A Highly Efficient CN-Like Scheme for the Transient Wigner Equation

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Abstract. The transient Wigner equation (TWE) plays an important role in modeling quantum effects of nano-scale semiconductor devices. The pseudo-differential term contained within the TWE provides quantum descriptions for the model, however, it is costly in numerical simulations. We develop a CN-like scheme for time integration of the TWE, based on the two-step method. Additionally, the spatial discretization is the hybrid finite-difference/sinc-Galerkin scheme [H. Jiang, T. Lu, W. Yao and W. Zhang, SIAM J. Sci. Comput. 45 (2023)]. Rigorous proofs are provided to show that the CN-like scheme is unconditionally L^2-stable and has second-order accuracy in time. More importantly, the computational efficiency of the new CN-like scheme could be considered to be higher than that of any explicit multi-stage one-step time integration scheme. Numerical experiments are also carried out to verify the accuracy, stability and efficiency of the new CN-like scheme. In addition to the verification experiments, resonant tunneling diodes (RTDs) with various sets of parameters are simulated. I-V characteristics and associated curves are obtained to demonstrate the resonant tunneling effect and the variations in I-V characteristic curves in relation to changes in structure parameters.

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1   Introduction

In 1932, E. Wigner [25] derived the Wigner equation by introducing quantum mechanical correction in the semi-classical Vlasov equation. Due to its similarity to the transport equation, the Wigner equation has natural advantages in dealing with the boundary conditions and scattering mechanism. It is widely used in fields such as quantum optics, chemistry [10], and nano-scale semiconductor devices [8], etc. The Wigner equation has always been a powerful tool to simulate quantum devices, including the resonant tunneling diode (RTD) [8], which is one of the most important quantum devices in semiconductor industry.

Numerical methods for the advection discretization of the Wigner equation are highly concerned. For the discretization of the advective term, many kinds of numerical methods could be considered. The first- and second-order upwind schemes [2,8,12,14] are usually considered, due to their simplicity in usage. Beyond the upwind schemes, the Lax-Wendroff scheme is adopted in [16], where the first-order upwind scheme is used when dealing with spatial discretizations near boundaries. For the case of strong quantum effects, it has been proven in [6] that the weighted essentially non-oscillatory (WENO) scheme, combined with adaptive momentum discretization, is able to capture the complex features of the device. Furthermore, a spectral element method by using the Gauss-Lobatto collocation points in the x-space is presented [21]. By employing the operator splitting approach, the Wigner equation can be divided into several sub-equations, where the sub-equation that represents the advective phenomenon can be readily solved using the characteristic line method, as discussed in [3]. In this paper, we follow [14] and use the finite-difference method to discretize the Wigner equation in the x-space.

Besides the advective term, the nonlocal pseudo-differential term makes it difficult and costly to solve the Wigner equation numerically. The pseudo-differential term is the key to the Wigner equation's ability to capture quantum effects [25]. In [5], a hyperbolic closed moment model of arbitrary order for the transient Wigner equation (TWE) is derived, and a numerical validation is provided in [17]. A Gaussian beam method is used to solve the Wigner equation with discontinuous potentials [27]. Spectral methods with high accuracy, e.g., the spectral collocation method [13,19,20], the Chebyshev spectral element method based on the cell averages [21,26], and the sinc-Galerkin method [14,15], have been proposed to discretize the Wigner equation in velocity space. In a recent work [23], the authors proved that the sinc-Galerkin discretization is equivalent to that using the Fourier pseudo-spectral method, which provides opportunities to further reduce the computational cost by leveraging the fast Fourier transform (FFT). In this paper, we follow [14,15] and use the sinc-Galerkin method to discretize the Wigner equation in k-space for two main reasons. First, the sinc basis is orthogonal in L^2-space and decays to zero as the velocity approaches infinity, which makes it suitable as a basis for expressing the Wigner function in the same L^2-space and has compact support. Furthermore, the sinc basis has interpolation properties that could be utilized by using the Whittaker-Shannon interpolation formula [22]. Second, and most importantly, [15] proved that the