Commun. Comput. Phys.
doi: 10.4208/cicp.080509.310310s

Vol. **9**, No. 3, pp. 711-739
March 2011

Adaptive Conservative Cell Average Spectral Element Methods for Transient Wigner Equation in Quantum Transport

Sihong Shao[1], Tiao Lu[1] and Wei Cai[2,*]

[1] *LMAM and School of Mathematical Sciences, Peking University, Beijing 100871, China.*
[2] *Department of Mathematics and Statistics, University of North Carolina at Charlotte, Charlotte, NC 28223, USA.*

Received 8 May 2009; Accepted (in revised version) 31 March 2010

Available online 17 September 2010

To the memory of David Gottlieb

Abstract. A new adaptive cell average spectral element method (SEM) is proposed to solve the time-dependent Wigner equation for transport in quantum devices. The proposed cell average SEM allows adaptive non-uniform meshes in phase spaces to reduce the high-dimensional computational cost of Wigner functions while preserving exactly the mass conservation for the numerical solutions. The key feature of the proposed method is an analytical relation between the cell averages of the Wigner function in the k-space (local electron density for finite range velocity) and the point values of the distribution, resulting in fast transforms between the local electron density and local fluxes of the discretized Wigner equation via the fast sine and cosine transforms. Numerical results with the proposed method are provided to demonstrate its high accuracy, conservation, convergence and a reduction of the cost using adaptive meshes.

AMS subject classifications: 65M70, 65M50, 42B20, 45K05, 81Q05

Key words: Wigner equation, quantum transport, spectral element methods, adaptive mesh.

1 Introduction

Ever since its invention in 1932 by Wigner in [1], the Wigner equation has found applications in many physical fields, such as optics, information theory and statistical physics and has constituted a new formulation of quantum mechanics [2,3]. The most appealing characteristic of the Wigner equation is that it describes the evolution of quantum states

*Corresponding author. *Email addresses:* `shaosihong@gmail.com` (S. Shao), `tlu@math.pku.edu.cn` (T. Lu), `wcai@uncc.edu` (W. Cai)

in the same way as the Boltzmann equation does for classical systems. Both of them are defined in a phase space and a physical interpretation can be given to terms appearing in their dynamical equations. Although it is not a real probability distribution function due to possible negative values as a result of the Heisenberg uncertainty principle, the Wigner function serves the role of a distribution [4,5], for example, in calculating number densities, current densities and etc. Using the Wigner equation to investigate quantum transport has become more popular [6,7] when the quantum behavior of semiconductor devices can not be neglected as their size is down to nano-scales.

Frensley succeeded in simulating the quantum transport in a resonant tunneling diode (RTD) by solving the Wigner equation with a first-order upwind scheme finite difference method (FDM) [8,9]. Since then, several second-order FDMs have been used [10] (for a detailed summary about FDMs for the Wigner equation, please refer to [11,12]). It has been shown that general FDMs are not very accurate for transient Wigner simulations and questions have been raised about the effect of the finite difference discretization of inflow/outflow boundary conditions proposed by Frensley in [9]. Moreover, in order to include the space charge effect, the Wigner equation should be coupled with a Poisson equation [13,14] and a self-consistent iteration is needed to solve the coupled system. Application of such models with FDM solvers can be found in [15–17] where the time-independent Wigner-Poisson system is considered. Recently, the Wigner function is extended to particle modeling accounting for various kinds of scatterings [18], where the Boltzmann equation and the Wigner equation are coupled in a unified framework so that simulation of actual quantum transport can be achieved by Monte Carlo methods [19,20].

In [21,22] a spectral method based on plane waves is used to discretize the transient Wigner equation in the k-space while FDMs are used in the x-space. In [23,24] an operator splitting method is used to calculate the coupled Wigner-Poisson system. The reason for using plane wave spectral methods is that the plane waves are the eigenfunctions of the pseudo-differential operator associated with the Wigner potentials. However, there are several issues in approximating the Wigner distributions in the k-space with periodic plane waves. The periodization in the k-space produces a numerical solution which resides in a different function space (periodic function) other than the original Wigner function space $L^2(-\infty,\infty)$ and more importantly, creates an unphysical interaction of the Wigner distribution with its periodic image frequencies in the k-space. Mathematically speaking, we need to handle carefully the infinite integral with respect to the dual variable y appearing in the pseudo-differential operator $\Theta_V[f]$ of (2.4). In [25,26], after assuming that $\widehat{f}(x,y,t)$ defined in (2.5) has a compact support in the y-space with a truncated domain in the y-space as $[-1/(2\Delta k),1/(2\Delta k)]$, the authors showed that the semi-discretized Wigner equation–finite difference discretization in the k-space in a uniform mesh–is well-posed and approaches the continuous problem when the mesh size Δk goes to zero.

Our main objective in this paper is to reduce the cost of computing the Wigner distribution in high-dimensional phase spaces. For this purpose, adaptive meshes will be our approach which concentrates the computational resources in regions of localized electron