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A HYBRID EXPLICIT-IMPLICIT SCHEME FOR THE TIME-DEPENDENT WIGNER EQUATION*

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Abstract

This paper designs a hybrid scheme based on finite difference methods and a spectral method for the time-dependent Wigner equation, and gives the error analysis for the full discretization of its initial value problem. An explicit-implicit time-splitting scheme is used for time integration and the second-order upwind finite difference scheme is used to discretize the advection term. The consistence error and the stability of the full discretization are analyzed. A Fourier spectral method is used to approximate the pseudo-differential operator term and the corresponding error is studied in detail. The final convergence result shows clearly how the regularity of the solution affects the convergence order of the proposed scheme. Numerical results are presented for confirming the sharpness of the analysis. The scattering effects of a Gaussian wave packet tunneling through a Gaussian potential barrier are investigated. The evolution of the density function shows that a larger portion of the wave is reflected when the height and the width of the barrier increase.

Mathematics subject classification: 65M06, 65M70.
Key words: Finite difference method, Spectral method, Hybrid scheme, Error analysis, Wigner equation.

1. Introduction

With the development of micro-manufacturing engineering and technology, the quantum effects (such as the tunnelling effects in Resonant Tunnelling Diodes) play an important role in transport property and can not be neglected. In order to clearly understand the quantum effects, quantum transport models have to be considered. One of such models is the Wigner equation, which was proposed by Wigner in 1932 as a quantum correction of the classical statistical mechanics in the phase space [1]. As its classical counterparts, the Boltzmann equation and the Vlasov equation are popular models in simulating of carrier transport in classical mechanics for clear description of scattering effects and boundary conditions. Thus, the Wigner equation has advantages over other quantum frameworks in handling scattering mechanisms and boundary

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conditions [2]. The Wigner equation is also suitable for describing time dependent dynamics and connecting quantum and semi-classical regimes [3], and it has been found many applications in different fields, e.g., quantum optics [4], nano-scale semiconductor devices [5].

The Wigner equation and its numerical solution have attracted more and more attention since Frensley successfully reproduced the negative differential resistance phenomenon of resonant tunnelling diodes (RTDs) in [5], where the first-order upwind finite difference method was used. Then the second-order upwind finite difference method was proposed and used to study the tunneling characteristics of double-barrier semiconductor structures [6, 7]. Many more numerical methods have developed for the Wigner equation, e.g., a WENO solver [8], a spectral method [9], a spectral collocation method [10], high-order upwind finite-difference methods [11], a Gaussian beam method [12], moment methods [13, 14] and a cell average spectral element method [15]. Many mathematicians also devoted to analyze the Wigner equation. Markowich proved the existence and uniqueness of the solution to the initial-value problem of the time-dependent Wigner equation by studying the equivalence between the quantum Liouville equation and the Schrödinger equation [16]. Jiang et al. studied the effect of the inflow boundary conditions of the stationary Wigner equation in [17, 18], and proposed a device adaptive inflow boundary condition in [19]. Readers interested in the research on the well-posedness of related problems can refer to, e.g., [16, 20–23].

There are also many works on the Wigner equation that focus on the numerical simulation and investigate the parallel computing, where the nonlinear iteration technique is used when the self-consistent potential is included. However, works on a detailed numerical analysis of the consistency, convergence and stability of numerical methods for the Wigner equation is still inadequate. In this paper, we propose a hybrid explicit-implicit scheme of finite difference methods and a Fourier spectral method for the time-dependent Wigner equation. We adopt the second-order upwind finite difference method for the discretization of the advection term as did in [6], which has gained its popularity comparing with the first-order upwind finite difference method used in [5]. The pseudo-differential term of the Wigner equation, which corresponds to the force field, is approximated by the Fourier spectral method. Because of the non-locality of the pseudo-differential operator of the Wigner equation, the semi-discretization in the phase space results a matrix with much more nonzero elements than that of the Vlasov equation. Thus the forward Euler method used in [5] is popular since a linear system (whose matrix is not very sparse) need not to be solved at every time step. However, the time step in the forward Euler method is restricted due to the CFL condition restraint. An implicit scheme can be used to alleviate the CFL restraint. For example, a backward Euler method is used in [9]. In order to take advantage of the computational efficiency of the explicit method and the big time step of the implicit method, we apply the implicit method for the advection term (which actually can be solved very efficiently) and the explicit method for the pseudo-differential operator term. A prediction-correction technique is implemented to achieve a second-order accuracy in time integration. For the discretization with respect to velocity, many methods have proposed, such as the collocation spectral method [9], the adaptive cell-average spectral element method [15], the moment method [13, 14]. In this paper, we adopt the collocation spectral method to approximate the pseudo-differential operator term as used in [9], which guarantees the conservative conditions automatically. The high-order truncation error of the proposed full discretization scheme is proved, and the stability is analyzed by using the von Neumann method. Finally, we give a proof of the convergence of the full discretization scheme.

This paper is arranged as following: Firstly, we introduce an initial boundary value prob-