Journal of Computational Mathematics
Vol.37, No.2, 2019, 170–183.

http://www.global-sci.org/jcm
doi:10.4208/jcm.1711-m2017-0097

SINGULARITY-FREE NUMERICAL SCHEME FOR THE STATIONARY WIGNER EQUATION*

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Abstract

For the stationary Wigner equation with inflow boundary conditions, the numerical convergence with respect to the velocity mesh size are deteriorated due to the singularity at velocity zero. In this paper, using the fact that the solution of the stationary Wigner equation is subject to an integral constraint, we prove that the Wigner equation can be written into a form with a bounded operator $\mathcal{B}[V]$, which is equivalent to the operator $\mathcal{A}[V]=\Theta[V]/v$ in the original Wigner equation under some conditions. Then the discrete operators discretizing $\mathcal{B}[V]$ are proved to be uniformly bounded with respect to the mesh size. Based on the theoretical findings, a singularity-free numerical method is proposed. Numerical results are provided to show our improved numerical scheme performs much better in numerical convergence than the original scheme based on discretizing $\mathcal{A}[V]$.

Mathematics subject classification: 65M06, 58J40, 81S30
Key words: Stationary Wigner equation, Singularity-free, Numerical convergence.

1. Introduction

The Wigner transport equation is one of the equivalent formulations of quantum mechanics. It is proposed by E. Wigner in 1932 as a quantum correction to the classical statistical mechanics [26]. Though the Wigner function may take negative values, it has a non-negative marginal distribution and can express system observables in the same way as the Boltzmann probability density function, thus it is called a quasi-probability density function. The strong similarity between the Wigner equation and the Boltzmann equation makes it convenient to borrow some describing tools of the latter, e.g., the boundary conditions and the scattering terms [7].

The Wigner equation has been used in many fields. For example, Frensley successfully reproduced the negative differential resistance phenomena of resonant tunneling devices by numerically solving the following one-dimensional Wigner equation

$$\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}-\Theta[V]f=0, \quad x\in(-l/2,l/2), \ \ v\in\mathbb{R}, \tag{1.1}$$

with inflow boundary conditions

$$f(-l/2,v)=f_L(v), \text{ if } v>0; \quad f(l/2,v)=f_R(v), \text{ if } v<0. \tag{1.2}$$

* Received April 14, 2017 / Revised version received September 7, 2017 / Accepted November 13, 2017 / Published online August 30, 2018 /

$\Theta[V]$ is a pseudo-differential operator that will be explained later. Since then, the Wigner equation has attracted many researchers in numerical simulation (e.g., [14] and references therein), and various numerical methods for the Wigner equation have been proposed, such as finite difference methods [4, 8, 12, 13], spectral methods [4, 22, 25], spectral element method [25], and Monte Carlo methods [20, 24]. When the Hartree potential is included, the Wigner-Poisson system can be solved self-consistently [2, 5, 11, 17, 28]. The nonlinear iteration for the coupled Wigner-Poisson system deserves a serious study and in [4] the Gummel method and the Newton method were compared for the RTD simulation in terms of efficiency, accuracy and robustness. As for the linear stationary Wigner equation with inflow boundary boundary conditions, there are still a lot of open problems, for example, the well-posedness, the numerical convergence, etc. In this paper, we focus on the linear problem.

Many mathematicians have been drawn to study the Wigner equation, e.g., [9, 10, 18, 19, 21]. The Wigner boundary value problem (the stationary Wigner equation with inflow boundary conditions) is a popular model in numerical simulation of the nano semiconductor devices. We note that some researchers have proved the well-posedness of the Wigner boundary value problem in some special cases, for example, [1] for a velocity semi-discretization version, [3] for an approximate problem by removing a small interval centered at velocity zero, and [15] for a periodical potential. However, it is reported that the Wigner boundary value problem may have more than one solution [23], though the authors have not given an exact definition of the solution by specifying a solution space.

Before the well-posedness issue of some problem is solved, one has to assume that there exists a unique smooth solution when designing some high-order numerical methods, for example, second-order upwind scheme [11, 12]. In this paper, we focus on designing a numerical scheme, thus we assume that the Wigner boundary value problem has a unique solution in $C_{Lip}(-l/2, l/2; L^2(\mathbb{R}_v))$ of all functions which are Lipschitz continuous with the position variable x and belong to $L^2(\mathbb{R}_v)$ at any fixed x. It seems not to be a very strong constraint in the quantum transportation, especially when the potential function $V(x)$ is a smooth function. When one discretizes the Wigner boundary value problem as Frensley did in [8], it is found that the numerical solution does not converge as the velocity mesh size goes to zero. The reason that one fails in obtaining a numerical convergence can be partially explained from the fact that the norm of the discretization operator $\mathcal{A}[V] = \frac{1}{v}\Theta[V]$ as a linear operator on $L^2(\mathbb{R}_v)$ increases to infinite as the velocity mesh size goes to zero. We are trying to solve this issue.

By observing the stationary Wigner equation (1.1) and taking the limit as v goes to 0, we find that the solution in $C_{Lip}(-l/2, l/2; L^2(\mathbb{R}_v))$ has a property that it is in a subspace $\mathcal{S}(x) \subset L^2(\mathbb{R}_v)$ where

$$\mathcal{S}(x) = \Big\{\phi \in L^2(\mathbb{R}_v)) : (\phi, V_w(x, \cdot)) = 0\Big\}, \quad \forall x \in (-l/2, l/2).$$

Restricting our problem in $C_{Lip}(-l/2, l/2; \mathcal{S}(x))$ is a natural idea to solve the problem, but it is hard technically to keep the numerical solutions in the subspace $\mathcal{S}(x)$ for all $x \in (-l/2, l/2)$ since the subspace changes with the position variable x. So we extend the $\mathcal{A}[V]$ to $L^2(\mathbb{R}_v)$, which does not change with the position variable. However, a natural and simple extension results in an unbounded operator $\mathcal{A}[V]$ on $L^2(\mathbb{R}_v)$. In this paper, we give another extension by defining a new operator $\mathcal{B}[V]f(x, v) = \frac{1}{v}\left(\Theta[V]f(x, v) - \Theta[V]f(x, 0)\right)$. We will prove that $\mathcal{B}[V] = \mathcal{A}[V]$ on the subspace $\mathcal{S}$, but is bounded on $L^2(\mathbb{R}_v)$. We obtain our new numerical method by discretizing $\mathcal{B}[V]$ (bounded on $L^2(\mathbb{R}_v)$) instead of $\mathcal{A}[V]$ (unbounded on $L^2(\mathbb{R}_v)$), and numerical convergence of our new method is validated by a numerical example.