Numer. Math. Theor. Meth. Appl. Vol. **5**, No. 2, pp. 278-296
doi: 10.4208/nmtma.2012.m1045 May 2012

Asymptotic Preserving Schemes for Semiconductor Boltzmann Equation in the Diffusive Regime

Jia Deng*

Department of Mathematical Sciences, Tsinghua University, Beijing 100084, P. R. China.

Received 12 December 2010; Accepted (in revised version) 1 July 2011

Available online 27 March 2012

Abstract. As is known, the numerical stiffness arising from the small mean free path is one of the main difficulties in the kinetic equations. In this paper, we derive both the split and the unsplit schemes for the linear semiconductor Boltzmann equation with a diffusive scaling. In the two schemes, the anisotropic collision operator is realized by the "BGK"-penalty method, which is proposed by Filbet and Jin [F. Filbet and S. Jin, J. Comp. Phys. 229(20), 7625-7648, 2010] for the kinetic equations and the related problems having stiff sources. According to the numerical results, both of the schemes are shown to be uniformly convergent and asymptotic-preserving. Besides, numerical evidences suggest that the unsplit scheme has a better numerical stability than the split scheme.

AMS subject classifications: 35Q20, 65M12

Key words: linear semiconductor Boltzmann equation, drift-diffusion limit, diffusive relaxation system, "BGK"-penalty method.

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1. Introduction

The semiconductor Boltzmann equation, serving as the mathematical model for the highly integrated semiconductor devices, has a diffusive scaling measured by the dimensionless parameter ϵ, i.e., the ratio of the mean free path of the particle with the typical length. When ϵ goes to zero, i.e, $\epsilon \to 0^+$, the kinetic equations lead asymptotically to the drift-diffusion equations.

In practical applications, it is often found that ϵ locates in the very different scale within one problem, which causes the difficulty of transition regime, i.e, a regime with ϵ too small for the kinetic equations to avoid numerical stiffness, and meanwhile, too large for the drift-diffusion equations to be accurate [15]. In this situation, one has to resolve the kinetic scaling and applies very fine grids to the kinetic equations when using the standard numerical methods. Clearly, the cost will be expensive. On the other hand, what we are concerned is actually the macroscopic observables of the system, such as the

*Corresponding author. *Email address:* dengj04@gmail.com (Jia Deng)

mass density and the bulk momentum, but not the phase distribution [4]. Hence, it is worthless to compute the kinetic models wherever and whenever the drift-diffusion limits are valid. To tackle this problem, one can apply such a class of multiscale, multi-physics type domain decomposition methods (see, e.g., [3, 5, 7, 20]). All of them have the same idea of solving the drift-diffusion equations in the diffusive regimes (where ϵ is small), and the kinetic equations in the rarefied regimes (where ϵ is big). However, these methods have the difficulties of determining the interface, including the location and the coupling condition. In the recent years, the domain decomposition methods are gradually replaced by the so-called asymptotic-preserving (AP) schemes in many areas.

The concept of AP was firstly summarized by Jin as follows. An AP scheme should possess the discrete analogy of the continuous asymptotic limit when $\epsilon \to 0^+$ (see, e.g., [9]). To derive a class of AP schemes for the kinetic equations having the drift-diffusion limits, Jin, Pareschi and Toscani proposed the diffusive relaxation system (DRS) and described the features of the diffusive relaxation schemes as follows (see, e.g., [9–12]):

- The numerical stability is independent of ϵ. Even in the worst case, it is merely restricted by the parabolic condition $\Delta t \sim O(\Delta x^2)$.

- For the fixed step sizes Δt and Δx, when $\epsilon \to 0^+$, the scheme becomes a good solver for the limiting drift-diffusion equation.

- The collision term, though applied with the implicit scheme, can be implemented explicitly.

Here, we employ the idea of DRS and derive two diffusive relaxation schemes in three steps. Firstly, we reformulate the kinetic equation into the DRS using the even- and odd- parities (see, e.g., [10–12]). Next, we apply the upwind scheme associated with the high-resolution method to the left hand side (LHS) of DRS, which corresponds to a standard nonstiff hyperbolic system. Finally, we perform the time discretization with the split and the unsplit techniques, respectively. In both the split and the unsplit schemes, the anisotropic collision term is dealt with the “BGK"-penalty method proposed by Filbet and Jin in [6], the velocity discretization is done with a quadrature method based on the Hermite polynomials and being essentially the moment method (see, e.g., [10, 14]).

In this paper, it is the first time for the “BGK"-penalty method applied to the Boltzmann equation with a diffusive scaling. Some other related works can be found in [8, 13], where the authors have verified the efficiency of the method for the Fokker-Planck-Landau and Quantum Boltzmann equations with the Euler limit. The outline of this paper is as follows. In Section 2, we give a brief introduction for the linear semiconductor Boltzmann equation, including the associated diffusive scaling and the reformulation of the DRS. In Section 3, we arrange three parts for the numerical schemes. Part 1 gives the quadrature method for the velocity discretization. Part 2 introduces the high-resolution method for the LHS of the DRS. Part 3 presents the split and the unsplit techniques for the time discretization, including the “BGK"-penalty method for the collision term. In Section 4, we apply both the split and the unsplit schemes to two transport problems in the slab geometry. According