COUPLING ONE-DIMENSIONAL TIME-DEPENDENT CLASSICAL AND QUANTUM TRANSPORT MODELS

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Abstract. A transient model for one dimensional charge transport in an open quantum system is proposed. In the semiclassical limit, it reduces to the inflow boundary value problem for the classical transport equation. On this basis, the coupling of classical and quantum transport models through an interface is investigated. Suitable interface conditions are derived through asymptotic formulae involving the quantum reflection-transmission coefficients and time delays.

1. Introduction

In this work, we propose and analyze a method for coupling classical and quantum transport models in a one-dimensional time-dependent setting. This paper is the follow-up of a previous work of one of the authors [4] where the one-dimensional stationary case was investigated. We shall see that the account of the time-dependence increases the complexity of the coupling methodology to a large extent.

The problem can be formulated as follows. We consider a particle system (such as certain semiconductor devices e.g. Resonant Tunneling Diodes) which consists of a small localized portion (denoted by Q) where the dynamics of the particles is quantum and a large area (denoted by C) where the behavior of the particles can be well approximated by classical mechanics. For computational efficiency, it is desirable to use a classical mechanics model for the particles as long as they are in region C and to shift to a quantum model only when they cross the border between the C and Q regions. Similarly, when a particle leaves the Q region, one should be able to shift back to a classical model.

The problems posed by this procedure are twofold. First, independently of the consideration of the classical region, the quantum region is an open quantum system, which may gain or lose particles. Boundary conditions for open quantum systems are not

easily derived. Such boundary conditions were proposed and analyzed in [7, 8] in the one-dimensional stationary case and in [16, 3] for the multidimensional stationary case (numerical studies of such boundary conditions can be found in [21, 22, 12, 13] ...). Approximate boundary conditions for the time-dependent case can be found in [23, 2, 11]. In the present paper, we shall present an alternative approach to the search for boundary conditions: the a priori construction of density matrices which are exact solutions of the quantum Von-Neumann equation, and which are consistent with the statistics of the particles coming into the quantum region.

However, there is not a unique such construction. This is due to the necessary 'delocalization' of the classical particles when they enter the quantum region. Indeed, the quantum-mechanical picture of a particle is a wave-packet. If there is only one classical limit of a given quantum wave-packet, the reciprocal is obviously untrue. A given classical particle may be the classical limit of many different wave-packets. Therefore, when a classical particle crosses the border of the quantum region, one has to choose into which wave-packet it will be transformed. Consequently, the construction depends on this arbitrarily chosen wave-packet.

In this work, the construction is restricted to the case of a time-independent potential. This is because it makes a large use of the scattering states of the quantum structure, which are well-defined only for time-independent potentials. This restriction will be waived in future work.

So far, we have discussed the problem of finding the correct solution of the quantum Von-Neumann equation, given the statistics of the incoming particles. Now, we have to examine the reverse question i.e. how the quantum behavior of the particles in the Q region affects the dynamics in the C region.

For that purpose, we consider the Wigner transform of the density matrix in the Q region and perform a semi-classical limit $\hbar \to 0$. We show that the formal limit of the Wigner distribution function satisfies the usual boundary value problem for the classical transport equation in Q with prescribed incoming data. Furthermore, the outgoing Wigner distribution function at the Q region boundary can be expressed in terms of the incoming data by means of quantum reflection-transmission probabilities and time delays. Since the incoming distribution in the Q region is the outgoing one of the C region and vice-versa, we can assign similar reflection-transmission conditions to the classical distribution function at the $C - Q$ interface. These conditions only depend on the scattering probabilities and time delays of the quantum structure, but not on the expression of the density matrix in the Q region. Therefore, they lead to a self-contained problem for the classical distribution function, decoupled from that of the quantum region.

In this paper, we first give a general presentation and justification of the above described procedure. Then, we concentrate on the quantum region Q and perform the semiclassical analysis of the the Wigner distribution function. Finally, we shall discuss

questions regarding current continuity through the interface. We shall only develop formal arguments, and will defer rigorous proofs to a forthcoming paper [6]. A summary of the present approach can be found in [5].

2. The coupling methodology: formal approach

2.1. **Setting of the problem.** We consider a one dimensional system consisting of a large number of independent particles moving along the whole real line. In the sequel, we shall consider electrons, since one of the potential application of the present work is to quantum semiconductor devices. However, the procedure would apply equally well to any other kind of particles. The electrons are subject to a given time independent potential $V(x)$. We suppose that the gradients of the potential are small apart in a tiny localized region contained in the interval $[a,b]$ where they are large. Therefore, we can consider that the dynamics is classical in the region $C = \mathbb{R} \setminus [a,b]$ and quantum in the region $Q = [a,b]$. What is the precise meaning of small and large in terms of dimensionless parameters and asymptotic analysis will be the subject of future work. In the present one, we shall take this for granted. Our aim is to find a procedure which couples a classical kinetic description of the particle system in the C region to a quantum statistical model in the Q region.

In $C = \mathbb{R} \setminus [a,b]$, the system is described by the classical particle distribution function $f(x,p,t)$ which is a function of position $x \in \mathbb{R}$, momentum $p \in \mathbb{R}$ and time $t > 0$. It it is a solution of the one-dimensional collisionless transport (or Vlasov) equation:

$$\partial_t f + v\partial_x f + e\frac{\partial V}{\partial x}\partial_p f = 0\,, \quad x \in \mathbb{R} \setminus [a,b]\,, \quad v = \frac{p}{m}\,, \tag{1}$$

where m and e are respectively the mass and charge, and v, the velocity. At the boundary $\partial C = \{a,b\}$, inflow boundary conditions must be prescribed. At $x = a$ (resp. $x = b$), an inflow velocity for C is such that $v < 0$ (resp. $v > 0$). We therefore prescribe the boundary conditions

$$f(a,p,t) = f_a(p,t)\,,\ p < 0 \quad ; \quad f(b,p,t) = f_b(p,t)\,,\ p > 0\,, \tag{2}$$

where f_a and f_b obviously depend on the dynamics of the Q region.

In $Q = [a,b]$, the system is modeled by the density matrix $\rho(x,x',t)$, which is a solution of the Von-Neumann equation. However, instead of prescribing boundary conditions for the Von-Neumann equation at the boundary of the quantum region Q, we take another route. We choose to solve the Von-Neumann equation on the whole real line, but with a modified potential $\tilde{V}$ which coincides with V in Q and which is constant in C:

$$\tilde{V}(x) = \begin{cases} V_a := V(a) & , \ x \le a\,, \\ V(x) & , \ a \le x \le b\,, \\ V_b := V(b) & , \ x \ge b\,. \end{cases} \tag{3}$$

Therefore, the Von-Neumann equation for ρ reads:

$$i\hbar\rho_t = (\tilde{H}_x - \tilde{H}_{x'})\rho, \quad (x,x',t) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R} \tag{4}$$

where

$$\tilde{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - e\tilde{V}(x)\,,$$

is the modified particle Hamiltonian in the potential $\tilde{V}$ and $\tilde{H}_x$, $\tilde{H}_{x'}$ are respectively the actions of $\tilde{H}$ on the x and x' variables. Now, which solution of the Von-Neumann equation we must consider of course depends of the distribution function in the C region. Therefore, the coupling problem can be summarized as follows: how f_a and f_b are linked with ρ and reciprocally how ρ is linked with f ?

We first note that we are not going to consider initial value problems for equations (1) and (4), but solutions for all times $t \in \mathbb{R}$ (so-called eternal solutions). The reason is the following. When entering the Q region, a classical particle must be delocalized into a wave-packet. However, a wave-packet has a finite extension in space and is in fact very unlikely to be compactly supported. In other words, even very far from the Q region, a classical particle interacts with it because of the tiny but non zero tail of its wave-packet representation. Therefore, the interaction of a classical particle with the Q region is non local in time and actually extends infinitely in the past and in the future.

Now, to understand our coupling methodology, it is illuminating to first consider a classical dynamics in the Q region and derive a classical-classical coupling methodology. Of course, this strange question (why not just use the same classical model everywhere) is investigated just for a clearer exposition of the true classical-quantum coupling.

2.2. **Classical-classical coupling.** In this section, we suppose that, in the Q region, the system is described by a classical distribution function g, solution of the Vlasov equation

$$\partial_t g + v\partial_x g + e\frac{\partial V}{\partial x}\partial_p g = 0\,, \quad x \in [a,b]\,, \quad v = \frac{p}{m}\,. \tag{5}$$

Of course, the boundary ∂Q of Q is $\partial Q = \partial C = \{a,b\}$. However, the incoming velocities for the domain Q at a (resp. b) are now such that $v > 0$ (resp. $v < 0$). Obviously, the boundary conditions for g at a and b must be

$$g(a,p,t) = g_a(p,t) := f(a,p,t)\,,\ p > 0 \quad ; \quad g(b,p,t) = g_b(p,t) := f(b,p,t)\,,\ p < 0\,, \tag{6}$$

where $f(a,p,t)$ (for $p > 0$) and $f(b,p,t)$ (for $p < 0$) are supposedly known from the resolution of f in the C region. Reciprocally, the boundary conditions (2) for f must obviously be completed by the condition that

$$f_a(p,t) := g(a,p,t)\,,\ p < 0 \quad ; \quad f_b(p,t) := g(b,p,t)\,,\ p > 0\,. \tag{7}$$

Now, we introduce the characteristic equations of (5):

$$\frac{dX}{dt} = \frac{P(t)}{m} \quad ; \quad \frac{dP}{dt} = e\frac{dV}{dx}(X(t)),$$

which are supposed to be uniquely solvable for a given set of initial conditions. This is certainly true, provided that the potential is smooth, which we shall assume from now on. We consider maximal solutions, which exist until the position X reaches one of the

boundaries a or b of the domain. We denote by $(X,P)_{(t;x,p)}$, the solution at time t such that $(X,P)(0)=(x,p)$. Now, it is readily seen that

$$\phi_{(a,p_0,t_0)}(x,p,t) = \delta\left((x,p) - (X,P)_{(t-t_0;a,p_0)}\right),$$

is the unique measure solution of (5) which satisfies the boundary condition

$$v\phi_{(a,p_0,t_0)}(a,p,t) = \delta(p-p_0)\delta(t-t_0)\,.$$

Here and in the remainder of the paper, δ denotes the Dirac delta measure. Writing g_a as a superposition of such elementary distributions:

$$\begin{aligned} g_a(p,t) &= \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^+} g_a(p_0,t_0)\,\delta(p-p_0)\delta(t-t_0)\,dt_0\,dp_0 \\ &= \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^+} (v_0 g_a(p_0,t_0))\,(v_0^{-1}\delta(p-p_0)\delta(t-t_0))\,dt_0\,dp_0\,, \end{aligned}$$

(with $v_0 = p_0/m$) and similarly for g_b:

$$g_b(p,t) = \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^-} (|v_0|g_b(p_0,t_0))\,(|v_0|^{-1}\delta(p-p_0)\delta(t-t_0))\,dt_0\,dp_0\,,$$

we can exactly represent g by the integral formula:

$$\begin{aligned} g(x,p,t) &= \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^+} (v_0 g_a(p_0,t_0))\,\phi_{(a,p_0,t_0)}(x,p,t)\,dt_0\,dp_0 \\ &\quad + \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^-} (|v_0|g_b(p_0,t_0))\,\phi_{(b,p_0,t_0)}(x,p,t)\,dt_0\,dp_0\,. \end{aligned} \tag{8}$$

The measures $\phi_{(a,p_0,t_0)}$ (resp. $\phi_{(b,p_0,t_0)}$) are elementary distributions which describe particles entering the Q region at time t_0 through point a with momentum $p_0>0$ (resp. through point b and momentum $p_0<0$).

Now, (8) can be used to compute the outgoing traces of g on ∂Q as functions of its incoming traces g_a and g_b, i.e. (by (6)), of the outgoing traces of f (with respect to C). On the other hand, outgoing traces of g on ∂Q are also incoming traces of f on ∂C by virtue of (7). Therefore, this operation will ultimately give us an expression of the incoming traces of f as functions of its outgoing traces, which will lead to a self-contained problem for f. Then, knowing f and in particular its outgoing traces by the resolution of this problem, we will find g by means of formula (8). We are now going to detail this programme.

We start with the computation of the outgoing traces of $\phi_{(a,p_0,t_0)}$ and $\phi_{(b,p_0,t_0)}$. Again, using the smoothness of the potential which rules out any pathology of the trajectories, the characteristic $(X,P)_{(t;a,p_0)}$ with $p_0>0$ exits the domain Q after a certain time $\tau(p_0)$ either by point a with momentum $-p_0$ (in which case, we say that the particle is reflected) or by point b with momentum

$$p_b(p_0) = \mathrm{sgn}(p_0)\sqrt{p_0^2 + 2me(V_b - V_a)}, \tag{9}$$

(then, the particle is transmitted). The expression (9) obviously follows from the energy conservation, itself a consequence of the time-independence of the potential. If the expression inside the square root defining $p_b(p_0)$ is negative, then reflection occurs certainly and the quantity $p_b(p_0)$ needs not be defined. We define reflection and transmission coefficients $R(p_0)$, $T(p_0)$ in such a way that

$$R(p_0) = 1 - T(p_0) = \begin{cases} 1 & , \text{ in the case of a reflection,} \\ 0 & , \text{ in the case of a transmission.} \end{cases}$$

Then we can write:

$$v\phi_{(a,p_0,t_0)}(a,p,t) = R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0))\,, \quad p<0\,, \tag{10}$$

$$v\phi_{(a,p_0,t_0)}(b,p,t) = T(p_0)\,\delta(p-p_b(p_0))\,\delta((t-t_0)-\tau(p_0))\,, \quad p>0\,. \tag{11}$$

Similar definitions can of course be given for characteristics starting from b with momentum $p_0 < 0$. In particular, we define

$$p_a(p_0) = \mathrm{sgn}(p_0)\sqrt{p_0^2 - 2me(V_b - V_a)}.$$

This leads to the following expressions:

$$v\phi_{(b,p_0,t_0)}(b,p,t) = R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0))\,, \quad p>0\,, \tag{12}$$

$$v\phi_{(b,p_0,t_0)}(a,p,t) = T(p_0)\,\delta(p-p_a(p_0))\,\delta((t-t_0)-\tau(p_0))\,, \quad p<0\,. \tag{13}$$

Now, from (10)-(13), we deduce, for $p<0$:

$$g(a,p,t) = \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^+} g_a(p_0,t_0)\,R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0))\,dt_0\,dp_0$$
$$+\int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^-}\frac{|p_0|}{|p_a(p_0)|}g_b(p_0,t_0)\,T(p_0)\,\delta(p-p_a(p_0))\,\delta((t-t_0)-\tau(p_0))\,dt_0\,dp_0\,.$$

or, after performing the integrations and noting that $p_0' = p_a(p_0) \Leftrightarrow p_0 = p_b(p_0')$:

$$g(a,p,t) = R(-p)\,g_a(-p,t-\tau(-p)) + T(p_b(p))\,g_b(p_b(p),t-\tau(p_b(p)))\,.$$

Similarly, for $p>0$, we have:

$$g(b,p,t) = \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^-} g_b(p_0,t_0)\,R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0))\,dt_0\,dp_0$$
$$+\int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^+}\frac{p_0}{p_b(p_0)}g_a(p_0,t_0)\,T(p_0)\,\delta(p-p_b(p_0))\,\delta((t-t_0)-\tau(p_0))\,dt_0\,dp_0\,,$$

or

$$g(b,p,t) = R(-p)\,g_b(-p,t-\tau(-p)) + T(p_a(p))\,g_a(p_a(p),t-\tau(p_a(p)))\,.$$

We note that, by time reversibility, $T(p_a(p)) = T(-p)$ and $\tau(p_a(p)) = \tau(-p)$, (for $p>0$ and when $p_a(p)$ is defined). Similarly, $T(p_b(p)) = T(-p)$ and $\tau(p_b(p)) = \tau(-p)$, (for $p<0$ and when $p_b(p)$ is defined). This finally leads to:

$$g(a,p,t) = R(-p)\,g_a(-p,t-\tau(-p)) + T(-p)\,g_b(p_b(p),t-\tau(-p))\,, \quad p<0\,, \tag{14}$$

$$g(b,p,t) = R(-p)\,g_b(-p,t-\tau(-p)) + T(-p)\,g_a(p_a(p),t-\tau(-p))\,, \quad p>0\,. \tag{15}$$

Now, eliminating g by (6) and (7), we use (14) and (15) to set up a self-contained reflection-transmission problem for f:

$$(16)\quad f(a,p,t) = R(-p)\, f(a,-p,t-\tau(-p)) + T(-p)\, f(b,p_b(p),t-\tau(-p))\,, \quad p<0\,,$$
$$(17)\quad f(b,p,t) = R(-p)\, f(b,-p,t-\tau(-p)) + T(-p)\, f(a,p_a(p),t-\tau(-p))\,, \quad p>0\,,$$

These boundary conditions express the incoming traces of f as functions of its outgoing traces. They are very likely to lead to a well-posed problem for f in C (existence of solutions for similar kinds of boundary conditions can be found in [9], [10]). With these boundary conditions, the Vlasov equation (1) can be solved in C without any reference to the distribution function in Q. Of course, via the reflection-transmission coefficients R, T and time delays τ, f depends on the potential in Q. Then, once f is found in C, formula (8) allows us to represent the solution in Q as an integral involving the boundary values of f at a and b.

We are going to duplicate the same methodology for the classical-quantum coupling in the next section.

2.3. **Classical-quantum coupling.** The first and non obvious point is to define the analogues of the elementary distributions $\phi_{(a,p_0,t_0)}$ and $\phi_{(b,p_0,t_0)}$ which characterize particles entering the Q region at time t_0 and point a with momentum $p_0>0$ (resp. at point b and momentum $p_0<0$). We start by recalling the definition of the scattering states of the potential $\tilde{V}$. These are solutions ψ of the stationary Schrödinger equation:

$$(18)\qquad \tilde{H}\psi = \mathcal{E}\psi\,,$$

(where $\mathcal{E}$ is the energy) which are bounded on the real line but not square-integrable. Elementary analysis [20] shows that for a given energy $\mathcal{E}$, the space of such solutions is of dimension zero, one or two according to the relative position of $\mathcal{E}$ with respect to V_a and V_b. A convenient basis of the solution space is provided by wave-functions describing the diffusion of a plane wave coming from infinity by the potential inhomogeneity. These are given by the solutions of the following boundary value problem in the interval $[a,b]$ [7]:

$$(19)\qquad \text{for } p>0,\quad \begin{cases} -\frac{\hbar^2}{2m}\psi_p'' - eV\psi_p = \left(\frac{p^2}{2m} - eV_a\right)\psi_p, \\ \hbar\psi_p'(a) + ip\psi_p(a) = 2ip, \\ \hbar\psi_p'(b) = ip_b(p)\,\psi_p(b), \end{cases}$$

$$(20)\qquad \text{for } p<0,\quad \begin{cases} -\frac{\hbar^2}{2m}\psi_p'' - eV\psi_p = \left(\frac{p^2}{2m} - eV_b\right)\psi_p, \\ \hbar\psi_p'(a) = -ip_a(p)\,\psi_p(a), \\ \hbar\psi_p'(b) + ip\psi_p(b) = 2ip\ . \end{cases}$$

Let us suppose, to fix the ideas that $V_b > V_a$. Then $p_b(p)$ is always well-defined. On the other hand, $p_a(p)$ is well-defined only if $|p| \geq \sqrt{2em(V_b-V_a)}$. For $p>0$, the two solutions ψ_p and $\psi_{-p_b(p)}$ form a basis of the solution space of (18) associated

with the energy $\mathcal{E} = \frac{p^2}{2m} - eV_a = \frac{p_b(p)^2}{2m} - eV_b$, which is therefore of dimension 2. ψ_p describes the scattering of a plane wave coming from $-\infty$ by the potential inhomogeneity, while $\psi_{-p_b(p)}$ describes the scattering of a plane wave coming from $+\infty$. For $p < 0$ and $|p| \leq \sqrt{2em(V_b - V_a)}$, then $p_a(p)$ in formula (20) has to be defined as a complex square root: $p_a(p) = \pm i\sqrt{2me(V_b - V_a) - p^2}$. Which sign must be chosen in this definition is unimportant because the solution space is of dimension 1 and the two solutions are then proportional. In this case, the solution (20) represents the pure quantum reflection of a plane-wave by a potential barrier.

The boundary conditions appearing in (19), (20) are consequences of the following explicit formula for ψ_p outside $[a,b]$ (this is because the potential $\tilde{V}$ is assumed constant in $\mathbb{R} \setminus [a,b]$):

$$\text{for } p > 0, \quad \begin{cases} \psi_p(x) = e^{ip\frac{(x-a)}{\hbar}} + A(p)\, e^{-ip\frac{(x-a)}{\hbar}}, & x < a \\ \psi_p(x) = B(p)\, e^{ip_b(p)\frac{(x-b)}{\hbar}}, & x > b \end{cases} \tag{21}$$

where

$$A(p) = \psi_p(a) - 1 \quad ; \quad B(p) = \psi_p(b), \quad p > 0\ , \tag{22}$$

and

$$\text{for } p < 0, \quad \begin{cases} \psi_p(x) = B(p)\, e^{i\frac{(x-a)}{\hbar}p_a(p)}, & x < a \\ \psi_p(x) = e^{i\frac{(x-b)}{\hbar}p} + A(p)\, e^{-ip\frac{(x-b)}{\hbar}}, & x > b \end{cases} \tag{23}$$

where

$$A(p) = \psi_p(b) - 1 \quad ; \quad B(p) = \psi_p(a), \quad p < 0. \tag{24}$$

In the above formulæ, $A(p)$ is the coefficient of the reflected wave (reflection amplitude) whereas $B(p)$ is that of the transmitted wave (transmission amplitude) and the factor in front of the incoming wave ensures that it has amplitude 1. If $p < 0$ and $|p| \leq \sqrt{2em(V_b - V_a)}$ (again assuming that $V_b > V_a$ to fix the idea), it must be noted that $p_a(p)$ in formula (23) is purely imaginary, so that the wave is evanescent in the region $x < a$.

We recall that the corresponding reflection and transmission coefficients

$$R(p) = |A(p)|^2\ , \qquad T(p) = \frac{\Re(p_{a,b}(p))}{p}|B(p)|^2, \tag{25}$$

(where $p_{a,b}(p)$ stands for p_a (resp. p_b) when $p < 0$ (resp. $p > 0$) and $\Re$, $\Im$ for the real and imaginary parts) satisfy

$$R(p) + T(p) = 1, \tag{26}$$

and the reciprocity identity

$$T(p) = T(-p_{a,b}(p)), \quad \text{for all } p \in \mathbb{R} \text{ such that } p_{a,b}(p) \in \mathbb{R}. \tag{27}$$

To any scattering state $\psi_p(x)$ corresponds a time-dependent wave-function

$$\Psi_p(x,t) = \psi_p(x) e^{-i\frac{\mathcal{E}(p)t}{\hbar}},$$

where we denote by $\mathcal{E}(p)$ the energy associated with ψ_p:

$$\mathcal{E}(p) = \frac{p^2}{2m} - eV_a, \text{ for } p > 0 \quad \text{and} \quad \mathcal{E}(p) = \frac{p^2}{2m} - eV_b, \text{ for } p < 0.$$

However, the probability density $|\Psi_p|^2$ associated with Ψ_p is time-independent (which is the definition of a stationary solution of the Schrödinger equation). Therefore, such a wave-function is unable to represent a dynamical process such as the motion of an isolated particle.

To do so, one has to call for the concept of wave-packet. Let $\Phi_\hbar(p_0, p_1)$ be a 'localizing function' which can be viewed as the typical shape of the wave-packet. This function is arbitrary, provided it satisfies a certain number of constraints which will be listed below. Let us think of $\Phi_\hbar$ as a non-negative real valued function, which "gets peaked" about $p_0 = p_1$ as $\hbar$ tends to zero. We shall make this definition more precise later on. We represent an electron coming into the domain Q at time t_0 with momentum p_0 by the following wave-packet:

$$\Psi_{p_0,t_0}(x,t) = \int_{\mathbb{R}} \Phi_\hbar(p_0,p_1)\, \psi_{p_1}(x)\, \exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right) dp_1\,. \tag{28}$$

An important example of wave-packet profile is the Gaussian wave-packet

$$\Phi_\hbar(p_0,p_1) = \sqrt{C_\hbar} \exp\left(-\frac{(p_0-p_1)^2}{4\sigma_\hbar}\right), \tag{29}$$

where $C_\hbar$ is a normalization constant about which we shall come back below and $\sigma_\hbar$ is the momentum variance of the wave-packet. Throughout the paper, $\Phi_\hbar$ will be assumed real-valued.

Although the above formula mixes states corresponding to incoming plane waves from either the left ($p_1 > 0$) or the right ($p_1 < 0$), a semi-classical analysis shows that Ψ_{p_0,t_0} corresponds to a particle entering Q at time t_0 through a and moving to the right if $p_0 > 0$ and entering Q through b and moving to the left if $p_0 < 0$. More specifically, applying the stationary phase theorem, a formal analysis [20] yields, for $p_0 > 0$:

$$\Psi_{p_0,t_0} \sim \begin{cases} \Psi^I_{p_0,t_0} + \Psi^R_{p_0,t_0} & , \quad x < a \\ \Psi^T_{p_0,t_0} & , \quad x > b \end{cases}$$

where the incident $\Psi^I_{p_0,t_0}$, reflected $\Psi^R_{p_0,t_0}$ and transmitted $\Psi^T_{p_0,t_0}$ wave-packets respectively represent classical particles moving according to equations

$$\begin{cases} x_I(t) = a + v_0(t-t_0), & x < a, \quad \text{(incident wave)}, \\ x_R(t) = a - v_0((t-t_0) - \tau_R(p_0)), & x < a, \quad \text{(reflected wave)}, \\ x_T(t) = a + v_0((t-t_0) - \tau_T(p_0)), & x > b, \quad \text{(transmitted wave)}. \end{cases}$$

Therefore, up to a limit $\hbar \to 0$, the incident wave-packet hits the boundary a at time t_0 coming from the left with momentum p_0. It gives rise to a reflected wave-packet which

departs from a at time $t_0 + \tau_R(p_0)$ where $\tau_R(p_0)$ is a quantum reflection time-delay, and to a transmitted wave-packet which departs from b at time $t_0 + \tau_T(p_0)$ with $\tau_T(p_0)$ is the transmission time-delay. These delays are given by the following formula (see also [20])

$$\tau_R(p) = \frac{1}{v}\frac{dS_R(p)}{dp}, \quad \tau_T(p) = \frac{1}{v}\frac{dS_T(p)}{dp}, \tag{30}$$

where $S_R(p)$ and $S_T(p)$ are smooth realizations of the complex phases of the scattering amplitudes:

$$A(p) = \sqrt{R(p)}e^{i\frac{S_R(p)}{\hbar}}, \quad B(p) = \sqrt{\frac{p}{\Re(p_{a,b}(p))}\,T(p)}e^{i\frac{S_T(p)}{\hbar}}.$$

In this paper, we shall give a more rigorous meaning to these statements.

The wave-packet Ψ_{p_0,t_0} is obviously a solution of the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \tilde{H}\Psi\ . \tag{31}$$

¿From these wave-packets, we construct a density matrix which is the quantum analogue of the elementary distributions $\phi_{(a,p_0,t_0)}$ or $\phi_{(b,p_0,t_0)}$. It is defined by

$$\begin{aligned}\rho_{q_0,t_0}(x,x',t) &= \Psi_{q_0,t_0}(x,t)\overline{\Psi_{q_0,t_0}(x',t)} \\ &= \int_{\mathbb{R}^2}\Phi_\hbar(q_0,p_1)\Phi_\hbar(q_0,p_2)\,\psi_{p_1}(x)\overline{\psi_{p_2}(x')}\,\exp\left(-\frac{i}{\hbar}(t-t_0)(\mathcal{E}(p_1)-\mathcal{E}(p_2))\right)dp_1\,dp_2\,.\end{aligned} \tag{32}$$

and represents a particle entering Q at time t_0 through point a if $q_0 > 0$ (resp. through point b if $q_0 < 0$). ρ_{q_0,t_0} is a truly time-dependent solution of the Von-Neumann equation (4).

Of course, for ρ_{q_0,t_0} to represent a physically admissible density matrix, it has to be of trace unity. We recall that the trace of a density matrix $\rho(x,x')$ is given by

$$\mathrm{Tr}\rho = \int_{\mathbb{R}}\rho(x,x)\,dx\,,$$

while $\rho(x,x)\,dx$ represents the probability density associated with ρ. In order to compute the trace of (32), it is convenient to highlight its relation with the scattering transform.

First, we recall that the definition of the Fourier transform of a function $g(p)$ is defined by:

$$\mathcal{F}g\,(\eta) = \frac{1}{2\pi}\int e^{i\eta p}g(p)\,dp\,, \tag{33}$$

while the inverse Fourier transform of a function $G(x)$ is given by:

$$\mathcal{F}^{-1}G\,(p) = \int e^{-i\eta p}G(\eta)\,d\eta\,. \tag{34}$$

The Plancherel identity states that:

$$\int\overline{\mathcal{F}g(\eta)}\,\mathcal{F}f(\eta)\,d\eta = \frac{1}{2\pi}\int\overline{g}\,f\,dp\,. \tag{35}$$

The scattering transform can be viewed as a Fourier transform in which the scattering states $\psi_p(x)$ are used instead of the exponentials e^{ipx}. In particular, it reduces to the Fourier transform (up to a change of variables) in the case of a constant potential. More precisely, we define the scattering transform $\mathcal{G}(g)$ according to:

$$\mathcal{G}g\,(x) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} g(p)\,\psi_p(x)\,dp\,,$$

and the inverse scattering transform:

$$\mathcal{G}^{-1}G\,(p) = \int_{\mathbb{R}} G(x)\,\overline{\psi_p(x)}\,dx\,,$$

It is immediately seen that, in the case of a constant potential, the scattering and Fourier transforms are related by:

$$\begin{aligned}\mathcal{G}g\,(x) &= \frac{1}{\hbar}\mathcal{F}g\left(\frac{x}{\hbar}\right) = \mathcal{F}\left[g(\hbar\cdot)\right](x)\,,\\ \mathcal{G}^{-1}G\,(p) &= \mathcal{F}^{-1}G\left(\frac{p}{\hbar}\right) = \hbar\mathcal{F}^{-1}\left[G(\hbar\cdot)\right](p)\,.\end{aligned}$$

In the general case, $\mathcal{G}^{-1}$ is an isomorphism of Hilbert spaces between $L^2_{\rm ac}$ onto $L^2(\mathbb{R})$, and $\mathcal{G}$ is the inverse isomorphism, where $L^2_{\rm ac}$ denotes the absolutely continuous subspace of $L^2(\mathbb{R})$ associated with the operator $\tilde{H}$. Therefore, we have the analogue of Plancherel's formula:

$$\int \overline{\mathcal{G}g(x)}\,\mathcal{G}f(x)\,dx = \frac{1}{2\pi\hbar}\int \overline{g}\,f\,dp\,, \tag{36}$$

The definition and properties of the scattering transform can be found in [1].

Now, in view of the scattering transform, Ψ_{p_0,t_0} can be written:

$$\Psi_{p_0,t_0}(x,t) = 2\pi\hbar\;\mathcal{G}_{p_1}\left[\Phi_\hbar(p_0,p_1)\,\exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right)\right](x)\,, \tag{37}$$

where $\mathcal{G}_{p_1}$ indicates that we take the scattering transform with respect to p_1. Then, using (36), we compute:

$$\begin{aligned}{\rm Tr}\rho_{q_0,t_0}(t) &= \int_{\mathbb{R}} |\Psi_{q_0,t_0}(x,t)|^2\,dx\\ &= (2\pi\hbar)^2\int_{\mathbb{R}}\left|\mathcal{G}_{p_1}\left[\Phi_\hbar(p_0,p_1)\,\exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right)\right](x)\right|^2\,dx\\ &= 2\pi\hbar\int_{\mathbb{R}}\left|\Phi_\hbar(q_0,p_1)\,\exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right)\right|^2\,dp_1\\ &= 2\pi\hbar\int_{\mathbb{R}}\left|\Phi_\hbar(q_0,p_1)\right|^2\,dp_1\,.\end{aligned}$$

Therefore, the density matrix $\rho_{q_0,t_0}(\cdot,\cdot,t)$ is of trace unity if and only if the wave-packet function $\Phi_\hbar$ satisfies the normalization condition

$$2\pi\hbar \int_{\mathbb{R}} |\Phi_\hbar(p,q)|^2 \, dq = 1\,, \tag{38}$$

which we shall assume satisfied from now on. We note that this normalization condition allows to define the probability density $P_\hbar(p,q)\,dq$ according to

$$P_\hbar(p,q)\,dq = 2\pi\hbar\, |\Phi_\hbar(p,q)|^2 \, dq\,. \tag{39}$$

We also complete the definition of the Gaussian wave-packet (29) by giving the expression of the normalizing constant, which, according to (38) must be equal to $C_\hbar = ((2\pi)^{3/2}\hbar\sqrt{\sigma_\hbar})^{-1}$.

Now, we recall that Q is an open quantum system where the statistics of incoming particles is described by two distribution functions $g_a(p,t)$ $(p>0)$ and $g_b(p,t)$ $(p<0)$. For simplicity, we define the boundary data $\underline{g}$ according to:

$$\underline{g}(p,t) = g_a(p,t) \text{ for } p>0 \quad \text{and} \quad \underline{g}(p,t) = g_b(p,t) \text{ for } p<0; \tag{40}$$

We postulate that the state of the quantum region Q is formed by the superposition of the elementary density matrices ρ_{q_0,t_0}, weighted by the statistics of incoming particles $\underline{g}(q_0,t_0)$. We therefore reproduce formula (8) and define the density matrix in Q by the formula:

$$\begin{aligned} \rho(x,x',t) &= \int_{\mathbb{R}^2} \frac{|q_0|}{m}\, \underline{g}(q_0,t_0)\, \rho_{q_0,t_0}(x,x',t)\, dt_0\, dq_0 \\ &= \int \frac{|q_0|}{m}\, \underline{g}(q_0,t_0)\, \Phi_\hbar(q_0,q_1)\, \Phi_\hbar(q_0,q_2)\, \psi_{q_1}(x)\, \overline{\psi_{q_2}}(x') \times \\ &\qquad \times \exp\left(-\frac{i}{\hbar}(t-t_0)(\mathcal{E}(q_1)-\mathcal{E}(q_2))\right) dt_0\, dq_0\, dq_1\, dq_2. \end{aligned} \tag{41}$$

This defines how the state of the quantum region Q is computed as a function of the inflow statistics g_a and g_b. Now, we turn to the classical distribution function f in the region C. Of course, it is understood that the inflow statistics for the quantum region Q coincides with the outgoing trace of f i.e. relation (6) is still valid:

$$g_a(p,t) = f(a,p,t)\,,\ p>0 \quad ; \quad g_b(p,t) = f(b,p,t)\,,\ p<0\,, \tag{42}$$

The problem is now to find the analogue of relation (7). Again, we take our inspiration from the classical case and more precisely, from the reflection-transmission boundary condition for f as given by (16) and (17). To use this relation in the quantum-classical coupling case, it is tempting to just replace the classical reflection-transmission coefficients and time delays by the quantum ones. However, this procedure is not current-conservative (see section 5). Furthermore, it does not take into account the fact that the quantum delocalization of a particle into a wave-packet mixes states of different momenta (or different energies).

In the remainder of this section, we make the following simplifying hypothesis:

$$\Phi_\hbar(p,q) = 0\,, \quad \text{if } p \text{ and } q \text{ have opposite signs.} \tag{43}$$

Under this hypothesis, we specify the following reflection-transmission condition for f at the interface between C and Q:

$$\begin{aligned} |p|f(a,p,t) &= \int_{q>0} P_\hbar(q,-p)\,R_\hbar(-p)\,f(a,q,t-\tau_R^\hbar(-p))\,|q|\,dq \\ &\quad + \int_{q<0} P_\hbar(q,p_b(p))\,T_\hbar(p_b(p))\,\frac{p}{p_b(p)} f(b,q,t-\tau_T^\hbar(p_b(p)))\,|q|\,dq\,, \quad p<0\,, \end{aligned} \tag{44}$$

$$\begin{aligned} |p|f(b,p,t) &= \int_{q<0} P_\hbar(q,-p)\,R_\hbar(-p)\,f(b,q,t-\tau_R^\hbar(-p))\,|q|\,dq \\ &\quad + \int_{q>0} P_\hbar(q,p_a(p))\,T_\hbar(p_a(p))\,\frac{p}{p_a(p)} f(a,q,t-\tau_T^\hbar(p_a(p)))\,|q|\,dq\,, \quad p>0\,, \end{aligned} \tag{45}$$

In these formulae, $P_\hbar(q,p)$ is the probability density defined by (39) and $(R_\hbar, T_\hbar)$, $(\tau_R^\hbar, \tau_T^\hbar)$ are the quantum reflection-transmission coefficients and time delays. Note that Hypothesis (43) implies that $P_\hbar(q,p) = 0$ if p and q have opposite signs. We also remark that the quantum time delays for reflection and transmission are not equal. In the classical formulae (16) and (17), only one of these times is relevant since, for a given value of p, reflection and transmission never occur simultaneously. The probabilistic nature of quantum mechanics however makes reflection and transmission occur simultaneously and the associated time delays are different.

We now explain the physics behind these conditions. For instance, let us examine (44), the discussion being obviously identical for (45). It expresses that the particles going out of the quantum zone Q through a (i.e. with momentum $p<0$) originate from particles having entered Q at an earlier time, either through a (i.e. with momentum $-p>0$) or through b (i.e. with momentum $p_b(p)<0$). However, the entering particles are transformed into wave-packets as they cross the border of the Q region, by means of $\Phi_\hbar$. Each entering particle through say a with momentum $q>0$ 'excites' a quantum wave of momentum $-p>0$ according to the probability density $P_\hbar(q,-p)$. Therefore the intensity of the wave entering at time t with momentum $-p>0$ per unit time is proportional to

$$\int_{q>0} P_\hbar(q,-p)\,f(a,q,t)\,|q|\,dq\,.$$

Only the fraction $R(-p)$ will be reflected back to a, the remaining part will be transmitted to b. Furthermore, for the wave to 'arrive' at a at time t, it needs to have entered Q at time $t-\tau_R^\hbar(-p)$. Collecting all these remarks leads to the flux of particles exiting Q through a at time t, originating from particles having entered Q through the same point, hence the first integral. The same analysis is valid for the second integral considering waves entering into Q through b and transmitted to a. Simply, the change of p to $p_b(p)$ (if

$V_a \neq V_b$) has to be taken into account. The ratio $p/p_b(p)$ takes into account the change of volume in momentum space in the map $p \to p_b(p)$.

Conditions (44), (45) maintain the positivity (i.e. if the outgoing distribution is positive, the incoming one is also positive). Note however that the Gaussian wave-packet (29) does not satisfy Hypothesis (43). It is worth mentioning that quantum time delays may be non positive. Analytical computations for specially unsmooth potentials like delta potentials indicate that time delays may become negative [24]. Nevertheless, for smooth enough potentials, we shall assume that time delays are positive, otherwise the well-posedness of the kinetic problem in C would not be guaranteed.

To summarize our coupling methodology, we first solve the self-contained problem (1) with the reflection-transmission boundary conditions (44) and (45) for f in the classical region C (provided that the quantum time delays are positive). Then, once f and its boundary values $f(a,p,t)$ (for $p>0$), $f(b,p,t)$ (for $p<0$) are known, we construct the density matrix in the quantum region Q according to (41) where $\underline{g}$ is given by (40) and (42).

2.4. **Classical-quantum coupling: summary of results.** We now outline how we can give a rigorous foundation to the above described coupling methodology. The main tool we will use is the Wigner transform [25]. The Wigner transform of the density matrix (41) is defined according to:

$$W^\hbar(x,p,t) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{i\eta p}\rho\left(x-\frac{\hbar}{2}\eta, x+\frac{\hbar}{2}\eta, t\right)\,d\eta\,.$$

Since the wave-packets Ψ_{q_0,t_0} are solutions of the Schrödinger equation (31), $W^\hbar$ is a solution of the Wigner equation

$$\partial_t W^\hbar + \frac{p}{m}\partial_x W^\hbar + \theta_\hbar[\tilde{V}].W^\hbar = 0\,,$$

where the pseudo-differential operator $\theta_\hbar$ is given by

$$\theta_\hbar[\tilde{V}]W^\hbar(x,p) = -\frac{ie}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{i\eta p}\delta_\hbar[\tilde{V}](x,\eta)\mathcal{F}_p^{-1}W^\hbar(x,\eta)\,d\eta\,,$$

with

$$\delta_\hbar[\tilde{V}](x,\eta) = \frac{\tilde{V}(x+\frac{\hbar}{2}\eta)-\tilde{V}(x-\frac{\hbar}{2}\eta)}{\hbar},$$

and $\mathcal{F}_p^{-1}$ denotes the inverse Fourier transform (34).

In the remainder of the paper, our goal is to prove that, in the semiclassical limit $\hbar \to 0$, $W^\hbar$ converges to a solution $g = g(x,p,t)$ of the Vlasov equation (5) in Q with the inflow boundary conditions (6) at a and b, namely:

$$g(a,p,t) = g_a(p,t)\,,\ p>0 \quad ; \quad g(b,p,t) = g_b(p,t)\,,\ p<0\,. \tag{46}$$

More precisely, we shall prove:

Formal Theorem. *Assuming that $\Phi_\hbar$ is real, we introduce $\Lambda_\hbar$ according to:*

$$\Lambda_\hbar(p,q,q') = 2\pi\hbar\,\Phi_\hbar\left(p, q+\frac{\hbar}{2}q'\right)\Phi_\hbar\left(p, q-\frac{\hbar}{2}q'\right)\,. \tag{47}$$

We note that

$$\Lambda_\hbar(p,q,0) = 2\pi\,\hbar\,|\Phi_\hbar\,(p,q)|^2 = P_\hbar(p,q)\,, \quad \int_{\mathbb{R}} \Lambda_\hbar(p,q,0)\,dq = 1\,. \tag{48}$$

We assume additionally that $\Lambda_\hbar$ satisfies:

$$\lim_{\hbar\to 0} \Lambda_\hbar(p,q,q') = \delta(p-q). \tag{49}$$

Then $W^\hbar$ formally converges as $\hbar \to 0$ towards g, the solution of

$$\begin{cases} \partial_t g + \frac{p}{m}\partial_x g + e\frac{dV}{dx}\partial_p g = 0\,, \\ g(a,p,t) = g_a(p,t), \qquad p>0, \\ g(b,p,t) = g_b(p,t), \qquad p<0. \end{cases}$$

Moreover we have asymptotically

$$W^\hbar(a,-p,t) = R_\hbar(p)W^\hbar(a,p,t-\tau_R^\hbar(p)) + T_\hbar(-p)W^\hbar(b,-p,t-\tau_T^\hbar(-p)), \quad p>0\,, \tag{50}$$

$$W^\hbar(b,-p,t) = R_\hbar(p)W^\hbar(b,p,t-\tau_R^\hbar(p)) + T_\hbar(-p)W^\hbar(a,-p,t-\tau_T^\hbar(-p)), \quad p<0\,, \tag{51}$$

where $R_\hbar(p)$, $T_\hbar(p)$ are the reflection-transmission coefficients (25) and $\tau_R^\hbar(p)$, $\tau_T^\hbar(p)$ are the time delays (30).

Condition (49) guarantees that, in the semi-classical limit, the wave-packet gets more and more localized in both position and momentum. For instance, in the case of the Gaussian wave-packet (29), we have

$$\Lambda_\hbar(p,q,q') = \frac{1}{2\pi\sigma_\hbar}\,\exp -\frac{(p-q)^2}{2\sigma_\hbar}\,\exp -\frac{\hbar^2 q'^2}{8\sigma_\hbar}\,.$$

Therefore, condition (49) is fulfilled as soon as we simultaneously have:

$$\sigma_\hbar \to 0 \quad \text{and} \quad \frac{\hbar^2}{\sigma_\hbar} \to 0 \quad \text{as} \quad \hbar \to 0\,.$$

For instance, $\sigma_h = O(\hbar)$ as $\hbar \to 0$ is convenient.

This 'formal' theorem justifies our methodology in that the Wigner transformed density matrix (41) converges in the semi-classical limit towards the solution of the inflow boundary value problem for the Vlasov equation in the region Q. In particular, as $\hbar \to 0$, the trace of the Wigner function at the boundary ∂Q satisfies the dual reflection-transmission problem to that imposed to the classical distribution function f. Indeed, substituting $f(a,p,t)$ to $W^\hbar(a,-p,t)$ and similarly at point b transforms (50), (51) into (16), (17).

Therefore, our definition of the density matrix seems established on a solid basis, in spite of the arbitrariness of the wave-packet function $\Phi_\hbar$.

The remainder of the paper is organized as follows. Section 3 develops the proof of theorem 2.4 in the case $V_a = V_b$. Then, in section 4, the extension of the result to the case $V_a \neq V_b$ will be outlined. In section 5, we prove that the reflection-transmission conditions (44), (45) satisfy the time-integrated current conservation principle. Finally, in section 6, we specialize to the stationary state in order to bridge the gap with earlier work of one of the authors [4].

3. Proof of theorem 2.4 in the case $V_a = V_b$

3.1. **Preliminaries.** First, we introduce some notations. We shall need to distinguish between the density matrices $\rho^{(a)}$ and $\rho^{(b)}$ of electrons injected at the boundaries a and b respectively:

$$\rho^{(a)}(x,x',t) = \int_{\mathbb{R}^+} dq_0 \int_{\mathbb{R}} dt_0 \, \frac{|q_0|}{m} \, g_a(q_0,t_0) \, \Psi_{q_0,t_0}(x,t) \, \overline{\Psi_{q_0,t_0}(x',t)}, \tag{52}$$

$$\rho^{(b)}(x,x',t) = \int_{\mathbb{R}^-} dq_0 \int_{\mathbb{R}} dt_0 \, \frac{|q_0|}{m} \, g_b(q_0,t_0) \, \Psi_{q_0,t_0}(x,t) \, \overline{\Psi_{q_0,t_0}(x',t)}, \tag{53}$$

so that $\rho = \rho^{(a)} + \rho^{(b)}$. We also decompose $W^\hbar = W_a^\hbar + W_b^\hbar$ with

$$W_{a,b}^\hbar(x,p,t) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\eta p} \rho^{(a,b)} \left(x - \frac{\hbar}{2}\eta, x + \frac{\hbar}{2}\eta, t \right) d\eta. \tag{54}$$

The major part of the computation concerns boundary conditions. Indeed, let $\theta(x,p,t)$ be a test function in $\mathcal{D}(\mathbb{R}_x \times \mathbb{R}_p \times \mathbb{R}_t)$. We have the following identity obtained by a simple integration by parts.

$$\int_{(x,p,t)\in[a,b]\times\mathbb{R}^2} \theta \left[\partial_t W^\hbar + \frac{p}{m}\partial_x W^\hbar + e\frac{dV}{dx}\partial_p W^\hbar \right] dx\,dp\,dt = I_b^\hbar - I_a^\hbar - I_{ab}^\hbar,$$

where

$$I_{ab}^\hbar = \int_{(x,p,t)\in[a,b]\times\mathbb{R}^2} W^\hbar \left[\partial_t\theta + \frac{p}{m}\partial_x\theta + e\frac{dV}{dx}\partial_p\theta \right] dx\,dp\,dt,$$

$$I_b^\hbar = \int_{\mathbb{R}^2} \frac{p}{m}\theta(b,p,t) W^\hbar(b,p,t)\, dp\,dt,$$

$$I_a^\hbar = \int_{\mathbb{R}^2} \frac{p}{m}\theta(a,p,t) W^\hbar(a,p,t)\, dp\,dt\ .$$

Standard results on semi-classical limits (see e.g. [17, 15, 14, 18, 19] etc.) allow to perform the $\hbar \to 0$ limit in the interior of the interval $[a,b]$, so that:

$$\lim_{\hbar\to 0} -I_{ab}^\hbar + I_b^\hbar - I_a^\hbar = 0\ . \tag{55}$$

In particular, we have:

Lemma 3.1.

$$\lim_{\hbar\to 0} I^\hbar_{ab} = \int_{(x,p,t)\in[a,b]\times\mathbb{R}^2} g\left[\partial_t\theta + \frac{p}{m}\partial_x\theta + e\frac{dV}{dx}\partial_p\theta\right] dx\,dp\,dt. \tag{56}$$

Next we need to calculate the $\hbar\to 0$ limit of the left boundary term $I^\hbar_a$. The right boundary term $I^\hbar_b$ can be treated analogously. To this aim, we introduce

$$U(p,t) = \frac{p}{m}\theta(a,p,t), \tag{57}$$

and we remark that $U(0,t)=0$ for all $t\in\mathbb{R}$. We compute:

$$\begin{aligned} I^\hbar_a &= \int_{\mathbb{R}^2} U(p,t)W^\hbar(a,p,t)\,dp\,dt \\ &= \int_{\mathbb{R}^2} U(p,t)W^\hbar_a(a,p,t)\,dp\,dt + \int_{\mathbb{R}^2} U(p,t)W^\hbar_b(a,p,t)\,dp\,dt, \end{aligned}$$

where $W^\hbar_a$ and $W^\hbar_b$ are defined at (54). Let us denote by $J^\hbar_a$ the first integral and $K^\hbar_a$ the second one. We have:

$$\begin{aligned} J^\hbar_a &= \int U(p,t)W^\hbar_a(a,p,t)\,dp\,dt \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^4} dp\,d\eta dt_0 dt \int_{\mathbb{R}+} dq_0 e^{i\eta p}U(p,t)\frac{|q_0|}{m}g_a(q_0,t_0)\overline{\Psi_{q_0,t_0}}(a+\frac{\hbar}{2}\eta,t)\times \\ &\qquad\qquad \times\Psi_{q_0,t_0}(a-\frac{\hbar}{2}\eta,t). \end{aligned} \tag{58}$$

On the other hand we have

$$\begin{aligned} &\overline{\Psi_{q_0,t_0}}(a+\frac{\hbar}{2}\eta,t)\Psi_{q_0,t_0}(a-\frac{\hbar}{2}\eta,t) \\ &= \int_{\mathbb{R}^2}\Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)\overline{\psi_{q_1}}\left(a+\frac{\hbar}{2}\eta\right)\psi_{q_2}\left(a-\frac{\hbar}{2}\eta\right)\times \\ &\qquad\qquad \times\exp\left[i\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)\right]\,dq_1\,dq_2. \end{aligned} \tag{59}$$

Before analyzing (58), we claim that the behavior of the right hand side of (59) as $\hbar$ tends to zero is left unchanged if we replace the integration set by $\mathbb{R}^2_+$.

$$\begin{aligned} &\overline{\Psi_{q_0,t_0}}(a+\frac{\hbar}{2}\eta,t)\Psi_{q_0,t_0}(a-\frac{\hbar}{2}\eta,t) \\ &\simeq \int_{\mathbb{R}^2_+}\Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)\overline{\psi_{q_1}}\left(a+\frac{\hbar}{2}\eta\right)\psi_{q_2}\left(a-\frac{\hbar}{2}\eta\right)\times \\ &\qquad\qquad \times\exp\left[i\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)\right]\,dq_1\,dq_2. \end{aligned} \tag{60}$$

This is a consequence of the fact that the wave packet "is peaked" around q_0 and q_0 is positive. This claim can be rigorously proven by applying the dominated convergence theorem and will be developed in [6].

3.2. **First approximation: using the asymptotics of ψ_q in the neighborhood of the boundary.** A simple rescaling of the Schrödinger equation (19) leads to:

$$\lim_{\hbar\to 0} \psi_q^\hbar\left(a+\frac{\hbar}{2}\eta\right) - e^{i\frac{q}{2}\eta} - A(q)e^{-i\frac{q}{2}\eta} = 0 \quad \text{for } q>0, \tag{61}$$

uniformly with respect to $\eta \in]-\infty, M]$ ($\forall\ M>0$). In what follows, we shall forget the subscripts $\hbar$ in the reflection-transmission coefficients and time-delays for clarity. Replacing $\psi_q\left(a+\frac{\hbar}{2}\eta\right)$ by $e^{i\frac{q}{2}\eta} + A(q)e^{-iq\eta}$ in (59) leads to the following approximate formula.

$$\overline{\Psi_{q_0,t_0}}\left(a+\frac{\hbar}{2}\eta, t\right)\Psi_{q_0,t_0}\left(a-\frac{\hbar}{2}\eta, t\right) \approx \mathrm{I}_\hbar + \mathrm{II}_\hbar + \mathrm{III}_\hbar + \mathrm{IV}_\hbar, \tag{62}$$

where

$$\mathrm{I}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\,\Phi_\hbar(q_0,q_2) e^{-i\frac{[q_1+q_2]}{2}\eta}\, e^{i\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)}\, dq_1\, dq_2, \tag{63}$$

$$\mathrm{II}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\,\Phi_\hbar(q_0,q_2)\overline{A(q_1)}\, A(q_2) e^{i\frac{q_1+q_2}{2}\eta}\, e^{i\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)}\, dq_1\, dq_2, \tag{64}$$

$$\mathrm{III}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\,\Phi_\hbar(q_0,q_2)\,\overline{A}(q_1)\, e^{i\frac{(q_1-q_2)}{2}\eta}\, e^{i\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)}\, dq_1\, dq_2, \tag{65}$$

$$\mathrm{IV}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\,\Phi_\hbar(q_0,q_2)\, A(q_2)\, e^{i\frac{q_2-q_1}{2}\eta}\, e^{i\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)}\, dq_1\, dq_2, \tag{66}$$

The first two terms correspond to the contributions of the two plane waves (corresponding to q_1 and q_2) traveling in the same direction, while the last two ones correspond to contributions of opposite traveling waves. We shall see later on that, because of the assumption (49) on the wave-packet function $\Phi_\hbar$, the last two integrals have vanishing $\hbar \to 0$ limits.

In order to compute these limits, we perform the change of variables

$$(z,y) = \left(\frac{q_1+q_2}{2}, \frac{q_1-q_2}{\hbar}\right), \quad (q_1,q_2) = (z+\frac{\hbar}{2}y,\, z-\frac{\hbar}{2}y), \quad \frac{q_1^2-q_2^2}{2m\hbar} = \frac{yz}{m}, \tag{67}$$

in (63)–(66). Introducing $\Lambda_\hbar$ according to (47), this leads to:

$$\mathrm{I}_\hbar = \frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)\; e^{-iz\eta}\, e^{i\frac{yz}{m}(t-t_0)}\, dz\, dy, \tag{68}$$

$$\mathrm{II}_\hbar = \frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)\; \overline{A}(z+\frac{\hbar}{2}y)\, A(z-\frac{\hbar}{2}y)\; e^{iz\eta}\, e^{i\frac{yz}{m}(t-t_0)}\, dz\, dy, \tag{69}$$

$$\mathrm{III}_\hbar = \frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)\; \overline{A}(z+\frac{\hbar}{2}y)\; e^{iy\hbar\eta} e^{i\frac{yz}{m}(t-t_0)}\, dz\, dy, \tag{70}$$

$$\mathrm{IV}_\hbar = \frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)\; A(z-\frac{\hbar}{2}y)\; e^{-iy\hbar\eta} e^{i\frac{yz}{m}(t-t_0)}\, dz\, dy\ . \tag{71}$$

We deduce from (58) that

$$J_a^\hbar \simeq \frac{1}{2\pi}\int e^{i\eta p} U(p,t)\,\frac{q_0}{m}\, g_a(q_0,t_0)\,[(\mathrm{I}_\hbar+\mathrm{II}_\hbar+\mathrm{III}_\hbar+\mathrm{IV}_\hbar)(q_0,t_0,\eta,t)]\, dp\, d\eta\, dt_0\, dt\, dq_0.$$

We first integrate with respect to p. This gives

$$J_a^\hbar = \int \mathcal{F}_p U(\eta,t)\,\frac{q_0}{m}\, g_a(q_0,t_0)\,[(\mathrm{I}_\hbar+\mathrm{II}_\hbar+\mathrm{III}_\hbar+\mathrm{IV}_\hbar)(q_0,t_0,\eta,t)]\, dq_0\, dt_0\, d\eta\, dt\,. \tag{72}$$

3.3. **Second approximation: using the asymptotics of the reflection amplitude.** Let us now work on $\mathrm{II}_\hbar$. We first recall that the reflection coefficient R and the phase S_R of the reflection amplitude are given by:

$$A(z) = \sqrt{R(z)}\; e^{i\frac{S_R(z)}{\hbar}}.$$

We suppose that S is a smooth (at least differentiable) determination of the phase and that it converges smoothly when $\hbar \to 0$. We then have:

$$\overline{A}\left(z+\frac{\hbar}{2}y\right) A\left(z-\frac{\hbar}{2}y\right) = R(z)e^{-iS'_R(z)y} + O(\hbar),$$

where

$$S'_R(z) = \frac{d}{dz}S_R(z)\ .$$

This finally leads to

$$\mathrm{II}_\hbar \simeq \frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y) R(z) e^{i\eta z} e^{-iS'_R(z)y} e^{i\frac{yz}{m}(t-t_0)}\, dy\, dz.$$

Now, going back to (72), we notice that t appears in $\mathrm{I}_\hbar$, $\mathrm{II}_\hbar$, $\mathrm{III}_\hbar$, $\mathrm{IV}_\hbar$ only through complex exponentials. Therefore, by integrating first with respect to t, we obtain Fourier transforms of U with respect to the time variable. We finally end up with the following formulæ:

$$J_a^\hbar = \mathrm{I}'_\hbar + \mathrm{II}'_\hbar + \mathrm{III}'_\hbar + \mathrm{IV}'_\hbar,$$

where

$$\mathrm{I}'_\hbar = \int \mathcal{F}_{p,t}U\left(\eta, \frac{yz}{m}\right) \frac{q_0}{m} g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y) e^{-i\eta z} e^{-i\frac{yz}{m}t_0}\, dy\, dz\, dt_0\, dq_0\, d\eta,$$

$$\mathrm{II}'_\hbar = \int \mathcal{F}_{p,t}U\left(\eta, \frac{yz}{m}\right) \frac{q_0}{m} g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y) R(z) e^{i\eta z} e^{-iS'_R(z)y} e^{-i\frac{yz}{m}t_0}\, dy\, dz\, dt_0\, dq_0\, d\eta,$$

$$\mathrm{III}'_\hbar = \int \mathcal{F}_{p,t}U\left(\eta, \frac{yz}{m}\right) \frac{q_0}{m} g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y) \overline{A}\left(z+\frac{\hbar}{2}\eta\right) e^{iy\hbar\eta} e^{-i\frac{yz}{m}t_0}\, dy\, dz dt_0\, dq_0\, d\eta,$$

$$\mathrm{IV}'_\hbar = \int \mathcal{F}_{p,t}U\left(\eta, \frac{yz}{m}\right) \frac{q_0}{m} g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y) A\left(z-\frac{\hbar}{2}\eta\right) e^{-iy\hbar\eta} e^{-i\frac{yz}{m}t_0}\, dy\, dz\, dt_0\, dq_0\, d\eta,$$

where the integration domain is $\mathbb{R}$ except for the variable q_0 where it is $\mathbb{R}_+$.

3.4. **Third approximation: using the assumption (49) on the wave-packets.** Formally, using (49), $\mathrm{I}'_\hbar$ converges in the sense of measures to:

$$\mathrm{I}'_\hbar = \frac{2\pi}{m} \int \mathcal{F}_{p,t}U\left(\eta, \frac{yz}{m}\right) z\, \overline{\mathcal{F}_t g_a\left(z, \frac{yz}{m}\right)}\, e^{-i\eta z}\, \mathbf{1}_{z>0}\, dy\, dz\, d\eta,$$

and the other terms are approximated by:

$$\mathrm{II}'_\hbar \simeq \frac{2\pi}{m} \int \mathcal{F}_{p,t}U\left(\eta, \frac{yz}{m}\right)\, z\, \overline{\mathcal{F}_t g_a\left(z, \frac{yz}{m}\right)}\, e^{i\eta z}\, R(z)\, e^{-iS'_R(z)y}\, \mathbf{1}_{z>0}\, dy\, dz\, d\eta,$$

$$\mathrm{III}'_\hbar \simeq \frac{2\pi}{m} \int \mathcal{F}_{p,t}U\left(\eta, \frac{yz}{m}\right)\, z\, \overline{\mathcal{F}_t g_a\left(z, \frac{yz}{m}\right)}\, \overline{A}\left(z+\frac{\hbar}{2}y\right)\, e^{iy\hbar\eta}\, \mathbf{1}_{z>0}\, dy\, dz\, d\eta,$$

where $\mathbf{1}_{z>0}$ denotes the characteristic function of the set $\{z>0\}$. The estimate for $\mathrm{IV}'_\hbar$ is similar as for $\mathrm{III}'_\hbar$.

Next, letting z fixed and integrating with respect to y leads, in view of the Parseval identity, to:

$$\mathrm{I}'_\hbar = \int_{(z,\eta,t)\in\mathbb{R}^+\times\mathbb{R}^2} \mathcal{F}_p U(\eta,t) g_a(z,t) e^{-i\eta z} dz\, d\eta\, dt = \int_{(z,t)\in\mathbb{R}^+\times\mathbb{R}} U(z,t) g_a(z,t)\, dt\, dz.$$

For $\mathrm{II}'_\hbar$, using the same computations, we get:

$$\mathrm{II}'_\hbar \simeq \int_{(z,t)\in\mathbb{R}^+\times\mathbb{R}} U(-z,t)\, g_a(z, t-\tau_R(z)) R(z)\, dt\, dz$$

where the reflection time delay $\tau_R(z)$ is given by (30).

Next, we claim that $\mathrm{III}'_\hbar$ tends to zero when $\hbar \to 0$. Indeed, integrating first with respect to η in the formula for $\mathrm{III}'_\hbar$, gives

$$\mathrm{III}'_\hbar = \frac{2\pi}{m} \int_{(z,y)\in\mathbb{R}^+\times\mathbb{R}} \mathcal{F}_t U\left(-\hbar y, \frac{yz}{m}\right)\, z\, \overline{\mathcal{F}_t g_a\left(z, \frac{yz}{m}\right)}\, \overline{A\left(z+\frac{\hbar}{2}y\right)}\, dy\, dz\ .$$

We just notice now that $|\overline{A}| \leq 1$, and that

$$\mathcal{F}_t U\left(-\hbar y, \frac{yz}{m}\right) \xrightarrow[\hbar \to 0]{} \mathcal{F}_t U\left(0, \frac{yz}{m}\right) = 0$$

since $U(0,t) = 0$. Since $\mathcal{F}_t U$, $\mathcal{F}_t g_a$ are smooth and sufficiently decaying at ∞, the dominated convergence theorem implies $\lim_{\hbar \to 0} \text{I\!I}'_\hbar = 0$. Therefore it follows that

$$\begin{aligned} J_a^\hbar &= \int_{\mathbb{R}^2} U(p,t) W_a^\hbar(a,p,t)\, dp\, dt \\ &\simeq \int_{(p,t)\in \mathbb{R}^+ \times \mathbb{R}} U(p,t) g_a(p,t)\, dp\, dt + \int_{(p,t)\in \mathbb{R}^+ \times \mathbb{R}} U(-p,t) g_a(p, t-\tau_R(p)) R(p)\, dp\, dt\ . \end{aligned}$$

Proceeding analogously for K_a^h, we find:

$$\begin{aligned} K_a^h &= \int_{\mathbb{R}^2} U(p,t) W_b^\hbar(a,p,t)\, dp\, dt \\ &\simeq \int_{(p,t)\in \mathbb{R}^- \times \mathbb{R}} T(p) U(p,t) g_b(p, t-\tau_T(p))\, dp\, dt, \end{aligned}$$

where the transmission time delay $\tau_T(z)$ is given by (30). This leads to the following asymptotic formulæ, restoring the dependence with respect to $\hbar$:

$$\begin{aligned} &W_a^\hbar(a,p,t) = g_a(p,t) \quad ; \quad W_a^\hbar(a,-p,t) = R_\hbar(p)\, g_a(p, t-\tau_R^\hbar(p)), \\ &W_b^\hbar(a,p,t) = 0 \qquad\quad ; \quad W_b^\hbar(a,-p,t) = T_\hbar(-p)\, g_a(-p, t-\tau_T^\hbar(-p)), \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{for } p>0. \end{aligned} \tag{73}$$

Analogously, we have the following asymptotic formulæ

$$\begin{aligned} &W_b^\hbar(b,p,t) = g_b(p,t) \quad ; \quad W_b^\hbar(b,-p,t) = R_\hbar(p)\, g_b(p, t-\tau_R^\hbar(p)), \\ &W_a^\hbar(b,p,t) = 0 \quad ; \quad W_a^\hbar(b,-p,t) = T_\hbar(-p)\, g_a(-p, t-\tau_T^\hbar(-p)), \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{for } p<0. \end{aligned}$$

Summing the asymptotic formulae for W_a^h and $W_b^\hbar$, we obtain relations (50) and (51), which concludes the proof of theorem 2.4 in the case $V_a = V_b$. □

4. The case $V_a \neq V_b$

In this section, we briefly describe how the proof should be adapted to the case $V_a \neq V_b$. The asymptotic analysis of $J_a^\hbar$ is unchanged while that of $K_a^\hbar$ needs to be adapted. We recall that

$$K_a^h = \int_{\mathbb{R}^2} U(p,t) W_b^\hbar(a,p,t)\, dp\, dt,$$

and is given by (58) in which g_a is replaced by g_b and the integration domain of the variable q_0 is $\mathbb{R}_-$. Besides, we can use (60) in which the integration domain is $\mathbb{R}^2_-$ for exactly the same reasons as those developed in the case $V_a = V_b$. Note that the phase

factor $i\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)$ is left unchanged since the energy $\mathcal{E}(q_1)$ and $\mathcal{E}(q_2)$ are shifted by the same amount, q_1 and q_2 having the same sign.

Next, we claim that the contribution of terms for which $p_a(q_1)$ (or $p_a(q_2)$) are imaginary is exponentially small as stated in Lemma B.3 of [4] (again a rigorous proof developed in [6] relies on the dominated convergence theorem). Now, using the asymptotic expansion

$$\psi_q(a+\frac{\hbar}{2}\eta) = B(q)e^{+i\frac{p_a(q)}{2}\eta} + O(\hbar)$$

leads to the asymptotic approximation (an analogue of (72)):

$$K_a^\hbar \simeq \int \mathcal{F}_p U(\eta,t)\,\frac{|q_0|}{m}\,g_b(q_0,t_0)\,\mathrm{I}_\hbar(q_0,t_0,\eta,t)\,dq_0\,dt_0\,d\eta\,dt\,,$$

where the integration domain is $\mathbb{R}$ for all variables except for q_0 where it is $\mathbb{R}_-$. The term $\mathrm{I}_\hbar$ is given by

$$\mathrm{I}_\hbar = \frac{1}{2\pi}\int_{\mathbb{R}^2_\hbar} \Lambda_\hbar(q_0,z,y)\,\overline{B}(z+\frac{\hbar}{2}y)B(z-\frac{\hbar}{2}y)e^{-i\frac{p_a(z+\frac{\hbar}{2}y)+p_a(z-\frac{\hbar}{2}y)}{2}\eta}\,e^{i\frac{yz}{m}(t-t_0)}\,dz\,dy,$$

where

$$\mathbb{R}^2_\hbar = \{(z,y)\in\mathbb{R}^2 \quad ,s.t. \quad (z\pm\frac{\hbar}{2}y)<0,\ \ p_a(z\pm\frac{\hbar}{2}y)\in\mathbb{R}\}.$$

Using the asymptotics of the transmission amplitude in the same way as in section 3.3, we find the asymptotic expression for $\mathrm{I}_\hbar$

$$\mathrm{I}_\hbar \simeq \int_{y\in\mathbb{R}}\int_{z<0,\ s.t.\ p_a(z)\in\mathbb{R}} \Lambda_\hbar(q_0,z,y)T(z)\frac{z}{p_a(z)}e^{-ip_a(z)\eta}e^{-i\frac{z}{m}\tau_T(z)y}e^{i\frac{yz}{m}(t-t_0)}dz\,dy\,.$$

This leads to

$$K_\hbar^a \simeq \int_{z<0,\ s.t.\ p_a(z)\in\mathbb{R}}\int_{(t,\eta)\in\mathbb{R}^2} \mathcal{F}_p U(\eta,t)g_b(z,t-\tau_T(z))T(z)\frac{z}{p_a(z)}e^{-i\eta p_a(z)}dz\;d\eta\,dt.$$

Letting $z'=p_a(z)$ which yields $z=p_b(z')$ and $zdz=z'dz'$, we obtain:

$$K_\hbar^a \simeq \int_{(z',t,\eta)\in\mathbb{R}_-\times\mathbb{R}^2} \mathcal{F}_p U(\eta,t)g_b(p_b(z'),t-\tau_T(p_b(z')))T(p_b(z'))e^{-i\eta z'}dz'\;d\eta\,dt.$$

The integration domain in z' is $\mathbb{R}_-$ because

- if $V_a \le V_b$, the set $\{z<0, \quad p_a(z)\in\mathbb{R}\}$ is nothing but $(-\infty,-\sqrt{2me(V_b-V_a)})$, which leads to $\mathbb{R}_-$ after the change of variable $z'=p_b(z)$
- if $V_a \ge V_b$, then $\{z<0, \quad p_a(z)\in\mathbb{R}\}=\mathbb{R}_-$ and the integration interval in z' should be $(-\infty,-\sqrt{2me(V_a-V_b)})$. Integrating on the whole half line $\mathbb{R}_-$ does not change the result since $T(p_b(z'))=0$ whenever $z'\in(-\sqrt{2me(V_a-V_b)},0)$.

Finally, making use of the reciprocity identities

$$T(p_p(p))=T(-p)\,, \quad \tau_T(p_b(p))=\tau_T(-p)$$

as well as the Parseval identity, we obtain

$$K_\hbar^a \simeq \int_{(p,t)\in\mathbb{R}_+\times\mathbb{R}} U(-p,t)T(-p_b(p))\, g_b(-p_b(p), t-\tau_T(-p_b(p)))\, dp\, dt\,,$$

which is the desired asymptotic result.

5. Time-integrated current conservation

In this section, we go back to the coupling methodology defined by equations (41)-(45). An important criterion for the validity of the coupling methodology is that it is current conservative, i.e. that there is no net creation or destruction of particles. Here, we show that our coupling approach is current conservative, in a time-integrated form. Instantaneous current conservation cannot be obtained because it would violate the time-energy uncertainty principle. Indeed, the quantum wave-packet description of a particle implies a certain time delocalization (which is at least equal to $\hbar$ over the energy delocalization). Therefore, it is not possible to a priori know how much of a given wave-packet has crossed the border between the C and Q region (or vice-versa) at a given time. However, we must be certain that, once an infinite time has elapsed, the whole wave-packet has crossed the border, hence a current conservation in time-integrated form.

Let us denote by $J_C(a,t)$ and $J_Q(a,t)$ the classical and quantum currents flowing through point a at time t. They are respectively defined by:

$$J_Q(a,t) = \frac{\hbar}{m}\Im\left(\frac{\partial\rho}{\partial x}(a,a,t)\right) = \frac{\hbar}{m}\int_{\mathbb{R}^2}\frac{|q_0|}{m}\,\underline{g}(q_0,t_0)\,\Im\left[\overline{\Psi_{q_0,t_0}}(a,t)\Psi'_{q_0,t_0}(a,t)\right]\,dq_0\,dt_0, \tag{74}$$

$$J_C(a,t) = \int_{\mathbb{R}}\frac{p}{m}f(a,p,t)\,dp, \tag{75}$$

with $\underline{g}$ defined by (40) and (42). Then:

Lemma 5.1. *Under Hypothesis (43), we have:*

$$\int_{\mathbb{R}} J_Q(a,t)dt = \int_{\mathbb{R}} J_C(a,t)dt\,, \quad \int_{\mathbb{R}} J_Q(b,t)dt = \int_{\mathbb{R}} J_C(b,t)dt\,. \tag{76}$$

Proof : We prove the first relation (76). The proof of the second one obviously follows the same method. We start with the computation of $J_Q(a,t)$. Inserting formula (28) in

(74) and performing the change of variables $q_1 = z + \frac{\hbar}{2}y$, $q_2 = z - \frac{\hbar}{2}y$, we get:

$$\begin{aligned}
&\int_{\mathbb{R}} J_Q(a,t)\,dt = \\
&= \Im\left\{ \frac{\hbar}{m^2} \int |q_0|\, \overline{\mathcal{F}_t \underline{g}\left(q_0, \frac{yz}{m}\right)}\, \Lambda_\hbar(q_0,z,y)\, \overline{\psi_{z+\frac{\hbar}{2}y}(a)}\, \psi'_{z-\frac{\hbar}{2}y}(a)\, e^{i\frac{yz}{m}t}\, dt\, dz\, dy\, dq_0 \right\} \\
&= \Im\left\{ \frac{2\pi\hbar}{m} \int \frac{|q_0|}{|z|}\, \overline{\mathcal{F}_t \underline{g}(q_0,0)}\, \Lambda_\hbar(q_0,z,0)\, \overline{\psi_z(a)}\, \psi'_z(a)\, dq_0\, dz \right\}
\end{aligned}$$

Since,

$$\Im\left(\overline{\psi_z}(a)\psi'_z(a)\right) = \frac{z}{\hbar}(1-R(z)) = \frac{z}{\hbar}T(z) \quad (z>0) \quad ; \quad \Im\left(\overline{\psi_z}(a)\psi'_z(a)\right) = \frac{z}{\hbar}T(z) \quad (z<0),$$

we deduce, with (48):

$$\begin{aligned}
\int_{\mathbb{R}} J_Q(a,t)\,dt &= \int_{\mathbb{R}} \frac{q_0}{m}\, \tilde{T}_\hbar(q_0)\, \mathcal{F}_t \underline{g}(q_0,0)\, dq_0 \\
&= \int_{\mathbb{R}^2} \frac{p}{m}\, \tilde{T}_\hbar(p)\, \underline{g}(p,t)\, dp\, dt,
\end{aligned}$$

where

$$\tilde{T}_\hbar(p) = \int P_\hbar(p,z)\, T_\hbar(z)\, dz, \quad \tilde{R}_\hbar(p) = \int P_\hbar(p,z)\, R_\hbar(z)\, dz\,. \tag{77}$$

Now, we turn to the computation of $J_C(a,t)$. Introducing

$$F(x,p) = \int_{\mathbb{R}} f(x,p,t)\, dt\,, \tag{78}$$

We have, with (44), (45), and dropping the indices $\hbar$ for simplicity:

$$\begin{aligned}
\int_{\mathbb{R}} J_C(a,t)dt &= \int_{p>0} p\,[F(a,p) - F(a,-p)]\,dp \\
&= \int_{p>0} p\,F(a,p)\,dp - \left\{ \int_{p>0}\int_{q>0} P(q,p)\, R(p)\, F(a,q)\, |q|\, dq\, dp \right. \\
&\qquad \left. + \int_{p>0}\int_{q<0} P(q,-p_b(p))\, T(-p_b(p))\, \frac{p}{p_b(p)}\, F(b,q)\, |q|\, dq\, dp \right\}
\end{aligned} \tag{79}$$

By exchanging the p and q variables in the integrals inside the curly brackets, we are led to:

$$\begin{aligned}
\int_{\mathbb{R}} J_C(a,t)dt &= \int_{p>0} |p|\, F(a,p)\, dp - \int_{p>0} F(a,p)\, |p| \left(\int_{q>0} P(p,q)\, R(q)\, dq \right) dp \\
&\quad - \int_{p<0} F(b,p)\, |p| \left(\int_{q>0} P(p,-p_b(q))\, T(-p_b(q))\, \frac{q}{p_b(q)}\, dq \right) dp\,.
\end{aligned} \tag{80}$$

Now, we have, using the normalization condition (38) together with relation (26):

$$1 - \int_{q>0} P(p,q)\, R(q)\, dq = \int_{q>0} P(p,q)\, T(q)\, dq = \tilde{T}(p), \quad p > 0,$$
$$\int_{q>0} P(p,-p_b(q))\, T(-p_b(q))\, \frac{q}{p_b(q)}\, dq = \int_{q>0} P(p,-q)\, T(-q)\, dq = \tilde{T}(p), \quad p < 0,$$

and therefore, (80) leads to:

$$\int_{\mathbb{R}} J_C(a,t)dt = \int_{p>0} |p|\, \tilde{T}(p)\, F(a,p)\, dp - \int_{p<0} |p|\, \tilde{T}(p)\, F(b,p)\, dp\,.$$

But, with (78) and the fact that the outgoing trace of f coincides with the incoming trace of g (see equ. (42)), we deduce that

$$\int_{\mathbb{R}} J_C(a,t)dt = \int_{\mathbb{R}^2} \tilde{T}(p)\, \underline{g}(p,t)\, p\, dp = \int_{\mathbb{R}} J_Q(a,t)dt\,,$$

which completes the proof. □

6. Classical-quantum coupling in the stationary case

In the present section, we specialize our method for the stationary case in order to bridge the gap with previous work [4]. We first state the:

Lemma 6.1. *Assume that the function $\underline{g}$ does not depend on time and that Hypothesis (43) holds true. Then the density matrix ρ defined by (41) does not depend on time and is given by*

$$\rho(x,x') = \int \tilde{g}(q)\psi_q(x)\overline{\psi_q}(x')\, dq \tag{81}$$

with

$$\tilde{g}(p) = 2\pi\hbar \int_{\mathbb{R}} \frac{|q|}{|p|} |\Phi_\hbar(q,p)|^2 \underline{g}(q)\, dq = \int_{\mathbb{R}} P(q,p)\, \frac{|q|}{|p|}\, \underline{g}(q)\, dq. \tag{82}$$

In a previous work, one of the authors [4] proposed a method for the stationary case based on (81) with $\underline{g}$ instead of $\tilde{g}$. We have seen that, given the conditions (49) on $\Phi_\hbar(q,p)$, $\tilde{g}$ is close to $\underline{g}$ in the limit $\hbar \to 0$. Therefore, these two constructions are consistent.

Proof : Performing the changes of variables $t_1 = t_0 - t$ and $(q_1, q_2) \to (z, y)$ (defined by (67)) in the expression (41) (in which $\underline{g}$ is now independent of t), we obtain

$$\rho(x,x',t) = \frac{1}{2\pi} \int \frac{|q_0|}{m}\, \underline{g}(q_0)\, \Lambda_\hbar(q_0,z,y)\, \psi_{z+\frac{\hbar}{2}y}(x)\, \overline{\psi_{z-\frac{\hbar}{2}y}(x')} \times$$
$$\times \exp\left(it_1 \frac{yz}{m}\right) dt_1\, dq_0\, dy\, dz\,,$$

which ensures that ρ does not depend on time. The integrations with respect to t_1 and y are respectively performed and lead to:

$$\begin{aligned}\rho(x,x') &= \int \frac{|q_0|}{|z|}\, \underline{g}(q_0)\, P(q_0,z)\, \psi_z(x)\, \overline{\psi_z(x')}\, dq_0\, dz \\ &= \int \tilde{g}(z)\, \psi_z(x)\, \overline{\psi_z(x')}\, dz\,,\end{aligned}$$

which leads to the result. □

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