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# ON ABSORBING BOUNDARY CONDITIONS FOR QUANTUM TRANSPORT EQUATIONS (*) 

by A. ARNOLD ( ${ }^{1}$ )

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#### Abstract

In this paper we derive a hierarchy of absorbing boundary conditıons for the Wigner equation of quantum mechanics and model extensions that have been used for semiconductor device simulatıons For these pseudo-differentıal equatıons we analyze the wellposedness of the resulting initial-boundary problems


Résumé. - Dans cet artıcle, nous établıssons une htérarchıe de conditıons aux lımıtes absorbantes pour l'équatıon de Wigner de la mécantque quantıque et des extenstons de ce modèle quı sont utllisées pour des simulations de composants électronqques Pour ces équatıons pseudo-dıfférentıelles, nous analysons comment cela conduit à des problèmes aux lımıtes bien posés

## 1. INTRODUCTION

This paper is concerned with the construction and well-posedness analysis of absorbing boundary conditions ( $A B C$ ) for kinetic quantum transport equations arising in the simulation of semiconductor devices. Many novel, ultra-integrated devices (e.g., resonant tunneling diodes) require quantum mechanical models for a correct description of their behavior. The most successful and accurate, transient simulations of quantum devices ([3], [10]) were based on the Wigner function formalism ([20]).

The real-valued Wigner function $w=w(x, v, t)$ describes the state of an electron ensemble in the $2 d$-dimensional position-velocity ( $x, v$ )-phase space. Its time evolution under the action of the electrostatic potential $V$ is governed by the Wigner equation, which reads in the collisionless, effective-mass approximation :

$$
\begin{gather*}
w_{t}+v \cdot \nabla_{x} w+\Theta[V] w=0, \\
x, v \in \mathscr{R}^{d}, \quad d=1,2 \text { or } 3, \tag{1.1}
\end{gather*}
$$

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with the pseudo-differential operator ( $P D O$ )

$$
\begin{align*}
& \Theta[V] w=i \delta V\left(x, \frac{1}{i} \nabla_{v}, t\right) w= \\
& =\frac{i}{(2 \pi)^{d}} \int_{\mathscr{R}_{\eta}^{d}} \int_{\mathscr{R}_{V^{\prime}}^{d}} \delta V(x, \eta, t) w\left(x, v^{\prime}, t\right) e^{t\left(v-v^{\prime}\right) \eta} d{Q^{\prime}}^{\prime} d \eta \\
&  \tag{1.2}\\
& \delta V(x, \eta, t)=V\left(x+\frac{\eta}{2}, t\right)-V\left(x-\frac{\eta}{2}, t\right)
\end{align*}
$$

This equation is already stated in a scaled form, and we refer the reader to [14] (and references therein) for a physical derivation and the discussion of many of its analytical properties. In order to account for electron-electron interactions in a simple mean-field approximation (1.1) has to be coupled to the Poisson equation

$$
\begin{equation*}
\Delta V(x, t)=n(x, t)-D(x), \tag{1.3}
\end{equation*}
$$

where $D$ denotes the doping profile of the semiconductor, and the particle density $n$ is obtained by $n=\int w d v$.

For the simulations of quantum devices most authors ([3], [7]) supplemented the Wigner equation, posed on a finite $x$-domain $\Omega \subseteq \mathscr{R}^{d}$, with inflow boundary conditions ( $B C$ ):

$$
\begin{equation*}
w(x, v, t)=w_{D}(x, v, t), \quad(x, v) \in \Gamma_{-}, \quad t>0 \tag{1.4}
\end{equation*}
$$

Here we denote by $\Gamma_{+}, \Gamma_{-}$the outflow and, respectively, inflow part of the boundary $\partial \Omega \times \mathscr{R}_{v}^{d}$ :

$$
\begin{equation*}
\Gamma_{ \pm}:=\left\{(x, v) \mid x \in \partial \Omega, \quad v \in \mathscr{R}^{d}, \quad v \cdot r(x) \geqq 0\right\} \tag{1.5}
\end{equation*}
$$

with $r(x)$ denoting the outward unit normal vector of $\partial \Omega$ at $x$. These $B C$ 's yield a well-posed problem ([13]) and their validity has recently been justified in the asymptotic analysis [15], when posed far enough away from the «source of quantum effects» (potential barriers, heterojunctions).

In typical semiconductors simulations, quantum effects are usually confined to small regions inside the device. Therefore, and due to the numerical complexity of the Wigner equation, it would be desirable to restrict the quantum model to rather small domains, introducing artificial boundaries. Along this boundary the Wigner equation would then be coupled to a numerically simpler model (e.g., hydrodynamics equation for semiconductors, [14]). In this situation, however, the inflow $B C$ 's (1.4) cause spurious numerical reflections of outgoing wave packets, which are due to the (in $v$ ) nonlocal nature of the $P D O \Theta[V]$. This behavior can be corrected
using $A B C$ 's for the Wigner equation, which were derived by Ringhofer et al. in [16] and employed in a self-consistent simulation of a quantum device in [10].

The outline of this paper is as follows : in § 2 we briefly motivate and recall from [16] the $A B C$ 's for the linear $1 D$-Wigner equation. These $B C$ 's are then reformulated and put into an analytic framework, needed for the well-posedness analysis of $\S 3$. In § 4, we discuss the model extensions, and their implications on the $B C$ 's, that are necessary for quantum device simulations : relaxation-time approximation, and $2 D$-simulation.

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## 2. ABSORBING BOUNDARY CONDITIONS FOR THE 1D-WIGNER EQUATION

In this section we will first outline the construction of $A B C$ 's for the $1 D$ Wigner equation (as presented in detail in [16]), and then reformulate them as to make them better tractable, both analytically and numerically.

When considering the half-space problem $(x \in \Omega=(0, \infty), v \in \mathscr{R})$ of (1.1), zero «physical inflow » cannot be modeled by prescribing $w=0$ on $\Gamma_{-}$, as right and left-traveling modes of the Wigner equation are not confined to $v>0$ and $v<0$, respectively. This parallels the situation in first order hyperbolic systems of the form

$$
\begin{equation*}
z_{t}+A z_{x}+B z=0 \tag{2.1}
\end{equation*}
$$

with the matrix $A=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{n}\right) ; \lambda_{1}, \ldots, \lambda_{k}>0 ; \lambda_{k+1}, \ldots, \lambda_{n}<0$, and $z=\left(z_{1}, \ldots, z_{n}\right)^{T}$. Since the inflow-BC $z_{j}(x=0, t)=0, j=1, \ldots, k$ disregards the coupling of in- and outgoing modes, $A B C$ 's are more appropriate for many numerical simulations ([6]).

The basic idea for obtaining an $A B C$ for the Wigner equation is to construct a transformation

$$
\begin{equation*}
u(x, v, t)=(M w)(x, v, t) \tag{2.2}
\end{equation*}
$$

with the (in $v$ and $t$ ) nonlocal operator $M=M\left(x, v, \partial_{v}, t, \partial_{t}\right)$, such that (1.1) is transformed to :

$$
\begin{equation*}
v u_{x}+\Phi u=0, \quad x>0, \quad v \in \mathscr{R}, \tag{2.3}
\end{equation*}
$$

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with the $P D O$

$$
\begin{align*}
& (\Phi u)(x, v, t)= \\
& =(2 \pi)^{-1} \iint \varphi\left(x, v, \eta, v^{\prime}, t, \partial_{t}\right) u\left(x, v^{\prime}, t\right) e^{i \eta\left(v-v^{\prime}\right)} d v^{\prime} d \eta  \tag{2.4}\\
& \varphi\left(x, v, \eta, v^{\prime}, t, \partial_{t}\right)=0 \text { for } v>0 \text { and } v^{\prime}<0
\end{align*}
$$

This form of $\Phi$ assures that incoming waves $(v>0)$ are decoupled from outgoing waves $\left(v^{\prime}<0\right)$, and hence a « perfectly $A B C »$ at $x=0$ is obtained by

$$
\begin{equation*}
u(0, v, t)=(M w)(0, v, t)=0, \quad v>0 \tag{2.5}
\end{equation*}
$$

Since this $B C$ is nonlocal in $t$, for practical reasons it has to be approximated by «highly $A B C$ 's », which are local in $t$ and asymptotically correct for high wave frequencies. For this purpose, $\Phi$ and $M$ are constructed using their asymptotic expansion with respect to $\partial_{t}$ in the sense of $P D O^{\prime}$ 's (see [18], e.g.) :

$$
\begin{equation*}
\Phi \sim \partial_{t} \circ \Phi_{-1}+\Phi_{0}+\partial_{t}^{-1} \circ \Phi_{1}+\cdots, \tag{2.6}
\end{equation*}
$$

with

$$
\begin{align*}
& \left(\Phi_{J} u\right)(x, v, t)= \\
& =(2 \pi)^{-1} \iint \varphi_{j}\left(x, v, \eta, v^{\prime}, t\right) u\left(x, v^{\prime}, t\right) e^{i \eta\left(v-v^{\prime}\right)} d v^{\prime} d \eta  \tag{2.7}\\
& \quad \varphi_{J}\left(x, v, \eta, v^{\prime}, t\right)=0 \text { for } v>0 \text { and } v^{\prime}<0
\end{align*}
$$

Similarly,

$$
\begin{equation*}
M \sim 1+\partial_{t}^{-1} \circ M_{1}+\partial_{t}^{-2} \circ M_{2}+\cdots, \tag{2.8}
\end{equation*}
$$

where the operators $M_{J}$ are local in $x$ and $t$ and (bounded - see § 3) Fourier integral operators in $v$. They only map negative onto positive velocities, satisfying

$$
\begin{equation*}
M_{J} w=M_{J}\left(w^{-}\right), \quad\left(M_{J} w\right)^{-}=0 \tag{2.9}
\end{equation*}
$$

with the notation

$$
\begin{equation*}
w^{ \pm}(v)=w(v) H( \pm v), \quad v \in \mathscr{R} \tag{2.10}
\end{equation*}
$$

therefore, $M_{j} \circ M_{k}=0, j, k \in \mathcal{N}$, and

$$
\begin{equation*}
M^{-1} \sim 1-\partial_{t}^{-1} \circ M_{1}-\partial_{t}^{-2} \circ M_{2}-\cdots \tag{2.11}
\end{equation*}
$$

follows.

We point out that for (in $t$ ) smooth potentials $V$, the operators $\Phi$ and $M$ are «standard» $P D O$ 's in $t$ of order 1 and 0 , respectively, what justifies their asymptotic expansions. In velocity direction, however, their symbols are not smooth, such that the composition formula for PDO's cannot be applied. Therefore, $M_{j}($ for $j \geqslant 2$ ) cannot be represented as a $P D O$, but only as a Fourier integral operator, again with non-smooth amplitude.

Using the expansions (2.6), (2.8), (2.11) in the Wigner equation, the operators $M_{j}$ can be calculated iteratively (see [16]) :

$$
\begin{align*}
& \left(M_{1} w\right)(x, v, t)= \\
& = \begin{cases}\frac{i}{2 \pi} \int_{\mathscr{R}} \int_{-\infty}^{0} \delta V(x, \eta, t) \frac{v^{\prime}}{v^{\prime}-v} w^{-}\left(x, v^{\prime}, t\right) e^{i \eta\left(v-v^{\prime}\right)} d v^{\prime} d \eta \\
0, & v>0 \\
v<0\end{cases} \tag{2.12}
\end{align*}
$$

$$
\left(M_{2} w\right)(x, v, t)=
$$

$$
=-\frac{i}{2 \pi} \int_{\mathscr{R}} \int_{-\infty}^{0}\left[\delta V_{t}(x, \eta, t)+\delta V_{x}(x, \eta, t) v^{\prime \prime}\right] \times
$$

$$
\times \frac{v v^{\prime \prime}}{\left(v-v^{\prime \prime}\right)^{2}} w^{-}\left(x, v^{\prime \prime}, t\right) e^{i \eta\left(v-v^{\prime \prime}\right)} d v^{\prime \prime} d \eta-
$$

$$
-(2 \pi)^{-2} \int_{\mathscr{R}^{3}} \int_{-\infty}^{0} \delta V(x, \eta, t) \delta V\left(x, \eta^{\prime}, t\right) h^{+}\left(v, v^{\prime}, v^{\prime \prime}\right) w^{-}\left(x, v^{\prime \prime}, t\right) \times
$$

$$
\times e^{\imath \eta^{\prime}\left(v^{\prime}-v^{\prime \prime}\right)+i \eta\left(v-v^{\prime}\right)} d v^{\prime \prime} d \eta^{\prime} d v^{\prime} d \eta, \quad v>0
$$

$$
\begin{equation*}
\left(M_{2} w\right)(x, v, t)=0, \quad v<0 \tag{2.13}
\end{equation*}
$$

with

$$
h^{+}\left(v, v^{\prime}, v^{\prime \prime}\right)= \begin{cases}\frac{v^{\prime \prime 2}}{\left(v-v^{\prime \prime}\right)\left(v^{\prime \prime}-v^{\prime}\right)}, & v^{\prime}>0  \tag{2.14}\\ \frac{v^{\prime \prime} v}{\left(v-v^{\prime \prime}\right)\left(v-v^{\prime}\right)}, & v^{\prime}<0\end{cases}
$$

Retaining a finite number of terms in the expansion (2.8) then yields a hierarchy of $A B C$ 's which approximate (2.5). The first and second order local-in- $t B C$ 's now read after differentiating with respect to $t$ :

$$
\begin{array}{rll}
w_{t}^{+}+M_{1} w^{-}=0, & x=0, & v>0 \\
w_{t t}^{+}+\partial_{t}\left(M_{1} w^{-}\right)+M_{2} w^{-}=0, & x=0, & v>0 . \tag{2.16}
\end{array}
$$

Under the assumptions $V, \mathscr{F}_{x} V \in L^{1}(\mathscr{R})$, the operator $M_{1}$ can be represented as a convolution $\left(\mathscr{F}_{x}\right.$ denotes the Fourier transform with respect
to $x$ ). If $w^{-}(0, ., t)$ lies in the weighted $L^{2}$-space $L^{2}\left(\mathscr{R}_{v}^{-},|v|^{\varepsilon}\right)$ for some $\varepsilon \in(1,3)$, then the integral in (2.12) converges absolutely and
$\left(M_{1} w^{-}\right)(0, v, t)=$

$$
\begin{align*}
=\frac{i}{\sqrt{2 \pi}} \int_{\mathscr{R}}\left(\mathscr{F}_{\eta} \delta V\right)\left(x=0, v^{\prime}\right. & -v, t) \times \\
& \times \frac{v^{\prime}}{v^{\prime}-v} w^{-}\left(0, v^{\prime}, t\right) d v^{\prime}, \quad v>0 \tag{2.17}
\end{align*}
$$

holds. If the initial Wigner function at $t=0$ satisfies $w^{l}, v w^{I} \in L^{2}\left(\Omega \times \mathscr{R}_{v}\right)$, then the boundary traces of the corresponding solution $w$ will indeed satisfy $w^{ \pm}(x, ., t) \in L^{2}\left(\mathscr{R}_{v}^{ \pm},|v|+|v|^{3}\right), x \in \partial \Omega$ (see §3). Thus (2.17) holds rigorously in this case. Throughout most of § 3 and $\S 4$, however, the considered initial functions $w^{I}$ will lie only in $L^{2}\left(\Omega \times \mathscr{R}_{v}\right)$, implying $w^{ \pm}(x, ., t) \in L^{2}\left(\mathscr{R}_{v}^{ \pm},|v|\right), x \in \partial \Omega$. For this limiting situation (2.17) represents the bounded (see Lemma 3.1, below) extension of $M_{1}$ to all of $L^{2}\left(\mathscr{R}_{v}^{-},|v|\right)$. Therefore, and because of the anyhow somewhat formal derivation of the $A B C$ 's, we will from now on consider (2.17) as the appropriate definition of $M_{1}$, even for $w^{-}$only in $L^{2}\left(\mathscr{R}_{v}^{-},|v|\right)$.

By the same reasoning the operator $M_{2}$ can be reformulated as

$$
\begin{align*}
& \left(M_{2} w^{-}\right)(0, v, t)= \\
= & -\frac{i}{\sqrt{2 \pi}} \int_{\mathscr{R}}\left[\left(\mathscr{F}_{\eta} \delta V_{t}\right)\left(0, v^{\prime \prime}-v, t\right)+\left(\mathscr{F}_{\eta} \delta V_{x}\right)\left(0, v^{\prime \prime}-v, t\right) v^{\prime \prime}\right] \times \\
& \times \frac{v v^{\prime \prime}}{\left(v-v^{\prime \prime}\right)^{2}} w^{-}\left(0, v^{\prime \prime}, t\right) d v^{\prime \prime}-  \tag{2.18}\\
& -\frac{1}{2 \pi} \int_{\mathscr{R}^{2}}\left(\mathscr{F}_{\eta} \delta V\right)\left(0, v^{\prime}-v, t\right)\left(\mathscr{F}_{\eta} \delta V\right)\left(0, v^{\prime \prime}-v^{\prime}, t\right) \times \\
& \times h^{+}\left(v, v^{\prime}, v^{\prime \prime}\right) w^{-}\left(0, v^{\prime \prime}, t\right) d v^{\prime \prime} d v^{\prime},
\end{align*}
$$

$$
v>0
$$

if the additional assumptions $V_{t}, \mathscr{F}_{x} V_{t}, V_{x}, \mathscr{F}_{x} V_{x} \in L^{1}(\mathscr{R})$ hold. Interchanging the sequence of integrations in the second term of the right hand side gives

$$
\begin{equation*}
\frac{1}{2 \pi} \int_{\mathscr{R}}\left[\lambda\left(v, v^{\prime \prime}\right)+\lambda\left(-v^{\prime \prime},-v\right)\right] v^{\prime \prime} w^{-}\left(0, v^{\prime \prime}, t\right) d v^{\prime \prime} \tag{2.19}
\end{equation*}
$$

with
$\lambda\left(v, v^{\prime \prime}\right):=\frac{v^{\prime \prime}}{v^{\prime \prime}-v} \int_{0}^{\infty}\left(\mathscr{F}_{\eta} \delta V\right)\left(0, v^{\prime}-v, t\right) \frac{\left(\mathscr{F}_{\eta} \delta V\right)\left(0, v^{\prime \prime}-v^{\prime}, t\right)}{v^{\prime \prime}-v^{\prime}} d v^{\prime}$.

With an eye towards the numerical application we will now rewrite the PDO $M_{1}$ using its right and left symbol, respectively, which then allows its evaluation through FFT's :

$$
\begin{align*}
& \left(M_{1} w^{-}\right)(0, v, t)= \\
& -\frac{1}{\sqrt{2 \pi}} \int_{\mathscr{R}} y(\eta, t) \mathscr{F}_{v^{\prime}}\left[v^{\prime} w^{-}\left(0, v^{\prime}, t\right)\right](\eta) e^{i v \eta} d n= \\
& =-\frac{v}{\sqrt{2 \pi}} \int_{\mathscr{R}_{-}} y(\eta, t)\left[\mathscr{F}_{v^{\prime}} w^{-}(0, ., t)\right](\eta) e^{i v \eta} d \eta+\left(\Theta[V] w^{-}\right)(0, v, t), \\
& v>0 \tag{2.21}
\end{align*}
$$

with

$$
\begin{equation*}
y(\eta, t)=\int_{-\infty}^{\eta} \delta V\left(0, \eta^{\prime}, t\right) d \eta^{\prime} \tag{2.22}
\end{equation*}
$$

When assuming $v^{-1}\left(\mathscr{F}_{\eta} \delta V\right)(v) \in L^{1}\left(\mathscr{R}_{v}\right)$, these representations can be obtained easily from (2.17) or (2.12) (cp. formula II-22 in [17], for PDO's with smooth symbols).

Since the operator $M_{2}$ cannot be written as a convolution, it is not clear yet if the improvement from using the second order $A B C$ can justify the increased numerical effort, involved in the evaluation of $M_{2}$.

When numerically coupling the Wigner equation at $x=0$ to some other kinetic model for $x<0$, an inhomogeneous $B C$, like

$$
\begin{equation*}
w^{+}(0, v, t)=f^{+}(v, t)-\int_{0}^{t}\left(M_{1} w^{-}\right)(0, v, \tau) d \tau, \quad v>0 \tag{2.23}
\end{equation*}
$$

has to be imposed. Here, $f^{+}, v>0$ and $w^{-}, v<0$ represent, respectively, the outflow and inflow-boundary data for the model on the left half-space.

## 3. WELL-POSEDNESS OF THE $1 D$ INITIAL-BOUNDARY VALUE PROBLEM

In the previous section, we derived a hierarchy of «highly $A B C$ 's » for the Wigner equation. It is well known that this kind of $B C$ 's for hyperbolic systems may lead to ill-posed initial-boundary value problems (IBVP) (see the example on the wave equation in [6]). In this section, and in § 4 we will analyze the well-posedness of various $A B C$ 's for the Wigner equation and related quantum transport models. Since we will also be interested in discontinuous potentials $V$, thus leading to (in $x$ ) non-smooth coefficients of the system, we cannot simply apply the normal mode analysis of Kreiss ([11]). Also, the two boundary conditions cannot be separated for short time intervals, as the Wigner equation includes infinite velocities.
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It will not be within our scope to estimate the error introduced by the $A B C$ 's, in comparison with the original whole space problem This question of «quality of the $A B C$ 's» is in the literature usually addressed by considering the reflection coefficients for outgoing waves ([6]) A rigorous error estımate for the wave equation, e $g$, has been derived in [9] by microlocal methods

First we will establish the well-posedness of the Wigner equation on the interval $-1<x<1, v \in \mathscr{R}$, supplemented with inhomogeneous $A B C$ 's of type (2 23) at $x= \pm 1$ First we collect the model equations when using first order ABC's

$$
\begin{gather*}
w_{t}+v w_{x}+\Theta[V] w=0, \quad|x|<1, \quad v \in \mathscr{R}, \quad t>0  \tag{31a}\\
w(x, v, t=0)=w^{\prime}(x, v),|x|<1, \quad v \in \mathscr{R} \tag{31b}
\end{gather*}
$$

$w^{+}(-1, v, t)=f^{+}(v, t)-$

$$
\begin{equation*}
-\int_{0}^{t}\left(M_{1} w^{-}\right)(-1, v, \tau) d \tau, \quad v>0, \quad t>0 \tag{array}
\end{equation*}
$$

$w^{-}(1, v, t)=f^{-}(v, t)-$

$$
\begin{equation*}
-\int_{0}^{t}\left(M_{1} w^{+}\right)(1, v, \tau) d \tau, \quad v<0, \quad t>0 \tag{array}
\end{equation*}
$$

where the data $V, w^{\prime}, f=\left(f^{+}, f^{-}\right)$are all real-valued We recall that $M_{1}$ is defined by ( 217 ), equally for $w^{+}$and $w^{-}$, and it maps outflow-data ( $w(x=-1), w^{+}(x=1)$ ) onto inflow-data $\left(w^{+}(x=-1), w^{-}(x=1)\right)$

One crucial ingredient to prove well-posedness of (31) is the boundedness of $M_{1}$, which will first be obtained for smooth, decaying potentials

Lemma 31 Let $V, \mathscr{F}_{x} V \in L^{1}(\mathscr{R})$ Then $M_{1}$ is bounded from $L^{2}\left(\mathscr{R}^{-},|v|\right)$ to $L^{2}\left(\mathscr{R}^{+},|v|\right)$ (and equivalently from $L^{2}\left(\mathscr{R}^{+},|v|\right)$ to $\left.L^{2}\left(\mathscr{R}^{-},|v|\right)\right)$

Proof Since the $x-$ and $t$ - dependence of $M_{1}$ are irrelevant here, we will suppress it We estimate (217) as

$$
\begin{align*}
& |v|^{\frac{1}{2}}\left|M_{1} u(v)\right| \leqslant \\
& \quad \leqslant \frac{1}{\sqrt{2 \pi}} \int_{\infty}^{0}\left|\left(\mathscr{F}_{\eta} \delta V\right)\left(v^{\prime}-v\right)\right| \frac{\left|v v^{\prime}\right|^{\frac{1}{2}}}{\left|v^{\prime}-v\right|}\left|v^{\prime}\right|^{\frac{1}{2}}\left|u \quad\left(v^{\prime}\right)\right| d v^{\prime} \tag{array}
\end{align*}
$$

where $\frac{\left|v v^{\prime}\right|^{\frac{1}{2}}}{\left|v^{\prime}-v\right|} \leqslant \frac{1}{2}$ holds for $v>0$ and $v^{\prime}<0$ Then Young's inequality
gives the result :

$$
\begin{equation*}
\left\||v|^{\frac{1}{2}}\left(M_{1} u^{-}\right)(.)\right\|_{L^{2}\left(\mathscr{R}^{+}\right)} \leqslant \frac{1}{\sqrt{2 \pi}}\left\|\mathscr{F}_{x} V\right\|_{L^{1}(\mathscr{R})}\left\||v|^{\frac{1}{2}} u^{-}(.)\right\|_{L^{2}\left(\mathscr{R}^{-}\right)} \tag{3.3}
\end{equation*}
$$

To derive this result, we have assumed $\mathscr{F}, V \in L^{1}(\mathscr{R})$, which implies $V \in C(\mathscr{R})$ and $\lim _{x \rightarrow \pm \infty} V(x)=0$. In the simulation of quantum devices it is, however, very important to include step potentials and to allow for a bias between the device contacts ([10]). We are, therefore, led to also consider a model potential of the form $V(x)=\operatorname{sgn}\left(2\left(x-x_{0}\right)\right)$. The boundedness of $M_{1}$ for a very general class of potentials can then be obtained by combining the following result with Lemna 3.1.

Lemma 3.2: Let $V=\operatorname{sgn}\left(2\left(x-x_{0}\right)\right)$. Then $M_{1}$ is bounded from $L^{2}\left(\mathscr{R}^{-},|v|\right)$ to $L^{2}\left(\mathscr{R}^{+},|v|\right)$.

Proof : Since $V, \mathscr{F}_{x} V \notin L^{1}(\mathscr{R})$, the representation (2.17) cannot be used and we have to resort to the original definition (2.12) of $M_{1}$. Like in $\S 2$ we will first reformulate $M_{1}$ for $u^{-} \in L^{2}\left(\mathscr{R}^{-},|v|+|v|^{\varepsilon}\right), \varepsilon>1$, and then extend $M_{1}$ to $L^{2}\left(\mathscr{R}^{-},|v|\right)$ by density. For fixed $v>0$ we have to consider the term

$$
\begin{align*}
& \int_{\mathscr{R}} \int_{-\infty}^{0} \operatorname{sgn}\left(\eta \pm \eta_{0}\right) \frac{v^{\prime}}{v^{\prime}-v} u^{-}\left(v^{\prime}\right) e^{i \eta\left(v-v^{\prime}\right)} d v^{\prime} d \eta= \\
&=-i \lim _{\substack{\alpha \rightarrow-\infty \\
\beta \rightarrow \infty}} \int_{-\infty}^{0} \frac{v^{\prime}}{v^{\prime}-v} u^{-}\left(v^{\prime}\right) e^{\mp i\left(v-v^{\prime}\right) \eta_{0}} \frac{1}{v-v^{\prime}} \times \\
& \quad \times\left[e^{i \beta\left(v-v^{\prime}\right)}+e^{i \alpha\left(v-v^{\prime}\right)}-2\right] d v^{\prime} \tag{3.4}
\end{align*}
$$

where the two integrations could be interchanged on bounded $\eta$-intervals. Since the last integrand is in $L^{1}\left(\mathscr{R}_{v^{\prime}}\right)$, the Riemann-Lebesgue lemma shows that the $\alpha-$ and $\beta$ - dependent terms both tend to zero as $\alpha \rightarrow-\infty$ and $\beta \rightarrow \infty$, respectively. Thus $M_{1}$ can be represented as

$$
\left(M_{1} u^{-}\right)(x, v)=\frac{2}{\pi} \int_{-\infty}^{0} \frac{v^{\prime}}{\left(v^{\prime}-v\right)^{2}} u^{-}\left(v^{\prime}\right) \cos \left(v^{\prime}-v\right) \eta_{0} d v^{\prime}
$$

$$
\begin{equation*}
v>0 \tag{3.5}
\end{equation*}
$$

with $\eta_{0}=2\left(x_{0}-x\right)$.
In order to now prove the boundedness of $\left\|\left||v|^{\frac{1}{2}} M_{1} u^{-} \|_{L^{2}\left(\mathscr{R}^{+}\right)}\right.\right.$in terms of $\left\||v|^{\frac{1}{2}} u^{-}\right\|_{L^{2}\left(\mathscr{R}^{-}\right)}$we will first consider this map from $L^{1}\left(\mathscr{R}^{-}\right)$to $L^{1}\left(\mathscr{R}^{+}\right)$and vol. 28, n ${ }^{\circ} 7,1994$
from $L^{\infty}\left(\mathscr{R}^{-}\right)$to $L^{\infty}\left(\mathscr{R}^{+}\right):$We estımate

$$
\begin{align*}
\left\||v|^{\frac{1}{2}} M_{1} u^{-}\right\|_{1} & \leqslant \frac{2}{\pi} \int_{0}^{\infty} \int_{-\infty}^{0} \frac{\left|v v^{\prime}\right|^{\frac{1}{2}}}{\left(v^{\prime}-v\right)^{2}}\left|v^{\prime}\right|^{\frac{1}{2}}\left|u^{-}\left(v^{\prime}\right)\right| d v^{\prime} d v= \\
& =C\left\|\left|v^{\prime}\right|^{\frac{1}{2}} u^{-}\right\|_{1} \tag{3.6}
\end{align*}
$$

Also, we obtain for $v>0$

$$
\begin{align*}
\left|v^{\frac{1}{2}}\left(M_{1} u^{-}\right)(v)\right| & \leqslant \frac{2}{\pi}\left\|\left|v^{\prime}\right|^{\frac{1}{2}} u^{-}\right\|_{\infty} \int_{-\infty}^{0} \frac{\left|v v^{\prime}\right|^{\frac{1}{2}}}{\left(v^{\prime}-v\right)^{2}} d v^{\prime}= \\
& =C\left\|\left|v^{\prime}\right|^{\frac{1}{2}} u^{-}\right\|_{\infty} \tag{3.7}
\end{align*}
$$

and the Riesz-Thorin interpolation theorem gives the result in $L^{2}$.
Using the boundedness of $M_{1}$ we will now derive an a priori estimate for (3.1). When considering a Wigner function $w \in L^{2}\left(\Omega \times \mathscr{R}_{v}^{d}\right)$, with bounded $\Omega$, the appropriate norms on the boundary are (see [4])

$$
\begin{equation*}
\|w\|_{\Gamma_{ \pm}}^{2}=\int_{\Gamma_{+}}|v \cdot r(x)| w(x, v)^{2} d \sigma d v \tag{3.8}
\end{equation*}
$$

( $d \sigma$ denotes the surface measure on $\partial \Omega$ ), and specifically for our situation :

$$
\begin{align*}
& \|w\|_{\Gamma_{+}}^{2}=\int_{-\infty}^{0}|v| w(-1, v)^{2} d v+\int_{0}^{\infty} v w(1, v)^{2} d v \\
& \|w\|_{\Gamma_{-}}^{2}=\int_{0}^{\infty} v w(-1, v)^{2} d v+\int_{-\infty}^{0}|v| w(1, v)^{2} d v \tag{3.9}
\end{align*}
$$

LEMMA 3.3: Let $V \in L^{\infty}\left((0, \infty) \times \mathscr{R}_{x}\right)$, such that $\left\|M_{1}(t)\right\| \leqslant \alpha$ holds for almost all $t>0$ in the $L^{2}\left(\mathscr{R}^{ \pm},|v|\right)$-operator norm. Then the following a priori estimate holds for a mild solution of (3.1) :

$$
\begin{align*}
& \|w(t)\|_{2}^{2}+\int_{0}^{t}\left[\|w(\tau)\|_{\Gamma_{+}}^{2}+\|w(\tau)\|_{\Gamma_{-}}^{2}\right] d \tau \leqslant \\
& \qquad \tag{3.10}
\end{align*}
$$

with $C$ depending continuously on $t$ and $\alpha$.

Proof: We first multiply (3.1a) by $w$, and then integrate over $x \in(-1,1)$, $v \in \mathscr{R}$, and $\tau \in(0, t)$, which immediately gives the inflow-outflow-balance

$$
\begin{equation*}
\|w(t)\|_{2}^{2}=\left\|w^{I}\right\|_{2}^{2}+\int_{0}^{t}\left[\|w(\tau)\|_{\Gamma_{-}}^{2}-\|w(\tau)\|_{\Gamma_{+}}^{2}\right] d \tau \tag{3.11}
\end{equation*}
$$

Here we used the fact that, for $V \in L^{\infty}\left(\mathscr{R}_{x}\right), \Theta[V]$ is skew-symmetric, i.e.,

$$
\begin{equation*}
\int_{\mathrm{R}} u_{1}(v)\left(\Theta[V] u_{2}\right)(v) d v=-\int_{\mathscr{R}} u_{2}(v)\left(\Theta[V] u_{1}\right)(v) d v \tag{3.12}
\end{equation*}
$$

for $u_{1}, u_{2} \in L^{2}(\mathscr{R})$ (see [13]). Strictly speaking, (3.11) is first derived for a classical solution, i.e., $w, v w_{x} \in C\left([0, t], L^{2}((-1,1) \times \mathscr{R})\right)$, for which a classical trace theorem ([4], Prop. 1) states that $\left.w(t)\right|_{\Gamma_{+}} \in L^{2}\left(\mathscr{R}^{ \pm},|v|\right)$ iff $\left.w(t)\right|_{\Gamma_{-}} \in L^{2}\left(\mathscr{R}^{ \pm},|v|\right)$. The result for mild solutions of (3.1) then follows from a density argument.

Using (3.1c, d), the inflow-data $\left.w\right|_{\Gamma}$ can be bounded by the outflow-data $\left.w\right|_{\Gamma_{+}}$. For $x=-1$ we estimate :

$$
\begin{align*}
& \left\|w^{+}(-1, ., t)\right\|_{L^{2}\left(\mathscr{R}^{+},|v|\right)}^{2} \leqslant \\
& \leqslant 2\left\|f^{+}(., t)\right\|_{L^{2}\left(\mathscr{R}^{+},|v|\right)}^{2}+2 t \int_{0}^{t}\left\|\left(M_{1} w^{-}\right)(-1, \ldots, \tau)\right\|_{L^{2}\left(\mathscr{R}^{+},|v|\right)}^{2} d \tau \leqslant \\
& \leqslant 2\left\|f^{+}(., t)\right\|_{L^{2}\left(\mathscr{R}^{+},|v|\right)}^{2}+2 t \alpha^{2} \int_{0}^{t}\left\|w^{-}(-1, ., \tau)\right\|_{L^{2}\left(\mathscr{R}^{-},|v|\right)}^{2} d \tau . \tag{3.13}
\end{align*}
$$

Together with the analogous result for $x=1$ this gives

$$
\begin{equation*}
\|w(t)\|_{\Gamma_{-}}^{2} \leqslant 2\|f(t)\|_{\Gamma_{-}}^{2}+2 t \alpha^{2} \int_{0}^{t}\|w(\tau)\|_{\Gamma_{+}}^{2} d \tau \tag{3.14}
\end{equation*}
$$

Now we will consider

$$
\begin{equation*}
z(t):=\|w(t)\|_{2}^{2}+\int_{0}^{t}\left[\|w(\tau)\|_{\Gamma_{+}}^{2}+\|w(\tau)\|_{\Gamma_{-}}^{2}\right] d \tau \tag{3.15}
\end{equation*}
$$

From (3.11), (3.14) we get
$z(t)=\left\|w^{I}\right\|_{2}^{2}+2 \int_{0}^{t}\|w(\tau)\|_{\Gamma_{-}}^{2} d \tau \leqslant$
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$$
\begin{align*}
& \leqslant\left\|w^{I}\right\|_{2}^{2}+4 \int_{0}^{t}\|f(\tau)\|_{\Gamma_{-}}^{2} d \tau+4 \alpha^{2} \int_{0}^{t} \tau \int_{0}^{\tau}\|w(s)\|_{\Gamma_{+}}^{2} d s d \tau \leqslant \\
& \leqslant\left\|w^{I}\right\|_{2}^{2}+4 \int_{0}^{t}\|f(\tau)\|_{\Gamma_{-}}^{2} d \tau+4 \alpha^{2} \int_{0}^{t} \tau z(\tau) d \tau \tag{3.16}
\end{align*}
$$

and the Gronwall inequality yields the result.
We point out that, even for homogeneous BC's, $\|w\|_{2}$ may not be globally bounded in $t$, which contrasts the (in $x$ ) periodic problem [2] and the whole space case [19]. Moreover, no dissipative energy functional for (3.1) has yet been derived (in [8] higher order energies for the wave equation with ABC's have been introduced). It is, therefore, not known yet if the nonlinear Wigner-Poisson equation, supplemented with ABC's admits a globally existing solution.

In order to show the existence of a mild solution of (3.1) we will analyze the fixed point operator $F$, defined by: for $u=\left(u^{+}, u^{-}\right) \in$ $L^{2}\left((0, T), L^{2}\left(\Gamma_{-},|v|\right)\right)$, with some fixed, finite $T$, solve the equation

$$
\begin{gather*}
y_{t}+v y_{x}+\Theta[V] y=0, \quad|x|<1, \quad v \in \mathscr{R}, \quad t \in(0, T), \\
y(t=0)=w^{I}, \\
\left.y(t)\right|_{\Gamma}=u(t), \quad t \in(0, T) . \tag{3.17}
\end{gather*}
$$

Then $F u=\left((F u)^{+},(F u)^{-}\right)$is defined as

$$
\begin{align*}
(F u)^{ \pm}(v, t)= & f^{ \pm}(v, t)- \\
& -\int_{0}^{t}\left(M_{1} y^{\mp}\right)(\mp 1, v, \tau) d \tau, \quad v \gtrless 0, \quad t \in(0, T) . \tag{3.18}
\end{align*}
$$

Lemma 3.4 : Let $w^{I} \in L^{2}((-1,1) \times \mathscr{R}), f^{ \pm} \in L^{2}\left((0, T), L^{2}\left(\mathscr{R}^{ \pm},|v|\right)\right)$, and let $V$ satisfy the assumptions of Lemma 3.3. Then, $F$ maps $L^{2}\left((0, T), L^{2}\left(\Gamma_{-},|v|\right)\right)$ into itself.

Proof: Our procedure to obtain the necessary regularity properties of the solution to (3.17) will be similar to the proof of Lemma 2.1 in [5]. The boundary data $u=\left(u^{+}(v, t), u^{-}(v, t)\right)$ can be extended to

$$
u_{D}(x, v, t)= \begin{cases}u^{+}\left(v, t-\frac{x+1}{v}\right), & v>0, \quad t>\frac{x+1}{v}  \tag{3.19}\\ u^{-}\left(v, t-\frac{x-1}{v}\right), & v<0, \quad t>\frac{x-1}{v} \\ 0, \text { else }\end{cases}
$$

$\mathbf{M}^{2}$ AN Modélısation mathématıque et Analyse numérique Mathematical Modelling and Numerical Analysis
and $u_{D} \in C\left([0, T], L^{2}((-1,1) \times \mathscr{R})\right)$ is a mild solution of $u_{t}+v u_{x}=0$ We now consider $z=y-u_{D}$, satısfying

$$
\begin{equation*}
z_{t}+v z_{x}+\Theta[V] z=-\Theta[V] u_{D} \tag{320}
\end{equation*}
$$

where the inhomogeneity appears in $L^{\infty}\left((0, T), L^{2}((-1) \times \mathscr{R})\right)$, since $\Theta[V]$ is bounded on $L^{2}\left(\mathscr{R}_{v}\right)$ for $V \in L^{\infty}\left(\mathscr{R}_{x}\right)(320)$ has a unique mild solution (see § 2 in [13]), which clearly satısfies $z(t=0)=w^{I}$ Also, $z$ has traces at $\Gamma_{ \pm} \times(0, T)$, with $\left.z\right|_{\Gamma}=0$ and $\left.z\right|_{\Gamma_{+} \in}$ $L^{2}\left((0, T), L^{2}\left(\Gamma_{+},|v|\right)\right)$. Like in Lemma 33 , this follows by first applying the trace theorem Prop 1, [4] to the classical solution of (320) (see TH. 2 in [13]) for smoother, approximatıng data, and a density argument.

Thus we conclude that (3.17) has a unique mild solution $y \in C\left([0, T], L^{2}((-1,1) \times \mathscr{R})\right)$, satisfyıng the inflow-outflow-balance (3.11). The assertion of the lemma then follows from (3.18) and the boundedness of $M_{1}$.

The following lemma will yield the existence of a unique local-in-t mild solution to (31)

Lemma 35 Undeı the assumptions of Lemma $34 F$ is contiactive for $T<\frac{\sqrt{2}}{\alpha}$.

Proof Given two inflow data $u_{1}, u_{2} \in L^{2}\left((0, T), L^{2}\left(\Gamma_{-},|v|\right)\right)$, the difference of the corresponding outflow data (as a result of solving (3.17)) can be estımated through (311)

$$
\begin{equation*}
\int_{0}^{t}\left\|y_{1}(\tau)-y_{2}(\tau)\right\|_{\Gamma_{+}}^{2} d \tau \leqslant \int_{0}^{t}\left\|u_{1}(\tau)-u_{2}(\tau)\right\|_{\Gamma_{-}}^{2} d \tau \tag{3.21}
\end{equation*}
$$

From (3 18) we then obtain

$$
\begin{align*}
\left\|F u_{1}(t)-F u_{2}(t)\right\|_{\Gamma_{-}}^{2} & \leqslant t \alpha^{2} \int_{0}^{t}\left\|y_{1}(\tau)-y_{2}(\tau)\right\|_{\Gamma_{+}}^{2} d \tau \leqslant \\
& \leqslant t \alpha^{2} \int_{0}^{t}\left\|u_{1}(\tau)-u_{2}(\tau)\right\|_{\Gamma_{-}}^{2} d \tau, \quad 0 \leqslant t \leqslant T \tag{3.22}
\end{align*}
$$

and the result follows by an integration with respect to $t$.
Since the contraction interval of $F$ depends only on $\alpha$, reflecting the linearity of problem (31), the local solution can always be continued in $t$. Thus we can formulate the main result of this section -

THEOREM $31 . \quad$ Let $\quad w^{t} \in L^{2}((-1,1) \times \mathscr{R}), \quad f^{ \pm} \in L_{\mathrm{loc}}^{2}((0, \infty)$, $\left.L^{2}\left(\mathscr{R}^{ \pm},|v|\right)\right)$, and let $V$ satısfy the assumptions of Lemma 3.3. Then (3 1) has a unique global mild solution $w \in C\left([0, \infty), L^{2}((-1,1) \times \mathscr{R})\right)$ with
boundary traces $\left.w\right|_{\Gamma_{ \pm}} \in L_{\text {loc }}^{2}\left((0, \infty), L^{2}\left(\Gamma_{ \pm},|v|\right)\right)$. The problem is strongly well-posed (in the sense of Kreiss, [12]), satisfying the estimate (3.10).

In the rest of this section, we will extend the above well-posedness result to second order $A B C$ 's. The Wigner equation ( $3.1 a, b$ ) is then supplemented with the $B C$ 's

$$
\begin{align*}
& w^{+}(-1, v, t)= \\
& =f^{+}(v, t)-\int_{0}^{t}\left[\left(M_{1} w^{-}\right)(-1, v, \tau)+\int_{0}^{\tau}\left(M_{2}^{+} w^{-}\right)(-1, v, s) d s\right] d \tau, \\
& v
\end{align*} \begin{array}{r}
\text { } \tag{3.23a}
\end{array}
$$

$$
\begin{align*}
& w^{-1}(1, v, t)= \\
& =f^{-}(v, t)-\int_{0}^{t}\left[\left(M_{1} w^{+}\right)(1, v, \tau)+\int_{0}^{\tau}\left(M_{2}^{-} w^{+}\right)(1, v, s) d s\right] d \tau, \\
& v<0, \quad t>0, \tag{3.23b}
\end{align*}
$$

Here $M_{2}^{+}: L^{2}\left(\mathscr{R}^{-},|v|\right) \rightarrow L^{2}\left(\mathscr{R}^{+},|v|\right)$ is given by (2.18), and $M_{2}^{-}$: $L^{2}\left(\mathscr{R}^{+},|v|\right) \rightarrow L^{2}\left(\mathscr{R}^{-},|v|\right)$ is defined by replacing in (2.18) $h^{+}$by $h^{-}$, with $h^{-}\left(v, v^{\prime}, v^{\prime \prime}\right)=h^{+}\left(-v,-v^{\prime},-v^{\prime \prime}\right)$.

Like before, the analysis relies crucially on the boundedness of $M_{2}^{ \pm}$, which is stated in

Lemma 3.6: Let $V, \mathscr{F}_{x} V, V_{t}, \mathscr{F}_{x} V_{t}, V_{x}, \mathscr{F}_{x} V_{x}$, and $v\left(\mathscr{F}_{x} V_{x}\right)(v) \in$ $L^{1}(\mathscr{R})$. Then $M_{2}^{ \pm}$are bounded operators.

Proof: We will only discuss the result for $M_{2}^{+}$, and suppress the $x$ - and $t$ dependence of its kernel, as it is irrelevent here. Also, since the situation here parallels the proof of Lemma 3.1 we only give the key estimates.

The boundedness of the first term in (2.18) is obtained by using the two estimates

$$
\begin{align*}
& \frac{|v|^{\frac{3}{2}}\left|v^{\prime \prime}\right|^{\frac{1}{2}}}{\left(v-v^{\prime \prime}\right)^{2}} \leqslant \text { const }, \quad v>0 \text { and } v^{\prime \prime}<0  \tag{3.24}\\
&\left|\left(\mathscr{F}_{\eta} \delta V_{x}\right)\left(v^{\prime \prime}-v\right)\right| \frac{\left|v v^{\prime \prime}\right|^{\frac{3}{2}}}{\left(v-v^{\prime \prime}\right)^{2}} \leqslant \\
& \leqslant \text { const }\left|v^{\prime \prime}-v\right| \cdot\left|\left(\mathscr{F}_{x} V_{x}\right)\left(v^{\prime \prime}-v\right)\right|,  \tag{3.25}\\
& v>0 \text { and } v^{\prime \prime}<0 .
\end{align*}
$$

For the second term of (2.18) one uses

$$
\begin{equation*}
\left|\frac{v}{v^{\prime \prime}}\right|^{\frac{1}{2}}\left|h^{+}\left(v, v^{\prime}, v^{\prime \prime}\right)\right| \leqslant \text { const }, \quad v>0, \quad v^{\prime} \in \mathscr{R}, \quad v^{\prime \prime}<0 \tag{3.26}
\end{equation*}
$$

and the boundedness then follows by applying the Young inequality twice.
With this boundedness, the Lemmata 3.3-3.5 carry over to the second order $A B C$ 's (in the proofs $\alpha$ just has to be replaced by $(1+t) \alpha$ ), and yield the strong well-posedness for this problem :

THEOREM 3.2: Let $\quad w^{I} \in L^{2}((-1,1) \times \mathscr{R}), \quad f^{ \pm} \in L_{\text {loc }}^{2}((0, \infty)$, $\left.L^{2}\left(\mathscr{R}^{ \pm},|v|\right)\right)$, and let $V \in L^{\infty}\left((0, \infty) \times \mathscr{R}_{x}\right)$, such that $\left\|M_{1}(t)\right\|+$ $\left\|M_{2}^{+}(t)\right\|+\left\|M_{2}^{-}(t)\right\| \leqslant \alpha$ holds for almost all $t>0$ in the $L^{2}\left(\mathscr{R}^{ \pm},|v|\right)-$ operator norm. Then $(3.1 a, b)$, (3.23) has a unique global mild solution $w \in C\left([0, \infty], L^{2}((-1,1) \times \mathscr{R})\right)$, and its boundary traces $\left.w\right|_{\Gamma_{+}} \in L_{\text {loc }}^{2}\left((0, \infty), L^{2}\left(\Gamma_{ \pm},|v|\right)\right)$ satisfy (3.10).

## 4. MODEL EXTENSIONS

For realistic device simulations at least a simple approximation for the electron-phonon scattering has to be included into the Wigner equation model ([10]). In this section we will analyze the $A B C$ ' $s$ for the $2 D$-Wigner equation and for the relaxation-time model. Since the proofs of the wellposedness results are based on the fixed point iteration of § 3 , we will only sketch them, mainly focusing on the a priori estimates.

## 4.1. $2 D$ Wigner Equation

Here we consider (1.1) on the slab $-1<x_{1}<1, x_{2} \in \mathscr{R}, v \in \mathscr{R}^{2}$, and we will now discuss appropriate ABC's at $x= \pm 1$. For the Wigner equation in two (spatial) dimensions the asymptotic construction of $\Phi$ and $M$ from $\S 2$ is generalized by requiring that the summands $\partial_{t}^{-J} \circ \tilde{\Phi}_{J}$ and $\partial_{t}^{-1} \circ \tilde{M}_{J}$ now be homogeneous of degree $-j$ in ( $\partial_{t}, \partial_{x_{2}}$ ) (see [16]). This procedure yields as the first order approximation

$$
\begin{align*}
& \left(\tilde{M}_{1} w\right)(x, v, t)= \\
& = \begin{cases}\frac{i}{(2 \pi)^{2}} \int_{\mathscr{R}^{3}} \int_{-\infty}^{0}\left[\frac{v_{1}^{\prime}-v_{1}}{v_{1}^{\prime}}+\frac{v_{2} v_{1}^{\prime}-v_{1} v_{2}^{\prime}}{v_{1}^{\prime}} \partial_{t}^{-1} \partial_{x_{2}}\right]^{-1} \times \\
\times \delta V(x, \eta, t) w^{-}\left(x, v^{\prime}, t\right) e^{\prime \eta\left(v-v^{\prime}\right)} d v_{1}^{\prime} d v_{2}^{\prime} d^{2} \eta, & v_{1}>0 \\
0, & v_{1}<0\end{cases} \tag{4.1}
\end{align*}
$$

which generalizes $M_{1},(212)$ to $2 D$ However, (41) is also a $P D O$ with respect to $t$ and $x_{2}$, thus not yet useful for numerical computations In order to obtain a local approximation, $\tilde{M}_{1}$ is expanded in powers of ( $\partial_{t}^{-1} \partial_{x_{2}}$ ), which corresponds to an expansion of the wave directions at the boundary about normal incidence (see [6], [16])

From the zero-order approximation one obtains the $B C$

$$
\begin{equation*}
w_{t}^{+}+\tilde{M}_{10} w^{-}=0, \quad v_{1}>0, \tag{42}
\end{equation*}
$$

with

$$
\begin{align*}
\left(\tilde{M}_{10} w^{-}\right)(x, v, t)= & \frac{l}{(2 \pi)^{2}} \int_{\mathscr{R}^{3}} \int_{-\infty}^{0} \frac{v_{1}^{\prime}}{v_{1}^{\prime}-v_{1}} \times \\
& \times \delta V(x, \eta, t) w^{-}\left(x, v^{\prime}, t\right) e^{t \eta}(v \quad v) d^{2} v^{\prime} d^{2} \eta \tag{43}
\end{align*}
$$

and the well-posedness analysis of § 3 immediately carries over to 2 D

Including the first order term in $\left(\partial_{t}{ }^{1} \partial_{x_{2}}\right)$ leads to the $A B C$

$$
\begin{equation*}
w_{t t}^{+}+\partial_{t}\left(\tilde{M}_{10} w\right)+\tilde{M}_{11} w^{-}=0, \quad v_{1}>0, \tag{44}
\end{equation*}
$$

with

$$
\begin{align*}
\left(\tilde{M}_{11} w^{-}\right)(x, v, t)= & \\
= & \frac{t}{(2 \pi)^{2}} \int_{\mathscr{R}^{3}} \int_{\infty}^{0} \frac{v_{1}^{\prime}}{v_{1}^{\prime}-v_{1}} \frac{v_{2} v_{1}^{\prime}-v_{1} v_{2}^{\prime}}{v_{1}^{\prime}-v_{1}} \times \\
& \times \delta V(x, \eta, t) w_{x_{2}}^{-}\left(x, v^{\prime}, t\right) e^{\prime \eta(\imath}() d^{2} v^{\prime} d^{2} \eta \tag{45}
\end{align*}
$$

which was first derived in [16] Using this type of $B C$ at $x= \pm 1$ for the Wigner equation (11) yields a very delicate $I B V P$, and it is not known yet if it is well- or ill-posed The difficulties here stem from the unboundedness of $\tilde{M}_{11}$ in the trace space $L^{2}\left(\mathscr{R}_{v_{1}}^{ \pm} \times \mathscr{R}_{x_{2}}^{2} v_{2},\left|v_{1}\right|\right)$ We will not pursue this question any further here, but instead improve the $B C$ (42) as to include $2 D$ effects at the boundary

When the given potential $V$ is independent of $x_{2}$, (11) decouples on the hyperplanes $v_{2}=$ const $T h e n$ the operator $\tilde{M}_{1}$ is local in $v_{2}$ and it corresponds, without further approximations, to the $B C$

$$
\begin{equation*}
\left(\partial_{t}+v_{2} \partial_{x_{2}}\right) w^{+}+\tilde{M}_{10} w^{-}=0, \quad v_{1}>0 \tag{46}
\end{equation*}
$$

This result motivates the following procedure for $x_{2}$-dependent potentials When first applying the operator $\left(1+v_{2} \partial_{t}^{-1} \partial_{x_{2}}\right)$ to the first order
$A B C w_{t}^{+}+\tilde{M}_{1} w^{-}=0$, and then taking the zero-order approximation with respect to $\partial_{t}^{-1} \partial_{x_{2}}$, one again obtains the $B C$ (4.6).

We will now formulate the well-posedness result for the Wigner equation on $(-1,1) \times \mathscr{R}^{3}$, supplemented with the inhomogeneous $B C$ 's

$$
\begin{equation*}
w^{ \pm}\left(\mp 1, x_{2}, v, t\right)=f^{ \pm}\left(x_{2}, v, t\right)-z^{ \pm}\left(x_{2}, v, t\right), \quad v_{1} \geqq 0, \tag{4.7}
\end{equation*}
$$

where $z^{ \pm}$solve the transport problems

$$
\begin{align*}
& \left(\partial_{t}+v_{2} \partial_{x_{2}}\right) z^{ \pm}= \\
& \quad=\left(\tilde{M}_{1,0} w^{\mp}\right)\left(\mp 1, x_{2}, v, t\right), \quad v_{1} \geqq 0, v_{2}, x_{2} \in \mathscr{R}, t>0,  \tag{4.8}\\
& \quad z^{ \pm}(t=0)=0 .
\end{align*}
$$

THEOREM 4.1: Let $\quad w^{I} \in L^{2}\left((-1,1) \times \mathscr{R}^{3}\right), \quad f^{ \pm} \in L_{\mathrm{loc}}^{2}((0, \infty)$, $\left.L^{2}\left(\mathscr{R}_{v_{1}}^{ \pm} \times \mathscr{R}^{2},\left|v_{1}\right|\right)\right)$, and let $\quad V \in L^{\infty}\left((0, \infty)_{t} \times \mathscr{R}_{x}^{2}\right)$, such that $\left\|\tilde{M}_{1,0}(t)\right\| \leqslant \alpha$ holds for almost all $t>0$ in the $L^{2}\left(\mathscr{R}_{v_{1}}^{ \pm} \times \mathscr{R}^{2},\left|v_{1}\right|\right)$ operator norm. Then (1.1), with the initial condition $w(t=0)=w^{I}$ and the $B C$ 's (4.7), (4.8), has a unique global mild solution $w \in C\left([0, \infty], L^{2}\left((-1,1) \times \mathscr{R}^{3}\right)\right)$ with boundary traces $\left.w\right|_{\Gamma_{ \pm}} \in L_{\mathrm{loc}}^{2}\left((0, \infty), L^{2}\left(\Gamma_{ \pm},\left|v_{1}\right|\right)\right)$.

Proof: The solution of (4.8) reads

$$
\begin{equation*}
z^{+}\left(x_{2}, v, t\right)=\int_{0}^{t}\left(\tilde{M}_{1,0} w^{-}\right)\left(-1, x_{2}-(t-\tau) v_{2}, v, \tau\right) d \tau \tag{4.9}
\end{equation*}
$$

and a straight forward estimate gives

$$
\begin{align*}
&\left\|w^{+}(-1, t)\right\|_{L^{2}\left(\mathscr{R}^{+} \times \mathscr{R}^{2},\left|v_{1}\right|\right)} \leqslant\left\|f^{+}(t)\right\|_{L^{2}\left(\mathscr{R}^{+} \times \mathscr{R}^{2},\left|v_{1}\right|\right)}+ \\
&+\alpha \int_{0}^{t}\left\|w^{-}(-1, \tau)\right\|_{L^{2}\left(\mathscr{R}^{-} \times \mathscr{R}^{2},\left|v_{1}\right|\right)} d \tau . \tag{4.10}
\end{align*}
$$

Hence, the results of $\S 3$ can be applied.

### 4.2. Relaxation-Time model

Most of the performed quantum device simulations in the Wigner formulation have used a relaxation-time approximation ([10], [3]), as no numerically tractable quantum scattering operator is available yet. We will here analyze $A B C$ 's for the equation

$$
\begin{equation*}
w_{t}+v w_{x}+\Theta[V] w=\frac{w_{0}-w}{\tau}, \quad|x|<1, \quad v \in \mathscr{R}, \quad t>0 \tag{4.11}
\end{equation*}
$$

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where $w_{0}=w_{0}(x, v)$ denotes a quantum steady state ([1]) and $\tau=\tau(x, v)>0$ the relaxation time. Since the relaxation term is local in $v$, the asymptotic construction of the «boundary operator» $M$ in $\S 2$ yields the same first order $A B C$ as for the collision-free Wigner equation (3.1a). Only for the second order $A B C, M_{2}$ in (2.21) has to be modified by an additional term, which is again bounded in the trace-space.

Extending Lemma 3.3, we will now derive an a priori estimate for the IBVP of (4.11).

Lemma 4.1: Let $V$ and $M_{1}$ satisfy the assumptions of Lemma 3.3. Also assume that $\tau^{-1} \in L^{\infty}((-1,1) \times \mathscr{R}) \quad$ with $\quad \tau(x, v) \geqslant \tau_{0}>0$, and $w_{0} \in L^{2}((-1,1) \times \mathscr{R})$. Then, a mild solution of $(4.11),(3.1 b, c, d)$ satisfies

$$
\begin{align*}
&\|w(t)\|_{2}^{2}+\int_{0}^{t}\left[\|w(s)\|_{\Gamma_{+}}^{2}+\|w(s)\|_{\Gamma_{-}}^{2}\right] d s \leqslant \\
& \leqslant C(t)\left[\left\|w^{I}\right\|_{2}^{2}+\int_{0}^{t}\|f(s)\|_{\Gamma_{-}}^{2} d s\right], \quad t \geqslant 0 \tag{4.12}
\end{align*}
$$

where $C$ depends continuously on $t, \alpha, \tau_{0}$ and $\left\|w_{0}\right\|_{2}$.
Proof: We first multiply (4.11) by $w$ and then integrate over $x \in(-1,1)$, $v \in \mathscr{R}$ and $\tau \in(0, t)$, which gives the estimate

$$
\begin{align*}
&\|w(t)\|_{2}^{2}-\left\|w^{I}\right\|_{2}^{2}+\int_{0}^{t}\left[\|w(s)\|_{\Gamma_{+}}^{2}-\|w(s)\|_{\Gamma_{-}}^{2}\right] d s \leqslant \\
& \leqslant \frac{2}{\tau_{0}}\left\|w_{0}\right\|_{2} \int_{0}^{t}\|w(s)\|_{2} d s \tag{4.13}
\end{align*}
$$

Next we will consider $z(t)$, as defined in (3.15). Using (4.13), (3.14) and the estimate $\lambda \leqslant 1+\lambda^{2}$ gives

$$
\begin{align*}
z(t) \leqslant\left\|w^{I}\right\|_{2}^{2}+2 \int_{0}^{t} \| w(s) & \left\|_{\Gamma_{-}}^{2} d s+\frac{2}{\tau_{0}}\right\| w_{0}\left\|_{2} \int_{0}^{t}\right\| w(s) \|_{2} d s \leqslant \\
& \leqslant\left\|w^{I}\right\|_{2}^{2}+4 \int_{0}^{t}\|f(s)\|_{\Gamma_{-}}^{2} d s+\frac{2}{\tau_{0}}\left\|w_{0}\right\|_{2} t \\
& +\int_{0}^{t}\left(4 \alpha^{2} s+\frac{2}{\tau_{0}}\left\|w_{0}\right\|_{2}\right) z(s) d s \tag{4.14}
\end{align*}
$$

and the Gronwall inequality yields the result.
To show the existence of a mild solution, one uses a fixed point iteration in $L^{2}\left((0, T), L^{2}\left(\Gamma_{-},|v|\right)\right)$, like in the analysis of $\S 3$. Here, only (3.17) has to
be replaced by the equation

$$
\begin{equation*}
y_{t}+v y_{x}+\Theta[V] y+\frac{y}{\tau}=\frac{w_{0}}{\tau}, \quad t \in(0, T), \tag{4.15}
\end{equation*}
$$

which admits a unique mild solution of the $I B V P$. This follows from the fact that $\tau^{-1}$, just like the operator $\Theta[V]$, is a bounded perturbation of the generator $v \partial_{x}$ (see [13] for the detailed reasoning), and the inhomogeneity $\frac{w_{0}}{\tau} \in L^{2}((-1,1) \times \mathscr{R})$.

The strong well-posedness of the relaxation-time Wigner equation with $A B C$ 's is now formulated in

THEOREM 4.2: Let $w^{I}, \quad w_{0} \in L^{2}((-1,1) \times \mathscr{R}), \quad f^{ \pm} \in L_{\mathrm{loc}}^{2}((0, \infty)$, $\left.L^{2}\left(\mathscr{R}^{ \pm},|v|\right)\right), \quad \tau(x, v) \geqslant \tau_{0}>0$, and let $V$ satisfy the assumptions of Lemma 3.3. Then (4.1), (3.1b, $c$, d) has a unique global mild solution $w \in C\left([0, \infty]\right.$, $\left.L^{2}((-1,1) \times \mathscr{R})\right)$ with boundary traces $\left.w\right|_{\Gamma_{ \pm}} \in L_{\mathrm{loc}}^{2}\left((0, \infty), L^{2}\left(\Gamma_{ \pm},|v|\right)\right)$.

## REFERENCES

[1] A. Arnold, P. A. Markowich, N. Mauser, 1991, The one-dimensional periodic Bloch-Poisson equation, $M^{3} A S, 1,83-112$.
[2] A. Arnold, C. Ringhofer, 1995, An operator splitting method for the WignerPoisson problem, to appear in SIAM J. Num. Anal.
[3] F. A. Buot, K. L. Jensen, 1990, Lattice Weyl-Wigner formulation of exact many-body quantum-transport theory and applications to novel solid-state quantum-based devices, Phys. Rev. B, 42, 9429-9457.
[4] M. Cessenat, 1985, Théorèmes de trace pour des espaces de fonctions de la neutronique, C. R. Acad. Sc. Paris, tome 300, série I, n ${ }^{\circ} 3$, 89-92.
[5] P. Degond, P. A. Markowich, 1990, A quantum transport model for semiconductors : the Wigner-Poisson problem on a bounded Brillouin zone, Modélisation Mathématique et Analyse Numérique, 24, 697-710.
[6] B. Engquist, A. Majda, 1977, Absorbing boundary conditions for the numerical simulation of waves, Math. Comp., 31, 629-651.
[7] W. R. Frensley, 1987, Wigner function model of a resonant-tunneling semiconductor device, Phys. Rev. B, 36, 1570-1580.
[8] T. Ha-Duong, P. Joly, 1990, On the stability analysis of boundary conditions for the wave equation by energy methods, Part I: The homogeneous case, Rapports de Recherche 1306, INRIA.
[9] L. HALPERN, J. RaUCh, 1987, Error analysis for absorbing boundary conditions, Numer. Math., 51, 459-467.
[10] N. Kluksdahl, A M Kriman, D. K. Ferry, C Ringhofer, 1989, Selfconsistent study of the resonant tunneling diode, Phys Rev B, 39, 77207735.
[11] H O. Kreiss, 1970, Inital boundary value problems for hyperbolic systems, Comm Pure Appl Math, 23, 277-298.
[12] H. O. Kreiss, J. Lorenz, 1989, Initıal-Boundary Value Problems and the Navier-Stokes Equatıons, Academic Press, San Diego.
[13] P. A. Markowich, C. Ringhofer, 1989, An analysis of the quantum Liouville equation, $Z$ angew Math Mech, 69, 121-127.
[14] P. A. Markowich, C. Ringhofer, C. Schmeiser, 1990, Semiconductor Equations, Springer-Verlag, Wien, New York.
[15] F. Nier, 1993, Asymptotic analysis of a scaled Wigner equation and quantum scattering, To appear in $M^{3} A S$
[16] C. Ringhofer, D. Ferry, N. Kluksdahl, 1989, Absorbing boundary conditions for the simulation of quantum transport phenomena, Transport Theory and Statustical Physics, 18, 331-346.
[17] D. Robert, 1987, Autour de l'Approximatıon Semi-classique, Bırkhauser, Boston.
[18] M. A. Shubin, 1987, Pseudodifferentıal Operators and Spectral Theory, Sprınger-Verlag, Berlın, Heidelberg.
[19] H Steinruck, 1991, The one-dımensional Wigner-Poisson problem and its relation to the Schrodinger-Poisson problem, SIAM J Math Anal, 22, 957-972.
[20] V. I. TatarskiI, 1983, The Wigner representation of quantum mechanics, Sov Phys Usp, 26, 311-327

