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A Hybrid Kinetic-Quantum Model for Stationary Electron Transport

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Interface conditions between a classical transport model described by the Boltzmann equation and a quantum model described by a set of Schrödinger equations are presented in the one-dimensional stationary setting. These interface conditions, derived thanks to an asymptotic analysis of the Wigner transform, are shown to be flux-preserving and are used to build a hybrid model consisting of a quantum zone surrounded by two classical ones. The hybrid model is shown to be well posed when the potential is either prescribed or computed self-consistently, and the semiclassical limit of the problem is shown to give the right interface conditions between two kinetic regions (the electrostatic potential being fixed). This model can be used to describe far-from-equilibrium electron transport in a resonant tunneling diode.

KEY WORDS: Boltzmann; Schrödinger; interface condition; Wigner transform; semiclassical limit; reflection-transmission coefficients.

1. INTRODUCTION

Due to the ongoing miniaturization in semiconductor technology, the very widely used Drift-Diffusion (DD) model ceases to correctly account for the more and more elaborate physical phenomena involved in many of nowadays devices.

To account for out of equilibrium phenomena in classical transport (ballistic electrons, energetic tails...), the Boltzmann equation (BE)

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represents the more precise model. However, its numerical cost is often prohibitive. The need of a coarser model, which is nevertheless more precise than the DD equation, has led to the introduction of the energy transport (ET), the spherical harmonic expansion (SHE) models,[40, 41] the extended hydrodynamic model.[2] The rigorous derivation of these models from the BE is investigated in refs. 5, 6, 36, and 39.

To model the quantum phenomena (the tunneling effect, etc) involved in devices such as the resonant tunneling diode (RTD) or superlattices and many others, the BE is of no use. A finer level of modeling is achieved via the Schrödinger or (equivalently the Wigner and the Von Neumann) equation. The collision processes (for example with phonons) can be modeled in this framework thanks to the quantum field theory[1, 10] or by deriving phenomenological "master equations" to compute the reflection-transmission coefficients (the interested reader can find in ref. 12 a detailed discussion and an extended bibliography on scattering assisted tunneling).

Hence, the designer is provided with a whole hierarchy of models among which he can chose the appropriate one, depending on the physical phenomena involved in the device operation. This situation is however not completely satisfactory, since the far from equilibrium phenomena, whose description needs an expensive model, often take place in localized regions of the device, while the remaining regions can be sufficiently well described by a coarser model. It is then necessary to develop a *hybrid* strategy: precise models used in out of equilibrium regions and coupled to coarser ones in the rest of the device. To achieve this goal, two mathematical issues have to be investigated. The first issue is the *mathematical derivation* of coarse models from finer ones, and the second one, which is not independent of the first, concerns the introduction of appropriate *interface conditions* for the coupling of the two models.

This program has been achieved for gas dynamics (reentry of the space shuttle in the atmosphere) by coupling the Boltzmann equation to the Euler or Navier Stokes equations and has been recently extended to the classical transport semiconductors by coupling the BE to the DD, the SHE and the ET models.[2] [14, 15, 23] Our purpose in this paper, is to propose and analyze a hybrid model which couples a quantum (**Q**) description to a classical one (**C**).

The Schrödinger equation applied to semiconductor modeling has been extensively analyzed in different contexts and settings (see for example refs. 9, 13, 31, and 32...). It has also been shown that its semiclassical limit leads to the Vlasov equation.[19, 26, 27, 37] The main tool to pass from the

[2] These references contain an extended bibliography on the Boltzmann–Euler (or Navier Stokes) coupling.

Schrödinger picture to the kinetic one is the Wigner transform introduced in ref. 42 and analyzed in refs. 19 and 26 and the Wigner series.[28] Hence, the first question, concerning the *mathematical derivation* of kinetic equations from the Schrödinger equation has been addressed in the literature and clear answers are available at least in the collisionless case (Vlasov). Let us note that all the mentioned semiclassical results concern whole space problems and are reviewed in ref. 20.

Interface conditions. When dealing with hybrid models, one has to consider boundaries, but a few results on the semiclassical limit in boundary value problems are available. However, in the very simple stationary one dimensional picture transparent boundary conditions have been introduced and analyzed in refs. 7 and 8. These boundary conditions have been shown to give rise in the semiclassical limit to the standard inflow boundary conditions for the Vlasov equation. Let us also note that a multidimensional version of these boundary conditions is introduced in ref. 25 (see also ref. 34 and analyzed in ref. 4). We shall take advantage of the analogy between quantum and classical inflow boundary conditions to introduce the appropriate **Q–C** interface conditions. Since the semiclassical limit of the Schrödinger picture to the kinetic one can be done uniquely, to our knowledge, in the collisionless case, we shall assume that the **Q** zone is purely ballistic, whereas collisions can take place in the **C** zone.

The outline of the paper is as follows. In the next section, we derive artificial boundary conditions for the Vlasov equation. Taking advantage of an analogous boundary condition in the Schrödinger picture, we write an appropriate **Q–C** interface condition and show that it is flux preserving. In Section 3, we write the hybrid **C–Q–C** model and show the existence of a self-consistent solution. In Section 4, we prove that the semiclassical limit of the hybrid model (with a prescribed electrostatic potential and a positive absorption term) gives the "good" artificial conditions for the Vlasov equation already derived in Section 2. We finally discuss in Section 5 the validity of the model and its application to the resonant tunneling diode.

2. THE APPROACH

2.1. Transparent Boundary Conditions for a Kinetic Equation

Let a beam of electrons be submitted to an electrostatic potential V in a region $[0, L]$ of the one dimensional space. In the stationary ballistic regime, the electron distribution function f satisfies the Vlasov equation

$$\frac{p}{m}\frac{\partial f}{\partial x} + e\frac{dV}{dx}\frac{\partial f}{\partial p} = 0 \qquad (2.1)$$

where e is the elementary charge, m is the effective electron mass and (x, p) are the position-momentum variables. The solution of (2.1) is constant along the characteristics defined by

$$\frac{dx}{dt} = \frac{p(t)}{m}, \qquad \frac{dp}{dt} = e \frac{dV}{dx}(x(t))$$

Note that the total energy $E(p, x) := (p^2/2m) - eV(x)$ is conserved along the above curves.

Since f is constant along the characteristics (that we plotted in Fig. 1), the knowledge of its value at incoming velocities ($x = 0$ and $p > 0$ or $x = L$ and $p < 0$) determines the value of f at those points of phase space belonging to open trajectories. On closed trajectories (trapped particles), f can be an arbitrary constant (see refs. 21 and 35).

Remark 2.1. To overcome the nonuniqueness problem, a minimal solution can be constructed by setting $f = 0$ on such closed trajectories. Mathematically speaking, this is done by adding an absorption term of the form νf in the left hand side of (2.1) (with $\nu > 0$), solving the modified Vlasov equation, and then letting ν tend to zero (see ref. 35). ∎

Let us now artificially split the interval $[0, L]$ into $[0, x_1]$ and $[x_1, L]$ as shown in Fig. 1, and solve the kinetic equation only on $[0, x_1]$. What are the boundary conditions to be prescribed at $x = x_1$ in order to the computed solution be the restriction on $[0, x_1]$ of the original problem's solution?

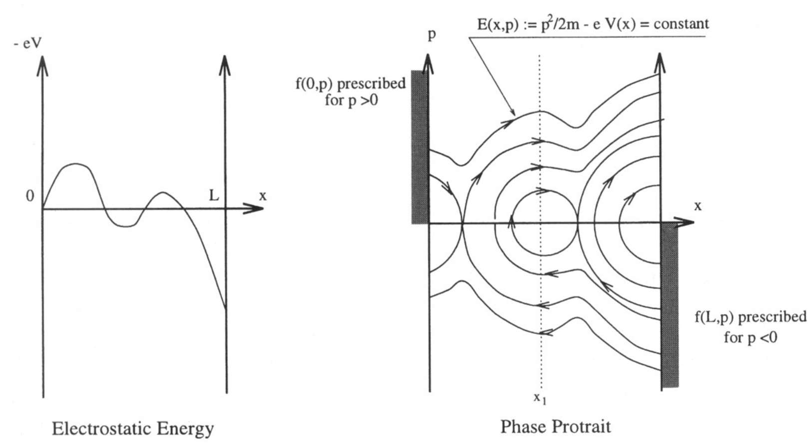

Fig. 1. Resolution by means of phase portrait.

In the one dimensional stationary case, a careful inspection of the phase portrait answers this question. Indeed, let $p>0$ be the momentum at $x=x_1$ of a particle going from $[0, x_1]$ to $[x_1, L]$. Two cases are possible

• Total reflection. If $p^2/2m - eV(x_1) < \max_{x\in[x_1,L]}\{-eV(x)\}$, the particle is reflected by a potential barrier located in $[x_1, L]$. Consequently, it reenters the interval $[0, x_1]$ with a momentum $-p$. For such p's, we have $f(x_1, -p) = f(x_1, p)$.

• Total transmission. If $p^2/2m - eV(x_1) > \max_{x\in[x_1,L]}\{-eV(x)\}$, the particle has enough energy to reach $x=L$. By symmetry, a particle entering the interval $[0, x_1]$ with a momentum $-p$ has been previously injected at $x=L$ with the momentum $-p_2 = -\sqrt{p^2 - 2emV(x_1) + 2emV(x_L)}$. This leads to $f(x_1, -p) = f(L, -p_2)$.

Both cases can be rewritten in a unique way

$$f(x_1, -p) = R_p f(x_1, p) + T_p f(L, -p_2) \tag{2.2}$$

where we have introduced the reflection and transmission coefficients $R_p = 1$ and $T_p = 0$ in the case of total reflection and conversely in the total transmission case. Let us also note that in the derivation of (2.2), the transport is assumed to be ballistic in $[x_1, L]$ only.

If the particles are in a quantum regime in $[x_1, L]$, it is sufficient to use (2.2) where R_p and T_p are computed from an appropriate quantum model. In ref. 7, a quantum model leading to (2.2) in the semiclassical limit is introduced and analyzed. It is based on the computation on a bounded domain of the scattering states of the Schrödinger operator. These scattering states play the role of the Vlasov equation's characteristics and allow the computation of the reflection-transmission coefficients needed to develop the **Q–C** coupling method. We shall recall in the following subsection the basic properties of these scattering states.

2.2. Scattering States and "Quantum Trajectories"

Let us consider an interval $[x_1, x_2]$ which we call the (quantum) device region $(x_1 < x_2)$ in which an electrostatic potential $V(x)$ is built. We assume that the electrostatic potential outside the device is constant (metallic contacts) and consider electrons injected into the device with a kinetic energy $p^2/2m$ either at x_1 or x_2.

Notation. All along this paper we shall denote $V_1 = V(x_1)$ and $V_2 = V(x_2)$.

• Electrons injected at $x = x_1$

An electron arrives at $x = x_1$ with a kinetic energy $p^2/2m$. The total energy at $x = x_1$ is equal to $E = p^2/2m - eV_1$. In a quantum framework, it can be described by a left scattering state of the Schrödinger with the energy E

$$-\frac{\hbar^2}{2m}\psi_p'' - eV(x)\,\psi_p = \left(\frac{p^2}{2m} - eV_1\right)\psi_p \qquad (p \geqslant 0)$$

The potential being constant outside the device, the wave function denoted by reads $\psi_p(x) = e^{ip(x-x_1)/\hbar} + r_p e^{-ip(x-x_1)/\hbar}$ for $x < x_1$ and $\psi_p(x) = t_p e^{i\sqrt{p^2+2em(V_2-V_1)}\,(x-x_2)/\hbar}$ for $x > x_2$ (see ref. 7). Let us note that the potential V_2 is assumed to be larger than V_1 in ref. 7 which yields that $\sqrt{p^2 + 2em(V_2 - V_1)}$ is real. Here we shall consider cases where this square root can be imaginary. We denote $\sqrt[+]{a}$ $(a \in \mathbb{R})$ the complex square root with nonnegative imaginary part and obtain $\psi_p(x) = t_p e^{i\sqrt[+]{p^2+2em(V_2-V_1)}(x-x_2)/\hbar}$ for $x > x_2$. Hence ψ_p solves

$$\begin{cases} -\dfrac{\hbar^2}{2m}\psi_p'' - eV(x)\,\psi_p = \left(\dfrac{p^2}{2m} - eV_1\right)\psi_p \qquad (p \geqslant 0) \\ \hbar\psi_p'(x_1) + ip\psi_p(x_1) = 2ip \\ \hbar\psi_p'(x_2) = i\sqrt[+]{p^2 + 2em(V_2 - V_1)}\,\psi_p(x_2) \end{cases} \tag{2.3}$$

The existence and uniqueness of solutions, is deduced from the Fredholm alternative:[4, 7] multiplying the Schrödinger equation by $\bar{\psi}_p$, integrating over $[x_1, x_2]$ and taking the imaginary part leads to

$$p\,|\psi_p(x_1)|^2 + \mathcal{R}e(\sqrt[+]{p^2 + 2em(V_2 - V_1)})\,|\psi_p(x_2)|^2 = 2p\,\mathcal{R}e(\psi_p(x_1))$$

The right hand side. being equal to zero if the boundary conditions of (2.6) are homogeneous, it is then clear that if $p \neq 0$, the solution is unique. Moreover since, for a real number a, the relation $\mathcal{R}e(\sqrt[+]{a}) = \sqrt{(a)^+}$ holds with $(a)^+ = \max(a, 0)$, then the reflection and transmission coefficients defined by

$$R_{p,1} = |\psi_p(x_1) - 1|^2, \qquad T_{p,1} = \frac{1}{p}\sqrt{(p^2 + 2em(V_2 - V_1)^+}\,|\psi_p(x_2)|^2 \tag{2.4}$$

satisfy the identity

$$R_{p,1} + T_{p,1} = 1 \tag{2.5}$$

• Electrons injected at $x = x_2$

In this case the electron arrives at $x = x_2$ with a negative momentum $-p$. Its energy is then equal to $E = p^2/2m - eV_2$. Hence the wave function φ_p is a right scattering state with energy E. The expressions $\varphi_p(x) = e^{-ip(x-x_2)/h} + r_p e^{ip(x-x_2)/h}$ for $x > x_2$ and $\varphi_p(x) = t_p e^{-i\,\sqrt[+]{p^2 - 2em(V_2 - V_1)}(x - x_1)/h}$ for $x < x_1$, lead to

$$\begin{cases} -\dfrac{h^2}{2m}\varphi_p'' - eV(x)\,\varphi_p = \left(\dfrac{p^2}{2m} - eV_2\right)\varphi_p \qquad (p \geqslant 0) \\ h\varphi_p'(x_1) = -i\ \sqrt[+]{p^2 + 2em(V_1 - V_2)}\,\varphi_p(x_1) \\ h\varphi_p'(x_2) - ip\varphi_p(x_2) = -2ip \end{cases} \tag{2.6}$$

Analogously to the first case, we have

$$R_{p,2} + T_{p,2} = 1 \tag{2.7}$$

$$R_{p,2} = |\varphi_p(x_2) - 1|^2, \qquad T_{p,2} = \frac{1}{p}\sqrt{(p^2 + 2em(V_1 - V_2))^+}\ |\varphi_p(x_1)|^2 \tag{2.8}$$

Remark 2.2. Note that with our choice of the index p, ψ_p and φ_p do not correspond in general to the same total energy for the Schrödinger operator (unless $V_1 = V_2$).

2.3. Adding an Absorption Term

In ref. 4, it has been noticed that the nonuniqueness of solutions near bound state energies leads in the multidimensional case to a difficulty in defining electron density because of a lack of integrability. This problem is solved by adding an absorption term to the Schrödinger equation. Although this problem does not occur in the one dimensional case, the introduction of an absorption term will help us in the study of the hybrid model and its semiclassical limit. Equations (2.6) and (2.3) are then replaced by

$$\begin{cases} -\dfrac{h^2}{2m}\psi_p'' - eV(x)\,\psi_p = \left(\dfrac{p^2}{2m} - eV_1 + ih\dfrac{\nu}{2}\right)\psi_p \qquad (p \geqslant 0) \\ h\psi_p'(x_1) + ip\psi_p(x_1) = 2ip \\ h\psi_p'(x_2) = i\ \sqrt[+]{p^2 + 2em(V_2 - V_1)}\,\psi_p(x_2) \end{cases} \tag{2.9}$$

$$\begin{cases} -\dfrac{h^2}{2m}\varphi_p'' - eV(x)\,\varphi_p = \left(\dfrac{p^2}{2m} - eV_2 + ih\dfrac{\nu}{2}\right)\varphi_p \qquad (p \geqslant 0) \\ h\varphi_p'(x_1) = -i\,\sqrt[+]{p^2 + 2em(V_1 - V_2)}\,\varphi_p(x_1) \\ h\varphi_p'(x_2) - ip\varphi_p(x_2) = -2ip \end{cases} \tag{2.10}$$

where ν is a positive constant. The reflection transmission coefficients $R^{\nu}_{p,1}$, $T^{\nu}_{p,1}$, $R^{\nu}_{p,2}$ and $T^{\nu}_{p,2}$ still given by (2.4) and (2.8) satisfy

$$R^{\nu}_{p,1} + T^{\nu}_{p,1} + \frac{\nu m}{p}\int_{x_1}^{x_2} |\psi_p(x)|^2\,dx = 1 \tag{2.11}$$

$$R^{\nu}_{p,2} + T^{\nu}_{p,2} + \frac{\nu m}{p}\int_{x_1}^{x_2} |\varphi_p(x)|^2\,dx = 1 \tag{2.12}$$

2.4. Quantum Inflow Boundary Conditions

In ref. 7, the quantum analogue of a one sided injection in a Vlasov boundary value problem was derived and studied. Let us write it in the case of an injection at both sides. Let $G_1(p)$ be the statistics of injected particles at $x = x_1$ and $G_2(p)$ that of particles injected at $x = x_2$ with a momentum $-p$ $(p > 0)$. The charge density and the current density are computed by the following formula

$$n(x) = \int_0^{+\infty} G_1(p)\,|\psi_p(x)|^2\,dp + \int_0^{+\infty} G_2(p)\,|\varphi_p(x)|^2\,dp$$

$$J(x) = \frac{h}{m}\int_0^{\infty} G_1(p)\,\mathscr{I}m(\bar{\psi}_p(x)\,\psi_p'(x))\,dp + \frac{h}{m}\int_0^{\infty} G_2(p)\,\mathscr{I}m(\bar{\varphi}_p(x)\,\varphi_p'(x))\,dp$$

To study the semiclassical limit of this system, we introduce the Wigner transform (see ref. 7)

$$f^h(x, p) = \int_0^{+\infty} G_1(q)\,\mathscr{W}_h[\mathscr{O}\psi_q](x, p)\,dq + \int_0^{+\infty} G_2(q)\,\mathscr{W}_h[\mathscr{O}\varphi_q](x, p)\,dq \tag{2.13}$$

with the notation

$$\mathscr{W}_h[\psi](x,p)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\eta p}\bar{\psi}\left(x+h\frac{\eta}{2}\right)\psi\left(x-h\frac{\eta}{2}\right)d\eta \qquad (2.14)$$

and where $\mathcal{O}$ is a localizing function

$$\mathcal{O}\in C_0^{\infty}(\mathbb{R}),\quad \mathcal{O}\geqslant 0,\quad \mathcal{O}=1,\qquad \text{on}\quad [x_1-\alpha, x_2+\alpha]$$

For some positive α. The macroscopic densities n, j can be shown to be the zero-th and the first moments of f^h

$$n(x)=\int_{-\infty}^{+\infty} f^h(x,p)\,dp,\qquad j(x)=j=\int_{-\infty}^{+\infty}\frac{p}{m}f^h(x,p)\,dp,\qquad x\in[x_1,x_2]$$

The role of the localizing function $\mathcal{O}$ is to provide a regular Wigner function for our problem. Let us note that the macroscopic quantities $n(x)$ and $j(x)$ do not depend on $\mathcal{O}$ for $x\in[x_1,x_2]$ and that the restriction to $[x_1,x_2]$ of the limit as h tends to zero of f^h does not depend on $\mathcal{O}$ (see ref. 20).

By the method used in ref. 7, it can be proven that as h tends to zero, f^h converges formally to the solution f of the Vlasov equation (2.1) with the boundary condition

$$f(x_1,p)=G_1(p)\quad \text{for } p>0,\qquad f(x_2,-p)=G_2(p)\quad \text{for } p>0 \qquad (2.15)$$

A rigorous proof in the case $G_2=0$ and G_1 small can be found in ref. 7. Let us recall how boundary conditions are recovered. For the sake of simplicity we first assume that $G_2=0$. To compute $f^h(x_1,p)$, we need to know $\psi_q(x_1+h(\eta/2))$. But it is readily seen by rescaling the Schrödinger equation that the formula $\psi_q(x_1+h\eta)=e^{iq\eta}+r_q e^{-iq\eta}$ which is rigorously satisfied for $\eta<0$ is a good approximation for $\eta>0$ lying in a bounded interval and h small enough. Using this asymptotic expression to compute $f^h(x_1,p)$ we find after some straightforward computations that

$$f^h(x_1,p)\simeq G_1(p),\qquad f^h(x_1,-p)\simeq R_{p,1}G_1(p)\qquad (p>0)\quad (2.16)$$

where $R_{p,1}$ is given by (2.4). Taking into account the fact that G_2 is not equal to zero, and by using the asymptotic expression $\varphi_p(x_1+h\eta)=t_p e^{-i\sqrt[+]{p^2-2em(V_2-V_1)}\,\eta}$ we find after some computations $f^h(x_1,-p)\simeq R_{p,1}G_1(p)+T_{p_2,2}G_2(p_2)$ where

$$p_2=\sqrt[+]{p^2+2em(V_2-V_1)} \qquad (2.17)$$

and with the convention $G_2(p_2) = 0$ when p_2 is imaginary. Consequently, we have the following asymptotic formula

$$f^{\hbar}(x_1, -p) \simeq R_{p,1} + f^{\hbar}(x_1, p) + T_{p_2,2} G_2(p_2)$$

To obtain a complete analogy with formula (2.2) we shall use the reciprocity of the transmission coefficients (see ref. 29).

Lemma 2.3. Let $p_2(p, V)$ be defined by (2.17). Assume that p_2 is real. Let ψ_p and φ_{p_2} be the unique solutions of the absorption Schrödinger equations (2.9) and (2.10). (p has to be replaced by p_2 in (2.10)). Then $T^{v}_{p,1} = T^{v}_{p_2,2}$.

Proof. First, we notice that in view of (2.17), ψ_p and φ_{p_2} solve the same Schrödinger equation. Hence their Wronskian is constant. Comparing its values at $x = x_1$ and $x = x_2$ leads to $p_2 \psi_p(x_2) = -p \varphi_{p_2(p, V)}(x_1)$ which yields the desired identity. ∎

In view of Lemma 2.3 we have the asymptotic formula

$$\begin{aligned} f^{\hbar}(x_1, -p) &\simeq R_{p,1} f^{\hbar}(x_1, p) + T_{p,1} G_2(p_2) \\ &= R_{p,1} f^{\hbar}(x_1, p) + T_{p,1} f^{\hbar}(x_2, -p_2) \end{aligned} \tag{2.18}$$

which is in complete analogy with (2.2).

3. A HYBRID MODEL FOR A 2-ZONE DEVICE

In this section we consider a device extending on an interval $[0, L]$ such that $[0, x_1]$ is a **C** zone and $[x_1, L]$ is a **Q** zone. We shall set $x_2 = L$ in all this section. In the **Q** zone, the description will rely on the wave functions ψ_p and φ_p defined by (2.9)–(2.10). Notice that the fundamental hypothesis to derive the boundary conditions involved in (2.9)–(2.10) is that the electrostatic potential V is constant outside the interval $[x_1, x_2]$. This hypothesis is fulfilled at $x = x_2$ if we consider that the medium $x > x_2$ has a very large conductivity (metal or highly doped region). At $x = x_1$, this argument does not hold since x_1 is an artificial boundary. However, x_1 is chosen to be a transition point between a classical description and a quantum one. Therefore, a WKB approximation should be appropriate near x_1 which implies that the potential variation is small. This gives an indication that the boundary conditions involved in (2.9)–(2.10) are reasonable. Of course, this assertion needs to be made more precise by looking at orders of magnitude in order to get a quantitative criterion for the location of the **Q**–**C** interface.

Let f_C be the distribution function in the **C** zone $[0, x_1]$ and f_Q be the Wigner function in the **Q** zone. According to the results of ref. 7 recalled in the previous section, f_Q is defined by

$$f_Q(x, p) = \int_0^{+\infty} f_C(x_1, q)\, \mathscr{W}_\hbar[\mathcal{O}\psi_q](x, p)\, dq + \int_0^{+\infty} G_2(q)\, \mathscr{W}_\hbar[\mathcal{O}\varphi_q](x, p)\, dq$$

where $G_2(p)$ is the statistics of particles emitted at $x = x_2 = L$. Inspired by the analogy between (2.2) and (2.18), we impose the following boundary condition on f_C at $x = x_1$

$$f_C(x_1, -p) = R_{p,1} f_C(x_1, p) + T_{p,1} G(p_2) \tag{3.1}$$

In order that the interface condition above to be physically admissible, the first thing that has to be checked is the current conservation at the interface $x = x_1$. This is done in the following Lemma

Lemma 3.1. The currents $J_C(x)$ and $J_Q(x)$ computed respectively in the **C** and the **Q** zone coincide at the **Q–C** interface $J_C(x_1) = J_Q(x_1)$.

Proof. We recall that

$$J_C(x) = \int_{\mathbb{R}} \frac{p}{m} f_C(x, p)\, dp$$

and

$$J_Q(x) = \int_{\mathbb{R}} \frac{p}{m} f_Q(x, p)\, dp = \frac{\hbar}{m} \int_0^{+\infty} f_C(x_1, p)\, \mathscr{I}m(\bar{\psi}_p(x)\, \psi'_p(x))\, dp$$
$$+ \frac{\hbar}{m} \int_0^{+\infty} G_2(p)\, \mathscr{I}m(\bar{\varphi}_p(x)\, \varphi'_p(x))\, dp$$

Using the boundary conditions of (2.9) and (2.10), we find

$$\hbar\, \mathscr{I}m(\bar{\psi}_p(x_1)\, \psi'_p(x_1)) = p(1 - R_{p,1}), \qquad \hbar\, \mathscr{I}m(\bar{\varphi}_p(x_1)\, \varphi'_p(x_1)) = -pT_{p,2}$$

This yields

$$J_Q(x_1) = \int_0^{+\infty} \frac{p}{m} (1 - R_{p,1})\, f_C(x_1, p)\, dp - \int_0^{+\infty} \frac{p}{m} T_{p,2} G(p)\, dp$$

In the last integral, we make the change of variable $p = p_2(p', V)$. Recalling that $p\,dp = p'\,dp'$ we claim that, dropping the primes, we have

$$J_Q(x_1) = \int_0^{+\infty} \frac{p}{m}(1 - R_{p,1})\, f_C(x_1, p)\, dp - \int_0^{+\infty} \frac{p}{m} T_{p_2,2} G(p_2)\, dp$$

Indeed, the above formula is obvious except for the lower bound of the last integral. To prove that it is equal to zero, we distinguish two cases.

- If $V_1 \leqslant V_2$, then $p_2(0, V) \in \mathbb{R}^+$ and consequently $T_{p,2}$ given by (2.10) is equal to zero if $p < p_2(0, V)$. Therefore

$$\int_0^{+\infty} \frac{p}{m} T_{p,2} G(p)\, dp = \int_{p_2(0,V)}^{+\infty} T_{p,2} G(p)\, dp$$

The change of variable $p = p_2(p', V)$ gives the desired lower bound (that is zero).

- If $V_2 \leqslant V_1$ then $p_2(0, V)$ is imaginary. We then have

$$\int_0^{+\infty} \frac{p}{m} T_{p,2} G(p)\, dp = \int_{\sqrt{2em(V_1 - V_2)}}^{+\infty} \frac{p}{m} T_{p_2,2} G(p_2)\, dp$$

and since p_2 is imaginary for $0 < p < \sqrt{2em(V_1 - V_2)}$, we have

$$\int_{\sqrt{2em(V_1 - V_2)}}^{+\infty} \frac{p}{m} T_{p_2,2} G(p_2)\, dp = \int_0^{+\infty} \frac{p}{m} T_{p_2,2} G(p_2)\, dp$$

Now it is readily seen from (3.1), that

$$\begin{aligned} J_C(x_1) &= \int_0^{+\infty} \frac{p}{m}(1 - R_{p,1})\, f_C(x_1, p)\, dp - \int_0^{+\infty} \frac{p}{m} T_{p,1} G(p_2)\, dp \\ &= J_Q(x_1) \end{aligned}$$

∎

In view of the interface conditions defined above, the hybrid model for a two zone device consists in solving for f_C and f_Q the following system

$$\frac{p}{m}\frac{\partial f_C}{\partial x} + e\frac{dV}{dx}\frac{\partial f_C}{\partial p} = \mathcal{Q}(f_C) \tag{3.2}$$

for $x \in [0, x_1]$ and $p \in \mathbb{R}$ with the boundary conditions

$$f_C(0, p) = G_\circ(p), \qquad f_C(x_1, -p) = R_{p,1} f_C(x_1, p) + T_{p,1} G_2(p_2) \tag{3.3}$$

where $R_{p,1}$ and $T_{p,1}$ are given by (2.8) and $p_2(p, V)$ is defined by (2.17). In the **Q** region, the electrons are described by the Wigner function

$$f_Q(x, p) = \int_0^{+\infty} G_2(q)\, \mathscr{W}_h[\mathscr{C}\varphi_q](x, p)\, dq + \int_0^{+\infty} f_C(x_1, q)\, \mathscr{W}_h[\mathscr{C}\psi_q](x, p)\, dq \tag{3.4}$$

Finally ψ_p and φ_p are given by (2.3) and (2.6). The collision operator $\mathscr{Q}$ is taken under the form

$$\begin{aligned}\mathscr{Q}(f) = \int_{\mathbb{R}} s(x, p, p')[M_T(p)\, f(x, p')(1 - \varepsilon f(x, p)) \\ - M_T(p')\, f(x, p)(1 - \varepsilon f(x, p'))]\, dp'\end{aligned} \tag{3.5}$$

where $M_T(p) = C \exp(-p^2/2mk_B T)$ is the Maxwellian with the lattice temperature. The Pauli exclusion principle can be taken or not into account ($\varepsilon \geqslant 0$). We assume (see ref. 33)

$$\begin{cases} s(x, p', p) = s(x, p, p') \geqslant 0 \\ M_T(p)\, s(x, p, p') \in L_x^\infty(L^2(\mathbb{R}^2)) \\ \sigma(x, p) = \int_{\mathbb{R}} s(x, p, p')\, M_T(p')\, dp' \in L^\infty([0, L] \times \mathbb{R}) \end{cases} \tag{3.6}$$

When $s > 0$ everywhere, the kernel of Q is equal to the set of Fermi–Dirac functions with the lattice temperature

$$\mathscr{F}_\mu(p) = \frac{1}{\varepsilon + \exp((p^2/2m - e\mu)/k_B T)} \tag{3.7}$$

In general, the problem (3.2)–(3.3) does not have a unique solution. By adding an absorption in the spirit of refs. 33 and 35 we obtain the following result.

Theorem 3.2. Let V be a given potential in $C^2([0, x_1])$ and continuous in the vicinity of x_2 and let $R_{p,1}$ and $T_{p,1}$ be nonnegative real functions of p such that $R_{p,1} + T_{p,1} \leqslant 1$. Assume there exists $\mu \in \mathbb{R}$ such that

$$0 \leqslant G_o(p) \leqslant \mathscr{F}_{\mu + V(0)}(p), \qquad 0 \leqslant G_2(p) \leqslant \mathscr{F}_{\mu + V_2}(p)$$

Then, for every positive ν the modified equation

$$\frac{p}{m}\frac{\partial f}{\partial x}+e\frac{dV}{dx}\frac{\partial f}{\partial p}+\nu f=\mathcal{Q}(f)$$

on $[0, x_1]$ with the boundary conditions (3.3) admits a unique solution f_C satisfying

$$0 \leqslant f_C(x, p) \leqslant \mathcal{F}_{\mu+V(x)}(p)$$

Proof. We first deduce from (2.17) that $G_2(p_2(p, V)) \leqslant \mathcal{F}_{\mu+V_1}(p)$. Let us now define

$$X=\{f(x, p)\ 0 \leqslant f(x, p) \leqslant \mathcal{F}_{\mu+V(x)}(p)\}$$

Starting from $g \in L^\infty(\mathbb{R}^+)$ (a guess for $f_C(x_1, p)$) such that $g(p) \leqslant \mathcal{F}_{\mu+V_1}(p)$, we look for a solution solution f in X of

$$\frac{p}{m}\frac{\partial f}{\partial x}+e\frac{dV}{dx}\frac{\partial f}{\partial p}+\nu f=\mathcal{Q}(f)$$

with the boundary conditions

$$\begin{cases} f(0, p)=G_\circ(p) & p>0 \\ f(x_1, -p)=R_{p,1}g(p)+T_{p,1}G(p_2) & p>0 \end{cases}$$

The relation $R_{p,1}+T_{p,1} \leqslant 1$ implies that $f(x_1, -p) \leqslant \mathcal{F}_{\mu+V_1}(p)$. We then apply Theorem 2.1 of ref. 33 and get a unique solution f in X. Let now $g^*(p)=f(x_1, p)$. Then f is a solution of the Boltzmann equation subject to the boundary conditions of Theorem 3.2 if and only if $g^*=g$. To prove the existence of such a g, we adopt a fixed point procedure. However, this cannot be done immediately because of the lack of compactness (with respect to p). To overcome this difficulty, we regularize g^* by a convolution procedure $g^*_\alpha=\rho_\alpha * g^*$ where ρ_α is a nonnegative C^∞ approximation of the Dirac measure. The kernel ρ_ε has to be chosen carefully in order to preserve the supersolution estimate

$$0 \leqslant g^*_\alpha(p) \leqslant \mathcal{F}_{\mu+V_1}(p)$$

Using the decay on $\mathbb{R}^+$ of the Fermi–Dirac distribution $\mathcal{F}_\mu$, it is readily seen that if supp $\rho_\alpha \subset \mathbb{R}_-$ then $[\rho_\varepsilon * \mathcal{F}_\mu](p) \leqslant \mathcal{F}_\mu(p)$ for $p \geqslant 0$. This gives compactness an allow to construct an approximate solution of the problem. Afterwards, we pass to the limit $\varepsilon \to 0$.

To prove uniqueness of solutions in X, we proceed like in ref. 33. We assume that f and g are two solutions, we write the difference between the two Boltzmann equations, multiply it by sgn(f−g) and integrate over x and p. Taking advantage of the inequality

$$\int_{\mathbb{R}} (\mathcal{Q}(f) - \mathcal{Q}(g)) \operatorname{sgn}(\mathrm{f}-\mathrm{g})\, \mathrm{dp} \leqslant 0$$

proven in ref. 33, we find

$$\nu \int |f-g|\, dx\, dp + \int_{-\infty}^{+\infty} \frac{p}{m} (|f(x_1, p) - g(x_1, p)| - |f(0, p) - g(0, p)|)\, dp \leqslant 0$$

Using the boundary conditions (3.1), we end with the following estimate

$$\nu \int |f-g|\, dx\, dp + \int_0^{+\infty} \frac{p}{m} (1 - R_{p,1})\, |f(x_1, p) - g(x_1, p)|\, dp - \int_{-\infty}^{0} \frac{p}{m} |f(0, p) - g(0, p)|\, dp \leqslant 0$$

which implies that $f = g$ since $R_{p,1} \leqslant 1$. ∎

4. A HYBRID MODEL FOR A 3-ZONE DEVICE

We consider now a device extending on the interval $[0, L]$ and let $0 \leqslant x_1 < x_2 \leqslant L$ such that $[0, x_1]$ and $[x_2, L]$ are the **C** zones and $[x_1, x_2]$ is the **Q** zone. We assume that the potential V is given, is regular in the **C** zones and satisfies $V(0) = 0$ and $V(L) = V_L \geqslant 0$. Before going on, we introduce a new notation

$$p_1(p, V) = \sqrt[+]{p^2 - 2emV_2 + 2emV_1} \tag{4.1}$$

It is readily seen that $-p_1$ is the momentum at $x = x_1$ of an electron injected at x_2 with a momentum $-p$ and which is submitted to the potential V. Analogously, the momentum $p_2(p, V)$ defined in (2.17) is that at x_2 of a particle having the momentum p at x_1. A direct application of Lemma 2.3 and the relation $p_1(p_2(p, V), V) = p_2(p_1(p, V), V) = p$, gives

Lemma 4.1. Let $p_1(p, V)$ be defined by (4.1) and assume it is real. Let φ_p and ψ_{p_2} be the unique solutions of the absorption Schrödinger equations (2.10) and (2.9). (p has to be replaced by p_1 in (2.9)). Then $T^{\nu}_{p_1,1} = T^{\nu}_{p,2}$.

Writing the interface conditions of the previous section at $x = x_1$ and their analogue at $x = x_2$, we obtain the following hybrid model

$$\begin{cases} \dfrac{p}{m}\dfrac{\partial f_C}{\partial x} + e\dfrac{dV}{dx}\dfrac{\partial f_C}{\partial p} + \nu f_C = \mathcal{Q}(f_C), \qquad x \in [0, x_1] \cup [x_2, L] \\ f_C(0, p) = G_\circ(p), \qquad f_C(L, -p) = G_L(p), \qquad p > 0 \\ f_C(x_1, -p) = R^{\nu}_{p,1} f_C(x_1, p) + T^{\nu}_{p,1} f_C(x_2, -p_2(p, V)), \qquad p > 0 \\ f_C(x_2, p) = R^{\nu}_{p,2} f_C(x_2, -p) + T^{\nu}_{p,2} f_C(x_1, p_1(p, V)), \qquad p > 0 \end{cases} \tag{4.2}$$

where $\nu \geqslant 0$ and the reflection transmission coefficients $R_{p,i}$ and $T_{p,i}$ $(i = 1, 2)$ are given by (2.4)–(2.8). Moreover the Wigner function in the **Q** zones is equal to

$$f_Q(x, p) = \int_{\mathbb{R}^+} f_C(x_1, q)\, \mathscr{W}_\hbar[\mathcal{O}\psi_q](x, p)\, dq + \int_{\mathbb{R}^+} f_C(x_2, -q)\, \mathscr{W}_\hbar[\mathcal{O}\varphi_q](x, p)\, dq \tag{4.3}$$

Here again, we can show that the currents computed in the quantum regions and classical regions have the same value at the interface. Also, thanks to the inequality $R_{p,i} + T_{p,i} \leqslant 1$, we can prove, in the same spirit as that of Theorem 3.2, existence and uniqueness of solutions of (4.2). More precisely,

Theorem 4.2. Let V be a given potential in $C^2([0, x_1] \cup [x_2, L])$ and let $R^{\nu}_{p,1}$, $T^{\nu}_{p,1}$, $R^{\nu}_{p,2}$ and $T^{\nu}_{p,2}$ be nonnegative real functions of p such that $R^{\nu}_{p,i} + T^{\nu}_{p,i} \leqslant 1$. Assume there exists $\mu \in \mathbb{R}$ such that

$$0 \leqslant G_o(p) \leqslant \mathscr{F}_{\mu + V(0)}(p), \qquad 0 \leqslant G_L(p) \leqslant \mathscr{F}_{\mu + V_L}(p)$$

Then, for every positive ν the system (4.2) admits a unique solution f_C satisfying

$$0 \leqslant f_C(x, p) \leqslant \mathscr{F}_{\mu + V(x)}(p)$$

Proof. The proof of uniqueness follows in analogy with that of Theorem 2.17. For existence, we shall only give the iteration procedure. Starting from an initial guess $g(p)$ for $f_C(x_2, -p)$ with $p > 0$ satisfying

$g(p) \leqslant \mathscr{F}_{\mu+V_2}$, we apply Theorem 3.2 and find a unique solution f_1 of the Boltzmann equation on $[0, x_1]$ with $G_\circ$ as inflow boundary condition at $x=0$ and with the boundary condition at x_1

$$f_1(x_1, -p) = R^{\nu}_{p,1} f_1(x_1, p) + T^{\nu}_{p,1} g(p_2(p, V))$$

Afterwards, we construct the unique solution f_2 of the Boltzmann equation on $[x_2, L]$ with the boundary condition

$$f_2(x_2, p) = R^{\nu}_{p,2} g(p) + T^{\nu}_{p,2} f_1(x_1, p_1(p, V)), \qquad p > 0$$

Then, we set $g^*(p) = f_2(x_2, -p)$. The functions f_1, f_2 are the solution of (4.2) if and only if $g^* = g$. To prove the existence of a solution, we regularize g^* like in the proof of Theorem 3.2 apply the Schauder fixed point theorem and then pass to the limit in the regularization. ∎

4.1. Existence Result for a Self-Consistent Potential

We consider the system (4.2)–(4.3) where the potential V is computed self consistently. Namely, we set $V = V_e + V_s$ where V_e is a given exterior potential, which includes the double barrier (if any), the doping effects and the applied voltage. The discontinuities of V_e (for instance due to a double barrier) are assumed to be strictly included in $[x_1, x_2]$ so that V_e is regular on the **C** zones. The self consistent potential V_s is the solution of the Poisson equation

$$-\frac{d}{dx}\left(\epsilon \frac{dV_s}{dx}\right) = -en(x), \qquad n(x) = \int_{\mathbb{R}} f(x, p)\, dp \tag{4.4}$$

with the homogeneous boundary conditions

$$V_s(0) = V_s(L) = 0 \tag{4.5}$$

In the above equation, ϵ is the permittivity of the material and is a function of x which may be discontinuous. We shall however assume that it is C^1 in the **C** zones. More precisely, we make the following hypotheses

(i) $V_e \in L^\infty([0, L]) \cap W^{2,\infty}([0, x_1] \cup [x_2, L])$ V_e is continuous at x_1, x_2 and $V_e(0) = 0$, $V_e(L) = V_L$

(ii) ϵ is in $L^\infty([0, L] \cap C^1([0, x_1] \cup [x_2, L])$ and $\epsilon(x) \geqslant c$ on $[0, L]$ for some $c > 0$.

Theorem 4.3. Under the hypotheses (i) (ii) and the hypothesis

$$0 \leqslant G_o(p) \leqslant \mathscr{F}_\mu(p), \qquad 0 \leqslant G_L(p) \leqslant \mathscr{F}_{\mu + V_L}(p)$$

the problem (4.1)–(4.5), (2.9), (2.10), (2.8), (2.4) admits a solution for each $\nu \geqslant 0$, which satisfies

$$0 \leqslant f_C(x, p) \leqslant \mathscr{F}_{\mu + V(x)}(p)$$

Proof. We shall only give the a priori estimates allowing to construct a fixed point mapping needed two prove existence of solutions.

• *Case of* $\nu > 0$. We shall prove that the potential V_s lies in a bounded set. First, we notice that V_s is nonpositive because the electron density n is nonnegative. This implies, in view of the supersolution estimate, that the electron density is in a bounded set of $L^\infty([0, x_1] \cup [x_2, L])$. Moreover, since n is given in the **Q** zone by

$$n(x) = \int_0^\infty f_C(x_1, p)\, |\psi_p(x)|^2\, dp + \int_0^\infty f_C(x_2, -p)\, |\varphi_p(x)|^2\, dp$$

and since by (2.11), (2.12) we have

$$0 \leqslant \int_{x_1}^{x_2} |\psi_p(x)|^2\, dp + \int_{x_1}^{x_2} |\varphi_p(x)|^2\, dp \leqslant \frac{2p}{\nu m}$$

we deduce from the bound of Theorem 4.2 on f that n is in a bounded set of $L^1((x_1, x_2))$ (depending on ν). As a conclusion, we have

$$\|n\|_{L^\infty([0, x_1] \cup [x_2, L])} \leqslant C, \qquad \|n\|_{L^1(x_1, x_2)} \leqslant \frac{C}{\nu} \tag{4.6}$$

where C is a constant independent of ν. Consequently, V_s is bounded in $W^{2,1}(0, L)$. This estimate allows to construct a fixed point mapping and gives by the Schauder fixed point theorem a solution of the hybrid model with $\nu > 0$.

• *Case of* $\nu = 0$. When $\nu \to 0$, the a priori estimate on V_s blows up. To obtain a better one, we begin by enumerating some simple facts that can be checked easily by noticing that $\epsilon V_s'(x)$ is increasing on $[0, L]$, that n is bounded in L^∞ in the **C** zones and that in the **C** zone, $n(x) \to 0$ if $V_s(x) \to -\infty$.

- **Fact 1.** V_s is bounded in L^∞ if and only if $V_s(x_1)$ is bounded
- **Fact 2.** $V_s(x_1)$ is bounded if and only if $V_s(x_2)$ is bounded.
- **Fact 3.** if V_s is not bounded in L^∞ then, min $V_s \sim V_s(x_1) \sim V_s(x_2) \sim V_s'(x_1) \sim -V_s'(x_2)$. By the notation $A \sim B$, we mean that $c \leqslant A/B \leqslant C$ for some positive constants c and C.

Lemma 4.4. Let θ be a function satisfying $|\theta''| \leqslant M^2 |\theta|$ on the interval $[0, A]$. Then θ satisfies the following bound

$$|\theta(x)| \leqslant (|\theta(0)| + A\,|\theta'(0)|)\, e^{Mx}, \qquad x \in [0, A]$$

Let us use the above lemma to give some bounds on ψ_p and φ_p. For this aim, we first remark that (2.11)(2.4) together with the boundary condition (2.9) imply

$$|\psi_p(x_1)| \leqslant 2, \qquad |\hbar\psi_p'(x_1)| \leqslant 2p$$

Applying Lemma 4.4 to equation (2.9) leads to the bound

$$\|\psi_p\|_{L^\infty(x_1, x_2)} \leqslant (1+p) \exp(C(1 + p + \sqrt{\|V\|_{L^\infty}}))$$

where C is a constant which does not depend on v. Analogously, one can prove that

$$\|\varphi_p\|_{L^\infty(x_1, x_2)} \leqslant (1+p) \exp(C(1 + p + \sqrt{\|V\|_{L^\infty}}))$$

Since the charge density in the **Q** zone is $n(x) = n_1(x) + n_2(x)$ where

$$n_1(x) = \int_0^{+\infty} f_C(x_1, p)\, |\psi_p(x)|^2\, dp, \qquad n_2(x) = \int_0^{+\infty} f_C(x_2, -p)\, |\varphi_p(x)|^2\, dp$$

we can use the estimate $f_C(x, p) \leqslant \mathscr{F}_{\mu + V(x)}(p)$ to get

$$\begin{aligned} \|n_1\|_{L^\infty(x_1, x_2)} &\leqslant \int_0^{+\infty} (1+p)^2\, e^{-(p^2/2m) + e\mu + eV_1 + 2C(1 + p + \sqrt{\|V\|_{L^\infty}})}\, dp \\ &\leqslant C e^{eV_1 + 2C\sqrt{\|V\|_{L^\infty}}} \end{aligned} \tag{4.7}$$

Let us now assume that V_s in not bounded. This means according to Facts 1, 2, 3 that

$$V_s(x_1),\ V_s(x_2) \to -\infty, \qquad \|V\|_{L^\infty} \sim -V_s(x_1) \sim -V_s(x_2)$$

This implies that the right hand side of (4.7) tends to zero. Proceeding analogously for n_2, we conclude that n is bounded in L^∞ whereas V_s is unbounded in L^∞. This is obviously in contradiction with the Poisson equation (4.4)(4.5).

Consequently, V_s is bounded in L^∞ which in turn implies the boundedness of n in L^∞ in view of (4.7). In view of the Poisson equation, V_s converges strongly in C^0 in the **Q** zone and in C^1 in the **C** zones. Passing to the limit $\nu \to 0$ leads to a solution of the self-consistent hybrid model (4.1)–(4.5), (2.6)(2.8), (2.3)(2.4). The details of the proof, especially proving that the formula giving the charge density in the **Q** zone passes to the limit, are left to the reader. ▮

4.2. Semiclassical Limit

We will pass to the limit h to zero in (4.2) and obtain a kinetic model on the whole interval $[0, L]$. Due to the lack of estimates induced by turning points, we shall prove the result when the electric potential V is given (and regular) and when the absorption ν is fixed and strictly positive. We let f^h, ψ_p^h, φ_p^h, be the solutions of Theorem 4.2. Before stating the main theorem of this section, we introduce the following Banach space $\mathscr{A} = \{\theta = \theta(x, v) \mid (\hat{\theta}(x, \eta) \in L^1(\mathbb{R}_\eta; C_0([x_1, x_2]_x))\}$, (see ref. 26), where $\hat{\theta}$ denotes the Fourier transform with respect to v

$$\hat{\theta}(x, \eta) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i\eta v} \theta(x, v)\, dv, \qquad \|\theta\|_{\mathscr{A}} = \int_{-\infty}^{+\infty} \sup_{x \in (x_1, x_2)} |\hat{\theta}(x, \eta)|\, d\eta$$

We shall assume the following hypothesis on the electrostatic potential

Hypothesis (H)

If $V_2 < V_1$, there exists an interval $\mathscr{I} = [x_2 - \varepsilon, x_2]$ on which $V \leqslant V_2$.
If $V_1 < V_2$, there exists an interval $\mathscr{I} = [x_1, x_1 + \varepsilon]$ on which $V \leqslant V_1$.

Theorem 4.5. Let $f^h = (f_C^h, f_Q^h)$ be the solution of the hybrid model (4.2), (4.3) with $\nu > 0$ fixed and $V \in C^2[0, L]$ and satisfies hypothesis (H). Then f^h converges weakly in $L^\infty([(0, x_1) \cup (x_2)] \times \mathbb{R})$ and in $\mathscr{A}'$ towards the unique solution f of

$$\begin{cases} \dfrac{p}{m} \dfrac{\partial f}{\partial x} + e \dfrac{dV}{dx} \dfrac{\partial f}{\partial p} + \nu f = \mathscr{Q}(f), & x \in [0, L] \\ f(0, p) = G_\circ(p), \qquad f(L, -p) = G_L(p), & p > 0 \\ \mathscr{Q}(f) = 0, \qquad x \in [x_1, x_2] \end{cases} \tag{4.8}$$

which satisfies $0 \leqslant f(x, p) \leqslant \mathscr{F}_{\mu + V(x)}$.

Proof. The proof is organized in three steps. First we prove the convergence in the **C** zones of f_C^h to a distribution function f_C satisfying the Boltzmann equation. Then we prove that in the **Q** zone f_Q^h converges to f_Q solution of the Vlasov equation. Finally we check that $f_C = f_Q$ at the interface. The first step is straightforward thanks to the supersolution estimate (the convergence of the collision operator is done like in ref. 33 by means of average compactness results).

To pass to the limit in the **Q** zone, we proceed analogously to ref. 7, but some additional effort has to be done because the wave functions ψ_p are only bounded in $L^2(x_1, x_2)$ whereas in ref. 7 they are bounded in L^∞. The L^2 bounds imply however the weak convergence in $\mathscr{A}'$ of f_Q^h to a positive measure f_Q on $[x_1, x_2] \times \mathbb{R}$. To derive the problem that the measure f solves, we proceed like in ref. 7 and compute the expression $(p/m)(\partial f^h/\partial x)$. By denoting

$$\mathscr{W}_h[a, b] = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i\eta p} \bar{a}\left(x + h\frac{\eta}{2}\right) b\left(x - h\frac{\eta}{2}\right) d\eta \tag{4.9}$$

we find after some simple algebra that

$$\begin{aligned}
\frac{p}{m}\frac{f_Q^h}{\partial x} = &\frac{-h}{m}\int_{\mathbb{R}^+} f_C^h(x_1, q)\, \mathscr{I}m\{\mathscr{W}_h[\mathcal{O}\psi_q'', \mathcal{O}\psi_q]\}\, dq \\
&-\frac{h}{m}\int_{\mathbb{R}^+} f_C^h(x_2, -q)\, \mathscr{I}m\{\mathscr{W}_h[\mathcal{O}\varphi_q'', \mathcal{O}\varphi_q]\}\, dq \\
&-\frac{h}{m}\int_{\mathbb{R}^+} f_C^h(x_1, q)\, \mathscr{I}m\{\mathscr{W}_h[\mathcal{O}''\psi_q, \mathcal{O}\psi_q] \\
&+ 2\mathscr{W}_h[\mathcal{O}'\psi_q', \mathcal{O}\psi_q]\}\, dq \\
&-\frac{h}{m}\int_{\mathbb{R}^+} f_C^h(x_2, -q)\, \mathscr{I}m\{\mathscr{W}_h[\mathcal{O}''\varphi_q, \mathcal{O}\varphi_q] \\
&+ 2\mathscr{W}_h[\mathcal{O}'\varphi_q', \mathcal{O}\varphi_q]\}\, dq
\end{aligned} \tag{4.10}$$

Since

$$\|\psi_q\|_{L^2(x_1, x_2)}^2, \qquad \|\varphi_q\|_{L^2(x_1, x_2)}^2 \leqslant \frac{q}{mv}$$

we deduce from the Schrödinger equation (2.9)–(2.10) that

$$\|\psi_q''\|_{L^2(x_1, x_2)}, \qquad \|\varphi_q''\|_{L^2(x_1, x_2)} \leqslant \frac{C}{h^2} q^{1/2}(1+q^2)$$

Hence

$$h^2 \|\psi_q'\|^2_{L^2(x_1, x_2)} + h^2 \|\varphi_q'\|^2_{L^2(x_1, x_2)} \leqslant Cq(1+q^2) \tag{4.11}$$

Since $\mathcal{O}$ is identically equal to 1 on $[0, L]$, the term

$$r^h(x, p) = \frac{-h}{m} \int_0^{+\infty} f_C^h(x_1, q)\, \mathcal{I}m\{\mathcal{W}_h[\mathcal{O}''\psi_q, \mathcal{O}\psi_q] + 2\mathcal{W}_h[\mathcal{O}'\psi_q', \mathcal{O}\psi_q]\}(x, p)\, dq$$

satisfies

$$\lim_{h \to 0} \int_{x_1}^{x_2} \int_{\mathbb{R}} r^h(x, p)\, \theta(x, p)\, dx\, dp = 0$$

for $\theta \in C_0^\infty(\mathbb{R} \times \mathbb{R})$. This result is obtained by applying corollary A.3. Indeed, the term $h\mathcal{W}_h[\mathcal{O}''\psi_q, \mathcal{O}\psi_q]$ can be written $\mathcal{W}_h[H\psi, \phi]$ where $H = \mathcal{O}''$, $\psi = h\psi_q$ and $\varphi = \mathcal{O}\psi_q$ satisfy the requirement of corollary A.3. The term $h\mathcal{W}_h[\mathcal{O}'\psi_q', \mathcal{O}\psi_q]$ is treated analogously. Hence, going back to (4.10) (where the fourth term of the right hand side is treated as above), we get

$$\frac{p}{m}\frac{\partial f_Q^h}{\partial x} = \frac{-h}{m} \int_0^{+\infty} f_C^h(x_1, q)\, \mathcal{I}m\, \mathcal{W}_h[\mathcal{O}\psi_q'', \mathcal{O}\psi_q]\, dq - \frac{h}{m} \int_0^{+\infty} f_C^h(x_2, -q)\, \mathcal{I}m\, \mathcal{W}_h[\mathcal{O}\varphi_q'', \mathcal{O}\varphi_q]\, dq + r'^{,h} \tag{4.12}$$

where $r'^{,h}$ satisfies

$$\lim_{h \to 0} \int_{x_1}^{x_2} \int_{\mathbb{R}} r'^{,h}(x, p)\, \theta(x, p)\, dx\, dp = 0$$

Let us now pass to the limit in $\mathcal{I}m\, \mathcal{W}_h[\mathcal{O}\psi_q'', \mathcal{O}\psi_q]$. For this aim we recall that the boundary conditions (2.9), imply that ψ_p is a solution on $(-\infty, x_1)$ of the same Schrödinger equation except that v has to be set to zero and $V(x)$ replaced by V_1. On $(x_2, +\infty)$ $V(x)$ has to be set to V_2. Introducing the notation

$$\bar{V}(x) = \begin{cases} V(x), & x_1 \leqslant x \leqslant x_2 \\ V_1, & x \leqslant x_1 \\ V_2, & x \geqslant x_2 \end{cases} \qquad H(x) = \begin{cases} 0, & x_1 \leqslant x \leqslant x_2 \\ 1, & x \leqslant x_1 \\ 1, & x \geqslant x_2 \end{cases} \tag{4.13}$$

we can write the equation satisfied by ψ_p on the whole real line

$$-\frac{h^2}{2m}\psi_p''(x) - e\bar{V}(x)\,\psi_p = \left(\frac{p^2}{2m} - e\bar{V}(x_1)\right)\psi_p + ih(1 - H(x))\frac{v}{2}\psi_p(x) \tag{4.14}$$

Using this equation, we obtain after some straightforward but lengthy calculations

$$\frac{-h}{m}\mathscr{I}m\,\mathscr{W}_h[\mathcal{O}\psi_q'', \mathcal{O}\psi_q] + e\frac{dV}{dx}\mathscr{W}_h[\mathcal{O}\psi_q] + v\mathscr{W}_h[\mathcal{O}\psi_q] = r_1^h + r_2^h$$

where

$$r_1^h(x, p) = \frac{-ie}{2\pi}\int_{-\infty}^{+\infty} e^{i\eta p}[\delta_h[\bar{V}](x, \eta) - \eta V'(x)]$$
$$\times\,\mathcal{O}\bar{\psi}_q\left(x + \frac{h}{2}\eta\right)\mathcal{O}\psi_q\left(x - \frac{h}{2}\eta\right)d\eta$$

$$\delta_h[\bar{V}](x, \eta) = \frac{\bar{V}(x + (h/2)\,\eta) - \bar{V}(x - (h/2)\,\eta)}{h}$$

$$r_2^h(x, p) = -v\,\mathscr{R}e\,\mathscr{W}_h[H\mathcal{O}\psi_q, \mathcal{O}\psi_q]$$

By applying Lemma A.1 for r_1 and Corollary A.3 for r_2 we have

$$\lim_{h \to 0}\int_{x_1}^{x_2}\int_{\mathbb{R}} r_i^h(x, p)\,\theta(x, p)\,dp = 0$$

For every $\theta \in C_\circ^\infty(\mathbb{R} \times \mathbb{R})$ (we can also prove that this limit is uniform with respect to q). Proceeding analogously for the φ_q and integrating with respect to q, we deduce from (4.12) that

$$\lim_{h \to 0}\int_{x_1}^{x_2}\int_{\mathbb{R}} \theta(x, p)\left[\frac{p}{m}\frac{\partial f_Q^h}{\partial x} + e\frac{dV}{dx}\frac{\partial f_Q^h}{\partial p} + vf_Q^h\right]dx\,dp = 0$$

for every test function θ in $C_c^\infty(\mathbb{R}\times\mathbb{R})$. This proves that the limit f_Q of f_Q^h is solution of the Vlasov equation on (x_1, x_2). Now we have to check that $f_Q = f_C$ at the interfaces. Let $\theta(x, p)$ be a test function in $C_c^\infty(\mathbb{R}_x \times \mathbb{R}_p)$ such that

$$\theta(0, -p) = \theta(L, p) = 0, \qquad p > 0 \tag{4.15}$$

Let us define the transport-absorption operator and its adjoint T^*

$$T = \frac{p}{m}\frac{\partial}{\partial x} + e\frac{dV}{dx}\frac{\partial}{\partial p} + v, \qquad T^* = -\frac{p}{m}\frac{\partial}{\partial x} - e\frac{dV}{dx}\frac{\partial}{\partial p} + v$$

Multiplying the Boltzmann equation (4.2), integrating by parts and taking into account (4.15), we obtain

$$\lim_{h\to 0} I_h + II_h + III_h = 0$$

where

$$I_h = \int_{\mathbb{R}^+} \frac{-p}{m}\left[\theta(L, -p)\, G_L(p) + \theta(0, p)\, G_o(p)\right] dp$$

$$II_h = \int_0^L \int_{\mathbb{R}} \left[\{f^h . T^*\theta\}(x, p) - \theta\mathcal{Q}(f^h)(x, p)\right] dx\, dp$$

$$III_h = \int_{\mathbb{R}} \frac{p}{m}\left[\{\theta f_C^h - \theta f_Q^h\}(x_1, p) - \{\theta f_C^h - \theta f_Q^h\}(x_2, p)\right] dp$$

In the above formula, we set $f^h = f_Q^h$ in the **Q** zone and $f^h = f_C^h$ in the **C** zone and $\mathcal{Q}(f^h) = 0$ in the **Q** zone. The term III_h represents the jump of the distribution function at the **Q**–**C** interfaces $x = x_1$ and $x = x_2$. We prove in Appendix B that this term tends to zero when h tends to zero, which shows that the limit distribution function does not have a jump at the **Q**–**C** interfaces.

Passing to the limit in I_h and II_h, we find that the limit distribution function satisfies

$$\int_0^L \int_{\mathbb{R}} \left[f . T^*\theta(x, p) - \theta\mathcal{Q}(f)(x, p)\right] dx\, dp$$
$$- \int_{\mathbb{R}^+} \frac{p}{m}\left[\theta(L, -p)\, G_L(p) + \theta(0, p)\, G_o(p)\right] dp = 0$$

for every θ satisfying (4.15), which is the weak formulation of (4.8). ∎

5. SOME REMARKS AND COMMENTS

The hybrid model that we have developed in this paper relies on three hypotheses. The first one is that the transport is purely on dimensional in the position momentum variables. The second hypothesis consists in assuming the quantum effect to be confined to a given zone $[x_1, x_2]$ of the device, while the third one stipulates that the quantum zone is purely ballistic. We shall briefly discuss the validity of these hypotheses.

The one dimensional picture relies on the fact that the geometry of the device has a privileged direction (say the x axis) and that the potential V depends only on this direction. This picture is however not completely correct when the classical zones are collisional. Indeed, the collisions with impurities or phonons break the independence of the distribution function with respect to the parallel (y and z) components of the momentum (or the velocity). Hence, the distribution function f in the **C** zones depends on one position variable x and three momentum variables $\mathbf{p} = (p, p_y, p_z)$. The Boltzmann equation reads

$$\frac{p}{m}\frac{\partial f_C}{\partial x} + e\frac{dV}{dx}\frac{\partial f_C}{\partial p} = \mathcal{Q}(f_C)$$

where

$$\mathcal{Q}(f) = (x, \mathbf{p}) = \int_{\mathbb{R}^3} s(x, \mathbf{p}, \mathbf{p}')[M_T(\mathbf{p})\, f(x, \mathbf{p}')(1 - \varepsilon f(x, \mathbf{p}))$$
$$- M_T(\mathbf{p}')\, f(x, \mathbf{p})(1 - \varepsilon f(x, \mathbf{p}'))]\, d\mathbf{p}'$$

This problem cannot be reduced to a one dimensional one. However, since the transport in the quantum zone does not act on the p_y and p_z variables, it is possible to write a hybrid model, where the interface conditions involve p_y and p_z only as parameters. The interface conditions at $x = x_1$ and $x = x_2$ are rigorously the same as proposed in the previous section except that p_y and p_z are added in the arguments of f. Finally, the Wigner function in the **Q** zone reads

$$f_Q(x, p, p_y, p_z) = \int_{\mathbb{R}^+} f_C(x_1, q, p_y, p_z)\, \mathscr{W}_h[\mathcal{O}\psi_q](x, p)\, dq$$
$$+ \int_{\mathbb{R}^+} f_C(x_2, -q, p_y, p_z)\, \mathscr{W}_h[\mathcal{O}\varphi_q](x, p)\, dq$$

Location of quantum effects. In the derivation of our model, we assumed that quantum phenomena occur only in the interval $[x_1, x_2]$. Also, the potential variation should be small in the vicinity of the interfaces. Although, we do not have a quantitative criterion to decide where to put the **Q–C** interfaces, we shall give some qualitative hints.

In resonant tunneling diodes, the tunneling effects often occur in the vicinity of the double barrier. Hence our model is valid when $[x_1, x_2]$ is a region including the double barrier. However, when the RTD is endowed with a spacer, the tunneling can extend far away from the double barrier (see for example ref. 30). Hence, the question of where to locate the **Q–C** interface requires a careful analysis, depending on the device configuration. To illustrate this difficulty, let us consider a potential barrier of height V extending on the interval $[a, b]$ and discuss the influence of the location of the interfaces x_1 and x_2. If $x_1 < a$ and $x_2 > b$ then the reflection transmission coefficients computed on $[x_1, x_2]$ are exactly equal to the reflection transmission of the potential barrier when the latter is analyzed on the whole real line. If $x_1 < a$ and $a < x_2 < b$, then it is readily seen that the transmission coefficient computed on $[x_1, x_2]$ is equal to zero for electron energies below the potential barrier. The second localization $(a < x_2 < b)$ gives obviously incorrect results if the tunneling effect is not negligible (when the length of the barrier is small the height being fixed). In this particularly simple situation, such a problem can be avoided by puting the interface x_2 beyond the point b. However, this issue might be tricky in the general case and needs a special care in the numerical implentation.

Finally, the third hypothesis stipulating that the quantum zone is purely ballistic is valid in an RTD in the positive resistance zone of the I–V curve and ceases to be correct in the valley region (see refs. 11 and 12). We think however, that the coupling strategy could be adopted in the valley region by using the master equation (introduced in refs. 11 and 12) which gives the values of the reflection-transmission coefficients. Note also, that our model is stationary and one dimensional. The extension to the time dependent case requires the derivation of inflow boundary conditions for the Schrödinger equation or the Wigner equation which leads to the standard inflow condition in the semiclassical limit. The reader can find in refs. 3, 16–18, 22, 24, and 38 some physical, mathematical and numerical aspects related to such boundary conditions.

APPENDIX A: WIGNER TRANSFORM ON BOUNDED SETS

Lemma A.1. Let (ψ_h, φ_h) be two sequences of functions bounded in L^2 and satisfying the following hypothesis

(i) $\lim_{h \to 0} h \, \|\psi_h\|_{L^\infty_{loc}} \|\varphi_h\|_{L^\infty_{loc}} = 0$.

Let Ω be a bounded open set of $\mathbb{R}^N$ with a boundary of finite surface measure and let F_h be a sequence of functions on $\mathbb{R}^N_x \times \mathbb{R}^N_\eta$ satisfying the following two hypotheses

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

$$\limsup_{h \to 0} \sup_{(x, \eta) \in \Omega \times \mathbb{R}^N} |F_h(x, \eta)|/(1 + |\eta|^k) < +\infty$$

(iii) There exists $\alpha > 0$ such that

$$\lim_{h \to 0} \sup_{(x, \eta) \in I_h(\Omega)} |F_h(x, \eta)| = 0$$

where $I_h(\Omega) = \{(x, \eta) \in \Omega \times \mathbb{R}^N \mid B_{\alpha h |\eta|}(x) \subset \Omega\}$, and $B_R(x)$ denotes the closed ball in $\mathbb{R}^N$ with radius R and centered at x.

Then for every $\theta(x, p) \in C_0^\infty(\mathbb{R}^N \times \mathbb{R}^N)$, we have

$$\lim_{h \to 0} \int_\Omega dx \int_{\mathbb{R}^N} d\eta\, F_h(x, \eta)\, \hat{\theta}(x, \eta)\, \bar{\psi}_h\left(x + \frac{h}{2}\eta\right) \varphi_h\left(x - \frac{h}{2}\eta\right) = 0$$

where $\hat{\theta}(x, \eta)$ is the Fourier transform with respect to p.

Proof. Let us denote the above integral by $J_h(\theta)$. We can split this integral in two ones depending on the modulus of η: $J_h = J_h^1 + J_h^2$ where

$$J_h^1 = \int_\Omega \int_{|\eta| < R} \cdots \qquad J_h^2 = \int_\Omega \int_{|\eta| > R} \cdots$$

The second integral can be made arbitrarily small by choosing R large enough. Indeed, some simple algebra in the spirit of ref. 26 lead to the following estimate

$$|J_h^2(\theta)| \leqslant \|\psi_h\|_{L^2} \|\varphi_h\|_{L^2} \int_{|\eta| > R} \sup_{x \in \Omega} |F_h \hat{\theta}(x, \eta)|\, d\eta$$

We conclude by taking into account (ii) and by noting that $\hat{\theta}$ is rapidly decaying since θ is in C_0^∞. Now we write

$$J_h^1 = \int_{\Omega \times B_R - I_h(\Omega)} \cdots + \int_{(\Omega \times B_R) \cap I_h(\Omega)} \cdots$$

The second integral is, like J_h^2, estimated by

$$C \|\psi_h\|_{L^2} \|\varphi_h\|_{L^2} R^N \sup_{(x,\eta) \in I_h(\Omega)} |F_h \hat{\theta}(x, \eta)|$$

which tends to zero in view of hypothesis (iii). The first integral can be estimated by

$$\sup |F_h \hat{\theta}| \; |\Omega \times B_R - I_h(\Omega)| \; \|\psi_h\|_{L^\infty(\Omega + B_R)} \|\varphi_h\|_{L^\infty(\Omega + B_R)}$$

for $h \leqslant 1$. Besides, it is readily seen that $|\Omega \times B_R - I_h(\Omega)| \leqslant Ch$ which in view of hypotheses (i) and (ii) imply that the above expression vanishes in the limit $h \to 0$. The proof is then complete. ∎

Remark A.2. Hypothesis (i) is satisfied when $h^{N+1} D^{N+1} \psi_h(\varphi_h)$ are bounded in L^2_{loc}. These bounds are satisfied when ψ_h is solution of a Schrödinger equation

$$\frac{-h^2}{2m} \Delta \psi_h - e V_h \psi_h = E \psi_h$$

with a potential V_h smooth enough (for example V_h bounded in $W^{N-1,\infty}_{loc}$ when h tend to zero. Hypothesis (iii) implies that $F_h \to 0$ a.e. $x \in \Omega$, $\eta \in \mathbb{R}^N$ but requires a little uniformity when x tends to the boundary. ∎

The following corollary is a direct application of Lemma A.1

Corollary A.3. Let H be an L^∞ function such that $H = 0$ a.e. on a regular bounded domain $\Omega \subset \mathbb{R}^N$. Let ψ_h, φ_h be a sequence of functions satisfying the hypotheses of Lemma A.1 Then for all $\theta \in C_\circ^\infty(\mathbb{R}^N \times \mathbb{R}^N)$, we have

$$\lim_{h \to 0} \int_\Omega dx \int_{\mathbb{R}^N} dp \; \theta(x, p) \; \mathscr{W}_h[\psi_h, H\varphi_h] = 0$$

where $\mathscr{W}_h[a, b]$ is defined by (4.9).

Remark A.4. The corollary remains true if we only assume that H is in L^∞_{loc}. ∎

Proof. The corollary is an application of Lemma A.1 with $F^h(x, \eta) = \bar{H}(x - (h/2)\eta)$. It is then easy to check the hypotheses (ii) and

(iii) of the lemma. For hypothesis (iii), we choose $\alpha = 1/2$. Therefore for $(x, \eta) \in I_h$, we have $x - (h/2)\eta \in \Omega$ and then $H(x - (h/2)\eta) = 0$. ∎

APPENDIX B: CONVERGENCE AT THE INTERFACE

In this appendix, we show that the quantum and classical distribution functions are asymptotically equal at the **C–Q** interfaces. Namely,

Lemma B.1. Let $f^h = (f_C^h, f_Q^h)$ be the solution of (4.2) (4.3) with a given potential $V \in C^2([0, L])$. Then for every θ such that $(\theta(p)/p) \in C_\circ^\infty(\mathbb{R}_p)$ the following limits hold

$$\lim_{h \to 0} \int_{\mathbb{R}} \theta(p)[f_C^h(x_1, p) - f_Q^h(x_1, p)]\, dp$$

$$= \lim_{h \to 0} \int_{\mathbb{R}} \theta(p)[f_C^h(x_1, p) - f_Q^h(x_2, p)]\, dp = 0$$

Proof. Let us prove that the first integral tends to zero. For this aim, we recall that the boundary conditions (2.9) imply that $\psi_p(x) = e^{ip((x-x_1)/h)} + r_p e^{-ip((x-x_1)/h)}$ for $x \leqslant x_1$ and $R_{p,1}^v = |r_p|^2$. For $x > x_2$, ψ_p reads $\psi_p(x) = t_p e^{i((x-x_2)/h)\, \overset{+}{\sqrt{p^2 + 2em(V_2 - V_1)}}}$ and $T_{p,1}^v = (1/p) \sqrt{(p^2 + 2em(V_2 - V_1))^+}\, |t_p|^2$. Rescaling the Schrödinger equation (2.9) in the vicinity of x_1 and x_2, we find that

$$\begin{cases} \psi_p(x_1 + h\eta) = e^{ip\eta} + r_p e^{-ip\eta} + o(1) \\ \psi_p(x_2 + h\eta) = t_p(e^{i\eta\, \overset{+}{\sqrt{p^2 + 2em(V_2 - V_1)}}} + o(1)) \end{cases} \tag{B.1}$$

where $o(1)$ is uniform when (p, η) lie in a bounded set. For a detailed proof, we refer the reader to ref. 7. In the same way, we can prove that

$$\begin{cases} \varphi_p(x_2 + h\eta) = e^{-ip\eta} + r'_p e^{+ip\eta} + o(1) \\ \psi_p(x_1 + h\eta) = t'_p(e^{-i\eta\, \overset{+}{\sqrt{p^2 + 2em(V_1 - V_2)}}} + o(1)) \end{cases} \tag{B.2}$$

where we have

$$R_{p,2}^v = |r'_p|^2, \qquad T_{p,2}^v = \frac{1}{p} \sqrt{(p^2 + 2em(V_1 - V_2))^+}\, |t'_p|^2$$

Let us now compute $I_1^h = \int_{\mathbb{R}} \theta(p)[f_C^h(x_1, p) - f_Q^h(x_1, p)]\, dp$. First, we write

$$I_1^h = \int_{\mathbb{R}^+} [\theta(p)\, f_C^h(x_1, p) + \theta(-p)\, f_C^h(x_1, -p)]\, dp - \int_{\mathbb{R}} \theta(p)\, f_Q^h(x_1, p)\, dp$$

$$= \int_{\mathbb{R}^+} [\theta(p) + R_{p,1}^v \theta(-p)]\, f_C^h(x_1, p)\, dp - \int_{\mathbb{R}} \theta(p)\, f_Q^h(x_1, p)\, dp$$

$$+ \int_{\mathbb{R}^+} T_{p,1}^v \theta(-p)\, f_C^h(x_2, -p_2(p, V))\, dp \tag{B.3}$$

Besides, we have

$$\int_{\mathbb{R}} f_Q^h(x_1, p)\, \theta(p)\, dp$$

$$= \int_{\mathbb{R}^+} f_C^h(x_1, q)\, \hat{\theta}(\eta)\, \overline{\psi_q}\left(x_1 + \frac{h}{2}\eta\right) \psi_q\left(x_1 - \frac{h}{2}\eta\right) d\eta\, dq$$

$$+ \int_{\mathbb{R}^+} f_C^h(x_2, -q)\, \hat{\theta}(\eta)\, \overline{\varphi_q}\left(x_1 + \frac{h}{2}\varphi\right) \varphi_q\left(x_1 - \frac{h}{2}\eta\right) d\eta\, dq \tag{B.4}$$

In order to analyze the first integral of the right hand side, we replace ψ_p by its asymptotic formula (B.1)

$$\overline{\psi_q}\left(x_1 + \frac{h}{2}\eta\right) \psi_q\left(x_1 - \frac{h}{2}\eta\right) = e^{-iq\eta} + R_{p,1}^v e^{iq\eta} + 2\mathscr{R}e(r_q) + o(1)$$

Hence

$$\lim_{\hbar \to 0} \int_{\mathbb{R}^+} \int_{\mathbb{R}} f_C^h(x_1, q)\, \hat{\theta}(\eta)\, \overline{\psi_q}\left(x_1 + \frac{h}{2}\eta\right) \psi_q\left(x_1 - \frac{h}{2}\eta\right) d\eta\, dq$$

$$= \lim_{\hbar \to 0} \int_{\mathbb{R}^+} \int_{\mathbb{R}} f_C^h(x_1, q)\, \hat{\theta}(\eta)[e^{-iq\eta} + R_{p,1}^v e^{iq\eta} + 2\mathscr{R}e(r_q)]\, d\eta\, dq$$

$$= \lim_{\hbar \to 0} \int_{\mathbb{R}^+} [\theta(q) + R_{p,1}^v \theta(-q)]\, f_C^h(x_1, q)\, dq \tag{B.5}$$

The last equality is recovered by back Fourier transforming (with respect to η) and by noticing that $\theta(0) = 0$. To prove rigorously the first equality, we use the Lebesgue dominated convergence theorem and we need the following lemma whose proof is postponed.

Lemma B.2. Let V is in $C^2([x_1, x_2])$ and satisfies Hypothesis (H) of subsection 4.3 holds. Then the following estimates hold

$$|\psi_p(x_2)|^2 \leqslant \frac{Cp}{\sqrt{|p^2 + 2emV_2 - 2emV_1|}}, \qquad \hbar^2 \, \|\psi_p'\|_{L^\infty}^2 \leqslant Cp(1+p)$$

$$|\varphi_p(x_1)|^2 \leqslant \frac{Cp}{\sqrt{|p^2 + 2emV_1 - 2emV_2|}}, \qquad \hbar^2 \, \|\varphi_p'\|_{L^\infty}^2 \leqslant Cp(1+p)$$

Indeed, this lemma implies that the integrand of the left hand side of (B.5) is bounded by $C\mathscr{F}_{\mu+V_1}(q)(1+q)^2(1+|\eta|)^2 |\hat{\theta}(\eta)|$. This function is in L^1 since $\mathscr{F}$ and $\hat{\theta}$ are rapidly decaying. To analyze the second integral of the right hand side of (B.4), we distinguish two cases:

- *Case* 1. $p_1(0, V) \in \mathbb{R}^+$. This means ($V_1 \geqslant V_2$). We make the change of variables $q = p_2(p, V)$ which implies that $p = p_1(q, V)$ and use the asymptotic expression (B.2). Since $p\,dp = q\,dq$, we find the asymptotic behavior

$$\begin{aligned} I_2 &= \int_{\mathbb{R}^+} f_C^\hbar(x_2, -q)\, \hat{\theta}(\eta)\, \overline{\varphi_q}\left(x_1 + \frac{\hbar}{2}\eta\right) \varphi_q\left(x_1 - \frac{\hbar}{2}\eta\right) d\eta\, dq \\ &= \int_{p_1(0,V)}^{+\infty} f_C^\hbar(x_2, -p_2(p, V))\, |t'_{p_2}|^2\, \theta(p) \frac{p}{p_2}\, dp + o(1) \end{aligned}$$

But since $(p/p_2)\,|t'_{p_2}|^2$ is nothing but $T^v_{p_2,2} = T^v_{p,1}$ (in view of Lemma 2.3) and since $T^v_{p,1} = 0$ when $p < p_1(0, V)$, the following identity holds

$$\begin{aligned} &\lim_{\hbar\to 0} \int_{\mathbb{R}^+} f_C^\hbar(x_2, -q)\, \hat{\theta}(\eta)\, \overline{\varphi_q}\left(x_1 + \frac{\hbar}{2}\eta\right) \varphi_q\left(x_1 - \frac{\hbar}{2}\eta\right) d\eta\, dq \\ &\quad = \lim_{\hbar\to 0} \int_{\mathbb{R}^+} T^v_{p,1} f_C^\hbar(x_2, -p_2(p, V))\, \theta(p)\, dp \end{aligned}$$

Combining the above formula with (B.3) (B.4) and (B.5) leads to the first identity of Lemma B.1.

- *Case* 2. $p_1(0, V) \in i\mathbb{R}^+$. This implies that $p_2(0, V) \in \mathbb{R}^+$. Hence we cut the integral I_2 into two integrals

$$I_2 = \int_{q \geqslant p_2(0,V)} \cdots + \int_{q \leqslant p_2(0,V)} \cdots$$

The first integral is treated exactly as in case 1 and leads after the change of variable to

$$\int_{\mathbb{R}^+} T^v_{p,1} f^h_C(x_2, -p_2(p, V))\, \theta(p)\, dp$$

To prove the result of Lemma B.1, we have to show that the second integral tends to zero. Here again, we use the Lebesgue's dominated convergence theorem. The integrand

$$f^h_C(x_2, -q)\, \hat{\theta}(\eta)\, \overline{\varphi_q}\left(x_1 + \frac{h}{2}\eta\right) \varphi_q\left(x_1 - \frac{h}{2}\eta\right)$$

is bounded by

$$C\, |\hat{\theta}(\eta)|\, \mathscr{F}_{\mu + V_2}(q) \left(\frac{q}{\sqrt{|q^2 + emV_1 - 2emV_2|}} + |\eta|^2\, q(1+q)\right) \in L^1(\mathbb{R}^+_q \times \mathbb{R}_\eta)$$

and converges pointwise to zero in view of the following lemma

Lemma B.3. Let $p > 0$ such that $p_1(p, V) \in i(0, +\infty)$. Then there exits an interval in the vicinity of x_1 on which φ_p solution of (2.10) converges uniformly to zero.

We then have proven the first part of Lemma B.1. The second part follows in complete analogy. We shall now give the proofs of Lemmas B.2 and B.3 ▌

Proof of Lemma B.2. For the sake of simplicity, we will only prove the estimate for ψ_p. The other estimate follows in analogy. We first recall that in view of (2.11)

$$|h\psi_p'(x_1)| \leqslant 2p, \qquad |\psi_p(x_1)| \leqslant 2$$

To look for a bound of ψ_p and ψ_p' at $x = x_2$, we distinguish two cases:

- $p_2(p, V) \in \mathbb{R}^+$; in this case we have in view of (2.11)

$$|\psi_p(x_2)|^2 \leqslant \frac{p}{\sqrt{p^2 + 2em(V_2 - V_1)}}, \qquad |h^2\psi_p'(x_2)|^2 \leqslant p\,\sqrt{p^2 + 2em(V_2 - V_1)}$$

• $p_2(p, V) \in i\mathbb{R}^+$. This implies that $V_2 < V_1$. Since, ψ_p solves (2.9), then it satisfies the following inequality on every interval in the vicinity of x_2 on which it does not vanish

$$\frac{h^2}{2m} |\psi_p|'' \geqslant \left(eV_1 - eV(x) - \frac{p^2}{2m} \right) |\psi_p|$$

Since the boundary condition (2.9) at $x = x_2$ yields $|\psi_p|'(x_2) \leqslant 0$, the above differential inequality implies that $|\psi_p(x)| \geqslant |\psi_p(x_2)|$ on the interval $\mathscr{I}$ (see Hypothesis (H) of subsection 4.3), because the multiplication term $(eV_1 - eV(x) - (p^2/2m))$ is nonnegative. Consequently, we have

$$|\mathscr{I}|\ |\psi_p(x_2)|^2 \leqslant \int_{x_1}^{x_2} |\psi_p(x)|^2\, dx \leqslant \frac{p}{vm}$$

We can group the results and get the following estimate on $\psi_p'(x_2)$, $\psi_p(x_2)$

$$\begin{cases} |\psi_p(x_2)|^2 \leqslant \dfrac{Cp}{\sqrt{|p^2 + 2em(V_2 - V_1)|}} \\ h^2\ |\psi_p'(x_2)|^2 \leqslant Cp\ \sqrt{|p^2 + 2em(V_2 - V_1)|} \end{cases} \tag{B.6}$$

where the constant C does not depend on p neither on h. This proves the first estimate of the lemma. Let us now introduce the function

$$G(x) = \frac{h^2}{2m} |\mathscr{R}e\psi_p'(x)|^2 + \left(\frac{p^2}{2m} + eV(x) - eV_1 \right) |\mathscr{R}e\psi_p(x)|^2$$

Using the Schrödinger equation (2.9), we have the following identity

$$\frac{dG}{dx} = eV'\ |\mathscr{R}e\psi_p|^2 - hv\mathscr{R}e(\psi_p')\ \mathscr{I}m(\psi_p)$$

Since $\|\psi_p\|_{L^2}^2 \leqslant Cp$ and $h^2\ \|\psi_p'\|_{L^2}^2 \leqslant Cp(1+p)$ (see (4.11), we deduce in view of (B.6) that G is bounded in L^∞ by $Cp(1+p)$. Let now, a point $x_M \in [x_1, x_2]$ on which $|\mathscr{R}e\psi_p'(x)|$ achieves its maximum. Assume, that $x_M \in (x_1, x_2)$ such that $\mathscr{R}e\psi_p''(x_M) = 0$. Using the Schrödinger equation (2.9), we deduce that

$$\begin{aligned} &\left| \frac{p^2}{2m} + eV(x_M) - eV_1 \right|\ |\mathscr{R}e\psi_p(x_M)|^2 \\ &\quad = h\frac{v}{2}\ |\mathscr{I}m\psi_p(x_M)\ \mathscr{R}e\psi_p(x_M)| \leqslant Cp(1+p) \end{aligned}$$

which implies in view of the bound on G, that

$$h^2 \, |\mathcal{R}e\psi_p'(x_M)|^2 \leqslant Cp(1+p)$$

Let us note that this estimate is still true if $x_M = x_1$ or x_2. Doing the same job for the imaginary part, we finally get

$$h^2 \, \|\psi_p'\|_{L^\infty}^2 \leqslant Cp(1+p)$$

and the lemma is proved. ∎

Proof of Lemma B.3. Since $p_1(p, V) \in i\mathbb{R}_*^+$, then

$$2meV_2 - 2meV(x) - p^2 \geqslant a^2 > 0$$

on an interval $\mathscr{I} = [x_1, x_1 + \delta]$ in the vicinity of x_1. By the same argument as in the proof of Lemma B.2, we deduce that

$$h^2 \, |\varphi|'' \geqslant a^2 \, |\varphi|, \qquad \text{on } \mathscr{I}$$

Since $|\varphi_p|' (x_1) \geqslant 0$ in view of the second equation of (2.10), we deduce that

$$|\psi_p(x)| \geqslant |\psi_p(x_1)| \; e^{(a/h)(x - x_1)}$$

and we conclude easily by using the bound $\|\varphi_p\|_{L^2}^2 \leqslant Cp$. ∎

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