k)] dk \\ &= \sum_{l=m}^{m_0} \int_{k_{m,l}^{i+\epsilon}}^{k_{m,l+1}^{i-\epsilon}} f_{i,m}^{+,N} k \vartheta_{i+1} dk + \sum_{l=m+1}^{m_0} \int_{k_{m,l}^{i-\epsilon}}^{k_{m,l}^{i+\epsilon}} f_{i,m}^{+,N} k \vartheta_{i+1} dk - \int_\epsilon^K f_{i,m}^{+,N} k \vartheta_i dk = \mathcal{D}. \end{aligned} \tag{3.35}$$

But

$$\begin{aligned} \int_\epsilon^K f_{i+1,m}^{+,N}(E(i+1, m, k)) k \vartheta(x_{i+1}, k) dk &= \int_\epsilon^K \left[\sum_{m' \leq M^i(E)} T_{i,m' \rightarrow m}^{+,N}(E(i+1, m, k)) f_{i,m'}^{+,N}(E) + \right. \\ &\left. + \sum_{m' \leq M^{i+1}(E)} R_{i,m' \rightarrow m}^{-,N}(E(i+1, m, k)) f_{i,m'}^{-,N}(E) \right] k \vartheta(x_{i+1}, k) dk, \end{aligned}$$

and using the change of variable $k^2 = (k')^2 + 2(E_m^i - E_m^{i+1})$

$$\begin{aligned} \int_\epsilon^K f_{i+1,m}^{+,N}(E(i+1, m, k)) k \vartheta(x_{i+1}, k) dk &= \int_\epsilon^K \left[\sum_{m' \leq M^i(E)} T_{i,m' \rightarrow m}^{+,N}(E(i, m, k')) f_{i,m'}^{+,N}(E) + \right. \\ &\left. + \sum_{m' \leq M^{i+1}(E)} R_{i,m' \rightarrow m}^{-,N}(E(i, m, k')) f_{i,m'}^{-,N}(E) \right] k' \vartheta \left(x_{i+1}, \sqrt{(k')^2 + 2(E_m^i - E_m^{i+1})} \right) dk' \\ &= \sum_{l=m}^{m_0} \int_{k_{m,l}^{i+\epsilon}}^{k_{m,l+1}^{i-\epsilon}} \dots dk' + \sum_{l=m+1}^{m_0} \int_{k_{m,l}^{i-\epsilon}}^{k_{m,l}^{i+\epsilon}} \dots dk'. \end{aligned}$$

Besides, we have by using the asymptotic behaviour of the reflection and transmission coefficients

$$\begin{aligned} & \int_{k_{m,l}^i}^{k_{m,l+1}^i} \left[\sum_{m' \leq M^i} T_{i,m' \rightarrow m}^+ f_{i,m'}^+ + \sum_{m' \leq M^{i+1}} R_{i,m' \rightarrow m}^- f_{i,m'}^- \right] k' \vartheta \left(x_{i+1}, \sqrt{(k')^2 + 2(E_m^i - E_m^{i+1})} \right) dk' \\ &= \int_{k_{m,l}^i}^{k_{m,l+1}^i} f_{i,m}^+(E(i, m, k')) k' \vartheta(x_{i+1}, k') dk' - \nu h_i \int_{k_{m,l}^i}^{k_{m,l+1}^i} f_{i,m}^+(E(i, m, k')) \vartheta(x_{i+1}, k') dk' - \\ & \quad - \int_{x_i}^{x_{i+1}} \int_{k_{m,l}^i}^{k_{m,l+1}^i} f_{i,m}^+(E(i, m, k')) \partial_x E_m(x) \partial_{k'} \vartheta(x_{i+1}, k') dk' dx + O_\epsilon(h_i^{5/4}), \end{aligned}$$

where for every fixed $\epsilon > 0$, $O_\epsilon(\xi) \rightarrow 0$ if $\xi \rightarrow 0$. Inserting these formulae in (3.35) yields

$$\begin{aligned} \mathcal{D} &= \int_\epsilon^K f_{i+1,m}^{+,N}(E(i+1, m, k)) k \vartheta(x_{i+1}, k) dk - \int_\epsilon^K f_{i,m}^{+,N}(E(i, m, k)) k \vartheta(x_i, k) dk + \\ & \quad + \sum_{l=m}^{m_0} \int_{x_i}^{x_{i+1}} \int_{k_{m,l}^i}^{k_{m,l+1}^i} f_{i,m}^{+,N}(E(i, m, k)) \partial_x E_m(x) \partial_k \vartheta(x_{i+1}, k) dk dx + \\ & \quad + \nu h_i \sum_{l=m}^{m_0} \int_{k_{m,l}^i}^{k_{m,l+1}^i} f_{i,m}^{+,N}(E(i, m, k)) \vartheta(x_{i+1}, k) dk + O(h_i^{5/4}) + \mathcal{L}, \end{aligned}$$

with

$$\begin{aligned} \mathcal{L} &= \sum_{l=m+1}^{m_0} \int_{k_{m,l}^i}^{k_{m,l+1}^i} \left\{ f_{i,m}^{+,N}(E(i, m, k)) k \vartheta(x_{i+1}, k) - \left[\sum_{m' \leq M^i} T_{i,m' \rightarrow m}^+ f_{i,m'}^+ + \right. \right. \\ & \quad \left. \left. + \sum_{m' \leq M^{i+1}} R_{i,m' \rightarrow m}^- f_{i,m'}^- \right] k \vartheta \left(x_{i+1}, \sqrt{k^2 + 2(E_m^i - E_m^{i+1})} \right) \right\} dk. \end{aligned}$$

Using Lemma 3.10 we get

$$\begin{aligned} \mathcal{L} &= \sum_{l=m+1}^{m_0} \int_{k_{m,l}^i}^{k_{m,l+1}^i} \left\{ f_{i,m}^{+,N}(E(i, m, k)) k \vartheta(x_{i+1}, k) - \right. \\ & \quad \left. - \left[\left(1 + \frac{1}{k_l^i} O(h_i) \right) f_{i,m}^{+,N}(E) + \frac{1}{k_l^i} O(h_i) \right] k [\vartheta(x_{i+1}, k) + O(h_i)] \right\} dk \\ &= \sum_{l=m+1}^{m_0} \int_{k_{m,l}^i}^{k_{m,l+1}^i} \left\{ \frac{1}{k_l^i} O(h_i) \right\} dk = O(h_i) \sum_{l=m+1}^{m_0} \int_{k_{m,l}^i}^{k_{m,l+1}^i} \frac{1}{k_l^i} dk. \end{aligned}$$

Therefore

$$|\mathcal{L}| \leq ch_i g\left(\frac{\epsilon}{\rho_0}\right).$$

Thus, by letting N tend towards ∞ (ϵ fixed), we deduce

$$\begin{aligned} \int_a^b \int_\epsilon^K f_m(x, k) k \partial_x \vartheta(x, k) dk dx &= - \int_\epsilon^K f_m(a, k) k \vartheta(a, k) dk + \\ & \quad + \sum_{l=m}^{m_0} \int_a^b \int_{k_{m,l}(x)+\epsilon}^{k_{m,l+1}(x)-\epsilon} f_m(x, k) \partial_x E_m(x) \partial_k \vartheta(x, k) dk dx + \\ & \quad + \nu \sum_{l=m}^{m_0} \int_a^b \int_{k_{m,l}(x)+\epsilon}^{k_{m,l+1}(x)-\epsilon} f_m(x, k) \vartheta(x, k) dk dx + O(1) g\left(\frac{\epsilon}{\rho_0}\right). \end{aligned}$$

The limit $\epsilon \rightarrow 0$ yields finally $\mathcal{T}_m(\vartheta) = 0$. Proceeding similarly with a test function $\vartheta \in C^1(\mathbb{R}^2)$, compactly supported in $(a, b] \times \mathbb{R}_*^-$, we get altogether that the limit functions $\{f_m\}_{m \leq m_0}$ satisfy

$$\begin{cases} p \frac{\partial f_m}{\partial x} - \frac{dE_m}{dx} \frac{\partial f_m}{\partial p} + \nu f_m = S_m(x) \delta(p=0) & \text{in } (a, b) \times \mathbb{R} \\ f_m(a, p) = f_{a,m}(p) \quad \text{for } p > 0; \quad f_m(b, p) = f_{b,m}(p) \quad \text{for } p < 0, \end{cases} \quad (3.36)$$

with

$$S_m(x) = -[f_m(x, 0^+) - f_m(x, 0^-)] \frac{dE_m}{dx}(x).$$

Step 3: Limit of the Schrödinger equation towards the Vlasov equation in the whole phase space.

The aim of this last step is to show, that $S_m \equiv 0$. Defining the functions

$$\begin{aligned} n_{i,m}^N(x, z) &= \int_0^\infty f_{i,m}^{+,N}(E(i, m, k)) |\psi_{\mathcal{I}}^+(x, z)|^2 dk + \int_0^\infty f_{i,m}^{-,N}(E(i+1, m, k)) |\psi_{\mathcal{I}}^-(x, z)|^2 dk \\ j_{i,m}^N(x, z) &= \int_0^\infty f_{i,m}^{+,N}(E(i, m, k)) \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^+}(x, z) \nabla \psi_{\mathcal{I}}^+(x, z) \right) dk + \\ &\quad + \int_0^\infty f_{i,m}^{-,N}(E(i+1, m, k)) \mathcal{I}m \left(\overline{\psi_{\mathcal{I}}^-}(x, z) \nabla \psi_{\mathcal{I}}^-(x, z) \right) dk. \end{aligned}$$

and following the proof of the Proposition 3.6, we obtain the relation

$$\nabla \cdot j_{i,m}^N(x, z) = -\nu n_{i,m}^N(x, z), \quad \text{for } (x, z) \in I_i, \quad \forall m.$$

Besides, we deduce from the boundary condition $\psi_{\mathcal{I}}^+(x, 0) = \psi_{\mathcal{I}}^+(x, 1) = 0, \forall x \in \Upsilon_i$, that

$$\int_0^1 \partial_z j_{i,m}^N(x, z) dz \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0,$$

which implies

$$\int_0^1 \partial_x j_{i,m}^N(x, z) dz \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \nu \int_0^1 n_{i,m}^N(x, z) dz = 0, \quad \forall x \in \Upsilon_i, \quad \forall i.$$

In terms of distributions, this gives

$$\int_0^1 \partial_x j_m^N(x, z) dz \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \nu \int_0^1 n_m^N(x, z) dz = \sum_{i=2}^N \delta_{x_i} s_{i,m}^N, \quad \text{in } \mathcal{D}'(a, b),$$

with $j_{i,m}^N = j_m^N|_{I_i}$, $n_{i,m}^N = n_m^N|_{I_i}$ and

$$s_{i,m}^N = \int_0^1 j_{i,m}^N(x_i, z) dz \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \int_0^1 j_{i-1,m}^N(x_i, z) dz \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Similar as for n^N and J^N , one can prove that

$$\begin{aligned} n_{i,m}^N &\rightarrow \int_{-\infty}^{\infty} f_m(x,p) dp |\chi_m(x,z)|^2, \quad \text{weak * in } L^\infty(\Omega) \\ j_{i,m}^N \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} &\rightarrow \int_{-\infty}^{\infty} p f_m(x,p) dp |\chi_m(x,z)|^2, \quad \text{weak * in } L^\infty(\Omega). \end{aligned}$$

We have only to show that

$$\sum_{i=2}^N \delta_{x_i} s_{i,m}^N \rightarrow 0, \quad \text{in } \mathcal{D}'(a,b), \quad \text{as } N \rightarrow \infty, \quad (3.37)$$

to get

$$\frac{d}{dx} \int_{-\infty}^{\infty} p f_m(x,p) dp + \nu \int_{-\infty}^{\infty} f_m(x,p) dp = 0.$$

This last equation enables us to finish the proof. Indeed, integrating the equation (3.36) with respect to p yields

$$\frac{d}{dx} \int_{-\infty}^{\infty} p f_m(x,p) dp + \nu \int_{-\infty}^{\infty} f_m(x,p) dp = S_m(x),$$

and consequently $S_m \equiv 0$.

Let us now prove (3.37). Similar as in the proof of Proposition 3.6, we deduce

$$\begin{aligned} s_{i+1,m}^N &= \int_0^\infty f_{i+1,m}^+(E) k (1 - R_{i+1,m}^+(E)) dk - \int_0^\infty f_{i+1,m}^-(E) k T_{i+1,m}^-(E) dk \\ &\quad - \int_0^\infty f_{i,m}^+(E) k T_{i,m}^+(E) dk - \int_0^\infty f_{i,m}^-(E) k (R_{i,m}^-(E) - 1) dk. \end{aligned}$$

Using Lemma 3.10 we obtain immediately (3.37). \blacksquare

Appendix A Proof of Lemma 3.9

The proof of this theorem is rather computational. The main idea is to derive some implicate expressions for ζ_r and ζ_r' and to deduce the necessary information from the asymptotic behaviour of these functions, as well as from the variational formulation of the Schrödinger equation. Inserting the decomposition (3.28) in (3.6), using the eigenvalue problem (3.3) and projecting the equation on the r^{th} mode, leads to the following coupled system for the longitudinal wave functions ζ_r :

$$\begin{cases} -\frac{1}{2}\zeta_r''(x) + E_r(x)\zeta_r(x) = \left(E + \mathbf{i}\frac{\nu}{2}\right)\zeta_r(x) + \sum_{l=1}^{\infty} \zeta_l(x)b_{lr}(x) + \sum_{l \neq r} \zeta_l'(x)a_{lr}(x) \\ \zeta_r'(x_i) + \tau_i k_r^i(E)\zeta_r(x_i) = 2\mathbf{i}k_m^i(E)\delta_{m,r} - \sum_{l \neq r} \zeta_l(x_i)a_{lr}(x_i) \\ \zeta_r'(x_{i+1}) - \tau_{i+1} k_r^{i+1}(E)\zeta_r(x_{i+1}) = -\sum_{l \neq r} \zeta_l(x_{i+1})a_{lr}(x_{i+1}) \end{cases} \quad (\text{A.1})$$

with

$$a_{lr}(x) = \int_0^1 \partial_x \chi_l(x, z) \chi_r(x, z) dz \quad ; \quad b_{lr}(x) = \frac{1}{2} \int_0^1 \partial_{xx} \chi_l(x, z) \chi_r(x, z) dz ,$$

and

$$\tau_i = \begin{cases} \mathbf{i} & \text{for } r \leq M^i(E) \\ -1 & \text{for } r > M^i(E). \end{cases}$$

We have reduced in this manner the 2D Schrödinger equation to a coupled system of one dimensional Schrödinger equations. In the following we will denote

$$\begin{aligned} S_1^r(x) &:= \sum_l \zeta_l(x) b_{lr}(x) \quad ; \quad S_2^r(x) := \sum_{l \neq r} \zeta_l'(x) a_{lr}(x) , \\ P_1^r &:= \sum_{l \neq r} \zeta_l(x_{i+1}) a_{lr}(x_{i+1}) \quad ; \quad P_2^r := \sum_{l \neq r} \zeta_l(x_i) a_{lr}(x_i) . \end{aligned}$$

Remark that using standard results for the 1D Schrödinger operator (3.3), we get

$$\max_{x \in [a, b]} \sum_{l \neq r} |a_{lr}(x)|^2 \leq c \quad ; \quad \max_{x \in [a, b]} \sum_l |b_{lr}(x)|^2 \leq c, \quad (\text{A.2})$$

with $c > 0$ a constant independent on r [8, 14, 17, 19].

Proceeding now like in the 1D case (see proof of Lemma 2.8) we rewrite the coupled system (A.1) for $r \leq M^i(E)$ in the form

$$\begin{cases} -\zeta_r''(x) - \left(k_r^i(E)\right)^2 \zeta_r(x) = 2 \left(E_r(x_i) - E_r(x) + \mathbf{i} \frac{\nu}{2}\right) \zeta_r(x) + 2S_1^r(x) + 2S_2^r(x) \\ \zeta_r(x_{i+1}) = \gamma_r \\ \zeta_r'(x_{i+1}) - \tau_{i+1} k_r^{i+1}(E) \gamma_r = -P_1^r , \end{cases} \quad (\text{A.3})$$

with γ_r some unknowns, and deduce the implicate formulae for ζ_r and ζ_r' , $r \leq M^i(E)$:

$$\begin{aligned} \zeta_r(x) &= \frac{1}{2} \gamma_r \left[e^{-\mathbf{i} k_r^i(x_{i+1}-x)} + e^{\mathbf{i} k_r^i(x_{i+1}-x)} \right] - \mathbf{i} \tau_{i+1} \frac{1}{2} \gamma_r \frac{k_r^{i+1}}{k_r^i} \left[e^{-\mathbf{i} k_r^i(x_{i+1}-x)} - e^{\mathbf{i} k_r^i(x_{i+1}-x)} \right] \\ &\quad + \frac{\mathbf{i}}{k_r^i} \int_x^{x_{i+1}} \left(e^{\mathbf{i} k_r^i(y-x)} - e^{-\mathbf{i} k_r^i(y-x)} \right) \left[\left(E_r(x_i) - E_r(y) + \mathbf{i} \frac{\nu}{2} \right) \zeta_r + S_1^r(y) + S_2^r(y) \right] dy \\ &\quad + \frac{\mathbf{i}}{2k_r^i} P_1^r \left[e^{-\mathbf{i} k_r^i(x_{i+1}-x)} - e^{\mathbf{i} k_r^i(x_{i+1}-x)} \right] ; \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} \zeta_r'(x) &= \frac{\mathbf{i} k_r^i}{2} \gamma_r \left[e^{-\mathbf{i} k_r^i(x_{i+1}-x)} - e^{\mathbf{i} k_r^i(x_{i+1}-x)} \right] + \tau_{i+1} \frac{1}{2} \gamma_r k_r^{i+1} \left[e^{-\mathbf{i} k_r^i(x_{i+1}-x)} + e^{\mathbf{i} k_r^i(x_{i+1}-x)} \right] \\ &\quad + \int_x^{x_{i+1}} \left(e^{\mathbf{i} k_r^i(y-x)} + e^{-\mathbf{i} k_r^i(y-x)} \right) \left[\left(E_r(x_i) - E_r(y) + \mathbf{i} \frac{\nu}{2} \right) \zeta_r(y) + S_1^r(y) + S_2^r(y) \right] dy \\ &\quad - \frac{1}{2} P_1^r \left[e^{-\mathbf{i} k_r^i(x_{i+1}-x)} + e^{\mathbf{i} k_r^i(x_{i+1}-x)} \right] . \end{aligned} \quad (\text{A.5})$$

Similar expressions can be deduced for $r > M^i(E)$. Moreover, the variational formulation (3.20) will be essential for the subsequent analysis. Choosing as test function $\varphi = \psi_{\mathcal{I}}^{\pm}$ and taking the imaginary respectively real parts, yields

$$\begin{aligned} \nu \int_{I_i} |\psi_{\mathcal{I}}^{\pm}|^2 dx dz + \sum_{l=1}^{M^i(E)} k_l^i(E) |\zeta_l(x_i)|^2 + \sum_{l=1}^{M^{i+1}(E)} k_l^{i+1}(E) |\zeta_l(x_{i+1})|^2 = \\ = 2k_m^i(E) \mathcal{R}e(\zeta_m(x_i)), \end{aligned} \quad (\text{A.6})$$

$$\begin{aligned} \int_{I_i} |\nabla \psi_{\mathcal{I}}^{\pm}|^2 dx dz + \sum_{l=M^i(E)+1}^{\infty} k_l^i(E) |\zeta_l(x_i)|^2 + \sum_{l=M^{i+1}(E)+1}^{\infty} k_l^{i+1}(E) |\zeta_l(x_{i+1})|^2 = \\ = 2 \int_{I_i} (E - V) |\psi_{\mathcal{I}}^{\pm}|^2 dx dz - 2k_m^i(E) \mathcal{I}m(\zeta_m(x_i)). \end{aligned} \quad (\text{A.7})$$

Omitting in the following the indices of the wave function $\psi_{\mathcal{I}}^{\pm}$, these equations imply

$$|\zeta_m(x_i)| \leq 2, \quad \|\psi\|_{L^2(I_i)} \leq c, \quad \|\nabla \psi\|_{L^2(I_i)} \leq c, \quad (\text{A.8})$$

and

$$\sum_{l=1}^{\infty} k_l^i(E) |\zeta_l(x_i)|^2 \leq c \quad ; \quad \sum_{l=1}^{\infty} k_l^{i+1}(E) |\zeta_l(x_{i+1})|^2 \leq c, \quad (\text{A.9})$$

where $c > 0$ is a constant independent on i , N , $E \leq M$, $m \leq m_M$, with $m_M \in \mathbb{N}$ such that $E_{m_M}(x) > M \forall x \in [a, b]$. Let us now consider the three different cases.

I. Case : $E \in \mathcal{A}^m(x_i, \alpha)$.

We shall make use, in this case, of the fact that we are far from turning points

$$k_l^i(E) = \sqrt{2|E - E_l^i|} \geq \sqrt{2\alpha} \quad \text{and} \quad k_l^{i+1}(E) = k_l^i(E) + O(h_i) \quad \forall l.$$

Thus, we have as a consequence of (A.9)

$$\sum_{l=1}^{\infty} |\zeta_l(x_i)|^2 \leq c \quad , \quad \sum_{l=1}^{\infty} |\gamma_l|^2 = \sum_{l=1}^{\infty} |\zeta_l(x_{i+1})|^2 \leq c. \quad (\text{A.10})$$

As

$$|\psi(x, z)|^2 = |\psi(x_i, z)|^2 + 2\mathcal{R}e \int_{x_i}^x \frac{\partial \psi}{\partial x}(t, z) \overline{\psi(t, z)} dt,$$

we get immediately the first estimate for the case $E \in \mathcal{A}^m(x_i, \alpha)$

$$\sum_{l=1}^{\infty} |\zeta_l(x)|^2 = \int_0^1 |\psi(x, z)|^2 dz \leq \sum_{l=1}^{\infty} |\zeta_l(x_i)|^2 + 2\|\nabla \psi\|_{L^2(I_i)} \|\psi\|_{L^2(I_i)} \leq c. \quad (\text{A.11})$$

A consequence of this inequality and of (A.2) is, that independently on r

$$\|S_1^r\|_{L^\infty(x_i, x_{i+1})} \leq c \quad , \quad |P_1^r| \leq c \quad , \quad |P_2^r| \leq c.$$

Furthermore, differentiating ψ with respect to x yields the equation

$$\sum_l \zeta_l'(x) \chi_l(x, z) = \partial_x \psi(x, z) - \sum_l \zeta_l(x) \partial_x \chi_l(x, z), \quad (\text{A.12})$$

implying

$$\int_{x_i}^{x_{i+1}} \sum_l |\zeta'_l(x)|^2 dx \leq c, \quad \|S_2^r\|_{L^1(I_i)} \leq c\sqrt{h_i}.$$

More exactly, we have even

$$\|S_2^r\|_{L^\infty(I_i)} = \max_{x \in [x_i, x_{i+1}]} \left| \sum_{l \neq r} \zeta'_l(x) a_{lr}(x) \right| \leq c \quad \forall r. \quad (\text{A.13})$$

This bound is based on the estimates

$$|\zeta'_l(x)| \leq c \quad \text{for } l \leq M^i(E); \quad |\zeta'_l(x)| \leq cl \quad \text{for } l > M^i(E),$$

deduced from (A.5) and the corresponding expression for $l > M^i(E)$, as well as on standard results [8, 16, 19], which permit to estimate the coefficients $a_{lr}(x)$ as follows

$$|a_{lr}(x)| \leq c \frac{1}{l|l^2 - r^2|}.$$

Let us deduce now the asymptotic behaviour of the coefficients γ_r , for $r \leq M^i(E)$, needed for the subsequent analysis. For this purpose we insert (A.4), (A.5) in the boundary condition $\zeta'_m(x_i) + \mathbf{i}k_m^i(E)\zeta_m(x_i) = 2\mathbf{i}k_m^i(E) - P_2^m$ to get

$$\begin{aligned} \mathbf{i}\gamma_m(k_m^i + k_m^{i+1})e^{-\mathbf{i}k_m^i h_i} &= 2\mathbf{i}k_m^i - P_2^m + P_1^m e^{-\mathbf{i}k_m^i h_i} \\ &\quad - 2 \int_{x_i}^{x_{i+1}} e^{-\mathbf{i}k_m^i(y-x_i)} \left[(E_m(x_i) - E_m(y) + \mathbf{i}\frac{\nu}{2})\zeta_m + S_1^m + S_2^m \right] dy. \end{aligned} \quad (\text{A.14})$$

After straightforward computations, we obtain

$$\mathbf{i}\gamma_m(k_m^i + k_m^{i+1})e^{-\mathbf{i}k_m^i h_i} = 2\mathbf{i}k_m^i + O(h_i).$$

implying $\gamma_m = 1 + O(h_i)$. Similarly, for $r \leq M^i(E)$ with $r \neq m$, we deduce $\gamma_r = O(h_i)$. Inserting these identities in (A.4) yields

$$\zeta_m(x) = \gamma_m + O(h_i) = 1 + O(h_i) \quad ; \quad \zeta_r(x) = O(h_i), \quad r \leq M^i(E), \quad r \neq m. \quad (\text{A.15})$$

Finally with (A.7), we get the inequalities

$$\|\nabla\psi\|_{L^2(I_i)}^2 \leq ch_i,$$

and

$$\sum_{l=M^i(E)+1}^{\infty} k_l^i(E)|\zeta_l(x_i)|^2 + \sum_{l=M^{i+1}(E)+1}^{\infty} k_l^{i+1}(E)|\zeta_l(x_{i+1})|^2 \leq ch_i.$$

Consequently, we deduce on the one hand, in view of (A.12)

$$\int_{x_i}^{x_{i+1}} \sum_l |\zeta'_l(x)|^2 dx \leq ch_i,$$

and on the other hand, in view of (A.11)

$$\sum_{l \neq m} |\zeta_l(x)|^2 \leq \sum_{l \neq m} |\zeta_l(x_i)|^2 + |\zeta_m(x_i)|^2 - |\zeta_m(x)|^2 + 2\|\nabla\psi\|_{L^2(I_i)}\|\psi\|_{L^2(I_i)} \leq ch_i.$$

There remains to prove the last estimate for $E \in \mathcal{A}^m(x_i, \alpha)$. This is done by considering

$$\sum_l \mathcal{I}m(\zeta_l'(x))\chi_l(x, z) = \partial_x \mathcal{I}m\psi(x, z) - \sum_l \mathcal{I}m(\zeta_l(x))\partial_x \chi_l(x, z),$$

which implies

$$\begin{aligned} \sum_l |\mathcal{I}m\zeta_l'(x)|^2 &= \int_0^1 |\partial_x \mathcal{I}m\psi(x, z)|^2 dz - 2 \int_0^1 \partial_x \mathcal{I}m\psi(x, z) \sum_l \mathcal{I}m(\zeta_l(x))\partial_x \chi_l(x, z) dz + \\ &+ \int_0^1 \left| \sum_l \mathcal{I}m(\zeta_l(x))\partial_x \chi_l(x, z) \right|^2 dz, \end{aligned}$$

turning to

$$\int_{x_i}^{x_{i+1}} |\mathcal{I}m\zeta_m'(x)|^2 + \sum_{l \neq m}^{x_{i+1}} |\mathcal{I}m\zeta_l'(x)|^2 dx = \int_{x_i}^{x_{i+1}} \int_0^1 |\partial_x \mathcal{I}m\psi(x, z)|^2 dz dx + O(h_i \sqrt{h_i}). \quad (\text{A.16})$$

To evaluate the integral on the right hand side, we will take the imaginary part of the Schrödinger equation (3.6), multiply it with $\mathcal{I}m(\psi_{\mathcal{I}}^{\dagger})$ and integrate by parts. This yields

$$\begin{aligned} \int_{I_i} |\nabla \mathcal{I}m\psi|^2 dx dz &\leq \{-2k_m^i(E)\mathcal{I}m(\zeta_m(x_i)) + k_m^i(E)\mathcal{R}e(\zeta_m(x_i))\mathcal{I}m(\zeta_m(x_i)) \\ &+ k_m^{i+1}(E)\mathcal{R}e(\zeta_m(x_{i+1}))\mathcal{I}m(\zeta_m(x_{i+1}))\} + O(h_i^2) \\ &\leq k_m^i(E) \int_{x_i}^{x_{i+1}} \mathcal{I}m(\zeta_m'(x)) dx + O(h_i^2). \end{aligned}$$

But equation (A.5) implies

$$\zeta_m'(x) = \mathbf{i}k_m^i(E) + O(\sqrt{h_i}).$$

Inserting these derived estimates in equation (A.16) yields

$$(k_m^i(E))^2 h_i + \int_{x_i}^{x_{i+1}} \sum_{l \neq m} |\mathcal{I}m\zeta_l'(x)|^2 + O(h_i \sqrt{h_i}) = (k_m^i(E))^2 h_i + O(h_i \sqrt{h_i}),$$

and we conclude the first part of the proof.

II. Case: $E \in \mathcal{C}_r^m(x_i, \alpha)$ with $r \neq m$.

Contrary to the previous case, we have this time to take into consideration the fact, that

$$k_r^i(E) = \sqrt{2|E - E_r^i|} < \sqrt{2\alpha},$$

whereas for $l \neq r$

$$k_l^i(E) \geq \sqrt{2\alpha} \quad \text{and} \quad k_l^{i+1}(E) = k_l^i(E) + O(h_i).$$

Thus we get in this case

$$\begin{aligned} \sum_l |\zeta_l(x_i)|^2 &= \sum_l \frac{1}{k_l^i(E)} k_l^i(E) |\zeta_l(x_i)|^2 \\ &\leq \frac{1}{k_r^i(E)} k_r^i(E) |\zeta_r(x_i)|^2 + c \sum_{l \neq r} k_l^i(E) |\zeta_l(x_i)|^2 \leq c \frac{1}{k_r^i(E)}. \end{aligned} \quad (\text{A.17})$$

Using inequality (A.17) instead of inequality (A.10) and repeating step by step the same computations as above, yields the formula (3.31).

III. Case: $E \in \mathcal{C}_m^m(x_i, \alpha)$.

Finally, in this case we will use the inequality $|\zeta_m(x_i)| \leq 2$ to get

$$\sum_l |\zeta_l(x_i)|^2 \leq 2 + \sum_{l \neq m} \frac{1}{k_l^i(E)} k_l^i(E) |\zeta_l(x_i)|^2 \leq c.$$

■

Appendix B Proof of Lemma 3.10

The proof of this theorem is a simple consequence of Lemma 3.9. The transmission coefficient writes

$$T_{i,m \rightarrow l}^+(E) := \frac{k_l^{i+1}(E)}{k_m^i(E)} |\zeta_l(x_{i+1})|^2, \quad \text{for } 1 \leq m \leq M^i(E), 1 \leq l \leq M^{i+1}(E), \quad (\text{B.18})$$

Let $E \in \mathcal{A}^m(x_i, \alpha)$. As we have seen in the previous proof (see equation (A.15)), we have for $l \neq m, l \leq M^i(E)$

$$|\zeta_l(x_{i+1})| = |\gamma_l| \leq ch_i,$$

thus leading to

$$|T_{i,m \rightarrow l}^+(E)| \leq ch_i^2 \quad l \neq m.$$

To get the asymptotic behaviour of $T_{i,m \rightarrow m}^+(E)$, we will need a more elaborate development of $|\gamma_m|^2$. For this we take the boundary condition (A.14) squared and deduce

$$\begin{aligned} |\gamma_m|^2 (k_m^i + k_m^{i+1})^2 &= 4(k_m^i)^2 + 4k_m^i \left[-\mathcal{I}m(P_2^m) + \mathcal{I}m(P_1^m e^{-ik_m^i h_i}) \right] \\ &\quad - 8k_m^i \mathcal{I}m \left(\int_{x_i}^{x_{i+1}} e^{-ik_m^i (y-x_i)} (S_1^m(y) + S_2^m(y)) dy \right) \\ &\quad - 4k_m^i \nu \mathcal{R}e \int_{x_i}^{x_{i+1}} e^{-ik_m^i (y-x_i)} \zeta_m(y) dy + O(h_i^2). \end{aligned}$$

Analyzing now term by term we get

$$|\gamma_m|^2 = \frac{4(k_m^i)^2}{(k_m^i + k_m^{i+1})^2} \left[1 - \nu \frac{h_i}{k_m^i} + O(h_i^{5/4}) \right],$$

leading thus to the asymptotic behaviour

$$|T_{i,m \rightarrow m}^{+,N}(E) - 1 + \frac{\nu h_i}{k_m^i(E)}| \leq Ch_i^{5/4} \quad \forall m \leq M^i(E).$$

Inserting this formula in the relation (3.14), yields $R_{i,m}^+(E) = O(h_i^{5/4})$ and we conclude the proof for $E \in \mathcal{A}^m(x_i, \alpha)$. The expressions for $E \in \mathcal{C}_r^m(x_i, \alpha)$, $r > m$ follow immediately. ■

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