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Numerical Validation for High Order Hyperbolic Moment System of Wigner Equation

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Abstract. A globally hyperbolic moment system upto arbitrary order for the Wigner equation was derived in [6]. For numerically solving the high order hyperbolic moment system therein, we in this paper develop a preliminary numerical method for this system following the NRxx method recently proposed in [8], to validate the moment system of the Wigner equation. The method developed can keep both mass and momentum conserved, and the variation of the total energy under control though it is not strictly conservative. We systematically study the numerical convergence of the solution to the moment system both in the size of spatial mesh and in the order of the moment expansion, and the convergence of the numerical solution of the moment system to the numerical solution of the Wigner equation using the discrete velocity method. The numerical results indicate that the high order moment system in [6] is a valid model for the Wigner equation, and the proposed numerical method for the moment system is quite promising to carry out the simulation of the Wigner equation.

AMS subject classifications: 82C10, 81-08, 47A57

Key words: Wigner equation, NRxx method, moment method.

1 Introduction

The Wigner equation was proposed by Wigner in 1932 to study the quantum corrections of the quantum statistical mechanics [41]. For its strong similarity with the classical counterpart of the Boltzmann equation, the Wigner equation has advantages in simulating the

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carrier transport in semiconductor devices [14]. Its applications are also found in quantum chemistry and quantum optics. So there has been an increasing interest in the Wigner equation.

The numerical methods for the Wigner equation have attracted many researchers from different fields. In [15], Frensley applied the upwind finite difference method to the Wigner equation, and successfully showed the negative differential resistance of the resonant tunneling diodes (RTD). Further, the finite difference methods for the Wigner equation have been used to investigate the Wigner-Poisson equations [23, 42]. Readers may refer [24, 28] for the comparison study of different finite difference methods for the Wigner equation. Besides the popular finite difference methods for the Wigner equation, many other numerical methods have been proposed. For example, [35] has given a new adaptive cell average spectral element method for the time-dependent Wigner equation. An operator splitting [1], a Fourier spectral method [34], and a Monte Carlo method [32] have also been put forward. Analysis and numerical solution for the discrete version of the transient Wigner equation have been given in [17, 18].

Though the Wigner functions have been successfully used in simulating one-dimensional devices, but are not expected to be directly used for the multi-dimensional devices simulation using deterministic numerical methods due to its formidable expense in memory storage and computation time. One practical approach to investigate higher dimensional devices where the quantum effects are relevant is to use the quantum hydrodynamics models which are moment systems derived from the Wigner equation. Because the close connection between the Wigner equation and the Boltzmann equation, many moment methods devised for the Boltzmann equation have been extended to the Wigner equation [13, 16]. The equations derived from the Wigner equation are called quantum drift-diffusion equations, quantum Euler equations and quantum hydrodynamics equations. Moreover, the numerical simulations based on such moment equations are extensively studied [12, 22, 26, 27, 43].

The moment method of the Boltzmann equation can be dated back to Grad [19] in 1940s. However, this 13-moment model proposed therein was soon found to be problematic [20]. Its major deficiencies include the appearance of subshocks in the structure of a strong shock wave and the loss of global hyperbolicity. A number of regularizations were raised to solve or alleviate these problems [25, 29, 37–39]. However, due to the complexity of the explicit expressions, systems with large number of moments are not investigated until recently (see, for examples, [2, 40]). In [4, 5], a new regularized model with global hyperbolicity is proposed by the correction of the characteristic speed and numerical methods solving large moment systems were proposed in [7, 8, 10].

Recently, we have extended the method of the hyperbolic regularization in [4, 5] to the Wigner equation, and obtained a new set of generalized quantum hydrodynamic models [6]. In this paper, we are aiming at developing an effective numerical solver for the quantum hydrodynamic models deduced therein. Since the quantum hydrodynamic model is a moment expansion, which may be truncated up to any order, our method can numerically solve it in a unified way which is actually able to be regarded as a kind