Asymptotic-preserving numerical schemes for the semiconductor Boltzmann equation efficient in the high field regime *

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Abstract

We present asymptotic-preserving numerical schemes for the semiconductor Boltzmann equation efficient in the high field regime. A major challenge in this regime is that there may be no explicit expression of the local equilibrium which is the main component of classical asymptotic-preserving schemes. Inspired by [14] and [13], our idea is to penalize the stiff collision term by a 'classical' BGK operator – which is not the local equilibrium in the high field limit – while treat the stiff force term implicitly by the spectral method. These schemes, despite being implicit, can be inverted easily, with a stability independent of the physically small parameter. We design these schemes for both nondegenerate and degenerate cases, and show their asymptotic properties. We present several numerical examples to validate the efficiency, accuracy and asymptotic properties of these schemes.

1 Introduction

In the semiconductor kinetic theory, the semi-classical evolution of the electron distribution function $f(t, x, v)$, in the parabolic band approximation, solves the kinetic equation:

$$\partial_t f + v \cdot \nabla_x f - \frac{q}{m_e} E \cdot \nabla_v f = \mathcal{Q}(f), \quad t > 0, x \in \mathbb{R}^{d_x}, v \in \mathbb{R}^{d_v}, \tag{1.1}$$

where q and m_e are positive elementary charge and effective mass of electrons, $E(t, x)$ is the electric field. The collision operator $\mathcal{Q}$ can be decomposed into three parts

$$\mathcal{Q} = \mathcal{Q}_{el} + \mathcal{Q}_{inel} + \mathcal{Q}_{ee}, \tag{1.2}$$

where $\mathcal{Q}_{el}$ and $\mathcal{Q}_{inel}$ describe the interactions between the electrons and the lattice imperfections, with the first one caused by ionized impurities and elastic part of the phonon collisions (or called crystal vibrations) and the second one by inelastic part of the phonon collisions. $\mathcal{Q}_{ee}$ characterizes the correlations between electrons themselves. For low electron densities, the general form of $\mathcal{Q}$ is [24]

$$\mathcal{Q}(f) = \int_{\mathbb{R}^{d_v}} \big(s(v', v) f(t, x, v') - s(v, v') f(t, x, v)\big) dv', \tag{1.3}$$

where s is the transition probability depending on the specific scattering mechanism described above, and satisfies the principle of detailed balance

$$s(v', v) M(v') = s(v, v') M(v), \tag{1.4}$$

where

$$M(v) = \left(\frac{2\pi K_B T}{m_e}\right)^{-\frac{d_v}{2}} e^{-\frac{v^2}{2v_{th}^2}} \tag{1.5}$$

*This research was partly supported by NSF grant DMS-1114546, NSF RNMS grant DMS-1107291. SJ was also supported by a Vilas Associate award from the University of Wisconsin-Madison.

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is the Maxwellian, v_{th} is the thermal velocity related to the lattice temperature T through $v_{th}^2 = \frac{K_B T}{m_e}$ and K_B is the Boltzmann constant. The null space of $\mathcal{Q}$ in (1.3) is spaned by the Maxwellian (1.5).

When the electron density is high, one should take Pauli's exclusion principle into account, and the collision operator $\mathcal{Q}$ becomes

$$\mathcal{Q}_{deg}(f) = \int_{\mathbb{R}^{N_v}} \big(s(v',v)f'(1-f) - s(v,v')f(1-f')\big)dv', \tag{1.6}$$

which is referred to as the degenerate case. Here f and f' are shorthanded notations for $f(t,x,v)$ and $f(t,x,v')$ respectively.

In principle, the electric field is produced self-consistently by the electrons moving in a fixed ion background with doping profile $h(x)$ through

$$\nabla_x(\varepsilon(x)\nabla_x\Phi) = \rho(x) - h(x), \qquad E = -\nabla_x\Phi, \tag{1.7}$$

where $\rho(x)$ is the electron density, Φ is the electrostatic potential and $\varepsilon(x)$ is the permittivity of the material.

The numerical computation of electron transport in semiconductors through the Boltzmann equation (BE) (1.1) is usually too costly for practical purposes since it involves the resolution of a problem rested on 7-dimensional time and space. Several macroscopic models based on the diffusion approximation were derived. The classical drift-diffusion (DD) [32] model was introduced, with the assumption that all the scatterings in $\mathcal{Q}$ are strong and that the electron temperature relaxes to the lattice temperature at the microscopic time scale. The connection between the BE and DD models has been well understood physically and mathematically [17, 27]. The case of the Fermi-Dirac statistics was investigated in [17] as well. However, in most situations, the momentum relaxation occurs much faster than temperature relaxation, thus results in an intermediate state at which the electrons have reached a local equilibrium with a different temperature other than the lattice temperature. The time evolution of this state is described by the Energy-Transport (ET) model, which is a system of diffusion equations for the electron density and energy. This model can be viewed as an augmented drift-diffusion model, and is derived asymptotically under the scaling that both the elastic $\mathcal{Q}_{el}$ and electron-electron $\mathcal{Q}_{ee}$ collisions are dominant [4]. Another model is the Spherical Harmonic Expansion (SHE) model which is obtained based on the observation that in some cases the electron-electron collision cannot constitute one of the dominant scattering mechanisms [29, 30]. This model, the only dominant collision mechanism of which is $\mathcal{Q}_{el}$, can be considered as a diffusion equation in the extended space: position and energy. In fact, the ET model was usually derived through the SHE model by taking the limit on the scaled electron-electron collision mean free path [10]. See also [11] for the new and simpler derivation of the ET model directly through the Boltzmann equation. [3] outlines a hierarchy between various macroscopic models as well as shows the macroscopic limit that links the two successive steps within the hierarchy.

However, due to the rapid progress in miniaturization of semiconductor devices, the standard drift diffusion models break down in some regime of hot electron transport. This regime concerns the physical situations where both the electric effects and collisions are dominant, which is called the high field regime. After rescaling of the variables, equation (1.1) can be written as

$$\partial_t f + v\cdot\nabla_x f - \frac{1}{\epsilon}E\cdot\nabla_v f = \frac{1}{\epsilon}\mathcal{Q}(f), \quad t>0, x\in\mathbb{R}^{d_x}, v\in\mathbb{R}^{d_v}, \tag{1.8}$$

where ϵ is the ratio between the mean free path and the typical length scale. It was first studied by Frosali *et.al* [16, 15], and later by Poupaud [28] for the nondegenerate case, where the limiting equation is a linear convection equation for the mass density with the convection proportional to the electric field. It also gives a necessary condition for the limit equation to embrace a unique solution, while if such a condition is not satisfied, a traveling wave solution will exist which is the so-called runaway phenomenon. When the electrostatic potential is obtained through the Poisson equation, [7] derives the high field limit for the BGK-type collision, and also reveals the boundary layer behavior when bounded domain is considered. The high field asymptotic for the degenerate case was carried out in [1], where the limit equation is a nonlinear convection equation for the macroscopic density which has a local in time regular solution. It was revisited in [2] where the convergence to entropy solutions and existence of shock profiles for the limit nonlinear conservation law were considered.

Considerable literature has been devoted to the design of efficient and accurate numerical methods for (1.1), such as [19, 5, 6, 8], to name just a few. These schemes become inefficient in the high field regime. Only recently, schemes efficient in the high field regime started to emerge [23, 9], in the framework of *Asymptotic Preserving* (AP) schemes. The AP schemes are efficient in the asymptotic regime since the scheme preserves a discrete analog of the asymptotic limit, so one does not need to numerically resolve the small scale of ϵ. It is often equipped with suitable time integrators in order to efficiently handle the numerical stiffness of the problem [20]. See a recent review on AP schemes [21].

In this paper, we are interested in designing AP schemes for Boltzmann equation of the type (1.8) with the high field scaling. So far the only AP schemes for the high field regime were those developed in [23, 9] in which $\mathcal{Q}(f)$ is the Fokker-Planck operator. In this case one can combine the forcing term and the collision term into a divergence form which cannot be done for other nonlocal collision operators to be studied in this paper.

As one can see, when ϵ is small, two terms of equation (1.8) become stiff and explicit schemes are subject to severe stability constraints. Implicit schemes allow larger time steps and mesh sizes, but it is usually expensive due to the prohibitive computational cost required by inverting a large algebraic system, even in the non-degenerate case where the collision operator is linear. Another remarkable difficulty is that there is no specific form of the *local equilibrium* M_h in the high field regime, which makes the modern asymptotic preserving methods such as [9, 12, 33] – all need the specific form of the local equilibrium – very hard to implement. To overcome the first difficulty, we follow the idea in [14] by penalizing the non-symmetric stiff term by a BGK operator which is much easier to treat implicitly. To overcome the second difficulty, inspired by the observation in [13] that one needs not to use the exact local equilibrium as a penalization but rather a "good" approximation of it might be enough, we only penalize the collision term by a 'classical' BGK operator with the Maxwellian defined in (1.5) instead of the real local equilibrium for the high field limit–which may not be available, and leave the stiff force term alone implicitly.

The rest of the paper is organized as follows. In the next section we give a brief review of the scalings in the high field regime and the corresponding macroscopic limit. Section 3 is devoted to the new schemes, as well as the study of their asymptotic properties. We consider three different cases: the nondegenerate isotropic case, the nondegenerate anisotropic case, and the degenerate case. Then we present several numerical examples to test the efficiency, accuracy and asymptotic properties of the schemes in section 4. At last, some concluding remarks are given in section 5.

2 Scalings and the high field limit

Since the transition probability in (1.3) satisfies the detailed balance principle, it is convenient to introduce a new function

$$\phi(v, v') = \frac{s(v', v)}{M(v)}, \quad \text{so that } \phi(v, v') = \phi(v', v). \tag{2.1}$$

Then the collision $\mathcal{Q}$ reads

$$\mathcal{Q}(f) = \int_{\mathbb{R}^{d_v}} \phi(v, v')\big(M(v)f(t, x, v') - M(v')f(t, x, v)\big)dv'. \tag{2.2}$$

Following [28], and also Chapter 2 in [24], introduce the rescaled variables:

$$\tilde{x} = \frac{x}{L}, \quad \tilde{t} = \frac{t}{T}, \quad \tilde{v} = \frac{v}{v_{th}},$$

where L and T are reference length and time. By the dimension argument, the collision term should be proportional to the reciprocal of a characteristic time, thus we define an average relaxation time τ and the rescaled collision $\tilde{\mathcal{Q}}$

$$\frac{1}{\tau} = \int_{\mathbb{R}^{d_v}} \phi(v, v')M(v)M(v')dvdv', \qquad \tilde{\mathcal{Q}} = \tau\mathcal{Q}.$$

Note here that for the degenerate case the definition of τ is a bit different but similar. The mean free path now can be defined as $l = \tau v_{th}$. Next define the thermal voltage U_{th} and the rescaled electric field $\tilde{E}$ as

$$U_{th} = \frac{m_e v_{th}^2}{q}, \qquad \tilde{E} = \frac{E}{E_0},$$

where E_0 is a reference field. Then the Boltzmann equation (1.1) takes the form

$$\frac{\tau}{T}\, \partial_{\tilde{t}} f + \frac{\tau v_{th}}{L}\, \tilde{v} \cdot \nabla_{\tilde{x}} f - \frac{\tau v_{th}}{U_{th}} E_0\, \tilde{E} \cdot \nabla_{\tilde{v}} f = \tilde{\mathcal{Q}}. \tag{2.3}$$

Now introduce the dimensionless parameter $\epsilon = \frac{l}{L}$ and consider the high field scalings

$$E_0 = \frac{U_{th}}{l}, \quad T = \frac{\tau}{\epsilon},$$

(2.3) becomes

$$\partial_t f + v \cdot \nabla_x f - \frac{1}{\epsilon} E \cdot \nabla_v f = \frac{1}{\epsilon} Q(f), \tag{2.4}$$

where we have dropped the tilde for convenience.

2.1 The high field limit: the nondegenerate case

In (2.4), when ϵ vanishes, the limiting equation is a linear convection equation for the macroscopic particle density with a convection proportional to the scaled electric field. That is,

$$f(t, x, v) \to \rho(t, x) F_{E(t,x)}(v), \tag{2.5}$$

where $F_{E(t,x)}(v)$ is the solution to

$$\int_{\mathbb{R}^{d_v}} F_E(v) dv = 1, \quad E \cdot \nabla_v F_E + \mathcal{Q}(F_E) = 0, \quad F_E \geq 0; \tag{2.6}$$

while the equation for the macroscopic density ρ is obtained by integrating (2.4) w.r.t. v

$$\partial_t \rho(t, x) + \int_{\mathbb{R}^{d_v}} v \cdot \nabla_x f = 0, \tag{2.7}$$

and then passing to the limit to get

$$\partial_t \rho(t, x) + \nabla_x \cdot (\rho(t, x) \sigma(E(t, x))) = 0, \quad \sigma(E) = \int_{\mathbb{R}^{d_v}} v F_E(v) dv. \tag{2.8}$$

Not all $\mathcal{Q}$ gives a unique solution of (2.6). Poupaud [28] gave a criteria for the transition probability s in the following theorem.

Theorem 1. *[28] Assume that the collision cross-section $\phi(v, v') > 0$ satisfies $\phi(v, v') \in W^{1,\infty}(\mathbb{R}^{2d_v})$, then the collision frequency*

$$\nu(v) = \int_{\mathbb{R}^{d_v}} s(v, v') dv' = \int_{\mathbb{R}^{d_v}} \phi(v, v') M(v') dv' \tag{2.9}$$

is bounded and positive. If it further satisfies

$$\int_0^\infty \nu(v + \eta E) d\eta = +\infty, \quad a.e., \tag{2.10}$$

and the initial data $f(0, x, v) = f^0(x, v)$ solves $E \cdot \nabla_v f^0(x, v) - \mathcal{Q}(f^0)(x, v) = 0$ a.e., then the solution to (2.4) converges to ρF_E in the following sense: $\exists$ a positive constant C_T that depends on the initial data such that for any time $t \leq T$, the following inequality

$$\| f(t, \cdot, \cdot) - \rho(t, \cdot) F_{E(t,\cdot)}(\cdot) \|_{L^1(\mathbb{R}^{d_x} \times \mathbb{R}^{d_v})} \leq C_T \epsilon$$

holds.

Remark 2. Equation (2.8) together with (2.6) can be regarded as the first order approximation of (2.4) which resembles the hydrodynamic approximation of the Boltzmann equation by the Euler equations. (2.8) that rules out all the diffusion effect, is nothing but Ohm's law. If one goes further to the second order approximation, a new drift diffusion equation can be derived, which again resembles the Navier-Stokes approximation of the Boltzmann equation.

Remark 3. The above result is obtained for the case where electrical field is given. The analytical result for the case when the electrical field is self-consistent through the Poisson equation is only derived by Cercignani, Gamba and Levermore in [7] for the BGK collision operator, while for general collision it is still open.

2.2 The high field limit: the degenerate case

Similar to the nondegenerate case, the transition probability $s(v, v')$ in (1.6) also satisfies the principle of detailed balance [26], so it can be reformulated in the same way as (2.2),

$$\mathcal{Q}_{deg}(f)(t,x,v) = \int_{\mathbb{R}^{d_v}} \phi(v',v)\Big(M(v)f(t,x,v')\big(1-f(t,x,v)\big) - M(v')f(t,x,v)\big(1-f(t,x,v')\big)\Big)dv', \quad (2.11)$$

where $M(v)$ and $\phi(v', v)$ are defined the same as before in (1.5) and (2.1). The null space of $\mathcal{Q}_{deg}(f)(t, x, v)$ is spaned by the Fermi-Dirac distribution

$$M_{FD} = \frac{1}{1 + e^{\frac{m_e v^2}{2K_B T} - \frac{\mu}{K_B T}}}, \quad (2.12)$$

where T is the lattice temperature and μ is the electron Fermi energy. The dimensionless form of the degenerate case is the same as (2.4), except that the collision $\mathcal{Q}$ is replaced by $\mathcal{Q}_{deg}$.

Assume B is either the Brillouin zone or the whole space $\mathbb{R}^{d_v}$. When sending ϵ to 0, f can no longer be decoupled into two functions with one depending on x and t and the other on v separately because of the nonlinearity of the collision operator, instead one has, under the hypothesis that $\phi \in W^{2,\infty}(B^2)$ and $\phi_0 \le \phi(v, v') \le \phi_1$ for some positive constant ϕ_0 and ϕ_1,

$$f \to F(\rho(t,x), E(t,x))(v)$$

where $F(\rho, E)(v)$ is the unique solution in space $D_E = \{F \in L^1(B);\ E \cdot \nabla_v F \in L^1(B)\}$ such that $0 \le F \le 1$ and

$$E \cdot \nabla_v F - \mathcal{Q}_{deg}(F) = 0, \quad \int_{\mathbb{R}^{d_v}} F(t,x,v)dv = \rho(t,x). \quad (2.13)$$

Moreover, the mapping

$$(\rho, E) \mapsto F(\rho, E) \quad (2.14)$$

from $\mathbb{R}^+ \times \mathbb{R}^{d_x}$ to $L^1(B)$ is C^2 differentiable. Then the macroscopic density ρ solves

$$\partial_t \rho(t,x) + \nabla_x\Big(j(\rho(t,x); E(t,x))\Big) = 0, \quad \rho(0,x) = \int_{\mathbb{R}^{d_v}} f^0(x,v)dv, \quad (2.15)$$

where $j(\rho; E) = \int_{\mathbb{R}^{d_v}} vF(\rho, E)(v)dv$. This result was proved in [1] for a given $E(x) \in \mathbb{R}^{d_x}$ on the time intervals such that the limit solution is regular.

Remark 4. Although there is no such condition (2.10) to insure the existence of the limit solution, the hypothesis that $\phi(v, v')$ should be uniformly bounded from below and above already implies it.

Remark 5. Due to the nonlinearity of the flux function in (2.15), only the existence and uniqueness of a local in time regular solutions were available and shock might be generated later [2]. This is different from the nondegenerate case, where the limit equation (2.8) is linear in ρ, thus a unique global in time solution exists.

3 A numerical scheme for the semiconductor Boltzmann equation

To design an asymptotic preserving method, one usually needs to treat the two stiff terms – the force term and the collision term implicitly. However, this would bring new difficulties to invert the algebraic system originated by the non-symmetric difference operator and the collision operator. In [23] and [9] when the collision is of the Fokker-Planck type, these two terms were combined and rewrote into one symmetric operator in velocity space. But unfortunately, this strategy cannot be implemented here because no symmetric combination of the two is available. Another remarkable difficulty is that one cannot write down the local equilibrium M_h in the high filed limit explicitly, thus we cannot use the existent asymptotic preserving method for kinetic equation in the hydrodynamic regime [9], nor can we use the even-odd decomposition [22] due to the fact that one cannot derive a "non-stiff" force term. Here we adopt the penalization idea introduced by Filbet and Jin [14]. In addition, inspired by the fact that functions that share the same conserved quantities with the exact local equilibrium can be used as candidates for penalty [13], we will only penalize the collision term by a BGK operator which conserves mass, and treat the stiff force term implicitly by the spectral method. To better illustrate our idea, we begin with the simplest case which is the so-called "time relaxation model".

Here for the sake of simplicity, we will explain our idea in the one dimensional case. The generalization to the multidimensional case can be done in a straightforward manner simply using the dimension-by-dimension discretization. Denote $f(x_l, v_m, t^n)$ by f^n_{lm}, where $0 \le l \le N_x$ and $0 \le m \le N_v$, and N_x and N_v are the numbers of mesh points in x and v directions respectively.

3.1 The nondegenerate isotropic case

In the low density approximation, if one only considers the collisions with background impurities, the collision opeator can be approximated by a linear relaxation time operator [7, 24]:

$$\mathcal{Q} = \int M f' - M' f dv' = M\rho - f, \tag{3.1}$$

which is the simplest case with $\phi(v', v) = 1$ in (2.2). This is usually called the "time-relaxation" model. In this model, one can directly treat both stiff terms implicitly. The first order scheme reads

$$\frac{f^{n+1} - f^n}{\triangle t} + v \cdot \nabla_x f^n - \frac{1}{\epsilon} E \cdot \nabla_v f^{n+1} = \frac{1}{\epsilon}(M\rho^{n+1} - f^{n+1}), \tag{3.2}$$

and we use the spectral discretization for the stiff force term. The scheme can be implemented as follows

- Step 1. Integrate (3.2) over v, note that the two stiff terms vanish, and one ends up with an explicit semidiscrete scheme for ρ^{n+1}:

  $$\frac{\rho^{n+1} - \rho^n}{\triangle t} + \nabla_x \cdot \int_{\mathbb{R}^{d_v}} v f^n dv = 0;$$

  – Step 1.1. If the electrical field is given by (1.7), then solve it by any Poisson solver such as the spectral method to get E^{n+1}.

- Step 2. Approximate the transport term $v \cdot \nabla_x f^n$ in (3.2) by a non-oscillatory high resolution shock-capturing method.

- Step 3. Use the spectral discretization for the stiff force term, i.e., (3.2) can be reformulated into

  $$\left[1 + \frac{\triangle t}{\epsilon} - \frac{\triangle t}{\epsilon} E \cdot \nabla_v \right] f^{n+1} = f^n - \triangle t v \cdot \nabla_x f^n + \frac{\triangle t}{\epsilon} M \rho^{n+1},$$

  then take discrete Fourier Transform w.r.t. v on both sides, one has

  $$\left[1 + \frac{\triangle t}{\epsilon} - i\frac{\triangle t}{\epsilon} E \cdot k\right] \hat{f}^{n+1} = \mathscr{F}\left(f^n - \triangle t v \cdot \nabla_x f^n + \frac{\triangle t}{\epsilon} M \rho^{n+1}\right), \tag{3.3}$$

  where $\hat{f}$ and $\mathscr{F}(f)$ denote the discrete Fourier Transform of f w.r.t. v.

- Step 4. Use the inverse Fourier transform on $\hat{f}^{n+1}$ to get f^{n+1}.

Remark 6. Although the force term $\frac{E}{\epsilon}\cdot\nabla_v f$ contains a derivative, which looks "more stiff" than the collision term, just treating it implicitly and leaving the collision explicit will not have the desired stability property. This can be seen from the simple Fourier analysis on the toy model

$$f_t + \frac{E}{\epsilon} f_v = -\frac{1}{\epsilon} f, \tag{3.4}$$

with the discretization

$$\frac{f^{n+1} - f^n}{\triangle t} + \frac{E}{\epsilon}\partial_v f^{n+1} = -\frac{1}{\epsilon} f^n,$$

where $f^n(v)$ denotes $f(t^n, v)$. Applying the Fourier Transform on $f^n(v)$ w.r.t. v to get $\hat{f}^n(k)$, then one has

$$\left|\hat{f}^{n+1}(k)\right|^2 = \frac{\left(1 - \frac{\triangle t}{\epsilon}\right)^2}{1 + \left(\frac{\triangle t}{\epsilon} E\cdot k\right)^2} \left|\hat{f}^n(k)\right|^2,$$

note that for stability the coefficient on the right hand side needs to be less than one for all values of k, that is $\frac{\triangle t}{\epsilon} < 2$, thus $\triangle t$ must be dependent of ϵ.

The scheme has the following AP property.

Proposition 7. *Assume all functions are smooth. Let*

$$\| f^n(x,\cdot) \|_{L^2(\mathbb{R}^{d_v})} = \sqrt{\int_{\mathbb{R}^{d_v}} f(t^n, x, v)^2 dv}, \tag{3.5}$$

then in the regime $\triangle t \gg \epsilon$ we have

$$\|f^n - M_h^n\|_{L^2(\mathbb{R}^{d_v})} \le \alpha^n \|f^0 - M_h^0\|_{L^2(\mathbb{R}^{d_v})} + O(\epsilon) \quad \textit{with } \alpha < 1 \textit{ uniformly in } \epsilon, \tag{3.6}$$

where $M_h^n = \rho^n F_E$ is the local equilibrium in the high field regime, with F_E being the solution to the limit equation (2.6) with $\mathcal{Q} = \rho M - f$.

Proof. Since M_h^{n+1} satisfies $-E\cdot\nabla_v M_h^{n+1} = \mathcal{Q}(M_h^{n+1}) = \rho^{n+1} M - M_h^{n+1}$, a simple manipulation of scheme (3.2) gives

$$\left(1 + \frac{\triangle t}{\epsilon} - \frac{\triangle t}{\epsilon} E\cdot\nabla_v\right)(f^{n+1} - M_h^{n+1}) = (f^n - M_h^n) - (M_h^{n+1} - M_h^n) - \triangle t v\cdot\nabla_x f^n. \tag{3.7}$$

Now take the Fourier Transform w.r.t. v on both sides, (3.7) reformulates to

$$\begin{aligned} & \hat{f}^{n+1} - \hat{M}_h^{n+1} \\ = \; & G\left[(\hat{f}^n - \hat{M}_h^n) - (\hat{M}_h^{n+1} - \hat{M}_h^n) - \triangle t \mathscr{F}(v\cdot\nabla_x f^n)\right], \end{aligned} \tag{3.8}$$

where

$$G = \frac{1}{1 + \frac{\triangle t}{\epsilon} - i\frac{\triangle t}{\epsilon} E\cdot k}. \tag{3.9}$$

Take the L^2 norm on both sides, one has, by the Minkowski inequality

$$\begin{aligned} & \| \hat{f}^{n+1} - \hat{M}_h^{n+1} \|_{L^2} \\ \le \; & \| G(\hat{f}^n - \hat{M}_h^n) \|_{L^2} + \left\| G\left((\hat{M}_h^{n+1} - \hat{M}_h^n) + \triangle t\mathscr{F}(v\cdot\nabla_x f^n)\right)\right\|_{L^2}. \end{aligned} \tag{3.10}$$

By smoothness assumption $\left|\hat{M}_h^{n+1} - \hat{M}_h^n\right| \le C_1 \triangle t \hat{M}_h$ and $\left\|G \triangle t\right\|_{L^\infty} \le C_2\epsilon$ for $\triangle t \gg \epsilon$, where C_1 and C_2 are two constants independent of $\triangle t$ and ϵ. Then (3.10) becomes

$$\| \hat{f}^{n+1} - \hat{M}_h^{n+1} \|_{L^2} \le \| G(\hat{f}^n - \hat{M}_h^n) \|_{L^2} + C\epsilon. \tag{3.11}$$

Since $\| G \|_{L^\infty} \le \alpha < 1$ uniformly in ϵ for $\triangle t \gg \epsilon$, applying Parseval's identity, one has

$$\|f^{n+1} - M_h^{n+1}\|_{L^2(\mathbb{R}^{d_v})} \le \alpha \|f^n - M_h^n\|_{L^2(\mathbb{R}^{d_v})} + O(\epsilon). \tag{3.12}$$

This leads to (3.6). □

3.2 The nondegenerate anisotropic case

This section is devoted to the nondegenerate anisotropic case. Recall that the collision operator takes the form

$$\mathcal{Q}(f) = \int_{\mathbb{R}^{N_v}} \phi(v,v')\big(M(v)f(t,x,v') - M(v')f(t,x,v)\big)dv' = \mathcal{Q}^+(f) - \nu(v)f. \tag{3.13}$$

Although $\mathcal{Q}$ is linear in f, due to the non-symmetric nature of the transition probability $s(v',v)$, treating it implicitly as what we did in the last section will make it difficult to invert, especially in higher dimensions. To overcome this difficulty, we adopt the idea introduced by Filbet and Jin in [14] by penalizing the collision term by a BGK operator, the simple structure of which makes it easy to be treated implicitly. Thus the first order scheme reads

$$\frac{f^{n+1} - f^n}{\triangle t} + v \cdot \nabla_x f^n - \frac{1}{\epsilon} E \cdot \nabla_v f^{n+1} = \frac{1}{\epsilon}\mathcal{Q}(f^n) - \frac{\lambda}{\epsilon}(\rho^n M - f^n) + \frac{\lambda}{\epsilon}(\rho^{n+1}M - f^{n+1}), \tag{3.14}$$

where M is the dimensionless form of (1.5)

$$M(v) = \frac{1}{(2\pi)^{\frac{d_v}{2}}} e^{-\frac{v^2}{2}}. \tag{3.15}$$

Then (3.14) has the similar implicit structure as (3.2), thus one can solve it by the same steps introduced in section 3.1, yielding a scheme that is implicit but can be implemented explicitly.

Notice that in [14], the penalty is the local equilibrium of the collision operator, which will drive f to the right Maxwellian if treated implicitly. However, as it has been mentioned, there is no explicit form of the "high field equilibrium" which is the solution to $E \cdot \nabla_v f = \mathcal{Q}(f)$, so we instead penalize the equation by the equilibrium ρM of the collision term $\mathcal{Q}(f)$, and this will indeed force f to the right local equilibrium by the following proposition. The cost of this "wrong Maxwellian" penalty is the extra $\triangle t$ error in (3.16). This was observed in [13] where the authors use the classical Maxwellian instead of the quantum one to penalize the quantum Boltzmann collision operator, and get a similar asymptotic property.

Proposition 8. *In (3.14), if $\mathcal{Q}$ takes the form of (3.1) and $\lambda > \frac{1}{2}$, then*

$$\|f^n - M_h^n\|_{L^2(\mathbb{R}^{d_v})} \le \alpha^n \|f^0 - M_h^0\|_{L^2(\mathbb{R}^{d_v})} + O(\epsilon + \triangle t) \quad \text{with } \alpha < 1, \tag{3.16}$$

where $M_h^n = \rho^n F_E$ is the local equilibrium in the high field regime, with F_E being the solution to the limit equation (2.6) with $\mathcal{Q}$ defined in (3.1).

The proof is very similar to the one for Proposition 11 in the next section and is omitted here.

Remark 9 (Choice of λ)**.** For the general collision (3.13), λ should be chosen to satisfy $\lambda > \max_v \mu(v)$, where ν is the collision frequency defined in (2.9). One can also refer to [33] for positivity concern.

Remark 10. This method can be easily extended to case with non-parabolic energy diagram such as Kane's model [5, 6, 8] since the convection term is treated explicitly.

3.3 The degenerate case

When the quantum effect is taken into account, the collision operator becomes nonlinear. Nevertheless, this can be dealt with in the same way as in section 3.2 at the same cost. Again inspired by [13], we use the classical Boltzmann distribution instead of the Fermi-Dirac distribution (2.12) as the penalty to avoid the complicated nonlinear solver for the Fermi-energy in (2.12) from mass density ρ, otherwise such nonlinear solver should be used at every time step and grid point, which is very time consuming. Since the $\triangle t$ error will be inevitable in the asymptotic property as we have seen in the last section, this change of penalty will only introduce new error of $O(\triangle t)$. Similar to (3.14), the first order scheme takes the form

$$\frac{f^{n+1}-f^n}{\triangle t}+v\cdot\nabla_x f^n-\frac{1}{\epsilon}E\cdot\nabla_v f^{n+1}=\frac{1}{\epsilon}\mathcal{Q}_{deg}(f^n)-\frac{\lambda}{\epsilon}(\rho^n M-f^n)+\frac{\lambda}{\epsilon}(\rho^{n+1}M-f^{n+1}), \tag{3.17}$$

where $\mathcal{Q}_{deg}$ is defined in (1.6) and M is the same as (3.15). In practice, similar to Remark 9, λ is chosen to be $\max_v \int_{\mathbb{R}^{d_v}} \phi(v',v)M(v')(1-f(v'))dv'$.

Because of the nonlinearity of $\mathcal{Q}_{deg}$, it is not easy to check the asymptotic property analytically. Instead we check it for the case where $\mathcal{Q}_{deg}$ is replaced by the "quantum BGK" operator "$M_{FD}-f$" in the following proposition.

Proposition 11. *Assume the solutions are smooth. If $\lambda>\frac{1}{2}$, then the scheme (3.17) with $\mathcal{Q}_{deg}$ replaced by "$M_{FD}-f$" has the asymptotic property*

$$\|f^n-M_{qh}^n\|_{L^2(\mathbb{R}^{d_v})}\le\alpha^n\|f^0-M_{qh}^0\|_{L^2(\mathbb{R}^{d_v})}+O(\epsilon+\triangle t) \tag{3.18}$$

with $0<\alpha<1$, where M_{qh} is the solution to the high field limit equation

$$-E\cdot\nabla_v M_{qh}=M_{FD}-M_{qh},\quad \int_{\mathbb{R}^{d_v}}M_{qh}dv=\int_{\mathbb{R}^{d_v}}f dv=\int_{\mathbb{R}^{d_v}}M_{FD}dv=\rho. \tag{3.19}$$

Proof. Since M_{qh} satisfies $-E\cdot\nabla_v M_{qh}^{n+1}=M_{FD}^{n+1}-M_{qh}^{n+1}$, the scheme (3.17) becomes

$$\begin{aligned}
&\left(1+\frac{\lambda\triangle t}{\epsilon}-\frac{\triangle t}{\epsilon}E\cdot\nabla_v\right)(f^{n+1}-M_{qh}^{n+1})\\
=&\left(1+\frac{(\lambda-1)\triangle t}{\epsilon}\right)(f^n-M_{qh}^n)-\left(1+\frac{(\lambda-1)\triangle t}{\epsilon}\right)(M_{qh}^{n+1}-M_{qh}^n)\\
&+\frac{\lambda\triangle t}{\epsilon}(\rho^{n+1}-\rho^n)M-\frac{\triangle t}{\epsilon}(M_{FD}^{n+1}-M_{FD}^n)-\triangle t v\cdot\nabla_x f^n.
\end{aligned} \tag{3.20}$$

After taking the Fourier Transform w.r.t. v on both sides, it reformulates to

$$\begin{aligned}
&\hat f^{n+1}-\hat M_{qh}^{n+1}\\
=&\frac{1+\frac{(\lambda-1)\triangle t}{\epsilon}}{1+\frac{\lambda\triangle t}{\epsilon}-i\frac{\triangle t}{\epsilon}E\cdot k}\big(\hat f^n-\hat M_{qh}^n\big)-\frac{1+\frac{(\lambda-1)\triangle t}{\epsilon}}{1+\frac{\lambda\triangle t}{\epsilon}-i\frac{\triangle t}{\epsilon}E\cdot k}\big(\hat M_{qh}^{n+1}-\hat M_{qh}^n\big)+\frac{\frac{\lambda\triangle t}{\epsilon}}{1+\frac{\lambda\triangle t}{\epsilon}-i\frac{\triangle t}{\epsilon}E\cdot k}(\rho^{n+1}-\rho^n)\hat M\\
&-\frac{\frac{\triangle t}{\epsilon}}{1+\frac{\lambda\triangle t}{\epsilon}-i\frac{\triangle t}{\epsilon}E\cdot k}\big(\hat M_{FD}^{n+1}-\hat M_{FD}^n\big)-\frac{\triangle t}{1+\frac{\lambda\triangle t}{\epsilon}-i\frac{\triangle t}{\epsilon}E\cdot k}\mathscr{F}\big(v\cdot\nabla_x f^n\big).
\end{aligned} \tag{3.21}$$

Let

$$G_1=\frac{1+\frac{(\lambda-1)\triangle t}{\epsilon}}{1+\frac{\lambda\triangle t}{\epsilon}-i\frac{\triangle t}{\epsilon}E\cdot k}, \tag{3.22}$$

take the L^2 norm for (3.21), and apply the same procedure as in Proposition 7, we have

$$\|\,\hat f^{n+1}-\hat M_{qh}^{n+1}\,\|_{L^2}\le\ \|G_1\|_{L^\infty}\|\,\hat f^n-\hat M_{qh}^n\,\|_{L^2}+O(\triangle t+\epsilon), \tag{3.23}$$

where the $O(\triangle t)$ terms come from the second, third and forth terms in (3.21) and form major difference compared to (3.8). If $\lambda>\frac{1}{2}$, $\|G_1\|_{L^\infty}\le\alpha<1$, the result (3.18) then follows. □

Remark 12. To get better asymptotic property than (3.16) and (3.18), we would like to extend the scheme to second order. Follow the idea in [18], using backward difference formula in time and MUSCL scheme [31] in space, we have

$$\begin{aligned} &\frac{3f^{n+1} - 4f^n + f^{n-1}}{2 \triangle t} + 2v \cdot \partial_x f^n - v \cdot \partial_x f^{n-1} + \frac{1}{\epsilon} E^{n+1} \cdot \partial_v f^{n+1} \\ &= \frac{2}{\epsilon}\mathcal{Q}(f^n) - \frac{1}{\epsilon}\mathcal{Q}(f^{n-1}) - \frac{2\lambda}{\epsilon}(\rho^n M - f^n) + \frac{\lambda}{\epsilon}(\rho^{n-1}M - f^{n-1}) + \frac{\lambda}{\epsilon}(\rho^{n+1}M - f^{n+1}). \end{aligned} \tag{3.24}$$

However, since the stiff terms contain a first derivative, it poses a very restrictive bound on λ for stability $\big($here one condition we derived is $|\nabla_v \mathcal{Q}(f)| \le \lambda \le \min(3, \frac{5}{2} + \frac{\epsilon}{\triangle t})|\nabla_v \mathcal{Q}(f)|$ $\big)$ which might not be applicable in general cases. A better second order discretization in time is planed in a future work.

4 Numerical examples

In this section, we perform several numerical tests for the semiconductor Boltzmann equations with different collisions and in different asymptotic regimes. In the one dimensional examples, we use the following settings unless otherwise specified. The computational domain for x and v is $[0, L_x] \times [-L_v, L_v] = [0, 1] \times [-8, 8]$ with $N_x = 128$ and $N_v = 32$. The time step is chosen to be $\triangle t = \frac{\triangle x}{10}$ to satisfy the CFL condition $\triangle t \le \frac{\triangle x}{\max_j |v_j|}$ in the transport part. Periodic boundary conditions in x will be used to avoid any difficulties that might be generated by the boundary. The "M" is the absolute Maxwellian

$$M(v) = \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}. \tag{4.1}$$

The permittivity $\varepsilon(x)$ in the Poisson equation (1.7) is taken to be $\varepsilon(x) \equiv 1$.

4.1 The time relaxation model

We first test the numerical method presented in section 3.1 for the simplest time relaxation model (2.4) with (3.1). The initial condition is taken as

$$\rho^0(x) = \frac{\sqrt{2\pi}}{2}\left(2 + \cos(2\pi x)\right), \quad \text{and } f^0(x, v) = \rho^0(x) M(v), \tag{4.2}$$

which is not at the local equilibrium. The electric field $E(t, x)$ satisfies the Poisson equation (1.7) with the doping profile

$$h(x) = \frac{\int_0^{L_x} \rho(x) dx}{1.2611} e^{\cos(2\pi x)}. \tag{4.3}$$

We show the time evolution of the asymptotic error defined as

$$errorAP^n = \sum_{l,m} |E_l \cdot \nabla_v f_l^n + M\rho_l^n - f_{lm}^n| \triangle x \triangle v, \tag{4.4}$$

where the derivative w.r.t. v is calculated by the spectral method. Figure 1 gives the error with ϵ decreasing by $\frac{1}{10}$ each time, which shows that the asymptotic error is of order ϵ, thus verifies the results in Proposition 7.

4.2 The nondegenerate anisotropic case

In this section, we consider the nondegenerate anisotropic case with collision cross-section defined as

$$\phi(v, v') = 1 + e^{-(v-v')^2}, \tag{4.5}$$

and the initial condition is chosen the same as (4.2).

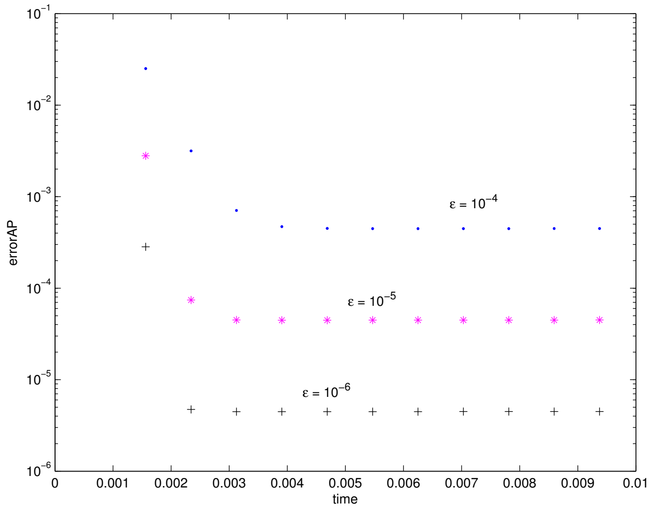

Figure 1: The time relaxation model coupled with the Poisson equation for the electric field. The time evolution of asymptotic error (4.4) for different ϵ with nonequilibrium initial data using the first order scheme in section 3.1.

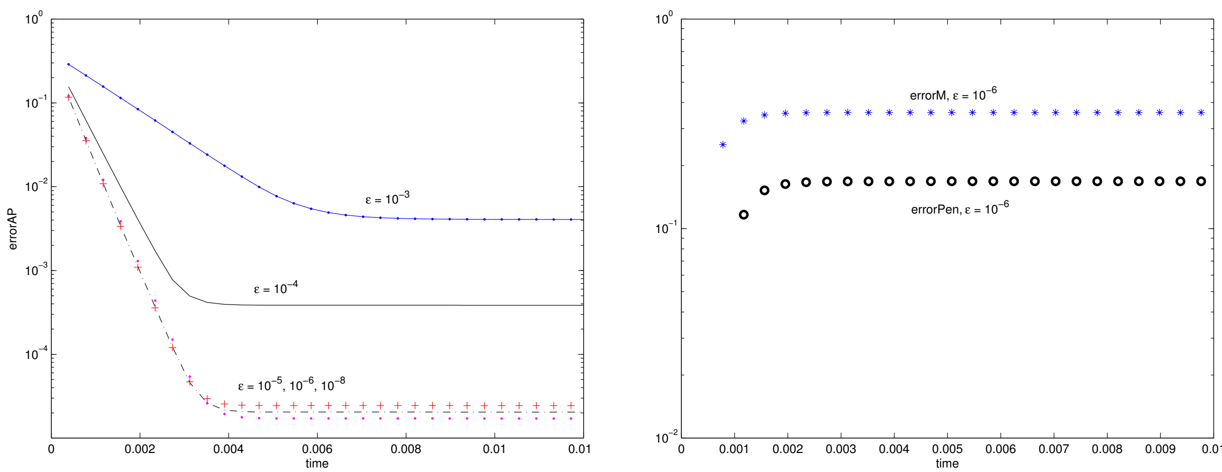

Figure 2: The nondegenerate anisotropic model with a fixed electrical field. The time evolution of asymptotic error (4.6) for different ϵ with nonequilibrium initial data (left), and a test of other errors (4.7) and (4.8) in comparison (right).

- Asymptotic property

Consider fixed $E = 0.2$ at the moment. Figure 2 gives the relations between ϵ and the asymptotic error defined as

$$errorAP^n = \sum_{l,m} \left| E_l \cdot \nabla_v f_l^n + \mathcal{Q}(f)_{l,m}^n \right| \triangle x \triangle v, \tag{4.6}$$

where the derivative w.r.t. v is again calculated by the spectral method. The initial data is away from the equilibrium. It can be seen in Figure 2 that when ϵ is relatively large, the error is dominated by ϵ. However, when ϵ is small enough, the time step $\triangle t = 3.9063e-4$ will play a role so that the error will not decrease with ϵ. The first order scheme is better performed asymptotically than we expected in Proposition 8 as the error observed in Figure 2 is smaller than $O(\triangle t)$.

To show that our scheme does not push f to the wrong Maxwellian, in Figure 2 we also plot the following two errors. One is defined as

$$errorPen^n = \sum_{l,m} |E_l \cdot \nabla_v f_l^n + \lambda(\rho M - f)| \triangle x \triangle v \tag{4.7}$$

to show that our penalization will not affect the asymptotic property. The other is the distance between f and the Maxwellian of the collision

$$errorM^n = \sum_{l,m} \left| f_{l,m}^n - \rho_l^n M \right| \triangle x \triangle v, \tag{4.8}$$

which is to show that our implicit treatment of the stiff force term necessarily accounts for the right asymptotic limit. It is shown that both errors stay large when ϵ is small, which means f will not be driven to either cases above when sending ϵ to 0.

- A piecewise constant initial data

Consider a piecewise constant initial data to test the efficiency of the method:

$$\begin{cases} (\rho_l, h_l) = (1/8, 1/2), & 0 \le x < 1/4; \quad (4.9a) \\ (\rho_m, h_m) = (1/2, 1/8), & 1/4 \le x < 3/4; \quad (4.9b) \\ (\rho_r, h_r) = (1/8, 1/2), & 3/4 \le x \le 1. \quad (4.9c) \end{cases}$$

Initially $f^0(x,v) = \frac{\rho}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}$ and let E be the solution of $-\nabla_x E = \rho - h$. Again periodic boundary condition in x direction is applied. ϵ is fixed to be 10^{-3}. For reference solution, we use the explicit second order Runge-Kutta discretization in time and MUSCL scheme for space discretization, with $N_x = 1024$, $N_v = 64$ and $\triangle t = \min(\triangle x/10, \epsilon \triangle v)/4 = 2.4414e-05$.

Define the flux and energy as the first and second moments of f:

$$\text{flux} = \int_{-L_v}^{L_v} f v dv, \quad \text{energy} = \int_{-L_v}^{L_v} f v^2 dv. \tag{4.10}$$

From Figure 3, one sees a good match between our solution and the reference solution.

4.3 The degenerate case

In this section, we consider the degenerate case where the collision $\mathcal{Q}_{deg}$ is defined as (1.6).

- Asymptotic property

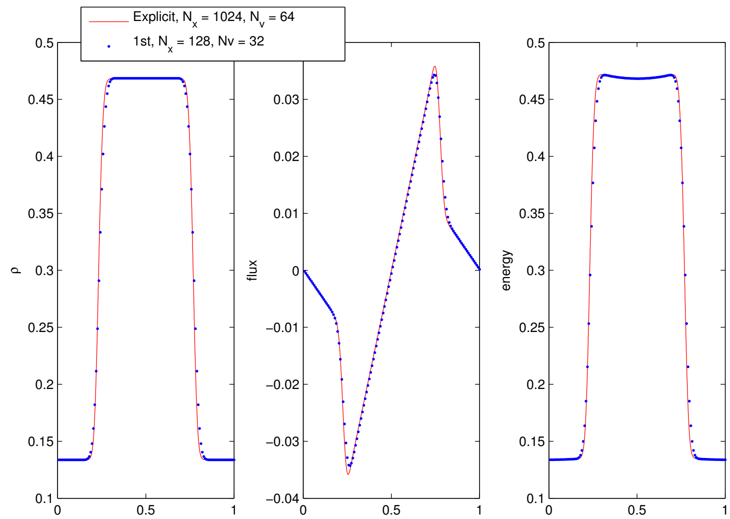

Figure 3: The plot of density, flux and energy at time $t = 0.2$ of the anisotropic nondegenerate case with (4.5) with E obtained from the Poisson equation. The initial data is given in (4.9).

The initial condition is taken as

$$\rho^0(x) = \frac{\sqrt{2\pi}}{4}(2+\cos(2\pi x)), \quad \text{and } f^0(x,v) = \rho^0(x)M(v) \tag{4.11}$$

to satisfy $0 \leq f \leq 1$. The electrical field E is obtained through the Poisson equation $-\nabla_x E = \rho - h$ with h given by (4.3). Again we compare the asymptotic error (4.6) with $\mathcal{Q}$ replaced by $\mathcal{Q}_{deg}$ for different orders of ϵ. As in the non-degenerate anisotropic case, the error is first dominated by ϵ and then by $\triangle t^\beta$ when ϵ is small enough, which is the same as was shown in section 3.3 (in section 3.3, β is shown to be 1, but numerically we get better results with $\beta > 1$), see Figure 4 where $\triangle t = 3.9063e-4$.

- Mixing scales

To test the ability of our scheme for mixing scales, consider ϵ taking the following form:

$$\epsilon(x) = \begin{cases} \epsilon_0 + \frac{1}{2}(\tanh(5-10x)+\tanh(5+10x)) & x \leq 0.3; \\ \epsilon_0 & x > 0.3, \end{cases} \tag{4.12}$$

where $\epsilon_0 = 0.001$ so that it contains both the kinetic and high field regimes, see Figure 5. The initial condition is taken to be

$$f^0(x) = \frac{1}{6}(2+\sin(\pi x))e^{-\frac{1}{2}v^2}. \tag{4.13}$$

Consider the anisotropic scattering where $\phi(v,v')$ is taken the same form as in (4.5). E is calculated through the Poisson equation (1.7) with h given by (4.3). We use the second order Runge-Kutta time discretization with the MUSCL scheme on a refined mesh to get the reference solution. Good agreements of these two solutions can be observed in Figure 6.

4.4 The electron-phonon interaction model

In this section, we consider a physically more realistic model, the electron-phonon interaction model, where the transition probability is

$$s(v,v') = K_0\delta\left(\frac{v'^2}{2}-\frac{v^2}{2}\right) + K\left[(n_q+1)\delta\left(\frac{v'^2}{2}-\frac{v^2}{2}+\hbar\omega_p\right) + n_q\delta\left(\frac{v'^2}{2}-\frac{v^2}{2}-\hbar\omega_p\right)\right], \tag{4.14}$$

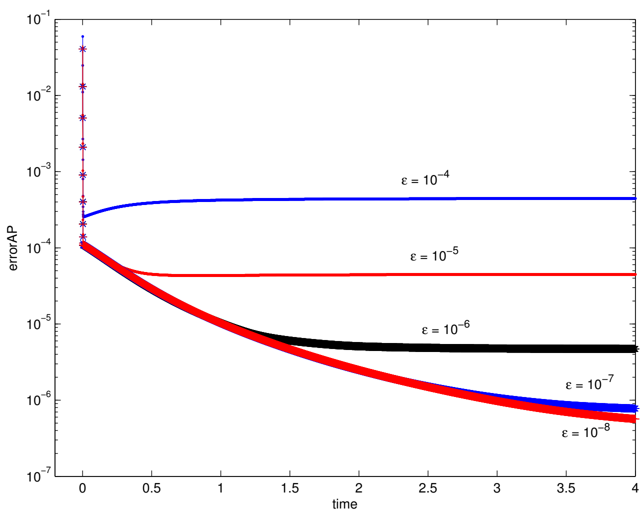

Figure 4: The degenerate isotropic model coupled with the Poisson equation. The time evolution of asymptotic error (4.6) with $\mathcal{Q}$ replaced by $\mathcal{Q}_{deg}$ for different ϵ with nonequilibrium initial data using the first order scheme in section 3.1.

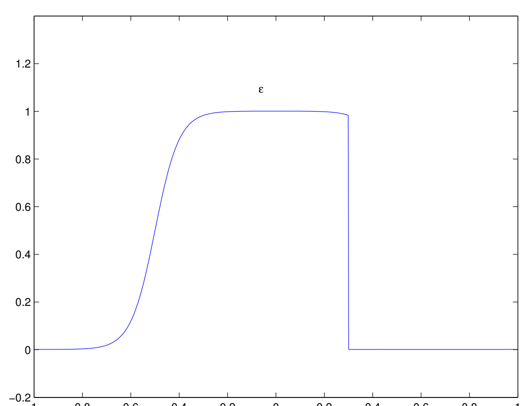

Figure 5: ϵ defined in (4.12).

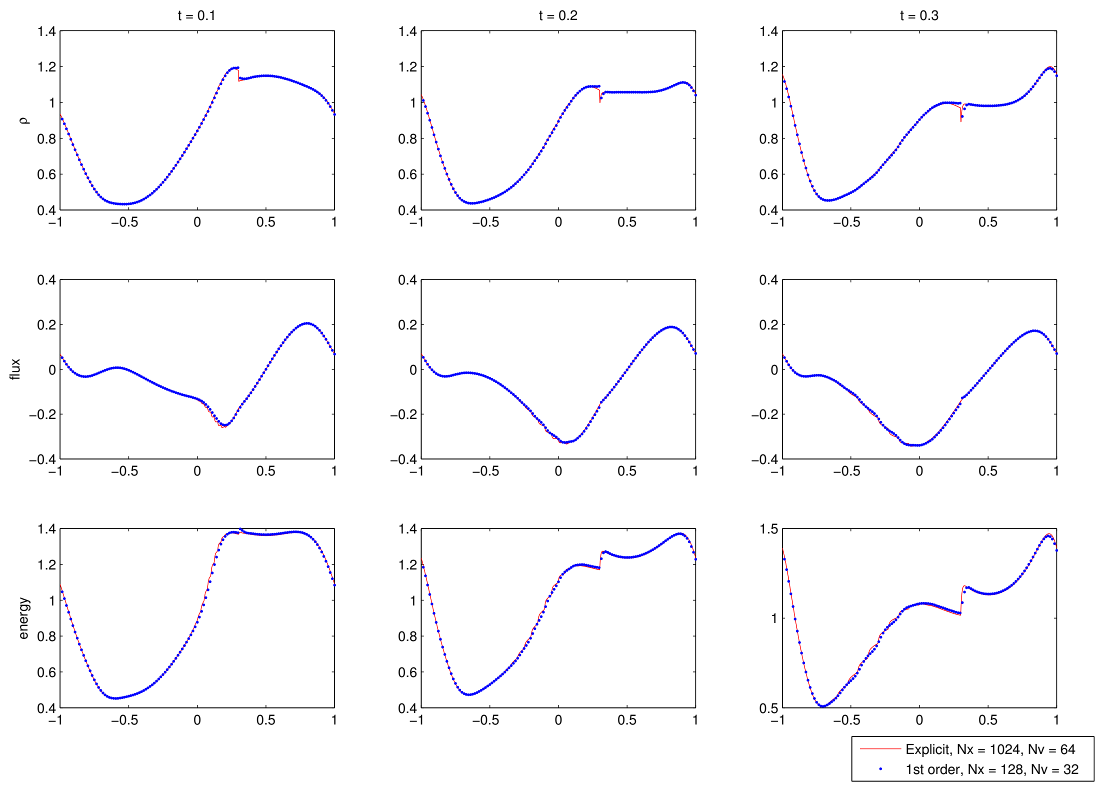

Figure 6: The degenerate anisotropic model coupled with the Poisson equation. Consider the mixing regimes with ϵ given in (4.12). Compare the first order scheme (3.2) on coarse mesh with an explicit method on refined mesh. We plot the macroscopic density, flux and energy at different times.

and n_q given by $n_q = \frac{1}{e^{\frac{\hbar\omega_p}{K_B T_L}}-1}$ is the occupation number of phonons. Here $\hbar$ is the planck constant, K_B is the Boltzmann constant, ω_p is the constant phonon frequency, T_L is the lattice temperature, K and K_0 are two constants for the material.

The singular nature of $s(v, v')$ makes the collision hard to compute numerically, but the cylindrical symmetry of s makes it possible to use polar coordinates so that the singularity in the delta function can be removed and the dimension of integral can be decreased by one [5, 6, 8]. However, this trick is not easy to be implemented here since we treat the stiff force term implicitly, and changing to polar coordinates will make it harder to invert. Instead, we use the spectral method [25] which can also remove the singularity.

In this numerical example, assume $d_x = 1$ and $d_v = 2$. Recall that the collision (1.3) can be written as

$$Q = Q^+(f)(t,x,v) - \nu(v)f(t,x,v). \tag{4.15}$$

Similar to [25], we restrict f on the domain $D_v = [-L_v, L_v]^2$ and extend it periodically to the whole domain. L_v is chosen such that the support of f is $\text{supp}(f) \subset B(0,R) = B_R$ and $L_v = 2R$. Approximate f by truncated Fourier serious

$$f(v) \approx \sum_{k=-Nv/2+1}^{N_v/2} \hat{f}_k e^{i\frac{\pi}{L_v}k\cdot v}, \qquad \hat{f}_k = \frac{1}{(2L_v)^2}\int_{D_v} f(v)e^{-i\frac{\pi}{L_v}k\cdot v}dv, \tag{4.16}$$

then $Q^+(f)$ is computed as follows

$$\begin{aligned} Q^+(f) &= \int_{B_R} S(v',v)f(t,x,v')dv' \\ &= \sum_{k=-Nv/2+1}^{N_v/2} \hat{f}_k \int_{B_R} e^{i\frac{\pi}{L_v}k\cdot v'}\left[(n_q+1)K\delta\left(\frac{1}{2}v^2 - \frac{1}{2}v'^2 + \hbar w_p\right)\right. \\ &\qquad \left. + n_q K\delta\left(\frac{1}{2}v^2 - \frac{1}{2}v'^2 - \hbar w_p\right) + K_0\delta\left(\frac{1}{2}v^2 - \frac{1}{2}v'^2\right)\right] dv'. \end{aligned} \tag{4.17}$$

Let $\xi' = \frac{1}{2}v'^2$, then change of variable $v' = \sqrt{2\xi'}(\cos\theta', \sin\theta')$ leads to

$$\begin{aligned} Q^+(f) &= \sum_{k=-Nv/2+1}^{N_v/2} \hat{f}_k \left[(n_q+1)K\int_0^{2\pi} e^{i|k|\sqrt{2(\xi+\hbar w_p)}\cos\theta'\frac{\pi}{L_v}}d\theta' \chi_{\xi+\hbar w_p\le\frac{1}{2}R^2}\right. \\ &\qquad + n_q K\int_0^{2\pi} e^{i|k|\sqrt{2(\xi-\hbar w_p)}\cos\theta'\frac{\pi}{L_v}}d\theta' \chi_{0\le\xi-\hbar w_p\le\frac{1}{2}R^2} \\ &\qquad \left. + K_0\int_0^{2\pi} e^{i|k|\sqrt{2\xi}\cos\theta'\frac{\pi}{L_v}}d\theta' \chi_{\xi\le\frac{1}{2}R^2}\right] \\ &= \sum_{k=-Nv/2+1}^{N_v/2} \hat{f}_k B(|k|,|v|), \end{aligned} \tag{4.18}$$

with

$$\begin{aligned} B(|k|,|v|) &= 2\pi\left[(n_q+1)KJ_0\left(\sqrt{2(\xi+\hbar w_p)}|k|\frac{\pi}{L_v}\right)\chi_{\xi+\hbar w_p\le\frac{1}{2}R^2}\right. \\ &\quad \left. + Kn_qJ_0\left(\sqrt{2(\xi-\hbar w_p)}|k|\frac{\pi}{L_v}\right)\chi_{0\le\xi-\hbar w_p\le\frac{1}{2}R^2} + K_0J_0\left(\sqrt{2\xi}|k|\frac{\pi}{L_v}\right)\chi_{\xi\le\frac{1}{2}R^2}\right], \end{aligned} \tag{4.19}$$

where J_0 is the Bessel function of order 0

$$J_0(\alpha) = \frac{1}{2\pi}\int_0^{2\pi} e^{i\alpha\cos\theta}d\theta.$$

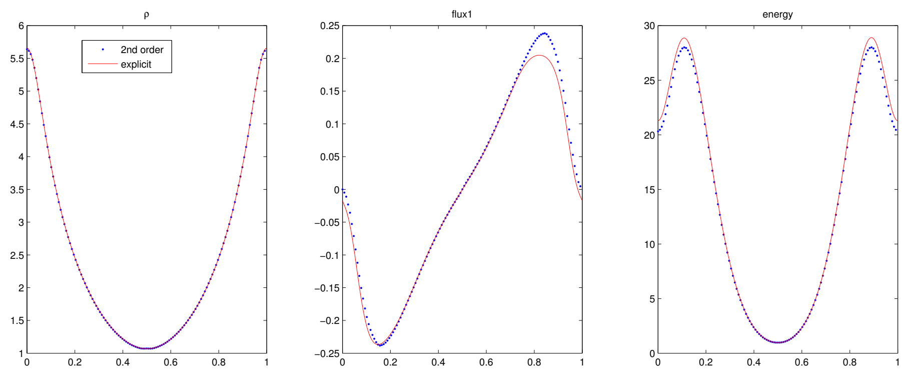

Figure 7: The macroscopic quantities for the electron-phonon interaction model with smooth initial data (4.2) and $\epsilon = 10^{-3}$: mass density (ρ), fluxes in v_1 (flux1) and v_2 (flux2) directions, and energy at time $T = 0.2$. $\epsilon = 10^{-3}$. Solid line: explicit method with $N_x = 1024$, $N_v = 32$. Dots: second order scheme (3.24) with $N_x = 128$, $N_v = 32$.

In the same way, the collision frequency $\nu(v)$ can be computed as

$$\begin{aligned}\nu(v) &= \int_{B(0,L_v)} s(v,v')dv \\ &= 2\pi\left[K(n_q+1)\chi_{0\le\xi-\hbar w_p\le\frac{1}{2}R^2} + Kn_q\chi_{\xi+\hbar w_p\le\frac{1}{2}R^2} + K_0\chi_{\xi\le\frac{1}{2}R^2}\right]. \qquad (4.20)\end{aligned}$$

Now let $L_v = 8$, $x \in [0,1]$, $K_BT_L = \frac{1}{2}$, $\hbar w_p = 1$, $K = 0$, and $K_0 = 1/5\pi$. Then the $2D$ Maxwellian is $M = \frac{1}{\left(\sqrt{\frac{\pi}{2K_BT_L}}\right)^2} e^{-\frac{v^2}{2K_BT_L}} = \frac{1}{\pi}e^{-v^2}$. We test two situations. One is for the pure high field regime with fixed $\epsilon = 10^{-3}$ and the initial data taking the form of (4.2) with M replaced by $\frac{1}{\pi}e^{-v^2}$. The macroscopic quantities at time $t = 0.2$ are given in Figure 7. The other is for mixing regimes problem, as ϵ defined the same as (4.12) but on the space interval $[0,1]$ and initial condition taken (4.13). To get better accuracy, we use (3.24) and choose $\lambda = \max_v \nu(v)$ in this case which does not violate the stability constraint. See Figure 8 for the time evolution of the macroscopic quantities. The reference solution is calculated by the forward Euler method with second order slope limiter method for space discretization on a much finer mesh.

It can be checked that the collision frequency (4.20) meets the condition (2.10), but $\phi(v,v') = \frac{s(v,v')}{M(v')}$ does not belong to $W^{1,\infty}(\mathbb{R}^4)$ as assumed in Theorem 1. To the authors' knowledge, no result is available numerically or analytically for the existence of the high field limit in this situation. From our numerical experiment, it seems to indicate that in this case, the solution does exist since our schemes capture it well in Figure 8. This is the first attempt to treat this problem in the high field regime, and we would like to put the designing of a fast efficient scheme in the future as well as the approximation of the runaway phenomenon that might be generated in this case.

5 Conclusion

Asymptotic-preserving numerical schemes for the semiconductor Boltzmann equation efficient in the high field regime have been introduced in this paper. One main difficulty in this problem is that there is no explicit form for the local equilibrium, which is the basic component of the classical asymptotic preserving methods. Our main idea is to penalize the collision term by a BGK operator – which is not the local equilibrium of the high field limit – and treat the stiff force term implicitly by the spectral method. The schemes are designed for both the nondegenerate (isotropic and anisotropic cases) and the degenerate case. We show that these methods have the desired asymptotic properties, and can be efficiently implemented with a uniform (in the

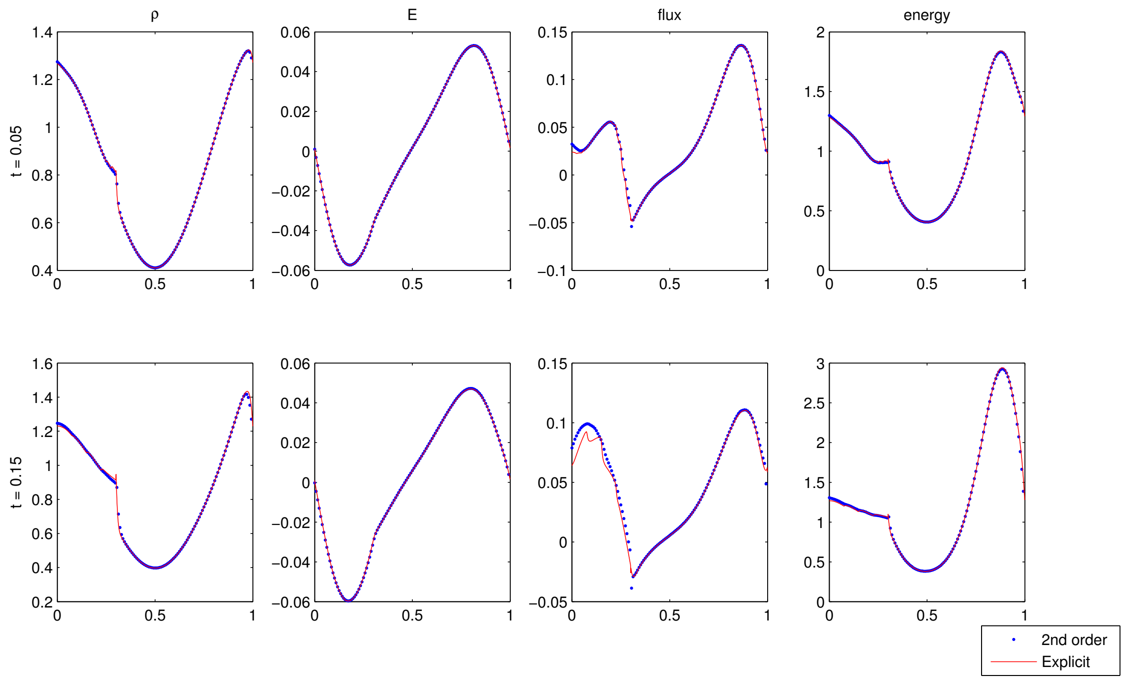

Figure 8: The time evolution of macroscopic quantities in electron-phonon interaction model in mix regimes (4.12) with initial data (4.13): mass density, electric field, flux in v_1 direction, and energy. Solid line: an explicit method with $N_x = 1024$, $N_v = 32$. Dots: the second order scheme (3.24) with $N_x = 128$, $N_v = 32$.

small parameter) stability. Numerical experiments also demonstrate the accuracy and the correct asymptotic behavior of these schemes.

Acknowledgements.
The second author would like to especially thank Dr. Bokai Yan, Prof. Francis Filbet and Dr. Jingwei Hu for fruitful discussions.

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