INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 11, Number 1, Pages 1–23

IMPLICIT ASYMPTOTIC PRESERVING SCHEMES FOR SEMICONDUCTOR BOLTZMANN EQUATION IN THE DIFFUSIVE REGIME

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Abstract. We design several implicit asymptotic-preserving schemes for the linear semiconductor Boltzmann equation with a diffusive scaling, which lead asymptotically to the implicit discretizations of the drift-diffusion equation. The constructions are based on a stiff relaxation step and a stiff convection step obtained by splitting the system equal to the model equation. The one space dimensional schemes are given with the uniform grids and the staggered grids, respectively. The uniform grids are considered only in two space dimension. The relaxation step is evolved with the BGK-penalty method of Filbet and Jin [F. Filbet and S. Jin, J. Comp. Phys. 229(20), 7625-7648, 2010], which avoids inverting the complicated nonlocal anisotropic collision operator. The convection step is performed with a suitable implicit approximation to the convection term, which gives a banded matrix easy to invert. The von-Neumman analysis for the Goldstein-Taylor model show that the one space dimensional schemes are unconditionally stable. The heuristic discussions suggest that all the proposed schemes have the correct discrete drift-diffusion limit. The numerical results verify that all the schemes are asymptotic-preserving. As far as we know, they are the first class of asymptotic-preserving schemes ever introduced for the Boltzmann equation with a diffusive scaling that lead to an implicit discretization of the diffusion limit, thus significantly relax to stability condition.

Key words. linear semiconductor Boltzmann equation, implicit asymptotic-preserving scheme, drift-diffusion limit, BGK-penalty method, time-splitting

1. Introduction

The semiconductor Boltzmann equation, serving as the mathematical model for the highly integrated semiconductor, has a diffusive scaling characterized by the Knudsen number δ (which denotes the ratio of the mean free path of the particle over a typical length) when the electric potential is weak. As $\delta \to 0^+$, the semiconductor Boltzmann equation leads asymptotically to the drift-diffusion equation, which is usually satisfactory for the region having both $\delta \ll 1$ and the initial solution around the local equilibrium state. In practical applications, it is often found that δ varies with very different scale of magnitude within one computational domain and the initial data is in the nonlocal equilibrium state. For the sake of accuracy and efficiency, one usually uses either the domain decomposition type methods [3, 4, 9, 18, 27, 28] or the asymptotic-preserving (AP) schemes [5, 11, 14, 15, 16, 20, 21] to describe the device.

The domain decomposition type methods have the idea of discretizing the kinetic equation in the rarefied regime (where δ is big) and the drift-diffusion equation in the diffusive regime (where $\delta \ll 1$). Such methods generally face the difficulty of determining the locations and the coupling conditions of the interfaces. The AP schemes, on the other hand, solve in the whole computational domain the kinetic equations and hence avoid the problems of interfaces. Specifically, as summarized in [11], an AP scheme possesses the discrete analogy of the continuous asymptotic limit when $\delta \to 0^+$ even with coarse grids Δt, $\Delta x \gg \delta^2$ (where Δt is the time step

Received by the editors May 5, 2012 and, in revised form, March 20, 2013.
2000 *Mathematics Subject Classification.* 82C05, 82D37, 65M12.

and Δx is the space step). A scheme that allows the use of coarse grids should be AP. For kinetic equation with a diffusive scaling, the previous AP schemes need $\Delta t = O(\Delta x^2)$ due to the explicit convection term [5, 11, 14, 15, 16, 20, 21] and typically have the following features [15]:

- The numerical stability is independent of δ. Even in the worst case, it is merely restricted to the parabolic condition $\Delta t \sim O(\Delta x^2)$.
- Given Δt and Δx, the scheme becomes a good explicit solver for the limiting drift-diffusion equation when $\delta \to 0^+$.
- The collision term, though implicit, can be implemented explicitly.

In this paper, we are interested in deriving the implicit AP schemes for the linear semiconductor Boltzmann equation with a diffusive scaling, which improve the first two features above. Specifically, these schemes allow $\Delta t = O(\Delta x)$ instead of $\Delta t = O(\Delta x^2)$ even in the diffusive regime. Moreover, they are good implicit solvers for the limiting drift-diffusion equation as $\delta \to 0^+$ without the electric field, i.e., Δt can be arbitrary for stability. The constructions are based on the BGK-penalty method and a suitable implicit approximation to the convection terms, which have been decoupled through splitting a stiff relaxation step from a stiff convection step. The BGK-penalty method, having the effect of solving the implicit complicated collision term explicitly, was first introduced by Filbet and Jin [7] for a class of hyperbolic system with stiff relaxation source term and the classical Boltzmann equation. The method only requires that the source term has the unique and stable local equilibrium state, and has been applied to the Boltzmann type equations with either the hydrodynamic limit [6, 10, 17] or the diffusive limit [5]. The implicit scheme in the convection step gives the banded matrix easy to invert. Additionally, the velocity discretization is done with the moment method, which has been proved to be stable and convergent in [24].

The paper is arranged as follows. In the next section, we introduce some basic facts about the linear semiconductor Boltzmann equation and its drift-diffusion limit. There we generalize δ to $\delta = \delta(\vec{x}) \in \mathbb{C}^1(\Omega)$, and rewrite the model equation into an equivalent system with respect to the even and odd parities as was done in [14, 16]. The schemes in this paper are actually based on this system. Moreover, the boundary conditions are simply assumed to be periodic. In section 3, we consider one space dimension and derive the implicit AP schemes with the uniform and staggered grids, respectively. For the sake of simplification, we denote the scheme using the uniform grids with IMUG and the other using the staggered grids with IMSG. To construct IMUG and IMSG, we split the system in a suitable way to obtain a stiff relaxation step and a stiff convection step. In the relaxation step, we handle the complicated nonlocal anisotropic collision operator with the BGK-penalty method, which allows the implicit scheme in this step implemented explicitly. The convection step is discretized by a suitable implicit approximation to the convection term, which gives a banded matrix easy to invert and meanwhile allows $\Delta t = O(\Delta x)$ rather than $\Delta t = O(\Delta x^2)$ as in previous approaches. By a comparison, IMSG helps to minimize the bandwith of the matrix in the convection step, while, IMUG has the benefit of easy generalization to the higher space dimension. Through the von-Neumman analysis, IMUG and IMSG are unconditionally stable for the Goldstein-Taylor model. Furthermore, the heuristic discussions suggest that both the one space dimensional schemes are consistent implicit discretiztations of drift-diffusion equation in the asymptotic sense. In section 4 where the electric potential is absent, we extend IMUG to two space dimension and discuss its asymptotic property heuristically. In section 5, the moment method for the velocity