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A DRIFT-COLLISION BALANCE FOR A BOLTZMANN–POISSON SYSTEM IN BOUNDED DOMAINS*

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Abstract. We consider a low density approximation to a Boltzmann–Poisson system for electrons in a semiconductor in regimes where strong forcing balances the collision terms. We compute the hydrodynamics corresponding to this regime by the Chapman–Enskog method and by a closure of moment equations as well. In both cases we obtain reaction diffusion systems, with anisotropic diffusions and convection coefficients that depend on the spatial derivatives of the anisotropic diffusion. In the case of a relaxation collision operator there is a recursion formula such that this self-consistent closure computes all the moments at all orders in the expanding parameter. The recursion procedure can be applied to field dependent relaxation time approximations, yielding a velocity saturated mobility. In addition we discuss boundary conditions for both the distribution function and the moments.

These nonequilibrium hydrodynamical regimes have been observed in the modeling of submicron doped semiconductor silicon devices and numerical evidence for them is presented.

Key words. mechanics of particles and systems, semiconductor models, time relaxation kernel, scaling limits, hydrodynamics

AMS subject classifications. 35, 70, 78, 82

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1. Introduction and basic equations.

Recent advances in submicron semiconductor devices have given rise to regimes of nonequilibrium hot-electron transport in which traditional drift-diffusion models break down. This failure is, in part, due to the small size of the devices and manifests itself with relatively larger carrier mean free path and stronger electric fields. This effect has made simulations of kinetic models (i.e., Monte Carlo based or discrete velocity methods) more accurate in reproducing the experimental current-voltage characteristics. However, they remain very costly computationally. For references on hot-electron transport we refer to Baranger and Wilkins [BW], Ferry and Grondin [FG], Laux and Fischetti [LF], Reggiani [Rg], Trugman and Taylor [TT], Thoernber [Th], and references therein.

Due to the need of faster computational methods away from equilibria and considering the inhomogeneities of a practical device (in particular effects due to heavily doped regions in submicron structures) a single device cannot be modeled with just one single set of partial differential equations derived from asymptotic methods to scaled kinetic-Poisson model. Different magnitudes of the scaling parameters might take over in different parts of the device (see Ferry and Grondin [FG]).

The present work is an attempt to produce a nonequilibrium hydrodynamic ap-

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proximation of self-consistent charged transport flow corresponding to regions where the flow gets accelerated due to the inhomogeneities of the geometry and local density levels. As a consequence, the collision terms balance the acceleration term in the transport equation yielding nonsymmetric distribution functions, far deviated from shift Maxwellians. Hence, it is important to discuss asymptotic models not only for the transport equation but also for the *full system* with the boundary data transfer from kinetic to macroscopic level. The regimes we describe would correspond to hot-electron transport transition from bulk phenomena to ballistic transport, given by an intermediate drift velocity scale in between both regimes. We call these a *drift-collision balance* (DCB) regime.

In the present paper we shall present a systematic hierarchy of self-consistent full models derived from the classical kinetic formulation of charged-particle transport when applied to strong force regimes due to local high electric fields. In addition, these models include boundary conditions and proper reduction to various augmented drift-diffusion regimes. We shall treat these ideas in the context of the following simplified model. We study a Boltzmann–Poisson system with a relaxation time operator modeling collisions (nondegenerate case). The relaxation term, to be called τ, may depend on the space and time variables. In particular they may depend on the electric field E. In this case, depending on the constitutive form of τ as a function of E, we obtain field saturated transport (mobilities) and diffusion coefficients at the macroscopic (fluid) level. This is an adequate approximation to low density regimes from the full semiclassical Boltzmann equation for statistical mechanical models of charged transport in solids. However, some of these ideas as well as methods can be applied in more general settings.

Here we present a high-field Chapman–Enskog expansion corresponding to a DCB regime, and a fluid (macroscopic) moment closure that matches the expansion at first order. This expansion yields distribution functions which are small perturbations of base functions (or ground states) that *are not* distributions in the null space of the collision operator for the transport equation.

In addition, we propose a boundary value problem at the kinetic level that yields neutral space charge boundary conditions at the ohmic contacts and the tangential flow condition at the insulating boundaries. Then, we also discuss the resulting boundary condition for the fluid model. Our formulation of the boundary conditions depends on the leading term of the expansion. They are valid for both weak and strong field scalings and consequently do not need any assumption on the scaling of the boundary data.

The resulting approximation is a first attempt to produce a full self-consistent model at the fluid level derived from a kinetic formulation that also may handle rough boundary effects and other geometrical constraints due to the design of the devices, as well as to provide a correction to fluid level models for those regions under moderate high field effects or other inhomogeneities. These macroscopic approximations model energy, transport, and diffusion coefficients that are field dependent and anisotropic. These models have appeared in the micro-electronic literature and are referred as augmented drift-diffusion equations. A simplified version was originally proposed by Thoernber [Th] as an ad-hoc approximation to hot-electron transport.

Recent computational work by Carrillo, Gamba, and Shu [CGS] shows that computational models for standard silicon diodes with channel sizes of the order of a half micron exhibit a DCB regime in the channel region, when there is moderate applied potential bias from 1 to 3 V. They are, under current technology, the simplest micro-

electronic devices that make up computer chips, as well as the standard test geometry for the modeling of submicron semiconductor devices. Some of these computations are included in section 6.

Our work follows that of Poupaud [P1], [P2], which considers a linear Boltzmann equation for charged-particle transport in a prescribed external electric field. There, the author shows the existence of a solution to the ground state equation for a high field scaling, which simply balances the drift velocity with the collision term, when the collision frequency is bounded from below. Then, he presents a Hilbert expansion (in small mean free path) about that solution and obtains a scalar drift-diffusion equation for the density in which the diffusion depends on the prescribed electric field. In [P2] he also proposes a moment closure. Here we do a similar systematic derivation for the case where the electric field is given self-consistently through a Poisson equation. We obtain closed systems that differ slightly from those of Poupaud. In a related work, Stichel and Strothmann [SS] consider other scaling assumptions on the initial and boundary data.

Some of the results worked out here have been announced in a short communication (see [CGL]).

Presentation of the problem. For simplicity's sake, we shall consider only electrons, because it is clear what modifications are needed when holes are to be taken into account.

The semiclassical Boltzmann equation for the electron gas in a semiconductor, in the parabolic band approximation (i.e., one carrier transport model), may be written as follows (see [MRS] and references therein):

$$\partial_t F + v \cdot \nabla_x F - \frac{e}{m} E(x,t) \cdot \nabla_v F = -\mathcal{C}(F)\,. \tag{1.1}$$

Here $F = F(x, v, t)$ is the density function for the electron of position x, velocity v, and time t. The constants e and m represent the electron charge and mass, respectively.

The electric field $E = E(x,t)$, sum of an external (applied and produced by an ion background $C(x)$) and a field produced by carriers, i.e.,

$$E = -\nabla\Phi \quad \text{with} \quad \nabla \cdot (\epsilon \nabla \Phi) = e\left(\int F\,dv - C(x)\right), \tag{1.2}$$

where ϵ is the permittivity of the material.

$\mathcal{C}$ is the collision operator. In general, the operator $\mathcal{C}(F)$ takes into consideration the interaction of electrons with background impurities and the electron-electron short range interactions.

Usually $\mathcal{C}$ is modeled as

$$\mathcal{C}(F) = \mathcal{L}(F) + \mathcal{B}(F)\,, \tag{1.3}$$

where $\mathcal{B}(\mathcal{F})$ describes the electron-electron interactions, conserves momentum and energy, and, in the absence of the other terms, drives the electrons toward thermal equilibrium, i.e., a Fermi–Dirac distribution with temperature fixed by energy conservation. $\mathcal{L}(\mathcal{F})$ describes the interaction with the lattice impurities and, in the absence of the other terms, also drives the electrons to equilibrium, but with a Maxwell–Boltzmann distribution having the temperature of the lattice.

Finally, the term $E \cdot \nabla_v F$ tends to heat up the electrons (by accelerating them).

When all the terms are present it is clear that, in general, the equations keep the distribution F away from equilibrium.

Here, we neglect $\mathcal{B}(\mathcal{F})$, as electron-electron interactions under the assumption of low density levels are not relevant.

In fact, as a first approximation, we shall assume (for instance, Markowich, Ringhofer, and Schmeiser [MRS] or Ferry and Grondin [FG]) the nondegenerate case and take

$$\mathcal{L}(F) = -\frac{M}{\tau} \int F(v')dv' + \frac{1}{\tau} F(v), \tag{1.4}$$

where $\tau = \tau(x,t)$, constant in v, is an approximation for the relaxation time $\tau(x,t,v)$ and M is the absolute Maxwellian at the temperature of the semiconductor given (in 3 dimensions) by

$$M = (2\pi\theta)^{-3/2}\, e^{-\frac{|v|^2}{2\theta}}, \tag{1.5}$$

where $\theta = \theta(x)$ is the temperature of the lattice, measured in units of specific energy, $\theta = k_B \frac{T}{m}$, where k_B is the Boltzmann constant and T the temperature of the lattice.

While this approximation is not sufficient to model all the inhomogeneities of an actual device, our primary goal is to investigate a boundary value problem corresponding to strong forcing regimes, because they will take over in some region of the device.

We obtain the fluid level approximation by two different methods: one uses a Chapman–Enskog expansion technique and the other gives a moment expansion where the closure is defined in a way that both methods yield the same model to the leading order the Chapman–Enskog expansion.

Both methods use the special structure of $\mathcal{L}(F)$ (as a BGK operator) and yield, at the lowest closure of the hierarchy, drift-diffusion models for the moment variables.

The resulting diffusion coefficients are anisotropic and quadratic in the electric field.

The drift terms are modified by a couple of terms not present in low-field expansions. Both terms are proportional to the relaxation time τ. One of them represents the acceleration induced by the electric field. This term is proportional to the divergence of the field. The other accounts for an internal magnetic effect, as it contains approximations of time derivatives of the field. This term is also proportional to the moment of the previous transport equation times a correction of the first moment by a new fluid variable.

After this introduction, section 2 describes a dimensionless formulation corresponding to high field scalings due to the balance of the drift term with the collision operator. We identify three dimensionless parameters, namely ε as the path, η the quotient between the scaled drift speed and the scaled thermal speed, and γ related to the characteristic Debye length.

Section 3 concerns the Chapman–Enskog expansion of the transport equation in the mean free path parameter $\varepsilon \ll 1$, to the first order. The expansion will be validated under the condition that the electric potential ϕ splits as a sum

$$\phi(x,t) = \phi_E(x) + \phi_I(x,t) \tag{1.6}$$

of an external, time independent potential ϕ_E with $|\nabla\phi_E| = \mathcal{O}(\frac{[\phi]}{L})$ and an internal, time-space (carrier) dependent potential ϕ_I with $|\nabla\phi_I| = \mathcal{O}(\gamma) \leq 1$. Here $[\phi]$ denotes the potential drop in a given reference length L, and γ a generalized characteristic Debye length.

Due to the linear structure of the collision operator in the nondegenerate case, we obtain a recursion relation for the terms in the expansion. We show that the lowest hierarchy for the first order of the expansion satisfies a drift-diffusion model with coefficients modified by the electric field, induced by the potential ϕ which solves the Poisson equation (1.2), and satisfies (1.6) for time independent boundary data given on a domain corresponding to a geometry adequate for a model of a metal oxide semiconductor field transport effect device.

This recursive relationship allows us to compute, in a simple fashion, higher order moment equations and then provides a fluid level description of the charged particle transport that models energies. We obtain a high hierarchy fluid system of diffusive equations with diffusion highly anisotropic.

Section 4 presents moment closures and the corresponding moment equations. We show that they agree with the ones obtained in section 3 by the Chapman–Enskog expansion procedure up to the order of the scaled mean free path for all the fluid moments.

Section 5 discusses the boundary conditions at the kinetic level for the contact regions of the boundary (i.e., regions where the macroscopic density $C(x)$ is to be prescribed), and the corresponding approximation to the boundary conditions at the fluid level.

Finally, in section 6, we include some computational work produced by Carrillo, Gamba, and Shu which numerically validates the expansion about a DCB state inside the channel. The computations correspond to a one dimensional simulation of electron transport in a model corresponding to a heavily doped silicon device with a channel of a half-micron in length and an applied voltage bias of 1V. We compute the distribution functions and compare them to the plots of Maxwellian distributions and the DCB distributions characterized by this high field scaling. Clearly, while in the region of high background density, the solution of the kinetic-Poisson system (see Figure 2) fits numerically a Maxwellian (upper left picture), the computations inside the channel indicate a clear fit with the later distributions. More related numerical work appears in [CGS], where a hybrid elementary domain decomposition technique was developed as a modification of that previously introduced in [CGJ2].

We close this introduction stating, for simplicity, only the equations for the lowest moments. The equations for higher moments can then be simply stated using the recursion relations derived in either section 2 or section 3.

Thus, let ρ and j denote

$$\rho = \int F(v)\,dv \qquad \text{and} \qquad j = \int v\,F(v)\,dv$$

at the lowest level, with an error of quadratic order in the asymptotic parameter (i.e., the scaled mean free path). The corresponding fluid-Poisson model reads as

$$0 = \partial_t \rho + \operatorname{div} j\,, \tag{1.7a}$$

$$\begin{aligned} j = -\tau\Big\{\nabla_x \cdot \big(\rho\,(\theta I + 2\mu^2\ E_{\otimes} E)\big)\Big\} - \mu\rho E \\ +\tau\mu E \operatorname{div}(\mu\, E\rho) - \tau\mu\rho\,\frac{e}{\epsilon}(\mu\rho E - \omega)\,, \end{aligned} \tag{1.7b}$$

$$\operatorname{div}\,\omega = 0 \qquad \text{and} \qquad \operatorname{curl}\,\omega = \mu\, E \otimes \nabla\rho\,, \tag{1.7c}$$

$$E = -\nabla\phi \qquad \text{and} \qquad \operatorname{div}(\epsilon\nabla\phi) = e(\rho - C(x))\,, \tag{1.7d}$$

where $\mu = \frac{e\tau(x)}{m}$ is the mobility coefficient associated with the drift-diffusion model for low electric fields when τ is constant. The constant θ is the background temperature of the lattice.

The state variable ω can be interpreted as the curl of a magnetic field associated with the electric current.

As stated above, a feature of the model is that the diffusion coefficient becomes a highly anisotropic tensor rather than a scalar. The same property characterizes the diffusive terms in the resulting moment and energy equations.

In addition, using the approximated boundary conditions derived in section 5 in the inner expansion, the boundary conditions for the fluid level system (1.7a)–(1.7d) are as follows. Denoting by n the outer unit normal to the boundary, and by s the unit tangential directions to the boundary at a given boundary point,

(i) *Insulating boundaries* $\Gamma_{\mathcal{N}}$*:* The current j and the electrostatic potential Φ, and ω satisfy

$$j \cdot n = 0, \qquad E \cdot n = -\nabla\Phi \cdot n = 0, \qquad \omega \cdot n = 0 \quad \text{on } \Gamma_{\mathcal{N}}, \tag{1.8a}$$

respectively.

(ii) *Contact boundaries* $\Gamma_{\mathcal{D}}$*:* The electric potential is constant in space and time on each connected component of the contact boundaries. In addition, at these contacts the neutral space charge condition at the kinetic level also delivers a neutral space charge plus a correction term of the order of the asymptotic parameter ε in the expansion (i.e., the scaled mean free path). That is, for a given background function $C(x)$,

$$\rho = C(x) + \mathcal{O}(\varepsilon), \qquad \Phi = \text{constant}, \qquad \omega \cdot s = 0 \quad \text{on } \Gamma_{\mathcal{D}}, \tag{1.8b}$$

respectively. The form of the term $\mathcal{O}(\varepsilon)$ is given in terms of the first order approximation of the first two moments of the asymptotic expansion of F. It is computed explicitly in section 5.

Remark. In the particular case of 2-space dimensional models, the macroscopic variable ω can be written as $\omega = (\nabla B)^{\perp}$, so that equations for ω in (1.7a)–(1.7d) become the single equation

$$\Delta B = \nabla(\mu\rho) \otimes E\,. \tag{1.9}$$

Then, the boundary condition $\omega \cdot n = 0$ becomes $\nabla B \cdot s = 0$ along insulating boundaries and $\nabla B \cdot n = 0$ along contacts, which can be obtained from the following boundary conditions for B,

$$B = \text{constant} \quad \text{on } \Gamma_{\mathcal{N}} \quad \text{and } \nabla B \cdot n = 0 \quad \text{on } \Gamma_{\mathcal{D}}\,. \tag{1.10}$$

Thus, the boundary value problem (1.9)–(1.10) has a unique regular solution B, for any regular field E and density ρ in any domain that is conformally transformed into a rectangle provided some compatibility conditions between the boundary data and the right-hand side of (1.10).

Thus, we expect the full model (1.7a)–(1.7d) and (1.8a)–(1.8b) to be a quasi-linear system of parabolic-elliptic equations and preliminary calculations and indicate that it provides well-posedness for the initial-boundary value problem. The existence of a solution for this boundary value problem will be part of future work.

We point out that Poupaud [P1] considered the linearized model for a given external electric field and derived a high field approximation from a one parameter (the scaled mean free path) dimensionless formulation of the kinetic equation by balancing the drift term with the collision integral. He obtained in the nondegenerate case a similar transport model with different transport coefficients in the correction terms to the standard drift-diffusion models which produced a reduced model given only by the transport equations (1.7a) and (1.7b) for a given external field. There the equations for ω are eliminated and $(\mu\,\rho\,E-\omega)$ is replaced by E_t.

However, we show here that $(\mu\,\rho\,E-\omega)=E_t+\mathcal{O}(\varepsilon)$ is valid for strong uniformly ε bounded solutions of a boundary value problem associated with the *full system* (1.7a)–(1.7d) and (1.8a)–(1.8b).

Hence, we indeed verify that to the first order in ε the continuity equation of the *full system* (1.7a)–(1.7d) agrees with the reduced transport scalar equation for a given external field as computed in [P1].

This presentation, which provides a complete boundary value problem to a full system of charged-particle transport derived from strong force asymptotics on the kinetic formulation, has not been found in the literature. The justification of the complete model requires existence proofs of solutions of (1.7a)–(1.7d) and (1.8a)–(1.8b) and also existence of solutions to the kinetic boundary value problem. Such studies are all under way and will be part of future presentations.

2. Scaling and dimensionless formulation. We start with an appropriate scaling, introducing dimensionless quantities, that isolates the relevant dimensionless parameters on which the model depends. We shall identify three dimensionless parameters, namely ε as the scaled mean free path, η the quotient between the scaled drift speed and the scaled thermal speed, and γ related to the characteristic Debye length.

Let L be the appropriate microscopic length scale of the device, $\bar\rho=\mathcal{O}(C(x))$, where $C(x)$ is the predefined doping profile, assumed strictly positive. The parameter $\bar\theta=k_B\frac{T_0}{m}$ is the reference magnitude of the temperature of the lattice, so that the thermal velocity has magnitude $\bar\theta^{1/2}$. Let $\bar\tau$ be the reference magnitude for the approximation of the relaxation time associated with $\mathcal{L}(x,v)$ and $\bar\epsilon$ be one for the permittivity. Then we define the new dimensionless variables, denoted by carets:

$$
\begin{aligned}
&x=L\hat x,\quad v=\bar\theta^{1/2}\,\hat v,\quad \theta(x)=\bar\theta\,\widehat\theta(\hat x),\\
&\tau=\bar\tau\,\hat\tau(\hat x),\quad \epsilon=\bar\epsilon\,\hat\epsilon(\hat x),\quad C(x)=\bar\rho\,\widehat C(\hat x).
\end{aligned}
\tag{2.1}
$$

Thus, a natural scaling for the distribution functions would be $\bar\rho\cdot\bar\theta^{-d/2}$, with d the space dimension. However, F will be scaled proportionally to the magnitude of the drift velocity $\frac{e}{m}\,\tau\nabla\phi$.

Now denoting $[\phi]$ the potential drop applied at the contacts of the device separated by a distance of order of L, we shall define U to be the reference magnitude for the drift velocity $u=-\tau\frac{e}{m}\,E$, with $E=-\nabla\phi$, where ϕ satisfies the Poisson equation (1.2). Then,

$$
U=\bar\tau\frac{e}{m}\,\overline{E}=\bar\tau\frac{e}{m}\,\frac{[\phi]}{L},\quad \phi(x,t)=[\phi]\widehat\phi(\hat x,\hat t\,)
\tag{2.2}
$$

and

$$
\nabla_x\phi=\frac{[\phi]}{L}\;\nabla_{\hat x}\hat\phi\,(\hat x,\hat t)=\overline{E}\;\widehat{E}\,(\hat x,\hat t\,).
$$

Notice that U and $\bar{\theta}^{1/2}$ are both measured in velocity units.

Next, in order to obtain a dimensionless Boltzmann–Poisson system, define

$$\delta = U\,\frac{\bar{\tau}}{L} = \frac{\bar{\tau}^2}{L^2}\;\frac{e}{m}\;[\phi] \tag{2.3}$$

and

$$\eta = \frac{U}{\bar{\theta}^{1/2}} = \frac{\bar{\tau}\,e\,[\phi]}{m\,L\,\bar{\theta}^{1/2}}. \tag{2.4}$$

Both parameters δ and η are dimensionless. Therefore, taking $T = \frac{L}{U}$ as the time scale $t = T\hat{t}$, we scale the drift velocity $u = U\hat{u}(\hat{x},\hat{t}\,)$ and the distribution function $F(x,t,v) = \bar{\rho}\cdot U^{-d}\widehat{F}\,(\hat{x},\hat{t},\hat{v}),\ x\in\mathbb{R}^d$. Then from (1.1), with (1.4) for the right-hand side, the transport equation scales as

$$\begin{aligned}\frac{\bar{\rho}}{U^{d-1}L}\;\widehat{F}_{\hat{t}} + &\frac{\bar{\rho}\bar{\theta}^{1/2}}{U^dL}\;\hat{v}\cdot\nabla_{\hat{x}}\,\widehat{F} + \frac{\bar{\rho}}{\bar{\theta}^{3/2}U^{d-1}}\;\frac{\widehat{u}}{\widehat{\tau}}\cdot\nabla_{\hat{v}}\,\widehat{F}\\ &= \frac{-\bar{\rho}}{\bar{\tau}\hat{\tau}U^d}\;\left(\widehat{F} - \widehat{M}\int\widehat{F}\,d\hat{v}\right).\end{aligned} \tag{2.5}$$

Multiplying (2.5) by $\frac{LU^d}{\bar{\rho}\bar{\theta}^{1/2}}$ yields the dimensionless equation

$$\frac{U}{\bar{\theta}^{1/2}}\;\widehat{F}_{\hat{t}} + \hat{v}\cdot\nabla_{\hat{x}}\widehat{F} + \frac{LU}{\bar{\theta}\bar{\tau}}\;\frac{\hat{u}}{\hat{\tau}}\cdot\nabla_{\hat{v}}\widehat{F} = -\frac{L}{\bar{\tau}\bar{\theta}^{1/2}}\;\left(\frac{\widehat{F} - \widehat{M}\int\widehat{F}\,d\hat{v}}{\widehat{\tau}}\right). \tag{2.6}$$

The Poisson equation yields

$$\begin{aligned}\nabla_{\hat{x}}\;\left(\hat{\epsilon}\,\nabla_{\hat{x}}\,\hat{\phi}\right) &= \frac{e\;L^2}{\bar{\epsilon}\,[\phi]}\;\left(\frac{\bar{\rho}}{U^d}\;\theta^{d/2}\;\int\widehat{F}(\hat{v}')\,d\hat{v}' - \bar{\rho}\widehat{C}(\hat{x})\right)\\ &= \frac{\bar{\rho}\,eL^2}{\bar{\epsilon}\,[\phi]}\;\left(\frac{1}{\eta^d}\;\int\widehat{F}\,(\hat{v}')dv' - \widehat{C}(\hat{x})\right).\end{aligned} \tag{2.7}$$

Introducing the last dimensionless parameter

$$\gamma = \frac{\bar{\rho}\,eL^2}{\bar{\epsilon}\,[\phi]}, \tag{2.8}$$

dropping the carets from (2.6) and (2.7) and combining with (2.3), (2.4), and (2.8) yield the dimensionless system

$$\eta\,F_t + v\cdot\nabla_x F + \frac{\eta}{\varepsilon}\;\nabla_x\phi\cdot\nabla_v F = -\frac{1}{\varepsilon}\;\frac{F - M\;\int\;F(v')dv'}{\tau}, \tag{2.9}$$

$$\nabla_x\cdot(\epsilon(x)\,\nabla_x\phi) = \gamma\;\left(\frac{1}{\eta^d}\;\int\;F(v')dv' - C(x)\right), \tag{2.10}$$

where $\varepsilon^{-1} = \frac{\eta}{\delta} = L/\bar{\tau}\theta^{1/2}$ is the inverse of the scaled mean free path.

Equations (2.9) and (2.10) yield the standard drift-diffusion (low-field) scaling when F is scaled using the thermal velocity reference parameter $\bar{\theta}^{1/2}$ instead of the drift velocity parameter U and $\delta = \eta^2$ with η small. In fact, taking standard expansions in η yields, at the fluid level, the drift-diffusion approximation with a small

scaled Debye length which is an adequate approximation for relative low-field regimes. See Poupaud [P1] and Golse and Poupaud [GP]. In addition, Poupaud [P1], [P2] considered a high field scaling comparable to ours in the case where the electric field E is given, so that the system is reduced to the linearized Boltzmann equation. [P1] contains a derivation of fluid equations by Hilbert expansion procedure and [P2] contains a discussion of moment closures.

Also, energy transport models have been derived from the Boltzmann transport equation of semiconductors [BDG], [DRS], under the hypothesis that the energy gain or loss of electrons by the phonon collisions is weak, leading to a different scaling that allows high relative local electric fields as well. These are essentially systems of standard isotropic diffusion equations that incorporate the total energy of the system as a state variable for the system.

Here, we are interested in a strong force regime, that is ε very small compared with η of order 1. In addition, such a regime requires that γ is of moderate small order, so that the contribution to the electric field coming from the internal potential ϕ_I does not override the applied external field which is of order $\frac{[\phi]}{L}$. This means that the scaled Poisson equation is not stiff.

Thus, by high field approximation we mean a regime where $\mathcal{O}(\varepsilon) \ll \mathcal{O}(\eta) = \mathcal{O}(1)$, or equivalently in devices of length L, such that for a given potential drop $[\phi]$, $\gamma = \frac{\bar{\rho}\, e\, L^2}{\bar{\epsilon}\,[\phi]} = \mathcal{O}(1)$.

From now on, we will work with equations of the dimensionless system (2.9), (2.10) for the parameters ε, η, and γ satisfying the above conditions.

Finally, we introduce the notation

$$\langle f \rangle = \int f \, dv \, .$$

Our full kinetic system becomes

$$\eta\, \partial_t F + v \cdot \nabla_x F + \frac{\eta}{\varepsilon}\, \nabla_x \phi \cdot \nabla_v F + \frac{1}{\varepsilon} \left(\frac{F - M\langle F \rangle}{\tau} \right) = 0 \, , \tag{2.11}$$

$$\nabla \cdot (\epsilon \nabla \phi) = \gamma \left(\frac{1}{\eta^d} \langle F \rangle - C(x) \right) . \tag{2.12}$$

Thus, the electron density $\rho = \langle F \rangle$ satisfies the local conservation law

$$\eta\, \partial_t \rho + \nabla_x \cdot \langle v F \rangle = 0 \, . \tag{2.13}$$

3. The Chapman–Enskog expansion.

3.1. The recursion relation. The Chapman–Enskog expansion of the transport equation consists of writing the distribution function F that solves problem (2.11)–(2.13) as a power series in ε, namely

$$F = \sum_{k \geq 0} \varepsilon^k \, F_k \, , \quad \text{with} \quad \langle F \rangle = \langle F_0 \rangle \quad \text{and} \quad \langle F_k \rangle = 0 \, , \ k > 0,$$

and expresses F, a solution of (2.11) and (2.12), as a function of ρ, τ, and u, and their spatial derivatives, in order to get rid of its time derivative using the mass equation (2.13) and the Poisson equation (2.12). Then we compute the corresponding equations

for the macroscopic variables defined as higher moments by balancing the order of each term in the expanding parameter.

Due to the linear structure of the collision operator, we find out a recursive relationship that defines F_{k+1} in terms of F_j $(j = 0 \dots k)$ and their moments. As a consequence we also show that the macroscopic equations for the higher order moments

$$\rho^{(n)} \equiv \langle v^{\otimes n} F \rangle$$

are given as a recursive relationship on $\rho^{(n)}_{k+1} \equiv \langle v^{\otimes n} F_k \rangle$ in terms of $\rho^{(m)}_j$ for $j = 0$, k, and $m = 0$, $n + 1$.

Finally, we write down the equations as a particular case of these relations for the corresponding moment equations when $n = 1$ and $k = 0$. These equations are the ones for system (1.7a)–(1.7d).

LEMMA 1. *Let* $(F,\ \phi)$ *be a solution of problem* (2.11)–(2.13) *such that* $F = \sum_{k\geq 0} \varepsilon^k\ F_k$ *with* $\langle F \rangle = \langle F_0 \rangle$ *and* $\langle F_k \rangle = 0$ *for* $k > 0$.

Then, for $u = \eta\tau \nabla_x \phi = -\eta\tau E$,

$$F_0 = \rho\, P\,,$$

where $P \geq 0$ *solves*

$$u \cdot \nabla_v P = -\mathcal{L}(P) = -P + M\,, \qquad \langle P \rangle = 1\,, \tag{3.1}$$

each term F_{k+1} *in the expansion satisfies the recursion relation*

$$u \cdot \nabla_v F_{k+1} + F_{k+1} = -\tau\, v \cdot \nabla_x F_k + \sum_{j=0}^{k} \tau \Big\{ D_\rho F_j \, \langle v \cdot \nabla_x F_{k-j} \rangle + \eta\tau\, D_u F_j \ \frac{\gamma}{\eta^d} \left(\langle v F_{k-j} \rangle + \omega_{k-j} \right) \Big\} \tag{3.2a}$$

$$\operatorname{div} \omega_{k-j} = 0, \qquad \operatorname{curl} \omega_{k-j} = -\operatorname{curl} \langle v\, F_{k-j} \rangle \tag{3.2b}$$

for $D_{\nabla\phi} = \eta\tau\, D_u$.

Proof. Because τ is time independent, the time dependence of F only enters through ρ and the gradient of ϕ. Thus for $F = F(\partial_x^k \rho,\ \partial_x^j \nabla\phi)$ where k and j denote the usual nonnegative multi-index $k = (k_i, \dots, k_d)$, $j = (j_1, \dots, j_d)$, d the space dimension and $x \in \mathbb{R}^d$,

$$F_t = \sum_{k\geq 0} \left(\frac{\partial F}{\partial \left(\partial_x^k \rho \right)}\ \partial_x^k \rho_t + \frac{\partial F}{\partial \left(\partial_x^{j+1} \phi \right)}\ \partial_x^{j+1}\, \phi_t \right)$$

which, by defining a new notation, we write as follows:

$$F_t = D_\rho\, F\, \partial_t \rho + D_{\nabla\phi} F\ \partial_t \nabla\phi. \tag{3.3}$$

We remark that at variance with the usual Chapman–Enskog expansion, the zeroth order approximation does not depend on space and time variables through the conserved moment only, but through the electric field as well; this new feature accounts for the presence of the second term in the above equations.

Differentiating (2.12) with respect to t and combining the result with (2.13) yield

$$\text{div}\ (\epsilon \cdot \partial_t \nabla\phi) = \nabla_x \cdot (\epsilon(x)\nabla\phi_t) = \frac{\gamma}{\eta^d}\,\partial_t\rho = -\frac{\gamma}{\eta^{d+1}}\,\nabla_x \cdot \langle vF\rangle. \tag{3.4}$$

Thus,

$$\nabla_x \cdot (\epsilon(x)\nabla\phi_t) = -\frac{\gamma}{\eta^{d+1}}\,\nabla_x \cdot \langle v\,F\rangle, \tag{3.5}$$

where $\phi_t\big|_{\partial\Omega} = \phi_{i,\,t}\big|_{\partial\Omega}$ because ϕ_E does not depend on t. Henceforth we let $\epsilon =$ constant to simplify the equations a bit. Combining (2.13), (3.3), and (3.5) yields

$$\eta F_t = -D_\rho\, F\,\langle v\cdot\nabla_x F\rangle - \frac{\gamma}{\eta^d} D_{\nabla\phi}F(\langle vF\rangle + \omega) \tag{3.6}$$

with $\text{div}\ \omega = 0$ and $\text{curl}\ \omega = -\text{curl}\langle vF\rangle$.

Hence, we seek solutions of

$$\begin{cases} v\cdot\nabla_x F - D_\rho F\,\langle v\nabla_x F\rangle - \frac{\gamma}{\eta^d}\ \left(D_{\nabla\phi}F\,\langle v_i F\rangle + D_{\nabla\phi}F\cdot\omega_i\right) \\ \qquad + \frac{\eta}{\varepsilon}\ \nabla_x\phi\,\nabla_v F + \frac{1}{\varepsilon}\ \frac{(F-\rho M)}{\tau} = 0 \\ \text{div}\,\omega_i = 0 \qquad \text{and} \quad \text{curl}\ \omega_i = -\text{curl}\ \langle vF\rangle. \end{cases} \tag{3.7}$$

Now, if $\varepsilon \ll 1$ and F is expanded as

$$F = F_0 + \varepsilon\, F_1 + \cdots + \varepsilon^k\, F_k \tag{3.8}$$

such that $\rho = \langle F_0\rangle$ and $\langle F_k\rangle = 0$ for $k \geq 1, 2, \ldots$, then to the order ε^{-1} we find

$$F_0 = \rho\ P, \tag{3.9}$$

where $P \geq 0$ solves (3.1).

For a given u, the solvability of (3.1) in L^1 can be found in Trugman and Taylor [TT] for the relaxation-type operator in one dimension and has also been discussed in Frosali, Van der Mee, and Paveri Fontana [FV] and in Poupaud [P1] for more general linear collision operators in higher dimensions.

In this case, with the relaxation operator $\mathcal{L}$ (the nondegenerate case), for given u, the distribution solution P_u satisfies the following explicit formula. Decompose v into a vector $v_\perp \in R^2$ (perpendicular to u) and a scalar $v_\parallel$ along u. Then

$$P_u(v) = \frac{1}{u} M_\theta(v_\perp) \exp\left(-\frac{\lambda(v_\parallel)}{u}\right) erf\left(\frac{\lambda(v_\parallel)}{\sqrt{2\theta}}\right) \tag{3.10}$$

with $u > 0$, $\lambda = v_\parallel - \frac{2\theta}{u}$ and $erf(x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{x} e^{-t^2}dt$.

For $u < 0$, the solution is given by $P_u(v) = P_{-u}(-v)$.

Though this formula is given explicitly, we do not need it here for the computation of the expansion and its moments.

Remark. For a given $u(t,x)$, the solvability (3.1) in $L^1(\mathbb{R}^3)$ follows naturally from spectral analysis of the operator $T_u = u\cdot\nabla_v - 1_{L^1}$, and it is shown in [FV] and [P1] in detail. In particular it is shown that the problem $T_u(G) = K$ is solvable in $L^1(\mathbb{R}^3)$ for $K \in L^1(\mathbb{R}^3)$ and in L^∞ in time t and space x.

However, the solution of the full system when incorporating (3.2b) for ω and the Poisson equation for u has not been addressed yet. It requires that we solve the

macroscopic model corresponding to this expansion and that we show both u and ω are L^∞ in time and space.

Thus, this regularity depends on the initial-boundary value problem associated with macroscopic formulation of the *full system*, which in the lowest hierarchy corresponds to system (1.7a)–(1.7d).

At this point it becomes imperative to move forward and obtain the moment equations which will deliver a macroscopic formulation for a well posed initial-boundary value problem for the full system.

In order to obtain the terms in the expansion given by the recursion relation (3.2a)–(3.2b), match the expansion of F to the order ε^k, $k = 0, 1, \ldots$, in system (3.7). Using that $\langle F_{k+1}\rangle = 0$ for $k \geq 1$, we obtain

$$\frac{u}{\tau}\cdot\nabla_v F_{k+1} + \frac{F_{k+1}}{\tau} = -v\cdot\nabla_x F_k + \sum_{j=0}^{k}\Big\{D_\rho F_j\,\langle v\cdot\nabla_x F_{k-j}\rangle + \eta\tau\, D_u F_j\,\frac{\gamma}{\eta^d}\left(\langle vF_{k-j}\rangle + \omega_{k-j}\right)\Big\}, \tag{3.11a}$$

where

$$\operatorname{div}\omega_{k-j} = 0, \qquad \operatorname{curl}\omega_{k-j} = -\operatorname{curl}\langle v\, F_{k-j}\rangle. \tag{3.11b}$$

Here $D_{\nabla\phi} = \eta\tau\, D_u$. Therefore, (3.2a) and (3.2b) both hold.

LEMMA 2 (the macroscopic variables). *Under the conditions of Lemma* 1, *the nth order moment of F given by $\rho^{(n)} \equiv \langle v^{\otimes n} F\rangle$ has a ε-power series representation $\rho^{(n)} = \sum_{k\geq 0}\varepsilon^k \rho_k^{(n)}$, where each $\rho_k^{(n)}$ is defined by the recursion relation*

$$\begin{aligned}\frac{1}{\tau}\,\rho_{k+1}^{(n)} &= -\frac{n}{\tau}\,u_{\otimes}\rho_{k+1}^{(n-1)} - \nabla_x\cdot\rho_k^{(n+1)}\\ &\quad + \sum_{j=0}^{k}\Big\{D_\rho\rho_j^{(n)}\nabla_x\cdot\rho_{k-j}^{(1)} + \eta\tau\, D_u\rho_j^{(n)}\,\frac{\gamma}{\eta^d}\left(\rho_{k-j}^{(1)} + \omega_{k-j}\right)\Big\},\end{aligned} \tag{3.12a}$$

where ω satisfies the equation

$$\operatorname{div}\omega_{k-j} = 0, \quad \operatorname{curl}\omega_{k-j} = -\operatorname{curl}\rho_{k-j}^{(1)} \tag{3.12b}$$

with the initial conditions

$$\rho_{k+1}^{(0)} = 0 \quad \textit{for } k\geq 0 \qquad \textit{and} \qquad \rho_0^{(n)} = \rho\,\langle v^{\otimes n} F_0\rangle \quad \textit{for } n\geq 0. \tag{3.12c}$$

Proof. From (3.1), compute the velocity moments of P given by

$$m_P^{(n)} \equiv \langle v^{\otimes n} P\rangle, \tag{3.13a}$$

which may be computed recursively, directly from (3.1) by

$$m_P^{(n)} - m_M^{(n)} = n\,u_{\otimes} m_P^{(n-1)} = n\eta\tau\,\nabla\phi_{\otimes} m_P^{(n-1)}. \tag{3.13b}$$

Here $m_M^{(n)}$ are the moments of the Maxwellian M_θ given by

$$m_M^{(2n+1)} = 0, \quad m_M^{(2n)} = \frac{(2n)!}{2^n n!}\,\theta^n I^{\otimes n}, \qquad n\geq 0. \tag{3.14}$$

Hence, the first five $m_P^{(n)}$ are

$$
\begin{aligned}
&m_P^{(0)} = 1, && m_P^{(1)} = u,\\
&m_P^{(2)} = \theta I + 2u_{\otimes}u,\\
&m_P^{(3)} = 3\theta I_{\otimes}u + 6\,u_{\otimes}u_{\otimes}u,\\
&m_P^{(4)} = 3\theta^2 I_{\otimes}I + 12\theta\, I_{\otimes}u_{\otimes}u + 24\,u_{\otimes}u_{\otimes}u_{\otimes}u.
\end{aligned}
\tag{3.15}
$$

Similarly, we do not need to solve (3.11a)–(3.11b) in order to get the moment equations. Defining the nth order moment of F_k by

$$
\rho_k^{(n)} \equiv \langle v^{\otimes n} F_k \rangle \tag{3.16}
$$

we compute from (3.11a)–(3.11b) the recursion relation

$$
\begin{aligned}
\frac{1}{\tau}\,\rho_{k+1}^{(n)} &= -\frac{n}{\tau}\,u_{\otimes}\rho_{k+1}^{(n-1)} - \nabla_x\cdot\rho_k^{(n+1)}\\
&\quad + \sum_{j=0}^{k}\left\{ D_\rho\rho_j^{(n)}\nabla_x\cdot\rho_{k-j}^{(1)} + \eta\tau\, D_u\rho_j^{(n)}\;\frac{\gamma}{\eta^d}\left(\rho_{k-j}^{(1)} + \omega_{k-j}\right)\right\}
\end{aligned}
\tag{3.17}
$$

along with

$$
\operatorname{div}\omega_{k-j} = 0, \quad \operatorname{curl}\omega_{k-j} = -\operatorname{curl}\rho_{k-j}^{(1)},
$$

and the initial conditions

$$
\rho_{k+1}^{(0)} = 0 \quad \text{for} \quad k \ge 0 \qquad \text{and} \qquad \rho_0^{(n)} = \rho\; m_P^{(n)} \quad \text{for} \quad n \ge 0. \tag{3.18}
$$

Then (3.12a)–(3.12c) hold.

3.2. A hierarchy for a full macroscopic model with strong forcing conditions. We now obtain a full system for the macroscopic description of the transport. For example, let $k = 0$ in (3.12a)–(3.12c) and solve recursively in n for $\rho_1^{(n)}$ to obtain

$$
\begin{aligned}
\frac{1}{\tau}\,\rho_1^{(n)} &= \frac{n}{\tau}\,u_{\otimes}\rho_1^{(n-1)} - \nabla_x\cdot\left(\rho m_P^{(n+1)}\right)\\
&\quad + m_P^{(n)}\nabla_x\cdot\rho_0^{(1)} + \eta\tau\rho\,\partial_u(m_P^{(n)})\,\frac{\gamma}{\eta^d}\left(\rho_0^{(1)} + \omega_0\right).
\end{aligned}
\tag{3.19}
$$

Then we approximate the nth moment of F by

$$
\rho^{(n)} \approx \rho_0^{(n)} + \varepsilon\rho_1^{(n)} = \rho m_P^{(n)} + \varepsilon\rho_1^{(n)}. \tag{3.20}
$$

In particular we obtain the lowest hierarchic model by taking the leading order of the expansion for $n = 1$ in (3.19)–(3.20). It yields the closure

$$
\frac{1}{\tau}\,\rho_1^{(1)} = -\nabla_x(\rho(\theta + 2u_{\otimes}u) + u\nabla_x\cdot(\rho u) + \eta\tau\left(D_u(\rho u)\,\frac{\gamma}{\eta^d}\,(\rho u + \omega_0)\right) \tag{3.21a}
$$

with

$$
\operatorname{div}\,\omega_0 = 0 \qquad \text{and} \qquad \operatorname{curl}\,\omega_0 = -\operatorname{curl}\,(\rho u). \tag{3.21b}
$$

Therefore, if $\rho^{(1)} = \langle v\, F\rangle$ denotes the first fluid level moment, which in thermodynamics is usually denoted by j, then j is approximated to the first order in the expansion by

$$j = \rho^{(1)} \approx \rho\, u + \varepsilon\, \rho_1^{(1)} = \rho\, u + \varepsilon\, \tau \left\{ -\nabla_x(\rho(\theta + 2u_{\otimes} u)) + u\, \nabla_x \cdot (\rho u) + \tau\, \eta\, \rho\, \frac{\gamma}{\eta^d}\, (\rho u + \omega_0) \right\}, \tag{3.22}$$

where ω_0 satisfies (3.21b).

The corresponding full system of equation at macroscopic or fluid level is

$$\eta \rho_t + \operatorname{div} j = 0, \tag{3.23a}$$

$$j = u\rho + \varepsilon\, \tau \left\{ -\nabla_x(\rho(\theta + 2u_{\otimes} u)) + u \nabla_x \cdot (\rho u) + \eta\, \tau\, \rho\, \frac{\gamma}{\eta^d}\, (\rho u + \omega) \right\} + \mathcal{O}(\varepsilon^2), \tag{3.23b}$$

with

$$u = \eta \tau \nabla \phi, \qquad \operatorname{div}\, (\nabla \phi) = \gamma \left(\frac{1}{\eta^d} \rho - C(x) \right), \tag{3.23c}$$

$$\operatorname{div}\, \omega = 0 \qquad \text{and} \qquad \operatorname{curl}\, \omega = -\operatorname{curl}\, (\rho u). \tag{3.23d}$$

The validation of this asymptotic expansion requires existence results that are beyond the scope of the present paper. Nevertheless it will be valid for regimes where $\varepsilon < 1$, provided the boundary value problem for the system of partial differential equations (3.23a)–(3.23d) has solutions ρ, u, and ω such that their L^∞ norms and those of their derivatives are all of $\mathcal{O}(1)$.

This very strong property depends on the regularity of the initial and boundary data. As we anticipated in the introduction, we shall propose a boundary condition at the kinetic level that yields the Dirichlet and Robin conditions for a standard boundary geometry. In addition to the standard boundary condition to determine the electric potential ϕ, the quantity ω must satisfy the following boundary value problem:

$$\begin{cases} \operatorname{div} \omega = 0, & \operatorname{curl} \omega = -\operatorname{curl}\, (\rho u), \\ \omega\big|_{\partial\Omega} = (\partial_t\, \nabla \phi - \rho\, u)\,\big|_{\partial\Omega}. \end{cases} \tag{3.24}$$

Moreover, in the case when the boundary data for the electric potential are time independent, the electric potential splits in an internal and external one satisfying

$$\begin{cases} \phi = \phi_I + \phi_E, & \\ \nabla \cdot (\epsilon \nabla \phi_E) = 0 \quad \text{and} & B(\phi) = g(x) \quad \text{on} \quad \partial\Omega, \\ \nabla \cdot \epsilon \nabla \phi_I = \gamma(\frac{1}{\eta^d} \rho - C(x)) \quad \text{and} & B(\phi) = 0 \quad \text{on} \quad \partial\Omega, \end{cases} \tag{3.25}$$

where $B(\phi)$ is a boundary operator defined on $\partial\Omega$ and $g(x)$ the corresponding boundary data.

We point out that in order to keep the rescaled electric field E of an order of one, because E will also split in an external one (of order of unity in the rescaled system), and an internal one E_I, the total field must be of order

$$|E| = |\nabla\phi| \geq \mathcal{O}(1) - \mathcal{O}\left(\gamma\|C\|_{L^\infty}, \frac{\gamma}{\eta^d}\|\rho\|_{L^\infty(x,t)}\right) \sim \mathcal{O}(1),$$

where $|E_I| = |\nabla\phi_I| = \mathcal{O}(\gamma\|C\|_{L^\infty}, \frac{\gamma}{\eta^d}\|\rho\|_{L^\infty(x,t)}) = \mathcal{O}(\gamma) + \mathcal{O}(\frac{\gamma}{\eta^d})$, where γ and $\frac{\gamma}{\eta^d}$ are small enough so that it does not overrule unity. In particular this means that the scaled Debye length γ compared with η (the ratio between the reference drift velocity and the background temperature) is of order of no more than a half. In particular, this configuration rules out scalings where the potential equation (3.23c) becomes very stiff.

Another important remark is that the nature of system (3.23a)–(3.23d) requires that the doping profile function $C(x)$ be a spatial smooth function if regular solutions are to be expected. This is due to the dependence of the coefficients of the resulting parabolic equation for the density ρ on the second derivatives of the electric field $E = -(\tau\eta)^{-1}u$.

Next we prove the following result which assumes the existence of smooth ε-independent bounded solutions to the boundary value problem associated with system (3.21a)–(3.21b). It compares the term in the closure that contains ω with the time derivative of the electric field E_t. We shall need this estimate when we propose the moment closure in the next section.

PROPOSITION 1. *Let (ρ, u, ω_0) be a solution to an initial-boundary value problem associated with system* (3.21a)–(3.21b) *such that its L^∞ bounds are independent of ε. Then*

$$\frac{\gamma}{\eta^d}(\rho\, u + \omega_0) = \tau\,\eta^2\,\rho\, E_t + \mathcal{O}(\varepsilon). \tag{3.26}$$

Proof. Let $\omega = \omega_0 + \varepsilon\omega_1$, where ω_0 and ω_1 are defined through system (3.21a)–(3.21b).

Then for $k = 0, n = 1$, the last term of (3.21a) satisfies

$$\tau\,\eta\,\rho\,\left(\frac{\gamma}{\eta^d}(\rho\, u + \omega_0)\right) = \tau\eta\rho\,\frac{\gamma}{\eta^d}\left(\langle v\, F\rangle - \varepsilon\rho_1^{(1)} + \omega - \varepsilon\omega_1\right), \tag{3.27a}$$

where

$$\text{div}\ \omega_1 = 0 \qquad \text{and} \qquad \text{curl}\ \omega_1 = -\text{curl}\ (\rho_1^{(1)}) \tag{3.27b}$$

with $\rho_1^{(1)}$ as in (3.21a).

Combining (2.12) and (2.13)

$$\frac{\gamma}{\eta^d}\left(\langle v\, F\rangle + \omega\right) = -\eta\, E_t.$$

Therefore, we may write

$$\tau\,\eta\,\rho\,\left(\frac{\gamma}{\eta^d}(\rho\, u + \omega_0)\right) = -\tau\,\eta^2\rho\, E_t - \varepsilon\tau\,\eta\,\rho\,\frac{\gamma}{\eta^d}\rho_1^{(1)} - \varepsilon\tau\,\eta\,\rho\,\frac{\gamma}{\eta^d}\omega_1$$

so that $\rho_1^{(1)}$ becomes

$$\rho_1^{(1)} = \frac{\tau}{1+\varepsilon\tau\,\eta\,\frac{\gamma}{\eta^d}\,\rho}\Big\{ -\nabla_x\cdot(\rho(\theta+2u_{\otimes}u)) - u\,\nabla_x\cdot(\rho u) \\ -\tau\,\eta^2\rho\,E_t - \varepsilon\tau\,\eta\,\rho\,\frac{\gamma}{\eta^d}\omega_1\Big\}, \tag{3.28a}$$

where ω_1 satisfies

$$\operatorname{div}\,\omega_1 = 0,$$

$$\operatorname{curl}\,\omega_1 = -\operatorname{curl}\,\Big(\tau\Big\{ -\nabla_x\cdot(\rho(\theta I+2u_{\otimes}u)) + u\nabla_x\cdot(\rho u) \\ -\tau\eta\rho\frac{\gamma}{\eta^d}\,(\rho u+\omega_0)\Big\}\Big). \tag{3.28b}$$

If $\tau\,\eta\,\frac{\gamma}{\eta^d}\rho = \mathcal{O}(1)$, then the solutions ω_1 of a boundary value problem associated with (3.28b) are of order $\mathcal{O}(1)$.

Therefore, the first moment $j = \langle v\,F\rangle$ can be also approximated by

$$\begin{aligned}\rho^{(1)} &\approx \rho\,u + \varepsilon\,\rho_1^{(1)}\\ &= \rho\,u + \varepsilon\,\tau\,\big\{(-\nabla_x\cdot(\rho\theta I) - 2\,\nabla_x\cdot\,(\rho u_{\otimes}u)) + u\,\nabla_x\cdot(\rho u) - \tau\,\eta^2\,\rho\,E_t\big\}\\ &\quad +\varepsilon^2\,\tau^2\eta\,\rho\,\frac{\gamma}{\eta^d}\,(1+\omega_1)\,,\end{aligned} \tag{3.29}$$

where ω_1 satisfies $\operatorname{div}\,\omega_1 = 0$ and (3.28b).

COROLLARY. *To the second order in the Chapman–Enskog expansion, the lowest closure for the first moment is given by either* (3.21b)–(3.22) *or by the one given above by* (3.28a)–(3.28b).

3.3. The dimensionalized lowest hierarchy full system with strong forcing. We complete this section by writing back system (3.23a)–(3.23d) in terms of the electric field E:

$$\eta\rho_t + \operatorname{div} j = 0, \tag{3.30a}$$

$$\begin{aligned}j = &-\tau\eta\,E\rho - \varepsilon\,\tau\,(\nabla_x\cdot(\rho(\theta I + 2(\eta\tau)^2\,E_{\otimes}E))) + \varepsilon\tau^2\,\eta E\,\operatorname{div}\,(\tau\eta\,E\rho)\\ &+\varepsilon\tau^2\,\rho\,\frac{\gamma}{\eta^d}\;\,(-\tau\,\eta\,\rho\,E+\omega)\,,\end{aligned} \tag{3.30b}$$

$$E = -\nabla\phi, \qquad \operatorname{div}\,(\nabla\phi) = \frac{\gamma}{\eta^d}(\rho - C(x)), \tag{3.30c}$$

$$\operatorname{div}\omega = 0 \qquad \text{and} \qquad \operatorname{curl}\,\omega = \operatorname{curl}\,(\tau\eta\rho E). \tag{3.30d}$$

To order $\varepsilon = \frac{\delta}{\eta}$ yields the parabolic-elliptic system

$$\eta\rho_t - \operatorname{div}\,(\tau\eta E\rho) + \tfrac{\delta}{\eta}\operatorname{div}\,\Big\{ -\tau\nabla_x(\rho(2\tau^2\eta^2E_{\otimes}E+\theta)) \\ +\tau^2\eta E\operatorname{div}\,(\tau\eta E\rho) + \tau^2\eta\,\rho\,\frac{\gamma}{\eta^d}(-\tau\,\eta\,\rho\,E+\omega)\Big\}, \tag{3.31a}$$

$$\operatorname{div}\omega = 0 \qquad \text{and} \qquad \operatorname{curl}\omega = \operatorname{curl}(\tau\eta\rho E), \tag{3.31b}$$

$$E = -\nabla\phi, \quad \operatorname{div}(\epsilon\nabla\phi) = \gamma\left(\frac{1}{\eta^d}\rho - C(x)\right). \tag{3.31c}$$

The corresponding dimensionalized strong force fluid level model, to the leading order, is also given by

$$0 = \partial_t\rho + \operatorname{div} j, \tag{3.32a}$$

$$\begin{aligned} j = &-\tau\{\nabla_x\cdot\left(\rho\left(\theta I + 2\mu^2\ E_{\circledcirc}E\right)\right)\} - \mu\rho E \\ &+ \tau\mu E\operatorname{div}(\mu\,E\rho) - \tau\mu\rho\,\frac{e}{\epsilon}(\mu\rho E - \omega), \end{aligned} \tag{3.32b}$$

$$\operatorname{div}\omega = 0 \qquad \text{and} \qquad \operatorname{curl}\omega = \mu\,E\otimes\nabla\rho, \tag{3.32c}$$

$$E = -\nabla\phi \qquad \text{and} \qquad \operatorname{div}(\epsilon\nabla\phi) = e(\rho - C(x)), \tag{3.32d}$$

where $\mu = \frac{e\tau(x)}{m}$ is the mobility coefficient associated with the drift-diffusion model for low electric fields when τ is constant.

Thus, the dimensionalized equations (1.7a)–(1.7d) hold.

Finally, we note that (3.32b) for the current can also be written in the form

$$\begin{aligned} j = &\left\{-\tau\nabla\rho\cdot\left(\left(\frac{\tau e}{m}\right)^2 E_{\circledcirc}E + \theta I\right)\right\} - \tau\rho\operatorname{div}\left(\left(\frac{e\tau}{m}\right)^2 E_{\circledcirc}E\right) \\ &-\tau\,\frac{\tau e}{m}\,E\,\rho\operatorname{div}\left(\frac{\tau e}{m}E\right) - \frac{\tau^2 e}{m}\,\frac{e}{\epsilon}\,\rho\left(\frac{\tau e}{m}\rho E - \omega\right). \end{aligned} \tag{3.33}$$

4. Moment closures. We propose a moment closure that yields fluid variables which agree, up to first order in ε, with the ones obtained in section 3 using the Chapman–Enskog procedure.

Defining the nth order moment of F by

$$\rho^n = \langle v^{\circledcirc n}F\rangle\,, \tag{4.1}$$

the nth order moment of the kinetic equation (2.11) yields (where $u = -\eta\,\tau\,E = \eta\,\tau\nabla\phi$)

$$\eta\,\partial_t\rho^{(n)} + \nabla_x\cdot\rho^{(n+1)} - \frac{n}{\varepsilon\,\tau}\,u_{\circledcirc}\rho^{(n-1)} + \frac{1}{\varepsilon\,\tau}\,\left(\rho^{(n)} - \rho m_M^{(n)}\right) = 0\,, \tag{4.2}$$

where $m_M^{(n)}$ are the moments of the Maxwellian given in (3.13a)–(3.13b) and $\varepsilon = \frac{\delta}{\eta}$.

In order to close these equations at level $n = N$, one must express $\rho^{(N+1)}$ in terms of the lower order moments. We propose a two-step closure. By balancing terms of order ε^{-1} in the moment equation of order $(N+1)$, we obtain our first approximation. By (4.2),

$$\tilde\rho^{(N+2)} = \rho m_M^{(N+2)} + (N+2)u_{\circledcirc}\rho^{(N+1)}\,. \tag{4.3}$$

Now consider the moment equation of order $N+1$,

$$\eta\,\partial_t\rho^{(N+1)} + \nabla_x\cdot\rho^{(N+2)} - \frac{N+1}{\varepsilon\,\tau}\,u_\otimes\rho^{(N)} + \frac{1}{\varepsilon\,\tau}\,\rho^{(N+1)} = 0\,. \tag{4.4}$$

Replace $\rho^{(N+2)}$ in (4.4) by $\rho^{(N+2)} = \tilde\rho^{(N+2)}$ from (4.3). That yields

$$\begin{aligned}&\eta\,\partial_t\rho^{(N+1)} + \nabla_x\cdot\left(\rho\,m_M^{(N+2)} + (N+2)u_\otimes\rho^{(N+1)}\right)\\ &-\frac{N+1}{\varepsilon\,\tau}\,u_\otimes\rho^{(N)} + \frac{1}{\varepsilon\,\tau}\left(\rho^{(N+1)} - \rho\,m_M^{(N+1)}\right) = 0\,.\end{aligned} \tag{4.5}$$

Now, the closure consists of taking the Chapman–Enskog procedure (3.16)–(3.17) to expand

$$\rho^{(N+1)} = \rho_0^{(N+1)} + \varepsilon\,\rho_1^{(N+1)} = \rho\,m_P^{(N+1)} + \varepsilon\,\rho_1^{(N+1)}\,,$$

and replace in (4.5) in order to obtain an expression for $\rho_1^{(N+1)}$. Therefore, replacing $\rho^{(N+1)}$ in (4.5) by $\rho\,m_P^{(N+1)} + \varepsilon\,\rho_1^{(N+1)}$ we obtain

$$\begin{aligned}&\eta\,\partial_t\left(\rho\,m_P^{(N+1)}\right) + \nabla_x\cdot\left(\rho\,m_M^{(N+2)} + (N+2)u_\otimes\rho\,m_P^{(N+1)}\right)\\ &-\frac{N+1}{\varepsilon\,\tau}u_\otimes\rho m_P^{(N)} + \frac{1}{\varepsilon\,\tau}\left(\rho\,m_P^{(N+1)} - \rho\,m_M^{(N+1)}\right)\\ &+\frac{1}{\tau}\rho_1^{(N+1)} - \frac{N+1}{\tau}u_\otimes\rho_1^{(N)}\\ &+\varepsilon\,\eta\,\partial_t\rho_1^{(N+1)} + \varepsilon\,\nabla_x\cdot\left((N+2)\,u_\otimes\rho_1^{(N+1)}\right) = 0\,.\end{aligned} \tag{4.6}$$

From (3.13a)–(3.13b) $(N+1)\,u_\otimes m_P^{(N)} = m_P^{(N+1)} - m_M^{(N+1)}$; then (4.6) gives

$$\begin{aligned}\rho_1^{(N+1)} = &-\tau\,m_P^{(N+1)}\eta\,\partial_t\rho - \tau\,\nabla_x\cdot\left(\rho\left(m_M^{(N+2)} + (N+2)u_\otimes m_P^{(N+1)}\right)\right)\\ &-\tau\eta\rho\partial_t m_P^{(N+1)} + (N+1)u_\otimes\rho_1^{(N)}\\ &-\varepsilon\left(\eta\partial_t\rho_1^{(N+1)} + \nabla_x\cdot\left((N+2)u_\otimes\rho_1^{(N+1)}\right)\right)\,.\end{aligned} \tag{4.7}$$

Replacing $\eta\,\partial_t\rho$ by $-\nabla_x(\rho u) + \mathcal{O}(\varepsilon)$ and $m_M^{(N+2)} + (N+2)u_\otimes m_P^{(N+1)} = m_P^{(N+2)}$, then (4.7) gives the second approximation of the $(N+1)$st moment

$$\begin{aligned}\rho_1^{(N+1)} = &\,\tau\,m_P^{(N+1)}\,\nabla_x(\rho u) - \tau\nabla_x\cdot\left(\rho m_P^{(N+2)}\right)\\ &-\tau\eta\rho\partial_u(m_P^{(N+1)})u_t + (N+1)u_\otimes\rho_1^{(N)} + \mathcal{O}(\varepsilon)\,.\end{aligned} \tag{4.8}$$

See that this expression coincides up to order ε with the $\rho_1^{(n)}$ given by the Chapman–Enskog procedure in (3.18) and the remark below (3.21a)–(3.21b).

Hence, the $(N+1)$st moment is given by

$$\begin{aligned}\rho^{(N+1)} &= \rho\, m_P^{(N+1)} \\ &+\varepsilon\Big\{\tau m_P^{(N+1)}\nabla_x\cdot(\rho u) - \tau\nabla_x\left(\rho m_P^{(N+2)}\right) \\ &\quad -\tau\eta\rho\partial_u m_P^{(N+1)}u_t + (N+1)u_{\otimes}\rho_1^{(N)}\Big\} + \mathcal{O}(\varepsilon^2)\,.\end{aligned} \tag{4.9}$$

Clearly, the moment variables obtained by the Chapman–Enskog expansion agree with the ones from these closures to first order in the scaled mean free path parameter ε.

Notice that for $N=0$ this becomes

$$\rho^{(1)} \approx \rho\, u + \varepsilon\,\tau\,\{-\nabla_x\cdot(\rho(\theta I + 2u_{\otimes}u)) + u\nabla_x\cdot(\rho u) - \eta\rho\partial_t u\}\,, \tag{4.10}$$

which recovers (3.22), with $u = -\tau\,\eta\,E$.

See that, by Proposition 1, $-u_t$ is approximated to order ε by $\tau\frac{\gamma}{\eta^d}(\rho\,u+\omega)$. Hence the moment equations for this closure are up to an order of ε^2 the same as those for the Chapman–Enskog expansion, i.e., system (3.21a)–(3.21b).

Higher order moments. For $N=1$ we obtain an approximation to the energy as the second moment of F. It becomes

$$\begin{aligned}W &= \rho^{(2)} \\ &= \rho(\theta I + 2u_{\otimes}u) + \varepsilon\tau\big\{-3\nabla_x\cdot(\rho\,u_{\otimes}\,(\theta I + 2u_{\otimes}u)) \\ &\qquad +\ (\theta\,I + 2u_{\otimes}u)\,\nabla_x\cdot(\rho\,u) - 4\tau\eta\,\rho u\partial_t u\big\} + \varepsilon 2u(\rho^{(1)} - \rho u) \\ &= \rho(\,\theta I + 2u_{\otimes}u\,) + \varepsilon\tau\big\{-2\nabla_x\cdot(\rho\,u_{\otimes}\,(2\theta I + 3u_{\otimes}u)) \\ &\qquad +2\rho\,(\theta\,I - u_{\otimes}u)\,\nabla_x\cdot u - \rho\,u\nabla_x(\theta I) - 6\eta\,\rho u\partial_t u\big\}\,.\end{aligned} \tag{4.11}$$

Similarly, $\rho^{(3)} = 3\rho(\theta I_{\otimes}u + 2u_{\otimes}u_{\otimes}u) + \rho_1^{(3)}$, with $\rho_1^{(3)}$ (4.8) for $N=2$, and $\rho_1^{(2)}$ from the ε order term in (4.11).

Writing the equations for the moments up to the second one we obtain a system that models mass, momentum, and energy, where $\rho^{(3)}$ provides the closure for the energy equation.

This closure yields drift-diffusive systems which are linear in the state variables due to the nondegeneracy property of the transport kinetic equation. However, the nonlinearity arises through the coupling with the electric field.

5. Boundary conditions for kinetic and macroscopic approximations. So far, we have not discussed the boundary conditions for the distribution function of the electrons and, indeed, this is a topic that is barely mentioned in the existing literature.

We start by remarking that the boundary conditions for the Boltzmann equation must be consistent with the boundary conditions for the electric field, which in turn reflect the physical nature of the boundary.

On those boundaries where the normal component of the electric field is zero (insulating boundaries), sometimes the situation is represented schematically by specularly reflecting the carriers, but this is not sufficiently accurate if (as is usually the case)

the carriers are not at the same temperature as the boundary and hence an energy exchange takes place there.

On those boundaries (electrodes), where the semiconductor is put into contact with a metal (ohmic contacts), the electric potential takes on an assigned value. Despite their importance, very little is known about ohmic contacts. Usually they are accompanied by heavily doped regions of the semiconductor, in which conditions of charge neutrality prevail.

In a previous paper [CGL] the authors propose a boundary condition at the kinetic level that yields charge neutrality at the ohmic contacts. The set of these boundary points will be denoted by Γ_D, where the suffix D stands for Dirichlet, because one would apply a Dirichlet boundary condition in the standard drift-diffusion approximation.

Let $P(\nabla\phi, v)$ be the ground state associated with an asymptotic expansion of (2.11)–(2.12) for either η or $\varepsilon = \frac{\delta}{\eta}$ small, and let N be a normalization factor and $C(x)$ the doping concentration (or background), then, for $v \cdot n < 0$, $F(x,t,v)$ is assumed to be proportional to $P(\nabla\phi, v)$ and hence to satisfy, at the ohmic contact points of the boundary in x-space:

$$F_- = P(\nabla\phi, v)\, N = \left(C(x) - \int_{v\cdot n>0} F_+\, dv\right) \frac{P(\nabla\phi, v)}{\int_{v\cdot n<0} P(\nabla\phi, v)\, dv} \quad (x \in \Gamma_D), \tag{5.1}$$

where $F_\pm$ denote the restrictions $F(x,t,v)\big|_{\pm v\cdot n>0}$ and n is the outer unit normal to the boundary section in x-space. Because this condition applies to heavily doped regions, we assume that $C(x)$ is strictly positive on the boundary. Should it vanish at some point, then F would also be forced to be zero there.

Let us check that the factor N, implicitly defined by (5.1), leads to charge neutrality. In fact, integrating over those velocities that are leaving a point of Γ_D, we obtain

$$C(x) = \int_{v\cdot n<0} F_-\, dv + \int_{v\cdot n>0} F_+\, dv\,, \quad x \in \Gamma_D\,. \tag{5.2}$$

Now, the electron density in x-space is given by $\rho(x,t) = \int F(x,t,v)\, dv$ and hence

$$\rho(x,t)\big|_\Gamma = \int_{v\cdot n<0} F_-\, dv + \int_{v\cdot n>0} F_+\, dv\,. \tag{5.3}$$

Comparing (5.2) with (5.3) immediately yields

$$\rho(x,t)\big|_{\Gamma_D} = C(x)\big|_{\Gamma_D}\,, \tag{5.4}$$

so that a charge neutrality condition is satisfied at the contacts.

This boundary condition was constructed in order to show that one can write a boundary condition yielding strict charge neutrality at ohmic contacts.

The boundary condition (5.1) is just a mathematical formulation of the phenomenological boundary conditions used in most simulations. In particular, it is explicitly mentioned by Baranger and Wilkins [BW] in a footnote. The main, but irrelevant, difference is only in the equilibrium density used (here P rather than the Maxwellian). The reason why we put P rather than M is theoretical consistency, but P will reduce to M near ohmic contacts, because there is no significant electric field. The reason why we mention again this kind of boundary condition is not to recommend but rather to criticize it. It has, in fact, at least two disadvantages:

(1) The larger the number of electrons arriving at the wall, the less the number of those leaving the wall. This is mainly a conceptual rather than a practical difficulty, because the electrons are not expected to come back once they have entered the drain and not many of them are going to arrive at the source.

(2) The usual boundary conditions are formulated in terms of particle flows and not of particle densities. Then the simplest boundary condition seems to be that of assigning the inflow as one usually does for a gas (vapor) at an evaporating surface. This boundary condition has been used previously [C2], [GK], [Kl], and [NP].

We remark that the exact form of the boundary condition at ohmic contacts is not so important, provided it ensures an approximate charge balance, because these contacts occur in a heavily doped region, where the electric field and the deviation from a Maxwellian are small. The corrections to the electron density will be small, because the mean free path is relatively small.

Next, we propose a similar condition for insulating boundaries in x-space (a subset denoted by Γ_N, where the suffix N stands for Neumann, as D stood for Dirichlet before):

$$F_- = NP(\nabla\phi, v) = \int_{v\cdot n>0} v\cdot n\, F_+\, dv\ \frac{P(\nabla\phi, v)}{\int_{v\cdot n<0} |v\cdot n| P(\nabla\phi, v)\, dv}\,. \tag{5.5}$$

Integrating over $v\cdot n<0$, (5.5) yields

$$j\cdot n\big|_{\Gamma_N} = \left(\int_{v\cdot n<0} v\cdot n\, F_-\, dv + \int_{v\cdot n>0} v\cdot n\, F_+\, dv\right)\Bigg|_{\Gamma_N} = 0\,, \tag{5.6}$$

where $j = \int\ v\, F(x,t,v)\, dv$ is the particle flow. One may well question the use of P in this boundary condition. In this case it is not irrelevant to use P rather than M; it will make a difference underneath the gate where the field does not vanish. Using P means imagining a mechanism that somehow allows the carriers to penetrate in a monatomic layer of the semiconductor and still feels the field there. We put the two choices (P and M) on the same level. Future simulations and comparisons should tell us which is preferable.

In order to solve the moment equations obtained in the previous section, we need, of course, appropriate boundary conditions. In order to obtain them in an exact form, we should solve an appropriate Milne problem [C2] and [BCN]. Because ohmic contacts occur in regions of low field, the previous treatments [GK] and [Kl] should suffice. The situation would of course be different if devices with high field near the ohmic contacts were to be studied. A sketch of an approximate treatment of this problem for the boundary condition (5.1) was previously given [CGL].

In the case of Neumann boundary conditions we obtain an exact boundary condition, i.e., the normal component of the electric current j vanishes.

Finally, we conclude by deriving appropriate boundary conditions for the macroscopic system (1.7a)–(1.7d) as follows.

Denoting by n the outer unit normal to the boundary and by s the unit tangential directions to the boundary at a given boundary point, we have the following.

(i) *Insulating boundaries* $\Gamma_{\mathcal{N}}$*:* The current j and the electrostatic potential Φ satisfy

$$j\cdot n = 0 \qquad \text{and} \qquad E\cdot n = -\nabla\Phi\cdot n = 0 \quad \text{on}\ \ \Gamma_{\mathcal{N}}, \tag{5.7a}$$

respectively, so that $E_t\cdot n = 0$ and $j_0\cdot n = \mu\rho\, E\cdot n = 0$; then

$$\omega\cdot n = (E_t + j_0)\cdot n = 0 \quad \text{on}\ \Gamma_{\mathcal{N}}\,. \tag{5.7b}$$

(ii) (*Ohmic*) *contact boundaries* $\Gamma_{\mathcal{D}}$*:* The electric potential is taken constant in space and time on each connected component of the contact boundaries.

We must expect charge neutrality, except for a small correction proportional to the density gradient. The coefficient will be of the order of the mean free path with a numerical factor depending on the specific boundary condition, that is, for a given doping profile function $C(x)$,

$$\rho = C(x) + \mathcal{O}(\varepsilon) \qquad \text{and} \qquad \Phi = \text{constant} \quad \text{on} \ \ \Gamma_{\mathcal{D}}\,. \tag{5.7c}$$

Then the condition for ω can be computed as

$$\begin{aligned} \omega \cdot s &= (E_t + j_0) \cdot s = (\nabla \Phi_t + \mu\rho E) \cdot s \\ &= (\nabla \Phi \cdot s)_t - \mu\rho \nabla\Phi \cdot s = 0 \quad \text{on } \Gamma_{\mathcal{D}}\,. \end{aligned} \tag{5.7d}$$

Before ending this section we would like to point out that there are kinetic layers which are to be studied. These are interior layers connecting regions of high and low field. These problems will be addressed in a separate paper.

6. Results of a numerical simulation. In this section we present computational evidence that the DCB scaling regime can be realized in a simulation of a semibulk model of a silicon diode of half-micron channel length at applied bias between 1 and 3 volts. In addition, a hybrid domain decomposition technique has been developed to incorporate the equations corresponding to the (DCB) scale. This work is based on a recent one by Carrillo, Gamba, and Shu [CGS], where a more comprehensive computational work is presented for a silicon and gallium arsenide full-device model.

The computational method used in [CGS] is a modification of the one from [CGJS2] in order to make a self-adaptive method of domain decomposition.

The computations shown here correspond to a one dimensional n^+-n structure of length $0.5\mu m$. They include the self-consistent field dependent relaxation kinetic-Poisson system showing the local nondimensional parameters ε, η, and δ introduced in section 2, the distribution functions at different positions of the channel region, and a comparison between current-voltage characteristics curves computed by the kinetic-Poisson system, by the classical drift-diffusion equation, and by a new adaptive method of domain decomposition that uses drift-diffusion models in the n^+ region and system (1.7a)–(1.7d) (augmented drift diffusion) inside the channel region.

Their global kinetic model is simulated with field dependent relaxation given by

$$\tau(E) = \frac{m}{e}\mu(|E|) = \frac{m}{e}\,\frac{2\mu_0}{1+\sqrt{1+4(\mu_0|E|/v_d)^2}}\,,$$

with $\mu_0 = 0.1323\mu m^2/(V\,ps)$ and $v_d = 0.13\ \mu m/ps$. Following [CGJS2], the parameter μ_0 is taken by the channel value extrapolation corresponding to bulk mobility of n^+ region, and v_d is taken to be the maximum of the velocity in the kinetic run with $vbias = 1.5$ and the channel extrapolated mobility which was calibrated by Monte Carlo simulations. The doping $C(x)$ is defined by $n_d(x) = 5\times 10^5/\mu m^3$ in $0 \le x \le 0.1$ and $0.5 \le x \le 0.6$; and $n_d(x) = 2\times 10^3/\mu m^3$ in $0.1 < x < 0.5$.

The numerical algorithm for the kinetic equation is a fourth order weakly essentially nonoscillatory (WENO) scheme. The high order accuracy of these algorithms can be achieved without introducing any oscillations near discontinuities or sharp gradient regions, and it allows use of relatively coarse grids while still obtaining very

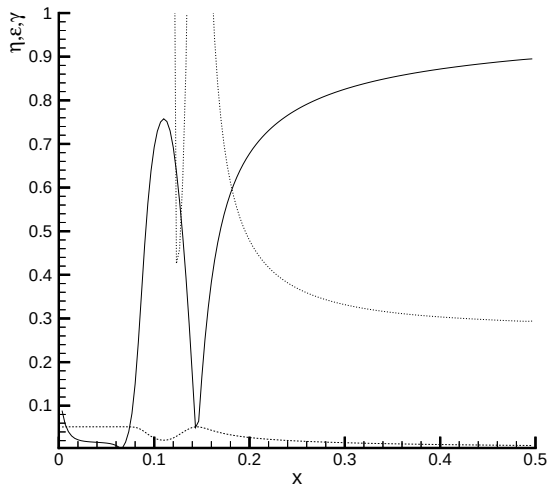

FIG. 1. *Local nondimensional parameters, calculated with $E(x)$ from the kinetic simulation results. Solid line: $\eta(x)$; dashed line: $\varepsilon(x)$; dotted line: $\gamma(x)$.*

accurate results. The algorithms are extremely stable and robust in all the numerical simulations. These kinetic numerical methods has been implemented in [CGJS1]. In all the numerical simulations, long time integration is performed until a steady state is reached. The collision integrals conserve particle number, hence $n(x,t)v(x,t)$ should be a constant in steady states. We take the average in the whole region $L = [a,b] = [0, 0.5]$ to compute I.

The data for the kinetic simulation is as follows. Velocity space is artificially cut at $-a \le u \le a$, where monitoring is needed in order to ensure that $f(x,u,t)$ is always very small at the boundary $u = \pm a$ for the final steady state results (it is more than enough in all runs to use $a = 3.5$). A uniform grid is used in x and u, with 160×150 points.

The kinetic boundary conditions in the n^+-n structure are at $x = 0$, take $\phi(0,t) = 0$, and $f(0,u,t) = n_d(0)\, M(u)$ if $u \ge 0$; and no boundary condition, by meaning extrapolation of the numerical solution from inside the domain to the boundary, if $u < 0$. At $x = 0.5$, take $\phi(0.5,t) = vbias$, and $f(0.5,u,t) = 0$ if $u \le 0$; and no boundary condition if $u > 0$. Also, at $u = -a$ and $u = a$, take no boundary condition in the sense given above. We point out that these are not the proposed boundary conditions in section 5, but the standard ones for kinetic computations.

Figure 1 contains plots of the dimensionless parameters introduced in section 2, the quotient between the scaled drift and thermal speeds η, the scaled mean free path ε, and the inverse of the Debye length γ. The drift-diffusion regime corresponds to $\gamma >> 1$, $\eta < \varepsilon << 1$. Because $\gamma >> 1$ then drift-diffusion regime is approximately dominant in $0 < x < 0.155$. The next regime, i.e., for γ and η of order one and $\varepsilon << 1$, corresponds to the DCB regime or augmented drift diffusion.

Figure 2 shows a comparison between the computed solution of the normalized kinetic system by its density ρ, a Maxwellian with temperature Θ centered at the origin, and the distribution $P_E(v)$ using formula (3.10).

In particular, the given example of a silicon device, with $v_d = 0.13$ and applied bias of 1 to 3 volts, is a "good parameter" case for domain decomposition of the drift-diffusion/augmented drift-diffusion coupling because it makes a quasi-perfect fit

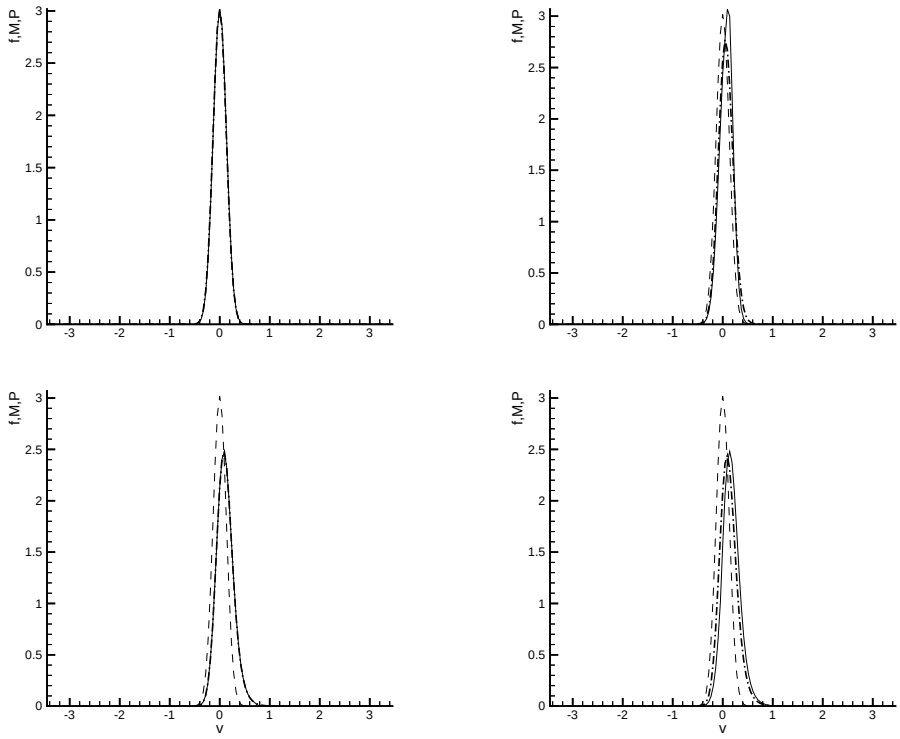

FIG. 2. *Normalized stationary distribution $f_\infty(x,v)/\rho_\infty(x)$ at several fixed x for $V_{bias} = 1V$, obtained from the kinetic simulation and compared to a Maxwellian at lattice temperature Θ, centered at zero velocity. Solid line: kinetic solution; dashed line: $M_\Theta(v)$; dash-dotted line: $P_E(v)$. Top left: at $x = 0.02\mu m$; top right: at $x = 0.13\mu m$; bottom left: at $x = 0.3\mu m$; bottom right: at $x = 0.46\mu m$.*

to the kinetic computation. The current voltage characteristic curves are improved considerably with respect to the drift-diffusion curves as the bias gets larger.

Figure 3 shows a comparison of the current-voltage characteristics, computed by the kinetic nonlinear system, by the standard drift-diffusion equations and by a hybrid method of domain decomposition combining drift-diffusion models in the highly doped region and the augmented drift-diffusion DCB hydrodynamic system (1.7a)–(1.7d) with boundary conditions (1.8a)–(1.8b) corresponding to the one dimensional case. Since in this case the equations yield ω constant, a suitable computational boundary condition for ω has been given in [CGJS1] and [CGJS2] by taking $\omega = (\mu\rho E)|_{x=x_0}$ at some point x_0 in the region where (1.7a)–(1.7d) is computed.

Finally, it can be observed in Figure 2 that the normalized kinetic solution and $P_E(v)$, at $x > 0.15$, agree at a high accuracy rate. This numerical evidence may indicate the large time asymptotic of the solution of the kinetic system approaches the P_E distribution solution of the DCB regime.

7. Concluding remarks. Our approximation is a first attempt to produce a full self-consistent model at the fluid level derived from a kinetic formulation that may also handle rough boundary effects and other geometrical constraints due to the design of the devices, as well as to provide a correction to fluid level models for those regions under moderate high field effects or other inhomogeneities. These macroscopic approximations model energy, transport, and diffusion coefficients that are field dependent and anisotropic. These models have appeared in the microelec-

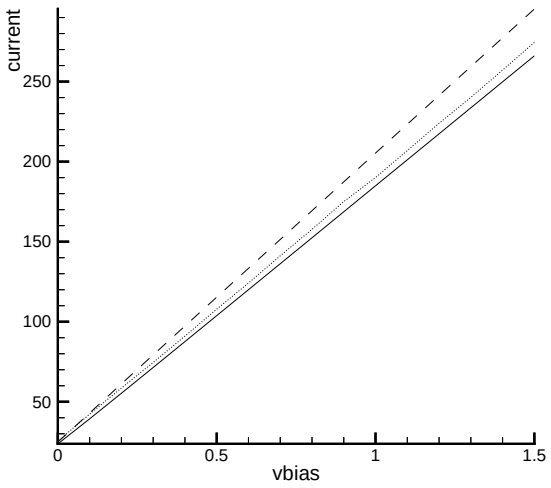

FIG. 3. *Current-voltage characteristics for the silicon n^+-n device. Solid line: the Boltzmann-Poisson system; dashed line: the drift-diffusion computation equation; dash-dotted line: the drift-diffusion/augmented drift-diffusion hybrid computation. Field dependent mobility $\mu(E)$.*

tronic literature and are referred as augmented drift-diffusion equations. A simplified version was originally proposed by Thoernber [Th] as an ad-hoc approximation to hot-electron transport.

For the reader's reference, other high field models that can model energies (energy transport models), have been obtained using spherical harmonic expansions (SHE) of the nonlinear Boltzmann equation by Dmitruck, Reyna, and Saul [DRS] and Ben Abdallah, Degond, and Genieys [BDG] under the hypothesis that the energy gain or loss of the electrons by the phonon collisions is weak, leading to a scaling that allows high relative local fields. Energy transport models are computed using expansions whose ground states are distributions in the null space of the collision operators under consideration (i.e., collision operators that take into account more physical phenomena other than linear interactions with the material). In all these cases their kernels are spanned by distributions which are field independent, so there are essentially isotropic drift-diffusion models that incorporate into the system a transport equation for the energy. See [BD1] and references therein for a detailed survey on derivations and hierarchies of macroscopic models for semiconductors.

Also, Ben Abdallah and Degond [BD2] worked out a stronger high field scaling corresponding to the Child–Langmuir asymptotic for the relaxation operator in the stationary one dimensional case. Though they developed a constitutive relation for the currents, no standard hydrodynamics are available yet for this regime. This asymptotic limit corresponds to a relative large ballistic speed with respect to the variance of the equilibrium distribution of the system at rest. The pure ballistic regime does not show in the kinetic simulation of submicron silicon heavily doped devices, though it localizes the magnitude of the mean velocity and currents as observed in the computations by Carrillo, Gamba, and Shu [CGS]. This is a different regime from the DCB regime.

An interesting numerical comparison of these models versus kinetic computations can be found in Laux and Fischetti [LF].

This presentation, although formal, has the goal to produce a diffusive closure for the full system and is presented in its simplest possible formulation in order to get a complete formulation of a boundary value problem for the full system that includes energy transport equations. Any formalism to justify the asymptotic expansion with the Chapman–Enskog procedure in a bounded domain would require solving a boundary value problem for the *full model* at the kinetic and its corresponding fluid level, as well as the corresponding Milne problem. Some portion of the program has been completed in problems of gas dynamics (see Cercignani [C1], Cercignani, Illner, and Pulverenti [CIP], and references therein). The Milne problem has been studied for gas dynamics by Cercignani [C2] and Bardos, Caflisch, and Nicolaenko [BCN].

However, many of the justifications to the problems associated with this expansion remain open for particle-charged transport models, in particular the boundary condition at the kinetic level that will deliver the expected boundary conditions at the fluid level under low and high forcing (see Markowich, Ringhofer, and Schmeiser [MRS] and references therein). Some recent numerical and analytical work on drift-diffusion equations has been done by Poupaud [P3], Golse and Klar [GK], and Klar [Kl]. In a forthcoming paper, Gamba, Klar, and Ben Abdallah treat the half-space problem for the scaling corresponding to the drift-collision balance regime presented in this paper.

The computational work by [CGS], done for a silicon diode of the order of a half-micron with a heavily doped channel, shows that the drift-collision balance regime takes over most through the channel while the classical Maxwellian distribution takes over the heavily doped regions. The largest discrepancy occurs in the depletion region most asymptotic hydrodynamic methods are expected to fail. However, their work numerically validates the expansion in the channel (section 6, Figure 2), and calls for the need of hybrid kinetic-fluid interfaces to handle regions of large energy gradients. They also implement an elementary hybrid domain decomposition improving the one developed by Cercignani et al. [CGJS2]. In addition, this new domain decomposition improves the comparison of the current-voltage characteristic curves (IV-curves) in a large factor (section 6, Figure 3).

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