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Discretization of the Multiscale Semiconductor Boltzmann Equation by Diffusive Relaxation Schemes

Shi Jin* and Lorenzo Pareschi*,†

*School of Mathematics, Georgia Institute of Technology, Atlanta, Georgia 30332-0160;
†Department of Mathematics, University of Ferrara, via Machiavelli 35, 44100 Ferrara, Italy
E-mail: jin@math.gatech.edu, pareschi@dm.unife.it

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In this paper we derive diffusive relaxation schemes for the linear semiconductor Boltzmann equation that work in both the kinetic and diffusive regimes. Similar to our earlier approach for multiscale transport equations, we use the even- and odd-parity formulation of the kinetic equation, and then reformulate it into the diffusive relaxation system (DRS). In order to handle the implicit anisotropic collision term efficiently, we utilize a suitable power series expansion based on the Wild sum, which yields a time discretization uniformly stable with any desired order of accuracy, yet is explicitly solvable with the correct drift-diffusion limit. The velocity discretization is done with the Gauss–Hermite quadrature rule equivalent to a moment expansion method. Asymptotic analysis and numerical experiments show that the schemes have the usual advantages of a diffusive relaxation scheme for multiscale transport equations and are asymptotic-preserving.

Key Words: semiconductor Boltzmann equation; drift-diffusion limit; diffusive relaxation schemes; Wild sums.

1. INTRODUCTION

Kinetic equations for highly integrated semiconductor devices have a diffusive scaling, measured by the mean free path, that lead asymptotically to the drift-diffusion equations as the mean free path goes to zero [Pou, MRS]. In practical applications, there is necessity to conduct numerical simulations in both resolved (when spatial grid size is smaller than the mean free path) and the underresolved (when spatial grid size is larger than the mean free path) regimes. In the former case, standard numerical methods for kinetic equations work effectively. In the latter case, one expects that the best possible numerical resolution is the approximation of the drift diffusion equation. However, even to achieve this goal is

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nontrivial for standard numerical methods applicable to the kinetic equations. In addition to the difficulty of numerical stiffness arising due to the small scaling, improper underresolved numerical solution often fail to capture the hydrodynamic drift-diffusion limit. Earlier study on numerical methods for transport or kinetic equations indicates that, in order for the underresolved numerical approximation to capture the correct diffusive behavior, the scheme should be *asymptotic preserving* (AP), in the sense that the asymptotic limit that leads from the transport or kinetic equations to the diffusion equations should be preserved at the discrete level [Ada, Jin, JL1, JL2, JPT1, JPT2, Kl1, Kl2, LMM, LM, Mil, NP1, NP2].

In an earlier work on discrete-velocity models [JPT] we handled this challenging numerical problem by reformulating the system into a form commonly used for a relaxation scheme for conservation laws [JX]. Such a reformulation allows us to use the splitting technique for relaxation schemes to design a class of implicit, yet *explicitly implementable*, schemes that work with high resolution uniformly with respect to the mean free path. Such a numerical technique was extended to general transport equations with isotropic collision kernels, by using parity formulation of the transport equation [JPT2].

Let ϵ be the dimensionless mean free path. The diffusive relaxation schemes, developed in [JPT1, JPT2] for kinetic and transport equations, have have the following features:

- they have an ϵ-independent ($\varepsilon \ll 1$), parabolic CFL condition $\Delta t \approx (\Delta x)^2$;
- the schemes, though implicit in the collision terms, can be implemented explicitly;
- they are asymptotic preserving (AP);
- they have a uniform accuracy with respect to ϵ.

In this paper, we will derive diffusive relaxation schemes for the linear semiconductor Boltzmann equation. Such a problem differs from those studied in [JPT2] in two aspects. First, this equation involves a derivative in the velocity, which requires a suitable velocity discretization. Here, as was previously done, we will use the Hermite quadrature rule [Ch, Kl2] which is equivalent to a moment expansion method [SZ, RSZ]. The main obstacle, however, is due to the anisotropic collision kernel. Since the diffusive relaxation schemes are implicit in the collision term, in this case, it becomes challenging to invert numerically the anisotropic collision term in an efficient way.

To this aim we utilize a power series expansion (a generalized Wild sum [Wil]), which has been used for nonlinear kinetic equation in the Euler scaling by Gabetta *et al*. [GPT]. A class of numerical schemes is derived by replacing the high order terms in the Wild sum by a Maxwellian, i.e., relaxing them to equilibrium.

Applying that to the diffusive relaxation system allows us to have an implicit time discretization for anisotropic collision that is uniformly stable with respect to the mean free path, is asymptotic-preserving, yet can be solved *explicitly*.

We mention here other approaches to the numerical solution of the semiconductor Boltzmann equation based on hydrodynamic models [ARR], spherical harmonics expansions [VGBO], and particle simulations [DD].

The rest of the paper is organized as follows. In Section 2 we present the kinetic semiconductor equation and its drift-diffusion limit. In Section 3 we formulate it into the parity systems and then the diffusive relaxation system. We then use the standard splitting method for such problem, which decouples the explicit convection step from the implicit relaxation step. In order to efficiently solve the implicit anisotropic collision term, in Section 4 we use the Wild sum and show that it has the desired properties. Section 5 discusses the

moment expansion method with the Hermite quadrature rule and the spatial discretization. In Section 6 some numerical examples are presented. We conclude in Section 7.

2. THE EQUATION AND ITS DRIFT-DIFFUSION LIMIT

We consider the linear Boltzmann equation for semiconductor devices under the diffusive scaling. Let $f(t, \mathbf{x}, \mathbf{v})$ be the probability density distribution for particles at space point $\mathbf{x} \in \mathbb{R}^d$ traveling with velocity $\mathbf{v} \in \mathbb{R}^d$, where $d = 1, 2, 3$ is the dimension, at time $t \geq 0$. f solves the kinetic equation [MRS]

$$\epsilon \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \frac{q}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}} f = \frac{1}{\epsilon} \mathbf{Q}(f) + \epsilon G. \tag{2.1}$$

In (2.1), $G = G(t, \mathbf{x}, \mathbf{v})$ is a source term that models the generation-recombination process, ϵ is the mean free path, $\mathbf{E} = -\nabla_{\mathbf{x}} \Phi(\mathbf{x}, t)$ is the electric field, with Φ the electric potential, and $\mathbf{Q}(f)$ is the anisotropic collision term defined by

$$\mathbf{Q}(f) = \int \sigma(\mathbf{v}, \mathbf{w}) \{M(\mathbf{v}) f(\mathbf{w}) - M(\mathbf{w}) f(\mathbf{v})\} \, d\mathbf{w},$$

where M is the normalized Maxwellian at the temperature $\theta/2$ of the semiconductor

$$M(\mathbf{v}) = \frac{1}{(\pi\theta)^{d/2}} \exp\left(-\frac{|\mathbf{v}|^2}{\theta}\right).$$

The constants q and m are the elementary charge and the effective mass of the electron, respectively. In this problem, the anisotropic scattering kernel σ is rotationally invariant and satisfies

$$\sigma(\mathbf{v}, \mathbf{w}) = \sigma(\mathbf{w}, \mathbf{v}) > 0.$$

This positivity assumption means that the collision operator is a regularized version of the physically relevant models.

We also assume that the collision frequency λ satisfies the following bound for some positive constant μ

$$\lambda(\mathbf{v}) = \int \sigma(\mathbf{v}, \mathbf{w}) M(\mathbf{w}) \, d\mathbf{w} \leq \mu. \tag{2.2}$$

The collision operator is bounded and nonnegative on a suitable Hilbert space H [Pou]. It has a one-dimensional kernel spanned by M.

Now let $h_i \in H$ be the unique solution to the problem

$$Q(h_i)(\mathbf{v}) = v_i M(\mathbf{v}), \qquad \int h_i(\mathbf{v}) \lambda(\mathbf{v}) \, d\mathbf{v} = 0, \qquad i = 1, \ldots, d.$$

Since σ is rotationally invariant, it follows that there is a positive constant D such that

$$\int v_i h_i(\mathbf{v}) \, d\mathbf{v} = D, \qquad i - 1, \ldots, d. \tag{2.3}$$

As $\epsilon \to 0$, one can show that $f(\mathbf{x}, \mathbf{v}, t)$ is approximated by $\rho(\mathbf{x}, t)M(\mathbf{v})$, where

$$\rho = \int f(\mathbf{v})\, d\mathbf{v}$$

satisfies the drift-diffusion equation [Pou, MRS]

$$\partial_t \rho = \nabla_{\mathbf{x}} \cdot (D\nabla_{\mathbf{x}}\rho + \eta\rho\mathbf{E}) + \tilde{G}. \tag{2.4}$$

In (2.4), D is the diffusion coefficient defined implicitly in terms of the cross section by (2.3), η is the mobility given by the Einstein relation $D = \eta m\theta/q$, and

$$\tilde{G}(x, t) = \int G(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{v}.$$

Remark 1. This drift-diffusion approximation can also be derived using the so-called even- and odd-parities, which gives the drift-diffusion equation in the leading order. This will be demonstrated in Section 3. To simplify notations, in the sequel we will always assume $q = m = \theta = 1$, hence $\eta = D$.

3. PARITY EQUATIONS AND DIFFUSIVE RELAXATION SYSTEM

We will derive in this section the diffusive relaxation system that corresponds to (2.1). To this aim we will make use of the even- and odd-parities formalism.

3.1. Parity equations. First, (2.1) is split into two equations, one for $\mathbf{v}$ and one for $-\mathbf{v}$,

$$\begin{aligned} \epsilon\partial_t f + \mathbf{v}\cdot\nabla_{\mathbf{x}} f - \mathbf{E}\cdot\nabla_{\mathbf{v}} f &= \frac{1}{\epsilon}Q(f) + \epsilon G, \\ \epsilon\partial_t f - \mathbf{v}\cdot\nabla_{\mathbf{x}} f + \mathbf{E}\cdot\nabla_{\mathbf{v}} f &= \frac{1}{\epsilon}Q(f) + \epsilon G. \end{aligned} \tag{3.1}$$

Next, introduce the even parity r and the odd parity j,

$$\begin{aligned} r(t, \mathbf{x}, \mathbf{v}) &= \frac{1}{2}[f(t, \mathbf{x}, \mathbf{v}) + f(t, \mathbf{x}, -\mathbf{v})], \\ j(t, \mathbf{x}, \mathbf{v}) &= \frac{1}{2\epsilon}[f(t, \mathbf{x}, \mathbf{v}) - f(t, \mathbf{x}, -\mathbf{v})]. \end{aligned}$$

Adding and subtracting the two equations in (3.1) lead to

$$\begin{aligned} \partial_t r + \mathbf{v}\cdot\nabla_{\mathbf{x}} j - \mathbf{E}\cdot\nabla_{\mathbf{v}} j &= \frac{1}{\epsilon^2}Q(r) + G, \\ \partial_t j + \tfrac{1}{\epsilon^2}(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \mathbf{E}\cdot\nabla_{\mathbf{v}} r) &= -\frac{1}{\epsilon^2}\lambda j, \end{aligned} \tag{3.2}$$

where we used the property that

$$\int \sigma(\mathbf{v}, \mathbf{w})\, j(\mathbf{w})\, d\mathbf{w} = 0,$$

since j is an odd function.

Note that the macroscopic variables mass ρ and mean velocity u can be expressed in terms of the new variables r and j using the identities

$$\begin{aligned} \rho &= \int f(\mathbf{v})\, d\mathbf{v} = \int r(\mathbf{v})\, d\mathbf{v}, \\ u &= \frac{1}{\epsilon\rho} \int f(\mathbf{v})\mathbf{v}\, d\mathbf{v} = \frac{1}{\rho} \int j(\mathbf{v})\mathbf{v}\, d\mathbf{v}. \end{aligned} \tag{3.3}$$

Remark 2. Since for all linear isometric mappings R we have

$$\sigma(R(\mathbf{v}), R(\mathbf{w})) = \sigma(\mathbf{v}, \mathbf{w}),$$

it is also possible to define the even and odd parities only for the positive components of $\mathbf{v}$ and $\mathbf{w}$ as in [JPT2].

3.2. Diffusive relaxation system. Now, as was done in [JPT2], we rewrite (3.2) into the following diffusive relaxation system

$$\begin{aligned} \partial_t r + \mathbf{v}\cdot\nabla_{\mathbf{x}} j - \mathbf{E}\cdot\nabla_{\mathbf{v}} j &= \frac{1}{\epsilon^2} Q(r) + G, \\ \partial_t j + \phi(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \mathbf{E}\cdot\nabla_{\mathbf{v}} r) &= -\frac{1}{\epsilon^2}[\lambda j + (1-\epsilon^2\phi)(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \mathbf{E}\cdot\nabla_{\mathbf{v}} r)], \end{aligned} \tag{3.4}$$

where $\phi = \phi(\epsilon)$ is a control parameter such that $0 \le \phi \le 1/\epsilon^2$. This restriction on ϕ guarantees the positivity of r and $1-\epsilon^2\phi$ so the splitting below remains well-posed uniformly in ϵ [JPT1, JPT2]. The simplest choice of ϕ is

$$\phi(\epsilon) = \min\left\{1, \frac{1}{\epsilon^2}\right\}. \tag{3.5}$$

The advantage of (3.4) is that it allows us to use the conventional splitting employed for this type of system [JPT1, JPT2]. In particular, a natural splitting on (3.4) consists of one relaxation step

$$\begin{aligned} \partial_t r &= \frac{1}{\epsilon^2} Q(r) + G, \\ \partial_t j &= -\frac{1}{\epsilon^2}[\lambda j + (1-\epsilon^2\phi)(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - \mathbf{E}\cdot\nabla_{\mathbf{v}} r)], \end{aligned} \tag{3.6}$$

followed by the transport step

$$\begin{aligned} \partial_t r + \mathbf{v}\cdot\nabla_{\mathbf{x}} j - E\cdot\nabla_{\mathbf{v}} j &= 0, \\ \partial_t j + \phi(\mathbf{v}\cdot\nabla_{\mathbf{x}} r - E\cdot\nabla_{\mathbf{v}} r) &= 0. \end{aligned} \tag{3.7}$$

One can easily verify that this splitting possesses the correct drift-diffusion limit. As $\epsilon \to 0$, (3.6) gives

$$\begin{aligned} Q(r) &= 0, \\ \lambda j &= -\mathbf{v}\cdot\nabla_{\mathbf{x}} r + \mathbf{E}\cdot\nabla_{\mathbf{v}} r. \end{aligned} \tag{3.8}$$

Solving the first equation in (3.8) gives

$$r = \rho(\mathbf{x}, t)M(\mathbf{v}). \tag{3.9}$$

The second equation of (3.8) then gives

$$j = \frac{1}{\lambda(\mathbf{v})}[-\mathbf{v} \cdot \nabla_{\mathbf{x}}\rho + \rho\mathbf{v} \cdot \mathbf{E}]. \tag{3.10}$$

Applying (3.9) and (3.10) in the first equation of (3.7) and integrating over $\mathbf{v}$, one gets the drift diffusion equation (2.4).

Since the transport equations (3.7) contain no small parameter, it can be solved using an explicit upwind scheme on the diagonal form

$$\begin{aligned} \partial_t U + \sqrt{\phi}(\mathbf{v} \cdot \nabla_{\mathbf{x}} U - E \cdot \nabla_{\mathbf{v}} U) = 0, \\ \partial_t V - \sqrt{\phi}(\mathbf{v} \cdot \nabla_{\mathbf{x}} V - E \cdot \nabla_{\mathbf{v}} V) = 0, \end{aligned}$$

where $U = r + j/\sqrt{\phi}$ and $V = r - j/\sqrt{\phi}$

The collision step (3.6), however, needs to be solved by an implicit scheme in order to achieve a numerical stability independent of ϵ.

4. TIME DISCRETIZATIONS OF THE RELAXATION STEP

From the previous section it is clear that the main difficulty now is to solve the collision step (3.6) implicitly in an efficient way. After the splitting of the diffusive relaxation system, we need to solve the relaxation step (where we take $G = 0$ for notation convenience)

$$\begin{aligned} \partial_t r &= \frac{1}{\epsilon^2} Q(r), \\ \partial_t j &= -\frac{1}{\epsilon^2}[\lambda j + (1 - \epsilon^2\phi)D(r)], \end{aligned} \tag{4.1}$$

with

$$D(r) = \mathbf{v} \cdot \nabla_{\mathbf{x}} r - E \cdot \nabla_{\mathbf{v}} r.$$

The use of the backward Euler method in time as in [JPT2] leads to

$$\begin{aligned} \frac{r^* - r^n}{\Delta t} &= \frac{1}{\epsilon^2} Q(r^*) + G, \\ \frac{j^* - j^n}{\Delta t} &= -\frac{1}{\epsilon^2}[\lambda j^* + (1 - \epsilon^2\phi)D(r^*)]. \end{aligned} \tag{4.2}$$

To compute r^* from the first equation one needs to invert numerically the integral operator $Q(r^*)$. This can be done easily in the case of isotropic collision whereas in the case of anisotropic collision it requires a suitable numerical method at, in general, a prohibitively expansive computational cost.

Following the approach presented in [GPT] we will derive a robust implicit scheme, that is explicitly implementable, for system (4.1).

First, rewrite this system of equations in the form

$$\begin{aligned} \partial_t r &= \frac{1}{\epsilon^2}[P(r) - \mu r], \\ \partial_t j &= -\frac{1}{\epsilon^2}[\lambda j + (1-\epsilon^2\phi)D(r)], \end{aligned} \tag{4.3}$$

where

$$P(r) = Q(r) + \mu r.$$

From the definition of λ we have

$$P(r) = \int \sigma(\mathbf{v}, \mathbf{w}) M(\mathbf{v}) r(\mathbf{w})\, d\mathbf{w} + (\mu - \lambda) r(\mathbf{v}).$$

Since $\mu \geq \lambda$, and $r \geq 0$, $P(r)$ is a nonnegative operator.

By introducing the new variables

$$\tau = 1 - \exp(-\mu t/\epsilon^2), \qquad R = r \exp(\mu t/\epsilon^2),$$

the first equation in (4.1) becomes

$$\partial_\tau R = \frac{1}{\mu(1-\tau)} P(R), \qquad 0 < \tau < 1.$$

Expanding it in Taylor series and setting $r^{(0)}(\mathbf{v}) = r(\mathbf{v}, 0)$ we have

$$R(\mathbf{v}, \tau) = \sum_{k=0}^{\infty} \tau^k r^{(k)}(\mathbf{v}),$$

with

$$r^{(k+1)}(\mathbf{v}) = \frac{1}{k+1} \sum_{n=0}^{k} \frac{1}{\mu} P\left(r^{(n)}\right), \qquad k \geq 1. \tag{4.4}$$

Upon reverting to the old notations, one gets

$$r(\mathbf{v}, t) = (1-\tau) \sum_{k=0}^{\infty} \tau^k r^{(k)}(\mathbf{v}). \tag{4.5}$$

Since the equation for j is linear, using the previous expansion we can write

$$\begin{aligned} j(\mathbf{v}, t) &= \exp^{-\lambda t/\epsilon^2} j(\mathbf{v}, 0) - (1 - \exp^{-\lambda t/\epsilon^2})(1-\epsilon^2\phi)\frac{D(r(\mathbf{v}, t))}{\lambda} \\ &= (1-\tau)^{\lambda/\mu}\left(j(\mathbf{v}, 0) + (1-\epsilon^2\phi)\frac{D(r(\mathbf{v}, t))}{\lambda} \right) - (1-\epsilon^2\phi)\frac{D(r(\mathbf{v}, t))}{\lambda}. \end{aligned} \tag{4.6}$$

The previous power series expansion (4.4)–(4.5) was first introduced by Wild [Wil] for the nonlinear Boltzmann equation in the Maxwellian case.

Now as in [GPT], we can construct a class of asymptotic preserving schemes by truncating the previous expansion and replacing the high order terms with the corresponding local equilibrium state. This leads to the so-called *time relaxed* (TR) schemes for the variable r

$$r^* = (1-\tau)\sum_{k=0}^{m} \tau^k r^{(k)} + \tau^{m+1} r^{(\infty)},$$

where the local equilibrium state is defined by

$$r^{(\infty)} = \rho^* M = p^n M.$$

For example, the first-order TR scheme is given by

$$r^* = (1-\tau)r^n + \tau(1-\tau)\frac{P(r^n)}{\mu} + \tau^2 \rho^n M; \tag{4.7}$$

the corresponding value for j is then obtained by solving

$$j^* = (1-\tau)^{\lambda/\mu}\left(j^n + (1-\epsilon^2\phi)\frac{D(r^*)}{\lambda}\right) - (1-\epsilon^2\phi)\frac{D(r^*)}{\lambda}. \tag{4.8}$$

These schemes, as proved in the more general setting in [GPT, PR], are stable uniformly in ϵ and are explicitly implementable provided that the spatial derivative that appears in $D(r^*)$ is discretized using linear schemes. It is also easy to check that they preserve mass and positivity (i.e., if $r^{(n)} \geq 0$, then $r^{(n+1)} \geq 0$). Finally, if $\epsilon \to 0$, then $\tau \to 1$ and

$$r^* \to \rho^n M, \qquad j^* \to -\frac{D(\rho^n M)}{\lambda}.$$

Thus the schemes are asymptotic-preserving. Hence, when combined with an explicit solver for the transport step, the zero mean free path limit of the time discretization becomes an explicit time discretization of the limiting drift-diffusion equation, possessing the AP property.

Remark 3. More general schemes can be derived using the arguments presented in [PR]. In particular, as an alternative to the previous first order discretization, one can use the TR scheme (4.7) coupled with a backward Euler scheme (4.2) for j^*

$$j^* = \frac{\epsilon^2}{\epsilon^2 + \lambda\Delta t} j^n - \frac{\Delta t(1-\epsilon^2\phi)}{\epsilon^2 + \lambda\Delta t} D(r^*). \tag{4.9}$$

It is straightforward to check that this hybrid discretization is also asymptotic-preserving.

5. FULLY DISCRETE SCHEMES

In order to derive fully discrete schemes we must discuss the discretizations of the velocity and the space variable. Here for the sake of simplicity we will present only the one-dimensional schemes. The generalization to the multi-dimensional case can be done in a straightforward manner simply using dimension-by-dimension discretization.

5.1. Velocity discretization. The velocity discretization is performed using the Hermite polynomials. This technique was previously used by several authors [Ch, Kl2] and is equivalent to a moment method [SZ, RSZ].

Set $r = \varphi M$, $j = \psi M$, with

$$\varphi(v) = \sum_{k=0}^{N} \varphi_k \tilde{H}_k(v), \qquad \psi(v) = \sum_{k=0}^{N} \psi_k \tilde{H}_k(v), \tag{5.1}$$

being the Hermite expansion. Here $\tilde{H}_k$ are the renormalized Hermite polynomials defined as $\tilde{H}_{-1} = 0$, $\tilde{H}_0 = 1/\pi^{1/4}$, and

$$\tilde{H}_{j+1} = v\sqrt{\frac{2}{j+1}}\tilde{H}_j - \sqrt{\frac{j}{j+1}}\tilde{H}_{j-1},$$

which satisfies

$$\partial_v \tilde{H}_j = \sqrt{2j}\,\tilde{H}_{j-1}.$$

The inverse Hermite expansion gives

$$\varphi_k = \sum_{j=0}^{N} \varphi(v_j)\tilde{H}_k(v_j)w_j, \qquad \psi_k = \sum_{j=0}^{N} \psi(v_j)\tilde{H}_k(v_j)w_j,$$

where (v_j, w_j) are the points and weights of the Gauss–Hermite quadrature rule. For the collision operator, we have

$$\begin{aligned} Q(r)(v) &= M(v)\sum_{j=0}^{N} \sigma(v, v_j)\varphi(v_j)w_j - \lambda(v)r(v), \\ \lambda(v) &= \sum_{j=0}^{N} \sigma(v, v_j)w_j. \end{aligned} \tag{5.2}$$

Thus, the derivatives with respect to v become

$$\partial_v r = M\partial_v\varphi - 2vM\varphi, \qquad \partial_v j = M\partial_v\psi - 2vM\psi,$$

and can be evaluated using

$$\partial_v\varphi = \sum_{k=1}^{N} \varphi_k\sqrt{2k}\tilde{H}_{k-1}(v) = \sum_{j=0}^{N} \varphi(v_j)c_j(v) \tag{5.3}$$

with

$$c_j(v) = \sum_{k=1}^{N} \sqrt{2k}\tilde{H}_k(v_j)\tilde{H}_{k-1}(v)w_j.$$

Similarly,

$$\partial_v \psi = \sum_{j=0}^{N} \psi(v_j) c_j(v).$$

Clearly the coefficients $c_j(v_i) = c_{ij}$ can be computed and stored in a matrix since they do not depend on the functions φ and ψ.

Finally, using the new variables φ, ψ the 1D velocity discretized DRS reads

$$\partial_t \varphi + v\partial_x \psi - E\partial_v \psi + 2v\psi = \frac{1}{\epsilon^2}\tilde{Q}(\varphi) + \tilde{G},$$

$$\partial_t \psi + \phi(v\partial_x \varphi - E\partial_v \varphi + 2v\varphi) = -\frac{1}{\epsilon^2}(\lambda\psi + (1-\epsilon^2\phi)(v\partial_x \varphi - E\partial_v \varphi + 2v\varphi)),$$

where $G = M\tilde{G}$ and

$$\tilde{Q}(\varphi)(v) = \sum_{j=0}^{N} \sigma(v, v_j)\varphi(v_j) w_j - \lambda(v)\varphi(v).$$

5.2. Spatial discretization. During the convection step (3.7), as was done in [JPT2], we use the second-order upwind scheme with slope limiters, dimension-by-dimension, to discretize the space derivative of r. In the meantime, the spatial derivative of r that appears in (4.1) is approximated using central difference as in [JPT2]. This choice allows one to explicitly implement the scheme and provides second-order accuracy without spurious oscillations across a discontinuity.

The space discretization of the electric potential Φ can be performed by standard method [Kl2, SZ]. In particular, in the drift-diffusion limit it is possible to obtain an analogue of the Scharfetter–Gummel type discretization of the drift-diffusion equation [Mar].

In fact, since the time discretization presented in Section 4 is asymptotic-preserving, similar to the analysis of [JPT2, Kl2], it is straightforward to show that the combination of time and space discretizations give a consistent explicit scheme for the drift-diffusion limit when $\epsilon \to 0$ and the discretization parameters hold fixed. We omit the details.

5.3. Boundary conditions. In the general case we have to deal with boundary conditions with respect to the space variable. We will restrict here only to the case of inflow boundary conditions. For a discussion of other types of boundary conditions we refer to [RSZ].

For example in the one-dimensional situation, with $x \in]x_L, x_R[$, $v \in \mathbb{R}$, problem (2.1) is complemented with the boundary conditions for $v > 0$

$$f(t, x_L, v) = F_L(v), \qquad f(t, x_R, -v) = F_R(v),$$

where F_L and F_R are assigned nonnegative functions.

Similarly to [JPT2], to get a boundary condition for r and j, we use relations (for positive v only)

$$r + \epsilon j|_{x=x_L} = F_L, \qquad r - \epsilon j|_{x=x_R} = F_R. \tag{5.4}$$

When $\epsilon \ll 1$, a reasonable approximation of the second equation in (3.2) is

$$\lambda_j = -v\partial_x r + E\partial_v r. \tag{5.5}$$

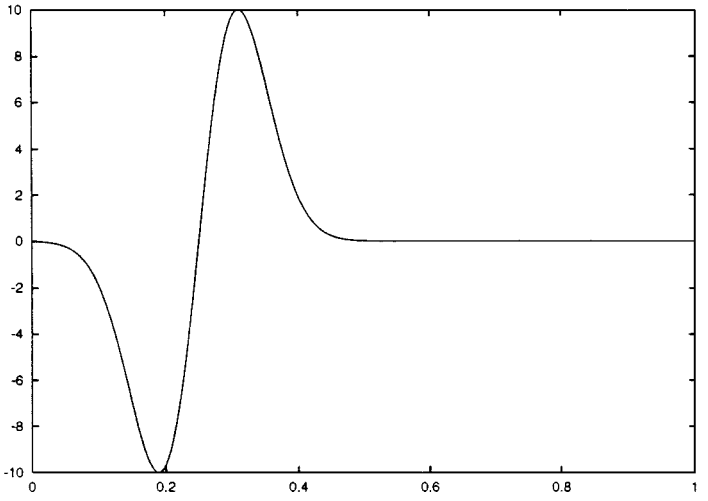

FIG. 1. The electric field E for Test 1.

Actually, (5.5) is exact for steady state solutions. Applying this in (5.4) one gets

$$r - \frac{\epsilon}{\lambda}(v\partial_x r - E\partial_v r)|_{x=x_L} = F_L, \qquad r + \frac{\epsilon}{\lambda}(v\partial_x r - E\partial_v r)|_{x=x_R} = F_R. \tag{5.6}$$

Thus by implementing (5.6) we get the desired boundary conditions. Other boundary conditions for time dependent problems have been developed in [Kl2].

Remark 4. A further approximation of the boundary conditions is obtained by observing that, from (5.4) we have

$$\partial_v r|_{x=x_L} = \partial_v F_L + O(\epsilon), \qquad \partial_v r|_{x=x_R} = \partial_v F_R + O(\epsilon),$$

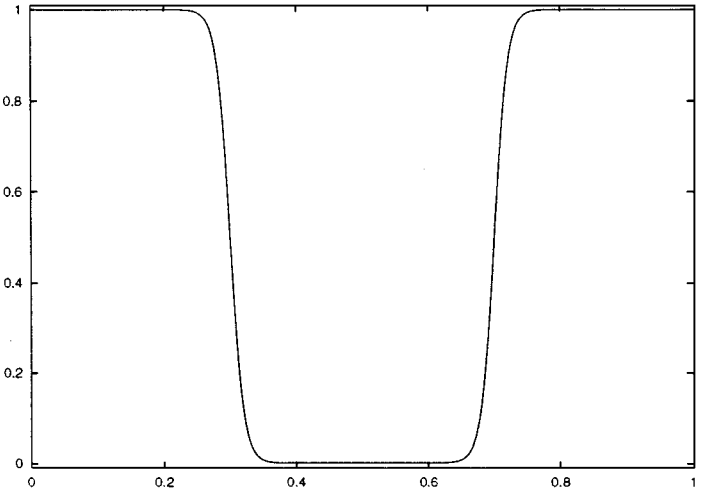

FIG. 2. The doping profile for Test 3.

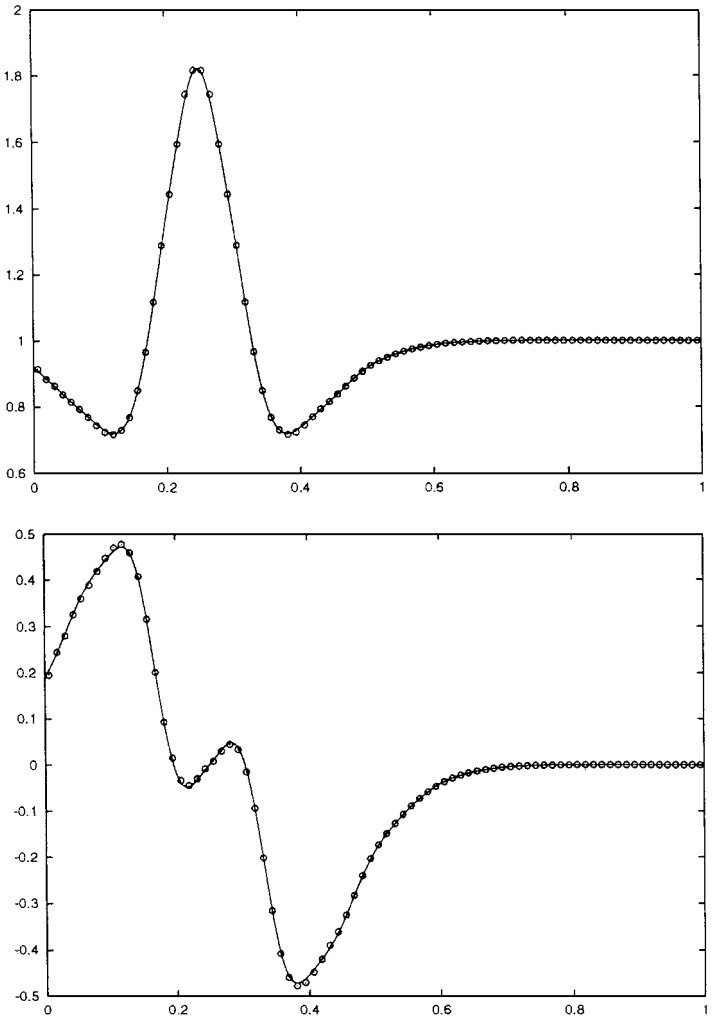

FIG. 3. Solution at $t = 0.08$ of Test 1 in the kinetic regime. Numerical solution is represented by circles, while the exact solution by solid lines. $\epsilon = 0.5$, $\Delta x = 0.0125$, and $\Delta t = 0.002$. Top, the mass density ρ; bottom, the mean velocity u.

and then up to $O(\epsilon^2)$

$$r - \frac{\epsilon}{\lambda}(v\partial_x r - E\,\partial_v F_L)|_{x=x_L} = F_L, \qquad r + \frac{\epsilon}{\lambda}(v\partial_x r - E\,\partial_v F_R)|_{x=x_R} = F_R. \quad (5.7)$$

This avoids the computation of $\partial_v r$ at the boundaries when $\partial_v F_L$ can be computed analytically.

6. NUMERICAL RESULTS

In this section, we present numerical results for several one-dimensional problems chosen to verify the performance of the schemes described above. In our computations we use two different scattering cross-sections. A simple isotropic case with a constant cross-section, $\sigma^{RTA}(\mathbf{v}, \mathbf{w}) = 1$, that corresponds to a relaxation time approximation (RTA) for which the

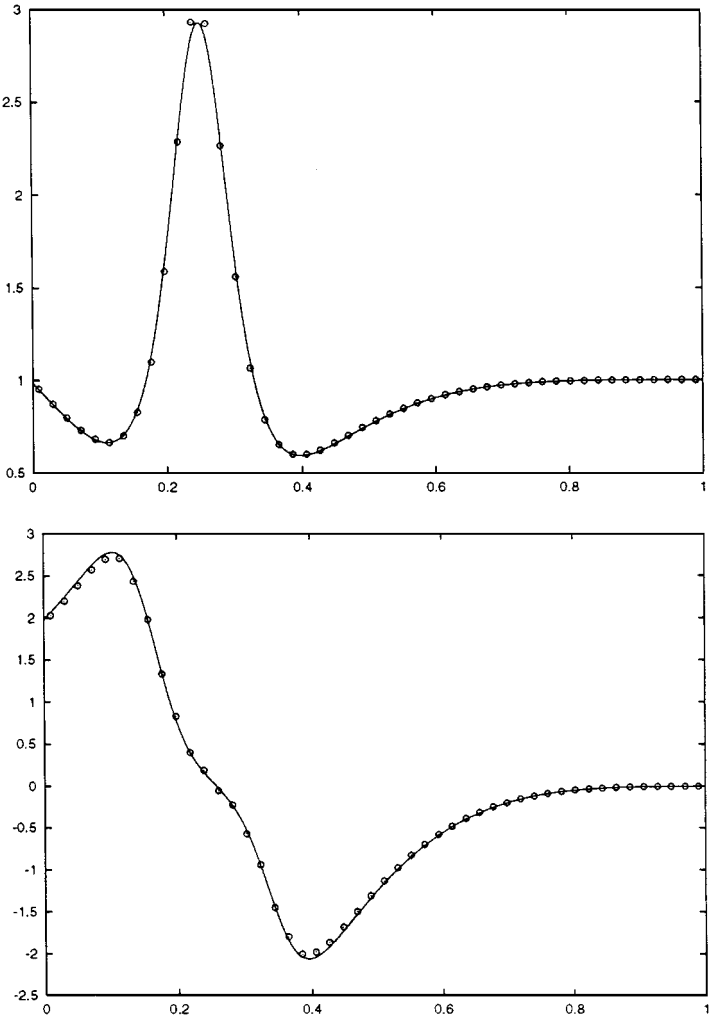

FIG. 4. Solution at $t = 0.03$ of Test 1 in the diffusive regime. Numerical solution is represented by circles, while the exact solution by solid lines. $\epsilon = 0.002$, $\Delta x = 0.02$, and $\Delta t = 5 \times 10^{-5}$. Top, the mass density ρ; bottom, the mean velocity u.

collision operator has the simple form $Q(f) = \rho(M - f)$, and regularized anisotropic cross section for electron–phonon interactions (EPI) of the form [MPS]

$$\sigma^{EPI}(\mathbf{v}, \mathbf{w}) = M(\mathbf{v})\tilde{\delta}(|\mathbf{v}|^2 - |\mathbf{w}|^2 + \omega) + M(\mathbf{w})\tilde{\delta}(|\mathbf{v}|^2 - |\mathbf{w}|^2 - \omega),$$

where $\tilde{\delta}(x) = \exp(-C|x|^2)$, $C \geq 1$, is a smoothed delta function and $\omega = 1$.

The boundary condition has been applied using a second-order implementation of Eqs. (5.6) and (5.7) based on central differences. In all the tests we have considered both approximations provide the same results. As usual, the reference solutions have been computed with very fine grids. The velocity discretization is done using the Gauss–Hermite discretization points with $N = 16$. For a numerical comparison of the influence of the number of quadrature points over the results we refer the reader to [Kl2]. The numerical results have been obtained using the scheme characterized by (4.7) and (4.8).

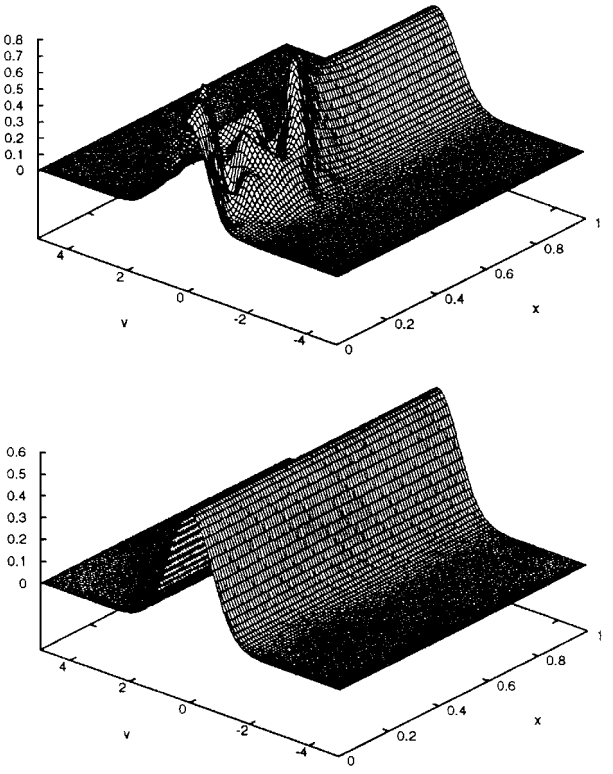

FIG. 5. Distribution function $f(x, v, t)$ for Test 1 on a grid of 100×100 points. Top, same data as in Fig. 3. Bottom, same data as in Fig. 4.

Remark 5. We point out that the second-order Runge–Kutta splitting developed in [CJR] cannot be applied directly with the time discretization defined by (4.7)–(4.8). Here we use the simple Strang splitting to achieve second-order accuracy in time in the non-stiff region. On the other hand for $\epsilon \ll 1$ and $D = O(1)$, we have a CFL condition of the type $\Delta t \approx (\Delta x)^2$ and hence second-order accuracy in time is not needed. A modified second-order Runge–Kutta splitting based on (4.7)–(4.8) which can handle the situation $\epsilon \ll 1$ and $D = O(\Delta x)$ is actually under study. However, in all our numerical tests $D \gg \Delta x$ and hence uniform second-order accuracy is guaranteed.

We shall consider several transport problems in slab geometry. Both transient as well as steady state solutions will be presented.

Test **1**,

$$x \in [0, 1], \qquad F_L(v) = M(v), \qquad F_R(v) = M(v),$$
$$G = 0, \qquad \Phi = \exp(-c(1/4 - x)^2), \qquad \epsilon = 0.5, 0.002,$$

with $c = 50 \exp(1)$.

The initial distribution is $f(x, v, t = 0) = M(v)$. In this problem we have a potential well in the left half of the slab with a maximum electric field equal to 10 (see Fig. 1). We consider only the RTA model. The numerical results for the mass density and the mean velocity, at $t = 0.1$ for $\epsilon = 0.5$ using 50 grid points, are reported in Fig. 3. This is a nonequilibrium solution in the kinetic regime. Next in Fig. 4 we report the results obtained for $\epsilon = 0.002$ at

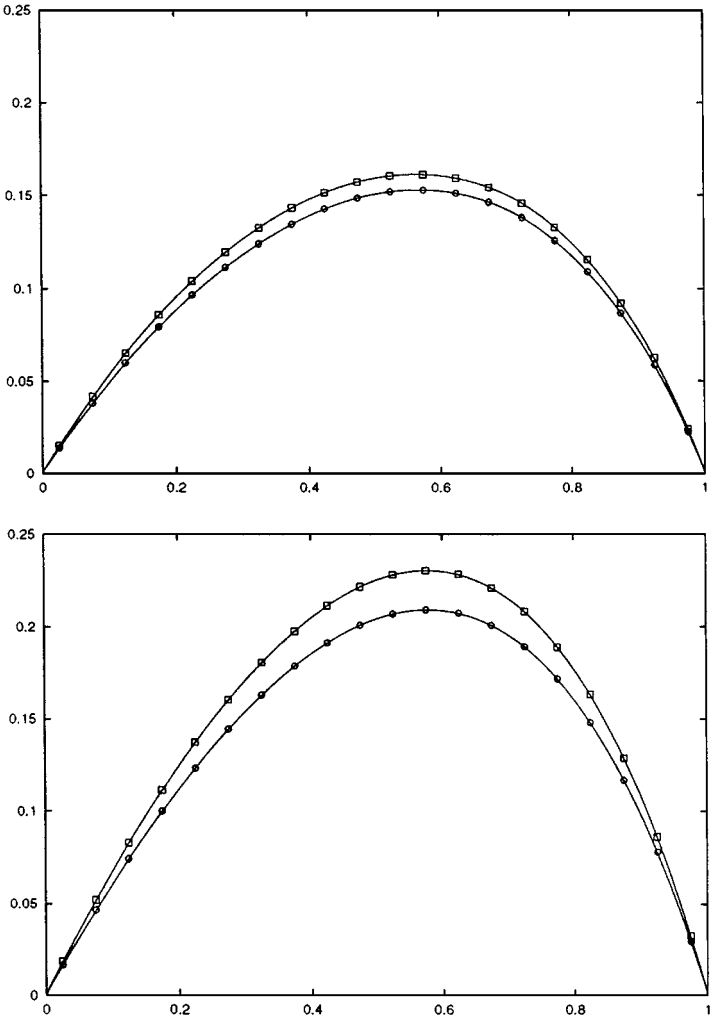

FIG. 6. Solution at $t = 0.2$ (top) and $t = 0.4$ (bottom) of Test 2. Numerical solution is represented by circles (RTA model) and squares (EPI model) while the exact solution by solid lines. $\epsilon = 0.001$, $\Delta x = 0.05$, and $\Delta t = 0.0001$.

$t = 0.03$ using the same grid points. In this case every cell contains 10 mean free path. The results clearly show that the scheme is able to capture the correct diffusive behavior even when $\Delta t, \Delta x \gg \epsilon$.

Finally the corresponding behavior of the distribution function $f(x, v, t)$ using a 100×100 grid obtained by reconstructing the velocity distribution through the Hermite interpolation is shown in Fig. 5.

Test **2**,

$$x \in [0, 1], \qquad F_L(v) = 0, \qquad F_R(v) = 0,$$
$$G = 1, \qquad \Phi = -x, \qquad \epsilon = 0.001.$$

The initial distribution is $f(x, v, t = 0) = 0$. The system consists of a diffusive slab with a flat interior source and a constant electric field equal to 1. In this test we compare the

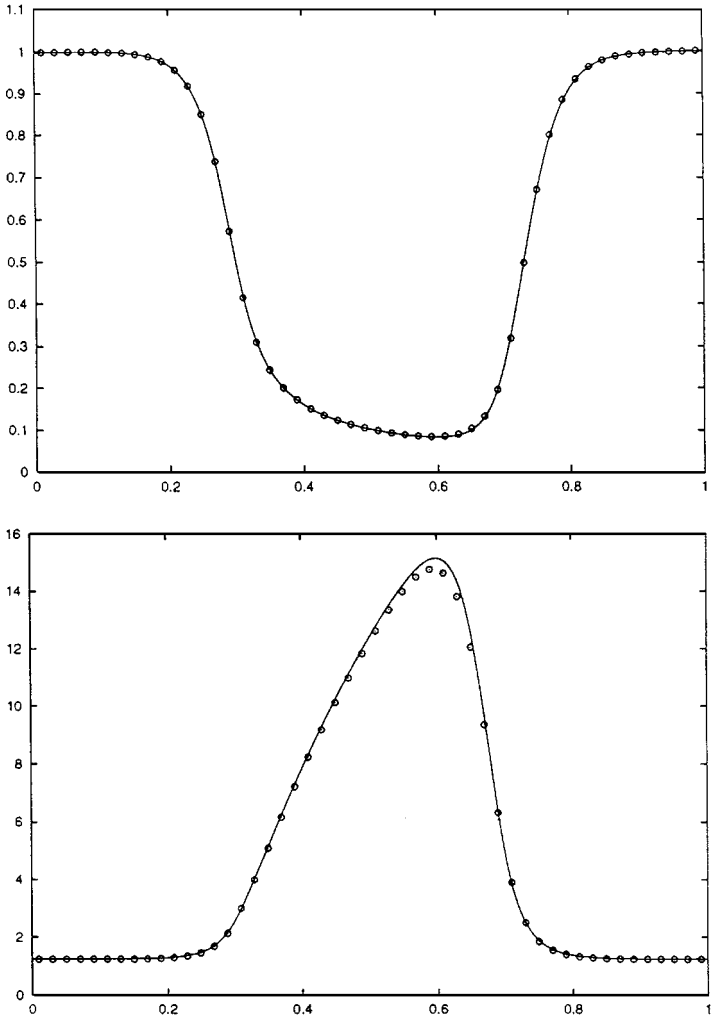

FIG. 7. Solution at $t = 0.05$ of Test 3. Numerical solution is represented by circles while the exact solution by solid lines. $\epsilon = 0.001$, $\Delta x = 0.02$, and $\Delta t = 0.0001$. Top, mass density ρ; bottom, the mean velocity u.

results for the mass density obtained with the two different collision models, namely the RTA and the EPI scattering kernels. The numerical solution at time $t = 0.2$ and $t = 0.4$ for $\epsilon = 0.001$ using 20 grid points is given in Fig. 6. One can clearly observe that even for coarse diffusive discretization the behavior of the system is described with good accuracy.

Test **3**,

$$x \in [0, 1], \qquad F_L(v) = M(v), \qquad F_R(v) = M(v),$$
$$G = 0, \qquad \epsilon = 0.001.$$

The initial distribution is $f(x, v, t = 0) = M(v)$. Here, we consider the problem for a unipolar diode of type $\rho^+\rho\rho^+$ in the diffusion regime. According to [FJO] at the boundary we assume

$$\partial_x j(0, t) = \partial_x j(1, t) = 0.$$

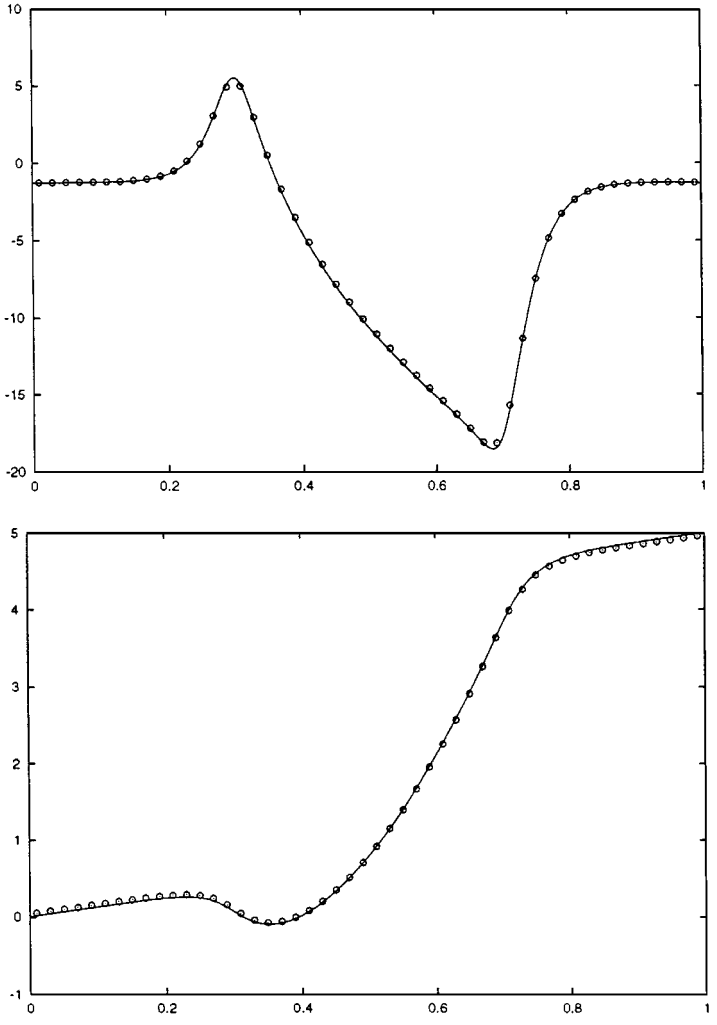

FIG. 8. Solution at $t = 0.05$ of Test 3. Numerical solution is represented by circles while the exact solution by solid lines. $\epsilon = 0.001$, $\Delta x = 0.02$, and $\Delta t = 0.0001$. Top, the electric field E; bottom, the potential Φ.

The electric potential is given by the solution of a Poisson equation

$$\beta \Delta_x \Phi = \rho - c(x), \qquad \Phi(0) = 0, \qquad \Phi(1) = V, \tag{6.1}$$

where β is the scaled Debye length, V the applied bias voltage, and $c(x)$ is the doping profile. Equation (6.1) can be easily solved by standard methods. The electric field is then computed by central difference. We point out that since ρ is constant during the relaxation step, the potential Φ, and so the electric field E, is constant during this step.

The discontinuities in the doping profile $c(x)$ has been smoothed by a hyperbolic tangent (see Fig. 2)

$$c(x) = (1 - M)\rho(0, t = 0)\left[\tanh\left(\frac{x - x_1}{s}\right) - \tanh\left(\frac{x - x_2}{s}\right)\right],$$

with $s = 0.02$, $M = (1 - 0.001)/2$, $x_1 = 0.3$, and $x_2 = 0.7$.

The results obtained with the two collision models are very similar and we report only the solution for the RTA approximation. The results for the mass density, mean velocity, electric field at $t = 0.05$ with $V = 5$, and $\beta = 0.002$ are given in Figs. 7 and 8.

For a comparison of the present results with previous results we refer the readers to [ARR, Kl2, NP2, SZ, RSZ].

7. CONCLUDING REMARKS

In this paper we derived a class of diffusive relaxation schemes for time-dependent multiscale kinetic semiconductor equations in any space dimension, based on the even-and odd-parity formulation of the kinetic equation. Key in the scheme is the use of a suitable implicit time discretization for the collision operator utilizing the Wild sum, which yields asymptotic-preserving diffusive relaxation schemes with mean-free-path-independent stability, yet can be implemented explicitly. Our scheme has a uniform accuracy with respect to the relaxation parameter, from the kinetic regime to the drift-diffusive regime, thus allowing the capturing of the hydrodynamic behavior with an underresolved numerical discretization, a property highly desirable for semiconductor device simulation using kinetic models.

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