Parity-decomposition and Moment Analysis for Stationary Wigner Equation with Inflow Boundary Conditions

Ruo Li∗, Tiao Lu†, Zhangpeng Sun‡

March 9, 2022

Abstract

We study the stationary Wigner equation on a bounded, one-dimensional spatial domain with inflow boundary conditions by using the parity decomposition in (Barletti and Zweifel, Trans. Theory Stat. Phys., 507–520, 2001). The decomposition reduces the half-range, two-point boundary value problem into two decoupled initial value problems of the even part and the odd part. Without using a cutoff approximation around zero velocity, we prove that the initial value problem for the even part is well-posed. For the odd part, we prove the uniqueness of the solution in the odd $L^2$-space by analyzing the moment system. An example is provided to show that how to use the analysis to obtain the solution of the stationary Wigner equation with inflow boundary conditions.

Keywords: Stationary Wigner equation, inflow boundary conditions, well-posedness.

1 Introduction

As the size of electronic devices approaches the nanometer scale, quantum effects, such as tunneling, have to be considered in study of the device properties. As a result, quantum models, including the Schrödinger equation, non-equilibrium Green function methods and the Wigner equation, have attracted increasing attentions. In these models, the Wigner equation has some advantages over other quantum models [7]. One advantage is that the inflow boundary conditions for the Boltzmann equation can be extended to the Wigner equation since the latter can be formulated as the former with a quantum correction term. Especially, the stationary Wigner equation with inflow boundary conditions is often adopted in numerical simulation of nanoscale devices. Starting from [8], simulations of nanoscale devices using such a model have provided a lot of encouraging numerical results [11, 19, 18, 16, 17, 5, 15].

Even though, rigorous mathematical theory on the well-posedness of the stationary Wigner equation with inflow boundary conditions is still an open problem, even for one dimensional case [2]. We note that there are some results in a semi-discrete version, such as [1]. In [14], the semi-discrete version of the Wigner equation is related to the truncated

∗HEDPS & CAPT, LMAM & School of Mathematical Sciences, Peking University, Beijing, China, email: rli@math.pku.edu.cn.
†CAPT, HEDPS, LMAM, IFSA Collaborative Innovation Center of MoE, & School of Mathematical Sciences, Peking University, Beijing, China, email: tlu@math.pku.edu.cn.
‡School of Mathematical Sciences, Peking University, Beijing, China, email: sunzhangpeng@pku.edu.cn.
Wigner equation proposed in [13] using the Shannon sampling theory. The truncation length is called a coherence length in many papers, e.g., [12].

The well-posedness of the stationary continuous Wigner equation with inflow boundary conditions is still a temptatious problem mathematically. We adopt the parity decomposition technique to study the stationary Wigner equation with inflow boundary conditions, which has been proposed in [3]. As in [3], the Wigner equation with inflow boundary conditions is a linear boundary value problem (BVP), and the even and odd parts are decoupled and each part is a solution of the Wigner BVP with corresponding boundary conditions. It was pointed out in [3] that: "It is worth to remark that we do not obtain a well-posedness result for the full problem (that is, with \( v \) in place of \( \eta_\epsilon(v) \)) by simply letting \( \epsilon \) go to 0. The analysis of the full problem must be carried out by means of more sophisticated techniques than those employed here. In particular, \( B(x) \) could be stud-

ied as an unbounded linear evolution operator in a suitable space, with the initial datum ((\( f_{b,e}^-((-l/2), f_{b,o}^+((-l/2)) \)) restricted to the appropriated domain." In [3], a small interval centered at \( v = 0 \) is removed to obtain the well-posedness result. Here we will try to clarify the questions put forward therein. Without a cutoff approximation around \( v = 0 \), we prove that the pseudo-differential operator \( B(x) \) (defined in (3.3)) is a bounded linear operator on the even \( L^2 \)-space, \( L^2_e(\mathbb{R}_v) \) (defined in (3.4)), only if the potential function is regular enough. Thus, we can obtain the well-posedness of the even part directly. Gener-

ally, \( B(x) \) is no longer a bounded operator on the odd \( L^2 \)-space, \( L^2_o(\mathbb{R}_v) \) (defined in (3.5)). However, we prove the uniqueness of the solution of the odd part in \( L^2_o(\mathbb{R}_v) \) by analyzing its moment system.

The rest of this paper is organized as follows. In Section 2, we present the governing equations and in Section 3, we introduce the parity decomposition. The equation with inflow boundary conditions is discussed in Section 4 and then a short conclusion closes the main text.

### 2 Wigner Equation

We consider the stationary, linear Wigner equation of the form [20]

\[
v \frac{\partial f(x,v)}{\partial x} - \Theta f(x,v) = 0, \quad x \in [-l/2,l/2], v \in \mathbb{R}_v.
\]  

For convenience, we have set the reduced Planck constant \( \hbar \), the electron charge \( e \) and the effective mass of electron \( m \) to be equal to unity. Here \( \Theta \) is an anti-symmetric pseudo-differential operator. Precisely,

\[
(\Theta f)(x,v) = i\mathcal{F}_{y\rightarrow x}^{-1} \left( (V(x+y/2) - V(x-y/2))\hat{f}(x,y) \right),
\]  

where \( V : \mathbb{R} \rightarrow \mathbb{R} \) is the potential. Using the convolution theorem of the Fourier transform, we have

\[
(\Theta f)(x,v) = \int_{\mathbb{R}_v} \mathcal{V}(x,v-v') f(x,v') dv',
\]  

where \( \mathcal{V}(x,v) \) is defined in (3.13). We use \( \mathcal{F}_{v\rightarrow y}(f(x,v)) \) to denote the Fourier transform of \( f(x,v) \), and

\[
\mathcal{F}_{v\rightarrow y}(f(x,v)) = \int_{\mathbb{R}_v} f(x,v) \exp(-ivy) dv.
\]
Correspondingly, the inverse Fourier transform of \( \hat{f}(x, y) \) is defined as
\[
\mathcal{F}_{y \rightarrow v}^{-1} \left( \hat{f}(x, y) \right) = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{f}(x, y) \exp(ivy) \, dy. \tag{2.5}
\]

The derivation of the Wigner equation from the Schrödinger equation can be found in many references, e.g., \cite{10, 13, 4}. Here, we only describe the Wigner-Weyl transform simply for completeness of the paper. A quantum system is described by the Schrödinger equation
\[
\left( -\frac{1}{2} \frac{d^2}{dx^2} + V(x) \right) \psi_n(x) = E_n \psi_n(x), \tag{2.6}
\]
where the eigen-function \( \psi_n(x) \) is called a pure state and the associated eigenvalue \( E_n \in \mathbb{R} \) is called an eigen energy. The density matrix \( \rho(x, x') \) for a mixed state is defined as
\[
\rho(x, x') = \sum_n P_n \psi_n^*(x) \psi_n(x'), \tag{2.7}
\]
where \( P_n \) is the probability of the electron occupying the state \( \psi_n \), and \( \sum_n P_n = 1 \). The stationary Liouville-von Neumann equation is then derived from (2.6) as
\[
\left[ -\frac{1}{2} \left( \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2} \right) + V(x) - V(x') \right] \rho(x, x') = 0 \tag{2.8}
\]
Introducing the quasi-probability distribution function
\[
f(x, v) = \mathcal{F}_{y \rightarrow v}^{-1} \left( \rho(x + y/2, x - y/2) \right), \tag{2.9}
\]
and applying a change of variables and the inverse Fourier transform of (2.8), we derive the Wigner equation governing \( f(x, v) \) as
\[
v \frac{\partial f(x, v)}{\partial x} - \Theta f(x, v) = 0, \quad x \in \mathbb{R}, v \in \mathbb{R}, \tag{2.10}
\]
where \( \Theta f \) is defined in (2.2).

We need to specify some conditions to ensure that (2.10) or (2.1) has a unique solution. Before the discussion on these conditions, let us to examine the properties of the stationary Wigner equation at first.

3 Parity Decomposition

Following \cite{3}, we take the point of view that the function \( f(x, \cdot) : \mathbb{R}_v \rightarrow \mathbb{R} \) belongs to the Hilbert space \( L^2(\mathbb{R}_v) \) for every fixed \( x \in \mathbb{R} \), equipped with the norm
\[
\|f(x, \cdot)\|_{L^2(\mathbb{R}_v)} = \left( \int_{\mathbb{R}_v} |f(x, v)|^2 \, dv \right)^{1/2}. \tag{3.1}
\]
Thus, \( f \) is regarded as a vector-valued function from \( \mathbb{R} \) to \( L^2(\mathbb{R}_v) \). To emphasize this, we will often use the notation \( [f(x)](v) \) instead of \( f(x, v) \) later on. With such notations, the Wigner equation (2.10) is recast into an equation for the unknown function \( f : \mathbb{R} \rightarrow L^2(\mathbb{R}_v) \) of the following form
\[
\frac{d}{dx} f(x) - B(x) f(x) = 0, \quad x \in \mathbb{R}. \tag{3.2}
\]
Here, \( \frac{d}{dx} \) is a differential operator on \( C^1(\mathbb{R}; L^2(\mathbb{R}_v)) \) and the operator \( B(x) \) is defined by

\[
[B(x)f(x)](v) = \frac{i}{v} F_{y\rightarrow v}^{-1} \left( D_{V}(x, y)[f(x)](y) \right),
\]  

where

\[
D_{V}(x, y) = V(x + y/2) - V(x - y/2), \quad [f(x)](y) = F_{v\rightarrow y} ([f(x)](v)).
\]

We decompose the space \( L^2(\mathbb{R}_v) \) into the direct sum \( L^2_e(\mathbb{R}_v) \oplus L^2_o(\mathbb{R}_v) \) where \( L^2_e(\mathbb{R}_v) \) and \( L^2_o(\mathbb{R}_v) \) are the subspaces of \( L^2(\mathbb{R}_v) \) defined by

\[
L^2_e(\mathbb{R}_v) = \{ u(v) \in L^2(\mathbb{R}_v) : u(v) = u(-v) \}, \quad (3.4)
\]

\[
L^2_o(\mathbb{R}_v) = \{ u(v) \in L^2(\mathbb{R}_v) : u(v) = -u(-v) \}. \quad (3.5)
\]

Clearly, for \( \forall f \in L^2(\mathbb{R}_v) \), \( f \) is uniquely decomposed into the sum

\[
f = f_e + f_o,
\]

where \( f_e \) and \( f_o \) are its even part and odd part, respectively, i.e.,

\[
f_e(v) = [P_e f](v) := \frac{1}{2} (f(v) + f(-v)), \quad f_o(v) = [P_o f](v) := \frac{1}{2} (f(v) - f(-v)),
\]

where \( P_e : L^2(\mathbb{R}_v) \rightarrow L^2_e(\mathbb{R}_v) \) and \( P_o : L^2(\mathbb{R}_v) \rightarrow L^2_o(\mathbb{R}_v) \) are two projection operators defined in the above equations.

As pointed out in [3], \( B(x) \) is an even operator which preserves the parity. Therefore, the subspace \( L^2_e(\mathbb{R}_v) \) and \( L^2_o(\mathbb{R}_v) \) are closed with exertion of \( B(x) \). This fact is formally expressed by the commutation relations

\[
P_e B(x) = B(x) P_e, \quad P_o B(x) = B(x) P_o, \quad \forall x \in \mathbb{R}.
\]

By applying the operators \( P_e \) and \( P_o \) on both sides of (3.2), we immediately split (3.2) into two identical decoupled equations for the even part and the odd part of the unknown \( f(x) \):

\[
\frac{d}{dx} f_e(x) - B(x) f_e(x) = 0, \quad x \in \mathbb{R}, \quad (3.6)
\]

\[
\frac{d}{dx} f_o(x) - B(x) f_o(x) = 0, \quad x \in \mathbb{R}. \quad (3.7)
\]

The equations (3.2), (3.6) and (3.7) are linear ordinary differential equations. This brings us to consider initial value problems at first.

We consider the following initial value problem (IVP)

\[
\frac{d}{dx} f(x) - B(x) f(x) = 0, \quad x \in \mathbb{R}, \quad (3.2)
\]

with the initial condition

\[
f(-l/2) = f_b \in L^2(\mathbb{R}_v). \quad (3.8)
\]

The initial value \( f_b \) can be uniquely decomposed into the sum

\[
f_b = f_{b,e} + f_{b,o},
\]
where \( f_{b,e} = P_e f_b \) and \( f_{b,o} = P_o f_b \). By the even property of the operator \( B(x) \), it is easy to verify that if \( f(x) \) is the solution of the IVP (3.2)+(3.8), then \( f_e = P_e f \) is the solution of the IVP (3.6) with the initial condition

\[
f_e(-l/2) = f_{b,e},
\]

(3.9)

and \( f_o = P_o f \) is the solution of the IVP (3.7) with the initial condition

\[
f_o(-l/2) = f_{b,o}.
\]

(3.10)

In order to study the IVP (3.2)+(3.8), we need only to analyze the IVP (3.6)+(3.9) and the IVP (3.7)+(3.10), respectively.

### 3.1 The even part

For the even part of the Wigner equation, i.e., the IVP (3.6)+(3.9), we rewrite it as

\[
\frac{df(x)}{dx} - B(x)f(x) = 0,
\]

(3.11)

with the initial condition

\[
f(-l/2) = f_b \in L^2_e(\mathbb{R}_v).
\]

(3.12)

Below we prove that under some assumptions, there exists a unique solution \( f(x) \in L^2_e(\mathbb{R}_v) \) of the IVP (3.11)-(3.12). As a preliminary step to prove the result, we give a lemma to declare that \( B(x) \) is a bounded linear operator on \( L^2_e(\mathbb{R}_v) \).

**Lemma 1.** Let

\[
\mathcal{V}(x,v) = iF_{y \rightarrow v}^{-1}(V(x+y/2) - V(x-y/2)).
\]

(3.13)

Assuming \( \mathcal{V}(x,v) \in H^1(\mathbb{R}_v) \), \( B(x) : L^2_e(\mathbb{R}_v) \rightarrow L^2_e(\mathbb{R}_v) \) defined in (3.3) can be rewritten into

\[
[B(x)f](v) = \frac{1}{v} \mathcal{V} \ast f(x,v).
\]

Then \( B(x) \) is a bounded linear operator on \( L^2_e(\mathbb{R}_v) \).

**Proof.** By the definition of \( \mathcal{V} \) in (3.13), we have \( \mathcal{V}(x) \in L^2_o(\mathbb{R}_v) \). Thus, for \( \forall f(x) \in L^2_o(\mathbb{R}_v) \), we have

\[
\int_{\mathbb{R}_v} \mathcal{V}(x,v) f(x,v) dv = 0.
\]

(3.14)

We introduce an linear operator \( A(x) : L^2(\mathbb{R}_v) \rightarrow L^2(\mathbb{R}_v) \)

\[
[A(x)f](v) = \int_{\mathbb{R}_v} \mathcal{V}(x,v-v') - \mathcal{V}(x,0-v') f(x,v') dv'.
\]

(3.15)

By (3.14), it is concluded that \( A(x) = B(x) \) on \( L^2_e(\mathbb{R}_v) \). We will prove that \( A(x) \) is a bounded linear operator on \( L^2(\mathbb{R}_v) \) by estimating it on regions \( |v| > 1 \) and region \( |v| \leq 1 \), respectively.

First, we consider the part with \( |v| > 1 \). Using \( \mathcal{V}(x,v) \in L^2(\mathbb{R}_v) \) and the Young’s inequality, we have

\[
\|\Theta f(x,v)\|_{L^\infty} = \|\mathcal{V}(x,v) \ast f(x,v)\|_{L^\infty(\mathbb{R}_v)} \leq \|\mathcal{V}(x,\cdot)\|_{L^2(\mathbb{R}_v)}\|f(x,\cdot)\|_{L^2(\mathbb{R}_v)}.
\]

(3.16)
By the Cauchy-Schwartz inequality, we then have

$$\left| \int_{\mathbb{R}_v} \mathcal{V}(x, 0 - v') f(x, v') \, dv' \right| \leq \| \mathcal{V}(x, \cdot) \|_{L^2} \| f(x, \cdot) \|_{L^2(\mathbb{R}_v)}. \quad (3.17)$$

It is obtained directly from (3.16) and (3.17) that

$$\int_{|v| > 1} \| [A(x)f](v) \|^2 \, dv = 2 \int_{|v| > 1} \left| \frac{\Theta f(x, v)}{v} \right|^2 \, dv + 2 \int_{|v| > 1} \frac{\| \mathcal{V}(x, \cdot) \|_{L^2}^2 \| f(x, \cdot) \|_{L^2(\mathbb{R}_v)}^2}{v^2} \, dv \leq 8 \| \mathcal{V}(x, \cdot) \|_{L^2}^2 \| f(x, \cdot) \|_{L^2}^2. \quad (3.18)$$

Then, we consider the part with $|v| \leq 1$. According to the Cauchy-Schwartz inequality again, we have

$$\| [A(x)f](v) \| \leq \int_{\mathbb{R}} \left| \frac{\mathcal{V}(x, v - v') - \mathcal{V}(x, 0 - v')}{v} \right| \left| f(x, v') \right| \, dv' \leq \frac{\left\| \frac{\mathcal{V}(x, v - v') - \mathcal{V}(x, 0 - v')}{v} \right\|_{L^2(\mathbb{R}_v)}}{\| f(x, \cdot) \|_{L^2}}, \quad v \in [-1, 1]$$

By using Theorem 3 in Chapter 5 of [6], we have

$$\left\| \frac{\mathcal{V}(x, v - v') - \mathcal{V}(x, 0 - v')}{v} \right\|_{L^2(\mathbb{R}_v)} \leq \left\| \partial_v \mathcal{V}(x, v') \right\|_{L^2(\mathbb{R}_v)}. \quad (3.19)$$

This fact, together with the Cauchy-Schwartz inequality, gives us the following estimate on the velocity interval $[-1, 1]$ that

$$\int_{|v| \leq 1} \| [A(x)f](v) \|^2 \, dv \leq \| f(x, \cdot) \|^2_{L^2} \| \partial_v \mathcal{V}(x, v) \|^2_{L^2(\mathbb{R}_v)} \quad (3.19)$$

Collecting (3.18) and (3.19) together results in

$$\| [A(x)f](v) \|^2_2 \leq C \| f(x, \cdot) \|^2_{L^2}$$

where

$$C = 8 \| \mathcal{V}(x, \cdot) \|^2_{H^1}. \quad$$

We have proved that $A(x)$ is a bounded operator on $L^2(\mathbb{R}_v)$. When it is restricted on the subspace $L^2(\mathbb{R}_v)$, we have $A(x) = B(x)$. This completes the proof that $B(x)$ is a linear bounded operator on $L^2(\mathbb{R}_v)$.

By Lemma 1, we immediately have

**Theorem 1.** Let $\mathcal{L} \left( L^2(\mathbb{R}_v) \right)$ denote the space of bounded linear operators on $L^2(\mathbb{R}_v)$. If the assumptions for Lemma 7 hold, then one has that

(a) If $B(x) \in L^1((-l/2, l/2), \mathcal{L} \left( L^2(\mathbb{R}_v) \right))$, then the IVP (3.11)-(3.12) has a unique mild solution $f \in W^{1,1}((-l/2, l/2), L^2(\mathbb{R}_v))$.

(b) If $B(x)$ is strongly continuous in $x$ on $[-l/2, l/2]$ and uniformly bounded in the norm of $\mathcal{L} \left( L^2(\mathbb{R}_v) \right)$ on $[-l/2, l/2]$, then the solution $f$ is a classical solution, i.e., $f \in C^1([-l/2, l/2], L^2(\mathbb{R}_v))$. 


3.2 The odd part

We rewrite the odd part of the Wigner equation, i.e., the IVP \((3.7)+(3.10)\), into
\[
\frac{df(x)}{dx} - B(x)f(x) = 0,
\]
with the initial condition
\[
f(-l/2) = f_b \in L^2_o(\mathbb{R}_v).
\]

We instantly declare that the solution of the IVP \((3.20)-(3.21)\) has to be an odd function.

Lemma 2. If \(f_b(v) \in L^2_o(\mathbb{R}_v)\) and \(f(x) \in L^2(\mathbb{R}_v)\) is the solution of the IVP \((3.20)-(3.21)\), then \(f(x) \in L^2_o(\mathbb{R}_v)\).

Proof. Let
\[
g(x)(v) = \frac{[f(x)](v) + [f(x)](-v)}{2},
\]
where \(f(x) \in L^2(\mathbb{R}_v)\) is the solution of the IVP \((3.20)-(3.21)\). One may directly verify that \(g(x) \in L^2_o(\mathbb{R}_v)\) and \(g(x)\) is the solution of the IVP \((3.11)\) with zero initial value. By Theorem [ ] we conclude that \(g(x) = 0\), thus \(f(x) \in L^2_o(\mathbb{R}_v)\).

However, whether there exists a solution \(f(x) \in L^2_o(\mathbb{R}_v)\) for \((3.20)-(3.21)\) is difficult to discuss. A necessary condition for the existence is derived as follow. We rewrite the Wigner equation into the form
\[
\frac{df(x)}{dx} - A(x)f(x) = \frac{1}{v} \int_{\mathbb{R}_v} \mathcal{V}(x,v') [f(x)](v')dv'.
\]
where \(A(x)\) defined in \((3.15)\) has been proved to be a bounded linear operator on \(L^2(\mathbb{R}_v)\). For a function \(f(x) \in L^2_o(\mathbb{R}_v)\) with \(\frac{df(x)}{dx} \in L^2_o(\mathbb{R}_v)\), we know that the left hand side of \((3.22)\) is in \(L^2(\mathbb{R}_v)\) by using the boundedness of the operator \(A(x)\), but the right hand side of \((3.22)\) is not in \(L^2(\mathbb{R}_v)\) unless the solution \(f(x,v)\) satisfies
\[
\int_{\mathbb{R}_v} \mathcal{V}(x,v) [f(x)](v)dv = 0.
\]

However, it is difficult to give a condition for the initial value \(f_b(v) \in L^2_o(\mathbb{R}_v)\) to ensure that there exists a solution \(f(x) \in L^2_o(\mathbb{R}_v)\) which satisfies the condition \((3.23)\). So we will assume the existence, and discuss the uniqueness from the viewpoint of moments of the distribution function.

Let us rewrite the Wigner equation \((3.20)\) into
\[
v \frac{\partial f(x,v)}{\partial x} - \int \mathcal{V}(x,v-v')f(x,v')dv' = 0.
\]
For \(n \in \mathbb{N}^+ := \{0, 1, 2, \cdots \}\), we define
\[
J_n(x) = \int_{\mathbb{R}_v} v^n f(x,v) dv, \quad \mathcal{V}_n(x) = \int_{\mathbb{R}_v} v^n \mathcal{V}(x,v) dv.
\]
If the moment generating function of \( f(x,v) \)
\[
M_v[f](x,t) = \int_{-\infty}^{\infty} e^{vt} f(x,v) \, dv = \sum_{n=0}^{\infty} \frac{t^n}{n!} J_n(x)
\]
exists for an open interval containing \( t = 0 \), then \( f(x,v) \) can be represented into the bilateral Laplace transform of \( M_v[f] \), i.e.,
\[
f(x,v) = \int_{-\infty}^{\infty} e^{-vt} M_v[f](x,t) \, dt,
\]
which implies \( f(x,v) \) is completely determined by all its moments.

Recalling that \( f(x,v) \) is an odd function of \( v \) according to Lemma 2, we have that
\[
J_n(x) = 0, \quad n = 0, 2, 4, \ldots.
\]

Noticing that \( V(x,v) \) is an odd function of \( v \), we integrate (3.24) with respect to \( v \) and obtain
\[
\frac{dJ_1(x)}{dx} = 0.
\]
Multiplying \( v^2 \) on both sides of (3.24), a simple calculation yields
\[
\frac{dJ_3(x)}{dx} - 2J_1(x)V_1(x) = 0.
\]
Similarly we can obtain the differential equations for \( n = 5, 7, \ldots \). Generally, we can write out the differential equations for \( J_n(x) \),
\[
\frac{dJ_n}{dx} - \sum_{k=1,3,\ldots,n-2} \binom{n-1}{k} V_k(x) J_{n-k}(x) = 0, \quad n = 1, 3, 5, \ldots,
\]
where for \( m \in \mathbb{N}^+, n \in \mathbb{N}^+ \),
\[
\binom{m}{n} = \begin{cases} \frac{m!}{n!(m-n)!}, & m \geq n, \\ 0, & m < n. \end{cases}
\]

Using (3.29) and (3.27), we obtain that if the initial value \( f_b = 0 \), then
\[
J_n(x) = 0, \quad \forall x \in \mathbb{R}, \quad \forall n \in \mathbb{N}^+.
\]
If \( f_b = 0 \) and \( f(x,\cdot) \in L^2(\mathbb{R}_v) \), then \( f(x,v) = 0 \). Otherwise, there exists an \( x \in (-l/2,l/2) \) such that \( f(x,v) \neq 0 \), which implies
\[
\int_{\mathbb{R}_v} |f(x,v)|^2 \, dv \neq 0.
\]
From (3.30), we have \( J_n(x) = 0 \) for all \( n \in \mathbb{N}^+ \). Since \( f(x,\cdot) \in L^2(\mathbb{R}_v) \), \( f(x,v) \) can be approximated by polynomial sequence \( P_n(v) \) that \( \|f(x,\cdot) - P_n(\cdot)\|_{L^2(\mathbb{R}_v)} \to 0 \) as \( n \to \infty \), and
\[
\int P_n(v)f(x,v) \, dv = 0.
\]
Taking the limit as \( n \to \infty \), we have
\[
\int |f(x,v)|^2 \, dv = 0,
\]
which contradicts with (3.31). This gives \( f(x,v) = 0 \) for all \( x \in (-l/2,l/2) \), which gives us the uniqueness that
Theorem 2. If \( f_b \in L^2_0(\mathbb{R}_v) \), \( f_1(x) \) and \( f_2(x) \in L^2_0(\mathbb{R}_v) \) are two solutions of the IVP (3.20)-(3.21), then \( f_1(x,v) = f_2(x,v) \).

4 Discussion on stationary Inflow Boundary Value Problem

With the results on the initial value problems, we are ready to study the stationary Wigner equation with inflow boundary conditions, i.e.,

\[
\frac{d}{dx} f(x) + B(x)f(x) = 0, \quad x \in (-l/2, l/2),
\]

and

\[
P^+ f(-l/2) = f_L, \quad P^- f(l/2) = f_R,
\]

where \( f_L \in L^2(\mathbb{R}_v^+) \) and \( f_R \in L^2(\mathbb{R}_v^-) \). Here \( P^\pm : L^2(\mathbb{R}_v) \to L^2(\mathbb{R}_v^\pm) \) are defined by

\[
[P^+ u](v) = u(v), \text{ if } v \in \mathbb{R}_v^+, \quad [P^- u](v) = u(v), \text{ if } v \in \mathbb{R}_v^-.
\]

where \( \mathbb{R}_v^+ = \{ v > 0 \} \) and \( \mathbb{R}_v^- = \{ v < 0 \} \).

Let us assume that there is a solution in \( L^2(\mathbb{R}_v) \) for the BVP (4.1)-(4.2). Due to the parity decomposition of the solution, the odd part of the solution has to satisfy the equations (3.29). The equations (3.29) actually give a one-to-one linear mapping between the odd part of the solution at the boundaries, which is denoted as

\[
[P_o f(l/2)](v) = Q_{l\to r}[P_o f(-l/2)](v), \quad [P_o f(-l/2)](v) = Q_{r\to l}[P_o f(l/2)](v).
\]

Here \( Q_{l\to r} \) is the map of the odd part of the solution from the left end to the right end, and \( Q_{r\to l} = Q_{l\to r}^{-1} \) is the inverse mapping of \( Q_{l\to r} \). Here we point out that actually \( Q_{r\to l} \) is given by the solution of system

\[
\frac{dJ_n}{dx} + \sum_{k=1,3,5,\cdots,n-2} \left( \frac{n-1}{k} \right) V_k(x) J_{n-k}(x) = 0, \quad n = 1, 3, 5, \cdots
\]

Meanwhile, by theorem [1] there is a one-to-one linear mapping between the even part of the solution at the boundaries, too. We denote this map as

\[
[P_e f(l/2)](v) = R_{l\to r}[P_e f(-l/2)](v), \quad [P_e f(-l/2)](v) = R_{r\to l}[P_e f(l/2)](v).
\]

Here \( R_{l\to r} \) is the map of the even part of the solution from the left end to the right end, and \( R_{r\to l} = R_{l\to r}^{-1} \) is the inverse mapping of \( R_{l\to r} \).

Then we have the relations that for \( v < 0 \),

\[
f_R(v) = [P_o f(l/2)](v) + [P_e f(l/2)](v)
\]

\[
= Q_{l\to r}[P_o f(-l/2)](v) + R_{l\to r}[P_e f(-l/2)](v)
\]

\[
= Q_{l\to r}[-P_o f(-l/2)](-v) + R_{l\to r}[P_e f(-l/2)](-v)
\]

\[
= -Q_{l\to r}[P_o f(-l/2)](-v) + R_{l\to r}[P_e f(-l/2)](-v),
\]

\[
f_L(-v) = [P_o f(-l/2)](-v) + [P_e f(-l/2)](-v).
\]

We can solve \([P_o f(-l/2)](-v),[P_e f(-l/2)](-v)\) from the equation:

\[
[P_e f(-l/2)](v) = \begin{cases} (Q_{r\to l}R_{l\to r} + I)^{-1}(Q_{r\to l}f_R(-v) + f_L(v)), & v > 0 \\ [P_e f(-l/2)](-v), & v < 0 \end{cases}
\]

(4.3)
and

$$[P_o f(-l/2)](v) = \begin{cases} f_L(v) - [P_e f(-l/2)](v), & v > 0 \\ -[P_o f(-l/2)](-v), & v < 0 \end{cases} \tag{4.4}$$

Thus the solution $[f(x)](v)$ of the BVP (4.1)-(4.2) can be solved, and it can be decomposed into the sum of $f_o(x) \in L^2_0(\mathbb{R}_v)$ and $f_e(x) \in L^2(\mathbb{R}_v)$,

$$f(x) = f_o(x) + f_e(x) \tag{4.5}$$

where $f_o(x)$ is obtained in the sense that all its moments can be obtained by solving the ODEs (3.29) with the initial value obtained through (4.4), and $f_e(x)$ can be obtained by solving (3.11) with the initial value given by (4.3).

Particularly, for a simple case that $V(x)$ is an even function, i.e., $V(-x) = V(x)$ (for example, $V(x) = \exp(-x^2/a)$ where $a > 0$ is a constant). In this case, we have that $V_n(x)$ is odd,

$$V_n(-x) = -V_n(x) \tag{4.6}$$

which can be verified by using (3.25) and (3.13).

Observing (3.29) and using (4.6), we can derive that $J_n(x)$ is even, i.e.,

$$J_n(-x) = J(x). \tag{4.7}$$

Especially,

$$J_n(-l/2) = J_n(l/2) \tag{4.8}$$

which means

$$f_o(-l/2) = f_o(l/2). \tag{4.9}$$

That is to say $Q_{l\rightarrow r} = Q_{r\rightarrow l} = I$. Using the symmetry analysis in [15], we can show that $R_{l\rightarrow r} = R_{r\rightarrow l} = I$. Then using (4.3) and (4.4), we obtain the initial values for the even part and the odd part of the Wigner equation. Finally, the solution of BVP (4.1)-(4.2) is constructed by the solutions of the two IVPs.

5 Conclusion

We studied the Wigner equation with inflow boundary conditions by parity decomposition. The pseudo-operation $\Theta[V]$ is proved to be bounded for the even $L^2$-space, so the propagator for the even Wigner IVP is invertible. For the odd part of the Wigner function whose moment generating function exists, we can calculate the Wigner function through calculating its moments. With the help of analysis in parity decomposition, we plan to design an implementable moment method for the Wigner equation.

Acknowledgements

This research was supported in part by NSFC (91230107, 11325102, 91434201).
References

[1] A. Arnold, H. Lange, and P.F. Zweifel. A discrete-velocity, stationary Wigner equation. *J. Math. Phys.*, 41(11):7167–7180, 2000.

[2] L. Barletti. A mathematical introduction to the Wigner formulation of quantum mechanics. *Bollettino dell’Unione Matematica Italiana*, 6-B(3):693–716, 10 2003.

[3] L. Barletti and P. F. Zweifel. Parity-decomposition method for the stationary Wigner equation with inflow boundary conditions. *Transport Theory and Statistical Physics*, 30(4-6):507–520, 2001.

[4] Z. Cai, Y. Fan, R. Li, T. Lu, and Y. Wang. Quantum hydrodynamics models by moment closure of Wigner equation. *J. Math. Phys.*, 53:103503, 2012.

[5] A.S. Costolanski and C.T. Kelley. Efficient solution of the Wigner-Poisson equations for modeling resonant tunneling diodes. *IEEE Trans. Nanotechnology*, 9(6):708 – 715, Nov. 2010.

[6] L.C. Evans. *Partial Differential Equations*. American Mathematical Society, Providence RI, 2nd edition, 2010.

[7] D.K. Ferry and S.M. Goodnick. *Transport in Nanostructures*. Cambridge Univ. Press, Cambridge, U.K, 1997.

[8] W.R. Frensley. Wigner function model of a resonant-tunneling semiconductor device. *Phys. Rev. B*, 36:1570–1580, 1987.

[9] A. Gehring and H. Kosina. Wigner function-based simulation of quantum transport in scaled DG-MOSFETs using a Monte Carlo method. *J. Comput. Electr.*, 4:67–70, 2005.

[10] M. Hillery, R.F. ÓConnell, M.O. Scully, and E.P. Wigner. Distribution functions in physics: Fundamentals. *Physics Reports*, 106(3):121–167, 1984.

[11] K.L. Jensen and F.A. Buot. Numerical aspects on the simulation of IV characteristics and switching times of resonant tunneling diodes. *J. Appl. Phys.*, 67:2153–2155, 1990.

[12] H. Jiang, W. Cai, and R. Tsu. Accuracy of the frensley inflow boundary condition for Wigner equations in simulating resonant tunneling diodes. *J. Comput. Phys.*, 230:2031–2044, 2011.

[13] H. Jiang, T. Lu, and W. Cai. A device adaptive inflow boundary condition for Wigner equations of quantum transport. *J. Comput. Phys.*, 248:773–786, 2014.

[14] R. Li, T. Lu, and Z.-P. Sun. Convergence of semi-discrete stationary Wigner equation with inflow boundary conditions. *Submitted to Communications in Mathematical Sciences*, 2014.

[15] R. Li, T. Lu, and Z.-P. Sun. Stationary wigner equation with inflow boundary conditions: Will a symmetric potential yield a symmetric solution? *SIAM J. Appl. Math.*, 70(3):885–897, 2014.
[16] D. Querlioz, J. Saint-Martin, V.-N. Do, A. Bournel, and P. Dollfus. A study of quantum transport in end-of-roadmap DG-MOSFETs using a fully self-consistent Wigner Monte Carlo approach. *Nanotechnology, IEEE Transactions on, 5*(6):737–744, Nov. 2006.

[17] S. Shao, T. Lu, and W. Cai. Adaptive conservative cell average spectral element methods for transient Wigner equation in quantum transport. *Commun. Comput. Phys.*, 9:711–739, 2011.

[18] J.J. Shih, H.C. Huang, and G.Y. Wu. Effect of mass discontinuity in the Wigner theory of resonant-tunneling diodes. *Phys. Rev. B*, 50(4):2399–2405, 1994.

[19] H. Tsuchiya and M. Ogawa. Simulation of quantum transport in quantum device with spatially varying effective mass. *IEEE Trans. Electron Devices*, 38(6):1246–1252, 1991.

[20] E. Wigner. On the quantum correction for thermodynamic equilibrium. *Phys. Rev.*, 40(5):749–759, Jun 1932.