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A Highly Efficient USOR-Like Iterative Method for the Stationary Wigner Equation with Scattering

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Abstract. The stationary Wigner equation (SWE) is often used to model the quantum transport in semiconductor devices. The discrete stationary Wigner equation is derived using the first-order upwind scheme and the sinc-Galerkin method [H. Jiang, T. Lu, and W. Zhang, J. Comput. Appl. Math. 409 (2022), 114152]. Based on the successive over relaxation (SOR) iterative method, we develop the basic SOR-like (BSOR-like) and updated SOR-like (USOR-like) iterative methods for solving the discrete stationary Wigner equation efficiently. The main difference between these two iterative methods is that the USOR-like iterative method aims to make more use of the updated components of the Wigner function by splitting the pseudo-differential term. The convergence range of the relaxation parameter in the USOR-like iterative method is numerically investigated. Compared with that of the BSOR-like iterative method, this interval is significantly enlarged. Numerical results have also shown that the USOR-like iterative method is more computationally efficient than the BSOR-like iterative method. As an application, the resonant tunneling effect and the effects of scattering are investigated by simulating a resonant tunneling diode (RTD) using the USOR-like iterative method.

AMS subject classifications: 65F10, 81S30

Key words: Stationary Wigner equation, iterative method, resonant tunneling diode, SOR method, convergence condition.

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1. Introduction

The Wigner equation was derived by Wigner [29] as a quantum correction of classical statistical mechanics for low temperatures. Given its similarity to the Boltzmann transport equation [13, 17], the Wigner equation can deal with the inflow boundary conditions [8] and the scattering mechanism well. The Wigner equation has been applied in many fields, such as quantum optics [11] and semiconductor devices [8]. In the steady-state simulation of a given quantum system, one needs to design schemes with good stability and high precision when utilizing the transient Wigner equation. By means of the stationary Wigner equation, one no longer pays attention to the transient state. Solving the SWE numerically is equivalent to solving a large system of equations. The computational complexity of direct solvers, such as the Gaussian elimination, could be significantly larger than that of excellent iterative methods. Therefore, constructing an efficient iterative method is crucial for numerically solving the SWE.

Numerical methods for solving the stationary Wigner inflow boundary value problem have been widely and deeply explored for decades. The finite difference methods [8, 13] and a weighted essentially non-oscillatory (WENO)-solver [7] are proposed for the discretization of the advection term in the Wigner equation. Many methods with high accuracy, e.g., the spectral collocation method [24], the spectral element method [25], and the sinc-Galerkin method [15], are adopted to discretize the Wigner equation in k-space. By employing the Fourier pseudo-spectral method, the authors derive the stationary discrete velocity Wigner equation and prove its well-posedness in [1]. The parity decomposition is adopted in [2, 19] to reduce the SWE with the inflow boundary conditions to an initial problem, and the partial problem is proved to be well-posed. In [20], the moment system for the Wigner equation derived in [4] is numerically solved using the NRxx method and the finite volume method. Considering the singularity at zero velocity, a singularity-free numerical scheme based on an equivalent form of the SWE is proposed, and the numerical convergence with respect to the velocity mesh size is obtained [21]. The SWE can be solved together with a Poisson equation. Convergence may be achieved via the decoupled Gummel method [3, 10] or the fully coupled Newton iterative method [3, 14]. Because of the similarity to the Boltzmann equation, the Wigner equation can be solved with the Monte Carlo (MC) method [18,22,27]. In [26], the authors model the stationary Wigner inflow boundary value problem as an optimization problem, which is solved with the shooting algorithm. The imaginary time propagation method combined the finite element method is used to solve an eigenvalue problem for the stationary Wigner function [31].

Analogous to solving a system of linear equations using an iterative method, constructing an iterative method for solving the discrete SWE is an alternative way. For some problems, the successive over relaxation iterative method, which immediately replaces the old component with the newly calculated one, could converge with a few iterations. The choice of the relaxation parameter ω has a significant influence on the convergence of the SOR iterative method. For solving a system of non-smooth equations, the SOR-Newton method is proposed and the choice of the relaxation parameter