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# Inflow boundary conditions for the time dependent one-dimensional Schrödinger equation

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**Abstract.** A transient quantum model for one-dimensional charge transport is derived and shown to lead in the semiclassical limit to the inflow boundary value problem for the Vlasov equation. Asymptotic formulae involving quantum reflection-transmission coefficients and time delays are used to construct a hybrid model coupling quantum descriptions to kinetic ones in a time-dependent one-dimensional setting. © 2000 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

***Conditions aux limites entrantes pour l'équation de Schrödinger unidimensionnelle dans le régime transitoire***

**Résumé.** *Un modèle transitoire de transport quantique monodimensionnel est proposé. L'analyse asymptotique de ce modèle conduit, dans la limite semi-classique, à l'équation de Vlasov avec condition au bord entrantes. Des formules asymptotiques faisant intervenir les coefficients de réflexion-transmission ainsi que les temps de retard quantiques sont obtenues et utilisées pour construire une modèle hybride* (*cinétique-quantique*) *transitoire mondimensionnel.* © 2000 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

## *Version française abrégée*

Nous présentons dans cette Note un modèle de transport quantique unidimensionnel transitoire, dont le pendant classique est l'équation de Vlasov avec condition de flux entrant au bord du domaine. Le modèle est transitoire en ce sens que les conditions d'injection dépendent du temps. Le potentiel électrostatique est, quant à lui, supposé stationnaire. L'analyse asymptotique de ce modèle repose sur l'utilisation de la transformée de Wigner [8,6,5] ainsi que sur l'étude de sa trace au bord [3]. Elle permet de construire un modèle hybride cinétique-quantique transitoire généralisant le modèle stationnaire développé dans [1].

**Note présentée par Pierre-Louis LIONS.**

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Seuls les constructions et les arguments formels sont présentés dans cette Note. Les théorèmes précis ainsi que leur démonstration seront exposés dans [2].

Le modèle que nous construisons est la version quantique de

$$\frac{\partial f}{\partial t} + p\,\frac{\partial f}{\partial x} - \frac{\mathrm{d}V}{\mathrm{d}x}\,\frac{\partial f}{\partial p} = 0; \quad f(x,p,t) = g(x,p,t), \quad t \in \mathbb{R},\ (x,p) \in \Sigma^-,$$

où $f = f(x,p,t)$ est la fonction de distribution dépendant de la position $x \in [a,b]$ de la particule, de son impulsion $p \in \mathbb{R}$ et du temps $t \in \mathbb{R}$. Le potentiel électrostatique $V$ est une fonction régulière à support dans $[a,b]$. Dans tout ce qui suit, pour simplifier, nous prendrons la masse de la particule égale à $1$ et sa vitesse égale à son impulsion $p$. La partie du bord correspondant aux vitesses entrantes est $\Sigma^- = (\{a\} \times \mathbb{R}_+^*) \cup (\{b\} \times \mathbb{R}_-^*)$ et $g(x,p,t)$ est une fonction donnée (fonction d'injection). On notera dans la suite

$$g_a(p,t) = g(a,p,t), \quad p > 0; \qquad g_b(p,t) = g(b,p,t),\ p < 0.$$

Pour construire le modèle quantique, on considère les états de scattering de l'opérateur de Schrödinger $H = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(x)$. Ce sont les fonctions d'onde $\psi_p^\hbar$ solutions de $H\psi_p^\hbar = E_p\psi_p^\hbar$ avec $E_p = p^2/2$ telles qu'il existe des coefficients $A_p^\hbar$ et $B_p^\hbar$ satisfaisant

$$\left.\begin{array}{r} \psi_p^\hbar(x) = \mathrm{e}^{ip\frac{x}{\hbar}} + A_p^\hbar\,\mathrm{e}^{-ip\frac{x}{\hbar}}, \quad x < a \\ \psi_p^\hbar(x) = B_p^\hbar\,\mathrm{e}^{ip\frac{x}{\hbar}}, \quad x > b \end{array}\right\} \quad \text{pour } p > 0,$$

ainsi que des expressions analogues pour $p < 0$ (en intervertissant les rôles de $a$ et $b$). À partir des amplitudes de réflexion et de transmission $A_p^\hbar$ et $B_p^\hbar$, on peut définir des coefficients de réflexion et de transmission $R_p^\hbar$ et $T_p^\hbar$ et des temps de retard $\tau_R^\hbar$ et $\tau_T^\hbar$ selon les formules (9) à (10). L'expression des temps de retard se déduit d'une analyse semi-classique développée dans la littérature physique [7,4] et démontrée dans [2].

La matrice densité $\rho^\hbar$ est donnée par :

$$\rho^\hbar(x,x',t) = \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}} p_0\, g(p_0,t_0)\rho^\hbar_{(p_0,t_0)}(x,x',t)\,\mathrm{d}p_0\,\mathrm{d}t_0,$$

où l'on désigne par $g(p,t)$ la fonction $g_a(p,t)$ pour $p > 0$ et $g_b(p,t)$ pour $p < 0$. La matrice densité élémentaire $\rho^\hbar_{(p_0,t_0)}$ a pour expression :

$$\rho^\hbar_{(p_0,t_0)}(x,x',t) = \frac{1}{2\pi}\int_{\mathbb{R}} \psi^\hbar_{p_0+\frac{\hbar}{2}\xi}(x)\overline{\psi^\hbar_{p_0-\frac{\hbar}{2}\xi}}(x')\,\mathrm{e}^{-i\xi(a+p_0(t-t_0))}\,\mathrm{d}\xi, \quad p_0 > 0,$$

ainsi qu'une expression similaire quand $a$ est remplacé par $b$ pour $p_0$ négatif. On montre alors que la transformée de Wigner $w^\hbar$ de $\rho^\hbar$ converge quand $\hbar$ tend vers zéro vers la solution de l'équation de Vlasov ci-dessus. L'analyse asymptotique fournit également les expressions asymptotiques (8) des traces en $a$ et $b$ de $w^\hbar$, pourvu que les coefficients de réflexion-transmission $R_p^\hbar$ et $T_p^\hbar$ et les temps de retard $\tau_R^\hbar$ et $\tau_T^\hbar$ possèdent des limites lorsque $\hbar \to 0$.

Nous utilisons ces résultats pour construire un modèle hybride transitoire de transport électronique (quantique dans $[a,b]$, et cinétique dans $[0,a] \cup [b,L]$) : le potentiel $V$ étant connu, on calcule les fonctions d'onde et on en déduit les coefficients de réflexion-transmission ainsi que les temps de retard. On résout ensuite l'équation de Vlasov (ou de Boltzmann) pour la fonction de distribution $f_C(x,p,t)$ dans la zone classique avec comme conditions d'interface

$$f_C(a,p,t) = R^\hbar_{-p} f_C\big(a,-p,t-\tau^\hbar_R(-p)\big) + T^\hbar_p f_C\big(b,p,t-\tau^\hbar_T(p)\big), \quad p<0,$$
$$f_C(b,p,t) = R^\hbar_{-p} f_C\big(b,-p,t-\tau^\hbar_R(-p)\big) + T^\hbar_p f_C\big(a,p,t-\tau^\hbar_T(p)\big), \quad p>0.$$

La matrice densité est ensuite donnée par (6) avec $g(p,t) = f_C(a,p,t)$ pour $p>0$ et $g(p,t) = f_C(b,p,t)$ pour $p<0$. Nous montrons que l'intégrale en temps du courant est continue aux interfaces $a$ et $b$ entre les zones classiques et quantiques.

## 1. Introduction

A correct modelling of electron transport in nanostructures such as resonant tunneling diodes, superlattices or quantum dots requires the use of quantum models like Schrödinger or Wigner equations. Quantum phenomena usually take place in localized regions of the devices, while the rest of the device is governed by classical mechanics. It is then important to design suitable boundary value problems for quantum models and adequate strategies to couple them to classical kinetic models such as the Vlasov or Boltzmann equation. In the one-dimensional stationary case, an adequate boundary value problem for the Schrödinger equation was introduced and analyzed in [3]. The semiclassical analysis of this model is used in [1] to derive interface conditions and define a hybrid quantum-kinetic model. The analysis was based on the standard results for the Wigner transform [8,6,5] and on a careful analysis of its trace on the boundary.

In this Note, we deal with the time-dependent one-dimensional case. The electrostatic potential is assumed to be stationary while electrons are injected into the device with a time-dependent profile. By using the notion of wave-packet, we construct the density matrix of electrons in terms of the injection profile and of the scattering states of the Schrödinger operator. We then show that this quantum model leads, in the semiclassical limit, to the inflow boundary conditions for the Vlasov equation. From the semiclassical limit, we recover the usual expressions of quantum reflection and transmission time delays [7,4] and construct a hybrid time-dependent model.

We have chosen to focus on the construction of density matrices, Wigner functions and on formal computations (boundary conditions, time delays) rather than on rigorous proofs. The precise setting, the rigorous theorems and proofs can be found in [2].

## 2. Setting of the problem

Let $a<b$, be two real numbers and $V(x)$, a smooth time independent potential defined on $\mathbb{R}$ and compactly supported in $[a,b]$. The aim of this note is to provide a quantum analogue of the boundary value problem for the distribution function $f(x,p,t)$, where $x\in[a,b]$, $p\in\mathbb{R}$ and $t\in\mathbb{R}$

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} - \frac{\mathrm{d}V}{\mathrm{d}x}\frac{\partial f}{\partial p} = 0; \quad f(x,p,t) = g(x,p,t), \quad t\in\mathbb{R},\ (x,p)\in\Sigma^-, \tag{1}$$

where $\Sigma^- = (\{a\}\times\mathbb{R}^*_+)\cup(\{b\}\times\mathbb{R}^*_-)$ is the part of the boundary corresponding to the incoming velocities and $g(x,p,t)$ is the incoming distribution function at the boundary. We shall denote

$$g_a(p,t) = g(a,p,t), \quad p>0; \qquad g_b(p,t) = g(b,p,t),\ p<0.$$

Note that, instead of looking at the Cauchy problem for (1), we are interested in solutions defined for all $t\in\mathbb{R}$ (eternal solutions). This is because our aim is the description of an open quantum system interacting with particles coming from the far outside in the past and leaving towards the far outside in the future. Because of the 'tail' of the quantum wave-packet representing these particles, their interaction with the quantum system is permanent (and not restricted to the interval in which the 'core' of the wave-packet only interacts with the quantum region).

More specifically, we are looking for a solution of the density matrix equation (DME)

$$i\,\hbar\rho_t = (H_x - H_{x'})\rho, \quad (x,x',t)\in\mathbb{R}^3 \tag{2}$$

(where $\rho = \rho(x,x',t)$ is the density matrix, $H = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(x)$ and $H_x,\ H_{x'}$ are respectively the actions of $H$ on the $x$ and $x'$ variables) which converges when $\hbar$ tends to zero, through a Wigner transform, to a solution of (1).

The ultimate goal of the study is to provide a scheme for coupling a classical description of particle motion (via (1)) outside the region $[a,b]$ and a quantum description of it (via (2)) inside $[a,b]$. For that purpose, the semiclassical limit will provide asymptotic formulae for the outgoing part of the distribution function at the boundary $\{a,b\}$, in terms of quantum expressions of the reflection and transmission coefficients and time delays.

## 3. Construction of the density matrix

Consider the scattering states associated with the potential $V$. These are the unique functions $\psi_p^\hbar(x)$ (where $p\in\mathbb{R}$) solving the stationary Schrödinger equation $H\psi_p^\hbar = E_p\psi_p^\hbar$ with $E_p = p^2/2$ and such that, there exist complex coefficients $A_p^\hbar,\ B_p^\hbar$ satisfying

$$\left.\begin{aligned}\psi_p^\hbar(x) &= \mathrm{e}^{ip\frac{x}{\hbar}} + A_p^\hbar\,\mathrm{e}^{-ip\frac{x}{\hbar}}, \quad x<a\\ \psi_p^\hbar(x) &= B_p^\hbar\,\mathrm{e}^{ip\frac{x}{\hbar}}, \quad x>b\end{aligned}\right\}\quad \text{for } p>0, \tag{3}$$

and similarly for $p<0$ by interchanging $a$ and $b$. We recall that $A_p^\hbar,\ B_p^\hbar$ are respectively the reflection and transmission amplitudes and that the reflection and transmission coefficients $R_p^\hbar = |A_p^\hbar|^2$, $T_p^\hbar = |B_p^\hbar|^2$ satisfy the conservation of probability current $R_p^\hbar + T_p^\hbar = 1$ and the reciprocity relation $T_p^\hbar = T_{-p}^\hbar$ (*see* [7]). Finally, we note that in the case where $V$ is identically vanishing on the whole real line, the $\psi_p^\hbar$'s are given by $\psi_p^\hbar(x) = \mathrm{e}^{ip\frac{x}{\hbar}}$.

Let us now define the "elementary" density matrix for $t_0\in\mathbb{R}$ and $p_0>0$ by

$$\rho^\hbar_{(p_0,t_0)}(x,x',t) = \frac{1}{2\pi}\int_{\mathbb{R}} \psi^\hbar_{p_0+\frac{\hbar}{2}\xi}(x)\overline{\psi^\hbar_{p_0-\frac{\hbar}{2}\xi}}(x')\,\mathrm{e}^{-i\xi(a+p_0(t-t_0))}\,\mathrm{d}\xi \tag{4}$$

and similarly with $a$ replaced by $b$ for $p_0$ negative. It is obvious to check that (4) is a particular solution of the DME equation (2). For $p_0>0$, $\rho^\hbar_{(p_0,t_0)}$ is the density matrix of a wave representing a particle hitting the plane $x=a$ at time $t=t_0$ with momentum $p_0$, while for $p_0<0$, it hits the plane $x=b$ at time $t_0$ with momentum $p_0$. This claim is readily seen in the case $V\equiv 0$ since

$$\rho^\hbar_{(p_0,t_0)}(x,x',t) = \mathrm{e}^{ip_0\frac{(x-x')}{\hbar}}\,\delta\!\left(\frac{x+x'}{2} - a - p_0(t-t_0)\right), \quad p_0>0, \tag{5}$$

and analogously for $p_0<0$ with $a$ replaced by $b$, and $\delta$ is the delta measure. We sketch below why it is also true for an arbitrary potential by looking at the limit $\hbar\to 0$.

Now, we denote $g(p,t) = g_a(p,t)$ for $p>0$ and $g(p,t) = g_b(p,t)$ for $p<0$. Starting from (5) we construct the quantum analogue of the solution of (1) by

$$\rho^\hbar(x,x',t) = \int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}} p_0\,g(p_0,t_0)\rho^\hbar_{(p_0,t_0)}(x,x',t)\,\mathrm{d}p_0\,\mathrm{d}t_0. \tag{6}$$

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By construction, $\rho^\hbar$ is a solution of the DME equation (2). It can be argued that the so-constructed $\rho^\hbar$ does not define a positive operator, as it should. However, it will be shown in [2] how a regularization of (4) using the concept of wave-packet satisfies this property.

## 4. Semiclassical limit

To investigate the semiclassical limit, we shall use the Wigner transform formalism. We first define the Wigner transform of a given density matrix $\rho$ by

$$\mathcal{W}^\hbar[\rho](x,p,t) = \frac{1}{2\pi}\int_{\eta\in\mathbb{R}} \rho\left(x - \frac{\hbar}{2}\eta, x + \frac{\hbar}{2}\eta, t\right)\mathrm{d}\eta. \tag{7}$$

Formally, $w^\hbar := \mathcal{W}^\hbar[\rho^\hbar]$ converges as $\hbar \to 0$ towards a solution $f(x,p,t)$ of (1) on $\mathbb{R}_x \times \mathbb{R}_p \times \mathbb{R}_t$. Furthermore, we have $f(x,p,t) = g(x,p,t)$ on $\Sigma^-$. To prove the latter, it is enough to check that

$$\lim_{\hbar\to 0} \mathcal{W}^\hbar\big[\rho^\hbar_{(p_0,t_0)}\big](a,p,t) = p_0^{-1}\delta(p-p_0)\otimes\delta(t-t_0), \quad \text{for } p>0,$$

and similarly for $x = b$ and $p < 0$. The proof proceeds by making $x = a$ in (7), multiplying it by a test function $\varphi(p)$ compactly supported in $\mathbb{R}_*^+$ and using the Ansatz (3) (which can be shown to be valid asymptotically for $x > a$ and close to $a$). To make the result a rigorous theorem, it is necessary to localize the Wigner transform as in [1] and introduce a small absorption term to insure uniform $L^2$ estimates on the $\psi_p$'s. The proof is detailed in [2].

Now, this methodology also provides asymptotic expressions of $w^\hbar(a,p,t)$ for $p < 0$ (outgoing distribution). Indeed, after some algebra, we obtain the following asymptotic expressions:

$$\begin{cases} w^\hbar(a,p,t) \simeq g_a(p,t), & p>0, \\ w^\hbar(a,p,t) \simeq R^\hbar_{-p} g_a(-p, t-\tau^\hbar_R(-p)) + T^\hbar_p g_b(p, t-\tau^\hbar_T(p)), & p<0, \end{cases} \tag{8}$$

and analogously for $w^\hbar(b,p,t)$, provided that the limits

$$(R_p, T_p) = \lim_{\hbar\to 0}(R^\hbar_p, T^\hbar_p), \qquad \big(\tau_R(p), \tau_T(p)\big) = \lim_{\hbar\to 0}\big(\tau^\hbar_R(p), \tau^\hbar_T(p)\big)$$

exist, and where

$$\tau^\hbar_R(p) = \frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}p}\alpha^\hbar(p), \qquad \tau^\hbar_T(p) = \frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}p}\beta^\hbar(p), \tag{9}$$

and $\alpha^\hbar(p)$, $\beta^\hbar(p)$ are smooth determinations of the complex phases of the scattering amplitudes

$$A^\hbar_p = \sqrt{R^\hbar_p}\,\mathrm{e}^{2iap/\hbar}\,\mathrm{e}^{i\alpha(p)/\hbar}, \qquad B^\hbar_p = \sqrt{T^\hbar_p}\,\mathrm{e}^{i(a-b)p/\hbar}\,\mathrm{e}^{i\beta(p)/\hbar}; \quad p>0, \tag{10}$$

and similarly for $p < 0$ by interchanging $a$ and $b$. It is to be noted that the above formulae for the reflection and transmission time delays $\tau^\hbar_R$ and $\tau^\hbar_T$ can be found in quantum physics text books ([7,4] for example).

## 5. Quantum-kinetic coupling

Formula (8) provides the coupling scheme that was referred to in Section 2. Indeed, let $0 < a < b < L$ represent an electronic device such that electrons are quantum in $[a,b]$ and behave like classical particles in $[0,a]\cup[b,L]$. Let $f_C(x,p,t)$ be the distribution function in the classical zone and $f_Q$ be the Wigner function in the quantum zone. Following the strategy developed in [1] for the stationary case, we define the coupling between $f_C$ and $f_Q$ as follows: first compute the wave functions $\psi_p^\hbar$ and deduce the reflection-transmission coefficients as well as transmission and reflection time delays. The classical distribution function is then computed by solving the Vlasov or the Boltzmann equation in the classical zone with appropriate boundary conditions at $x = 0$ and $x = L$ (e.g., inflow boundary conditions) and the following interface conditions at $x = a$ or $x = b$

$$f_C(a,p,t) = R^\hbar_{-p} f_C\big(a,-p,t-\tau^\hbar_R(-p)\big) + T^\hbar_p f_C\big(b,p,t-\tau^\hbar_T(p)\big), \quad p<0,$$
$$f_C(b,p,t) = R^\hbar_{-p} f_C\big(b,-p,t-\tau^\hbar_R(-p)\big) + T^\hbar_p f_C\big(a,p,t-\tau^\hbar_T(p)\big), \quad p>0.$$

Once $f_C$ is known, $f_Q$ is computed as the Wigner transform of the density matrix (6) in which $g(p,t) = f_C(a,p,t)$ for $p > 0$ and $g(p,t) = f_C(b,p,t)$ for $p < 0$.

To be effective, this procedure has to be current conservative, which we prove in time integrated form. The "quantum" and "classical" currents are respectively given by

$$J_Q(a,t) = \hbar\left[\left(\frac{\mathrm{d}}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x'}\right)\rho^\hbar(x,x',t)\right]_{x=x'=a} = \int_{\mathbb{R}} p\, f_Q(a,p,t)\,\mathrm{d}p, \tag{11}$$

$$J_C(a,t) = \int_{\mathbb{R}} p\, f_C(a,p,t)\,\mathrm{d}p. \tag{12}$$

Although (12) is an approximation of (11) by virtue of (8), we have *exactly*, for any $\hbar > 0$,

$$\int_{\mathbb{R}} J_Q(a,t)\,\mathrm{d}t = \int_{\mathbb{R}} J_C(a,t)\,\mathrm{d}t$$

and similarly at the point $x = b$.

For the sake of simplicity, the results of this Note are restricted to the case $V(a) = V(b) = 0$. The extension to the general case $V(a) \neq V(b)$ is straightforward. Rigorous results are stated and proven in the general case in [2].

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