A High Field Approximation to a Boltzmann–Poisson System in Bounded Domains

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Abstract. We consider the Boltzmann-Poisson system for electrons in a semiconductor in the case of high fields and small devices. We discuss closures of moment equations and boundary conditions for both the distribution function and the moments.

1. Introduction and Basic Equations.

Recent advances in submicron semiconductor devices led to regimes of hot electron transport in which traditional drift–diffusion models break down. This failure is, in part, due to small size of the devices and manifests itself with relatively larger carrier mean free path and stronger electric fields. Moreover, boundary value problems for these models are essential issues in the actual modeling of devices, as well as the understanding of macroscopic level of modeling which are reliable and computationally efficient (for instance, see Barenger and Wilkins [B1], Ferry and Grondin [FG] and Reggiani [Rg], and references therein.)

Considering the inhomogeneities of a practical device (in particular effects due to heavily doped regions in submicron structures) a single device can not be modeled with just one single set of partial differential equations derived from kinetic charged–particle transport, as different magnitudes of the scaling parameters might take over in different parts of the device (see Ferry and Grondin [FG]). Therefore it is imperative not only to discuss asymptotic models for the transport equation, but also for the *full system* with the boundary data transfer from kinetic to macroscopic level as well.

We shall present a systematic hierarchy of self consistent full models derived from 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 drift–diffusion regimes. We shall treat these ideas in the context of a simplified model, although these ideas as well as methods can be applied in more general settings. These regimes would correspond to hot–electron transport transition from bulk phenomena to ballistic transport, given by an intermediate drift velocity scale in between both regimes.

In the present paper we analyze the Boltzmann–Poisson system. We present a high field Chapman–Enskog expansion and a fluid (macroscopic) moment closure that matches the

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expansion at first order. 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 discuss the resulting boundary condition for the fluid model as well.

The resulting approximation is a first attempt to produce a full model at the fluid level derived from a kinetic formulation that can 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 high field effects (see Barenger and Wilkins[B1] and [B2], Trugman and Taylor [TT]). These macroscopic approximations model energy, transport and diffusion coefficients that are field dependent and anisotropic.

In fact, we present a *full boundary value problem* for a nonlinear system of partial differential equations that can also handle some geometrical constraints of the domain. These constraints correspond to devices when modeled in 2 or 3 space dimensions. For example, drift–diffusion models with constant transport and isotropic diffusion coefficients do not yield a well posed problem in a nonconvex spatial geometry with realistic boundary conditions unless special compatibility conditions are given between the jump in the data, the angle of the junction and the scaled Debye length. This is due to the fact that the corresponding electric field becomes infinity at the intersections of contacts with oxides or insulating boundaries and also at rough boundaries.

Our work follows the one initiated by Poupaud, [P1], [P2] and Stichel and Strothmann [SS]. Poupaud [P1] considers a linear Boltzmann equation for charged–particle transport for a given external electric field with a linear collision frequency operator. He solves the existence problem of a solution for the ground state equation for high field scalings, which consists in balancing the drift velocity with the collision term, and shows solvability (i.e. no runaway phenomena) when the collision frequency is bounded from below. In addition, he presents a Hilbert expansion for a small mean free path in a high field scaled linear Boltzmann equation, and computes a scalar drift–diffusion equation for the density, with a diffusion that depends on the given electric field. [P2] proposes a moment closure that models energies.

Stichel and Strothmann [SS] address the asymptotic expansion by the Hilbert method, for initial–boundary value problems under different scaling assumptions on the initial and boundary data.

Other high field models (energy transport models) that can model energies, have been obtained by Dmitruck, Reyna and Saul [DRS] and Ben-Abdallah, Degond and Genieys [BDG] under the hypothesis that the energy gain or loss of the electron 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). However their kernels are spanned by distributions which are field independent, so there are essentially drift–diffusion models that incorporate into the system a transport equation for the energy. See [BD] and references therein for a detailed survey on derivations and hierarchies of macroscopic models for semiconductors. In particular, these models cannot handle rough boundaries and reentrance corners or other nonconvex geometries with discontinuous data, with the exception of straight angles separating contacts from insulating walls as in a simple diode or other stiff constraints between the data. They have the same analytical difficulties of standard drift–diffusion models when the electric field becomes infinite.

Here, we take a Boltzmann–Poisson system with a relaxation time operator modeling collisions (non-degenerate case). We concentrate on two different aspects of this system. First, we look at the asymptotic macroscopic model that produces an approximation to the solution of the Boltzmann-Poisson system when the small parameter under consideration is the scaled mean free path, but in a regime of transport under large electric fields. Second, we concentrate on the boundary value problem for the kinetic problem and the corresponding one for the fluid level problem. Our formulation of the boundary conditions depends on the leading term of the expansion. They are valid on weak or strong field scalings and consequently do not need any assumption on the scaling of the boundary data as in [SS].

Hence, we use a high field (strong force) scaling for the full system and compute the formal Chapman–Enskog expansion for the asymptotic problem, and also get a moment closure. We show that both coincide up to terms of order of the mean free path. In addition we present a kinetic boundary condition that only requires the existence of a ground state (for either low or high fields) and delivers a density at the boundary of the inner expansion with an error of order of the mean free path.

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 to solve 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 these program has been completed in some 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 [BCK].

However most of these justifications remain open for the problem of particle–charged transport, in particular the boundary condition at the kinetic level that will deliver the expected boundary conditions at the fluid level (see Markowich [M1] and Markowich, Ringhofer and Schmeiser [MRS] and references therein). Some recent numerical and analytical work on drift–diffusion equations has been done by Golse and Klar[GK] and Klar [Kl]; however they use different boundary conditions from those proposed here.

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

For simplicity sake, we shall only consider electrons, since 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):

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

$F = F(x,v,t)$ 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

$$\mathcal{C}(F) = \mathcal{L}(F) + \mathcal{B}(F) \tag{1.4}$$

where $\mathcal{B}(F)$ 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. $\mathcal{L}(F)$ 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 $\mathcal{B}(F)$, 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 et al. [MRS], (& 1), or Ferry and Grondin [FG], (& 2)) the non–degenerate case and take

$$\mathcal{L}(F) = -\frac{M}{\tau} \int F(v')dv' + \frac{1}{\tau}\, F(v), \tag{1.5}$$

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

$$M = (2\pi\theta)^{-3/2}\, e^{-\frac{|v|^2}{2\theta}} \tag{1.6}$$

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, since they will take over 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 C-E 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 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 moment of the previous transport equation and to the divergence of the mobility and 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 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.

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

$$\phi(x,t) = \phi_E(x) + \phi_I(x,t),$$

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 non–degenerate 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 (1.7) 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 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 whose diffusion are 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 introduces the following boundary conditions at the kinetic level contact regions of the boundary (i.e. regions where the macroscopic density $C(x)$ is to be prescribed), and provides the corresponding approximation to the boundary conditions at the fluid level.

Denoting by $P(\nabla\phi,\, v)$ the ground state associated with an asymptotic expansion of a non–dimensionalized Boltzmann–Poisson system, for either low or strong forcing scales, and $C(x)$ the doping concentration (or background) then, for $v \cdot n < 0$, the condition consists in assuming $F(x,t,v)$ to be proportional to $P(\nabla\phi,\, v)$ times a normalizing factor $N(x)$, and hence to satisfy, at the contact points of the boundary in x-space,

$$F_- = P(\nabla\phi, v)\, N = \left(C(x) - \int_{v\cdot n>0} F_+\, dv \right) \frac{P(\nabla\phi, v)}{\int_{v\cdot n<0} P(\nabla\phi, v) dv} \quad (x \in \Gamma_D) \tag{1.7}$$

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. Since this condition applies to high background density 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.

The factor $N(x)$, implicitly defined by (1.7), leads to charge neutrality at the contact boundary.

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 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

$$0 = \partial_t \rho + \operatorname{div} j \tag{1.8.1}$$

$$j = -\tau \Big[\nabla_x \left(\rho \left(\theta + \mu^2\ E_{\otimes} E \right) \right) \Big] - \mu\rho E + \tau\mu E \rho \operatorname{div}(\mu\, E) - \tau\mu\rho\, \frac{e}{\epsilon} (\mu\rho E - \omega), \tag{1.8.2}$$

$$\operatorname{div}\, \omega = 0 \qquad \text{and} \qquad \operatorname{curl}\, \omega = \mu\, E \otimes \nabla\rho, \tag{1.8.3}$$

$$E = -\nabla\phi, \qquad \text{and} \qquad \operatorname{div}(\epsilon\nabla\phi) = e(\rho - C(x)), \tag{1.8.4}$$

where $\mu = \frac{e\tau}{m}$ is the mobility coefficient associated with the drift diffusion model for low electric fields. 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 we stated above, a feature of the model above 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 (1.8) 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

$$j \cdot n = 0, \qquad E \cdot n = -\nabla\Phi \cdot n = 0, \qquad \omega \cdot n = 0 \quad \text{on } \Gamma_{\mathcal{N}} \tag{1.9.1}$$

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 delivers also 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 $C(x)$,

$$\rho = C(x) + \mathcal{O}(\varepsilon), \qquad \Phi = constant, \qquad \omega \cdot s = 0 \quad \text{on } \Gamma_{\mathcal{D}} \tag{1.9.2}$$

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 (1.8) become the single equation

$$\Delta B = \nabla(\mu\rho) \otimes E \tag{1.10.}$$

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, or equivalently,

$$B = constant \quad \text{on } \Gamma_{\mathcal{N}} \quad \text{and } \nabla B \cdot n = 0 \quad \text{on } \Gamma_{\mathcal{D}} \tag{1.11}$$

Thus, we expect the full model (1.8)-(1.9) to be a quasi–linear system of parabolic–elliptic equations and preliminary calculations 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 non-degenerate 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 (1.8.1) and (1.8.2) 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 (Lemma 3) $(\mu\,\rho\,E-\omega)=E_t+\mathcal{O}(\varepsilon)$ is valid for strong uniformly ε bounded solutions of a boundary value problem associated with the *full system* (1.8)-(1.9).

Hence, we indeed verify that to the first order in ε the continuity equation of the *full system* (1.8) 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 be found in the literature. The justification of the complete model requires existence proofs of solutions of (1.8)–(1.9) and also existence of solutions to the kinetic boundary value problem as well. 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 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 $\bar\tau$ 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 (1.5) for the right hand side, the transport equation scales

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

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 equations (2.6), (2.7) and combining with (2.3), (2.4) and (2.8) yields the dimensionless system

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

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

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] Golse-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],[DSR], under the hypothesis that the energy gain or loss of electrons by the phonon collisions is weak, leading to a different scaling that allow

s high relative local electric fields as well. These are essentially systems of standard diffusion equations. Such regimes would be valid on large devices (i.e. L large) if the voltage drop $[\phi]$ is relatively small.

However, 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, under 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 $[\phi]$, $\gamma = \frac{\bar{\rho}\, e\, L^2}{\bar{\epsilon}\, [\phi]} = \mathcal{O}(1)$

In particular, our interest is concentrated in deriving a fluid approximate model under the assumption that the magnitude of the drift velocity U is of the same order as the magnitude of the thermal velocity $\bar{\theta}^{1/2}$ (i.e. $\eta = O(1)$) but the length scale of the device is very small compared with $U\bar{\tau}$ (i.e. $\varepsilon^{-1} = \eta/\delta \gg 1$).

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

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

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

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

$$(2.13) \qquad \eta \partial_t \rho + \nabla_x \cdot \langle vF \rangle = 0.$$

3. The Chapman-Enskog Expansion.

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

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

and express 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 (1.8).

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

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

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

$$u \cdot \nabla_v F_{k+1} + F_{k+1} = - \tau \, v \cdot \nabla_x F_k + \sum_{j=0}^{k} \tau \left\{ D_\rho F_j \, \langle v \cdot \nabla_x F_{k-j} \rangle \right.$$
$$(3.2.1) \qquad \left. + \, \eta \tau \, D_u F_j \, \frac{\gamma}{\eta^d} \left(\langle v F_{k-j} \rangle + \omega_{k-j} \right) \right\}$$

$$\text{(3.2.2)} \qquad \operatorname{div}\omega_{k-j} = 0 \qquad \operatorname{curl}\omega_{k-j} = -\operatorname{curl}\langle v\, F_{k-j}\rangle.$$

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

Proof: Since τ is time independent, the time dependence of F only enters through ρ and the gradient of ϕ.T thus for $F = F(\partial_x^k\rho,\, \partial_x^j\nabla\phi)$ where k and j denote the usual nonnegative multi index $k = (k_i, \ldots, k_d), j = (j_1, \ldots, j_d)$, 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 synthetically write as follows

$$\text{(3.3)} \qquad F_t = D_\rho\, F\,\partial_t\rho + D_{\nabla\phi}F\ \partial_t\nabla\phi.$$

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), yields

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

Thus

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

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

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

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

Hence, we seek solutions of

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

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

$$\text{(3.8)} \qquad F = F_0 + \varepsilon\,F_1 + \ldots + \varepsilon^k\,F_k$$

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).

The solvability of (3.1) in L^1 can be found in Trugman and Taylor [TT] for the relaxation type operator in one dimension, has also been discussed in Frosali, Van der Mee and Paveri Fontana [FV] and Poupaud [P1] for more general linear structures of collision operators in higher dimensions. Given our simple form for $\mathcal{L}$ (the non-degenerate case), indeed we may solve for P explicitly, but we do not need it here.

Indeed, in order to obtain the next terms in the expansion, match the expansion of F to the order ε^k, $\quad k = 0, 1, \ldots$ in system (3.7). Using that $\langle F_{k+1} \rangle = 0$ for $k \geq 1$, we obtain the recursion relation

$$\begin{aligned} \frac{u}{\tau} \cdot \nabla_v F_{k+1} + \frac{F_{k+1}}{\tau} = -v \cdot \nabla_x F_k + \sum_{j=0}^{k} \Big\{ & D_\rho F_j \, \langle v \cdot \nabla_x F_{k-j} \rangle \\ & + \eta\tau \, D_u F_j \, \frac{\gamma}{\eta^d} \left(\langle v F_{k-j} \rangle + \omega_{k-j} \right) \Big\} \end{aligned} \tag{3.10}$$

where

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

Here $D_{\nabla\phi} = \eta\tau\, D_u$. Therefore, (3.2.1) and (3.2.2) both hold.

Remark: The solvability (3.10) in $L^1(\mathbb{R}^3)$ follows naturaly 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 follows that the problem 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 equation (3.11.2) for ω and the Poisson equation for u has not been addressed yet. It will require to solve the macroscopic model corresponding to this expansion and show that both u and ω are L^∞ in time and space.

Thus, this regularity will depend on the initial–boundary value problem associated with macroscopic formulation of the full system, which in the lowest hierarchy corresponds to system (1.8). At this point becomes imperative to move forward and obtain the moment equations which will deliver a macroscopic formulation for the full system.

Lemma 2. *(The macroscopic or state variables) Under the conditions of Lemma 1, the* n^{th} *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*

$$\begin{aligned} \frac{1}{\tau}\, \rho_{k+1}^{(n)} = & -\frac{n}{\tau}\, u_{\otimes} \rho_{k+1}^{(n-1)} - \nabla_x \cdot \rho_k^{(n+1)} + \\ & + \sum_{j=0}^{k} \Big\{ D_\rho \rho_j^{(n)} \nabla_x \cdot \rho_{k-j}^{(1)} + \eta\tau\, D_u \rho_j^{(n)} \, \frac{\gamma}{\eta^d} \left(\rho_{k-j}^{(1)} + \omega_{k-j} \right) \Big\} \end{aligned} \tag{3.12.1}$$

where ω satisfies the equation

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

with the initial conditions

(3.12.3) $$\rho^{(0)}_{k+1} = 0 \quad \textit{for } k \geq 0 \qquad \textit{and} \qquad \rho^{(n)}_0 = \rho\,\langle v^{\otimes n} F_0\rangle \quad \textit{for } n \geq 0$$

As stated above, given the simple form for $\mathcal{L}$, we may solve for P explicitly. However, we will have no need for an explicit formula in order to obtain the moment equations. Thus we defer its computation till we discuss boundary conditions. Here we shall only need its velocity moments,

(3.13) $$m^{(n)}_P \equiv \langle v^{\otimes n} P\rangle,$$

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

(3.13) $$m^{(n)}_P - m^{(n)}_M = n\, u_{\otimes} m^{(n-1)}_P = n\eta\tau\, \nabla\phi_{\otimes} m^{(n-1)}_P.$$

Here $m^{(n)}_M$ are the moments of the Maxwellian M given by

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

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

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

Similarly, we do not need to solve (3.11) in order to get the moment equations. Defining the n^{th} order moment of F_k by

(3.16) $$\rho^{(n)}_k \equiv \langle v^{\otimes n} F_k\rangle$$

we compute from (3.11) the recursion relation

$$\begin{aligned} \frac{1}{\tau}\,\rho^{(n)}_{k+1} &= -\frac{n}{\tau}\, u_{\otimes}\rho^{(n-1)}_{k+1} - \nabla_x \cdot \rho^{(n+1)}_k + \\ &+ \sum_{j=0}^{k} \Big\{ D_\rho \rho^{(n)}_j \nabla_x \cdot \rho^{(1)}_{k-j} + \eta\tau\, D_u \rho^{(n)}_j \;\frac{\gamma}{\eta^d}\, \Big(\rho^{(1)}_{k-j} + \omega_{k-j}\Big)\Big\} \end{aligned} \tag{3.17}$$

along with

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

and the initial conditions

$$\rho^{(0)}_{k+1} = 0 \quad \text{for} \quad k \geq 0 \qquad \text{and} \qquad \rho^{(n)}_0 = \rho\, m^{(n)}_P \quad \text{for} \quad n \geq 0. \tag{3.18}$$

Then (3.12.1)–(3.12.3) hold so that the proof of lemma 1 is now completed.

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 (3.12.1)–(3.12.3) and solve recursively in n for $\rho^{(n)}_1$ to obtain

$$\begin{aligned}\frac{1}{\tau}\,\rho^{(n)}_1 &= \frac{n}{\tau}\,u_{\otimes}\rho^{(n-1)}_1 - \nabla_x \cdot \left(\rho m^{(n+1)}_P\right) + \\ &\quad + m^{(n)}_P \nabla_x \cdot \rho^{(1)}_0 + \eta\tau\rho\,\partial_u(m^{(n)}_P)\,\frac{\gamma}{\eta^d}\left(\rho^{(1)}_0 + \omega_0\right).\end{aligned} \tag{3.19}$$

Then we approximate the n^{th} moment of F by

$$\rho^{(n)} \approx \rho^{(n)}_0 + \varepsilon\rho^{(n)}_1 = \rho m^{(n)}_P + \varepsilon\rho^{(n)}_1 \tag{3.20}$$

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

$$\frac{1}{\tau}\,\rho^{(1)}_1 = -\nabla_x(\rho(\theta + 2u_{\otimes}u) + u\nabla_x\cdot(\rho u) + \eta\tau\left(D_u(\rho u)\,\frac{\gamma}{\eta^d}\,(\rho u + \omega_0)\right), \tag{3.21.1}$$

with

$$\operatorname{div}\,\omega_0 = 0 \qquad \text{and} \qquad \operatorname{curl}\,\omega_0 = -\operatorname{curl}\,(\rho u). \tag{3.21.2}$$

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

$$\begin{aligned} j = \rho^{(1)} \approx \rho\, u + \varepsilon\,\rho^{(1)}_1 = \rho\, u + \varepsilon\ \tau\,\{&-\nabla_x(\rho(\theta + 2u_{\otimes}u)) + u\,\nabla_x\cdot(\rho u) + \\ &+\tau\,\eta\,\rho\,\frac{\gamma}{\eta^d}\,(\rho u + \omega_0)\Big\}\end{aligned} \tag{3.22}$$

where ω_0 satisfies (3.21.2).

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

$$\eta\rho_t + \operatorname{div} j = 0, \tag{3.23.1}$$

(3.23.2)
$$j = u\rho + \varepsilon\,\tau\,\left\{ -\nabla_x(\rho(\theta + 2u_{\otimes}u)) + u\nabla_x\cdot(\rho u) + \eta\,\tau\,\rho\,\frac{\gamma}{\eta^d}\,(\rho u + \omega)\right\} + \mathcal{O}(\varepsilon^2),$$

with

(3.23.3)
$$u = \eta\tau\nabla\phi, \qquad \mathrm{div}\ (\nabla\phi) = \gamma(\frac{1}{\eta^d}\rho - C(x)),$$

(3.23.4)
$$\mathrm{div}\ \omega = 0 \qquad \text{and} \qquad \mathrm{curl}\ \omega = -\mathrm{curl}\ (\rho u).$$

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 (3.23) 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

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

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

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

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 order of one, since 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 $|E_I| = |\nabla\phi_I| = \mathcal{O}\left(\gamma\|C\|_{L^\infty}, \frac{\gamma}{\eta^d}\|\rho\|_{L^\infty(x,t)}\right) = \mathcal{O}(\gamma) + \mathcal{O}\left(\frac{\gamma}{\eta^d}\right)$ where γ and $\frac{\gamma}{\eta^d}$ is 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 (3.23.3) becomes very stiff.

Another important remark is that the nature of system (3.23) 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 (3.21). 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.

Lemma 3. *Let (ρ, u, ω_0) be a solution to an initial–boundary value problem associated with system (3.21) 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 in through system (3.2.1)–(3.2.2).

Then for $k = 0, n = 1$, the last term of (3.21.1) satisfies

$$\tau\, \eta\, \rho\, \left(\frac{\gamma}{\eta^d}(\rho\, u + \omega_0)\right) = \tau\eta\rho\, \frac{\gamma}{\eta^d}\left(\langle v\, F\rangle - \varepsilon\rho_1^{(1)} + \omega - \varepsilon\omega_1\right) \tag{3.27.1}$$

where

$$\text{div}\ \omega_1 = 0 \qquad \text{and} \qquad \text{curl}\ \omega_1 = -\text{curl}\ (\rho_1^{(1)}) \tag{3.27.2}$$

with $\rho_1^{(1)}$ as in (3.21.1).

Combining (2.12) and (2.13)

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

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

$$\begin{aligned} \rho_1^{(1)} = \frac{\tau}{1 + \varepsilon\tau\, \eta\, \frac{\gamma}{\eta^d}\, \rho}\{ &- \nabla_x(\rho(\theta + 2u_{\otimes}u)) - u\, \nabla_x \cdot (\rho u) + \\ &- \tau\, \eta^2 \rho\, E_t - \varepsilon\tau\, \eta\, \rho\, \frac{\gamma}{\eta^d}\omega_1\} \end{aligned} \tag{3.28.1}$$

where ω_1 satisfies

$$\begin{aligned} &\text{div } \omega_1 = 0 \\ &\text{curl } \omega_1 = -\text{curl } \left(\tau \Big\{ -\nabla_x(\rho(\theta + 2u_{\otimes}u)) + u\nabla_x \cdot (\rho u) \right. \\ &\qquad\qquad \left. - \tau\eta\rho\frac{\gamma}{\eta^d}\,(\rho u + \omega_0) \Big\} \right) \end{aligned} \tag{3.28.2}$$

If $\tau\,\eta\,\frac{\gamma}{\eta^d}\rho = \mathcal{O}(1)$ then the solutions ω_1 of a boundary value problem associated with (3.28.2) are of order $\mathcal{O}(1)$.

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

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

where ω_1 satisfies div $\omega_1 = 0$ and (3.28.2).

Corollary. *To the second order in the C–E expansion, the lowest closure for the first moment is given by either (3.21.2)–(3.22) or by the one given above by (3.28.1)–(3.28.2).*

3.3. The dimensionalized lowest hierarchy full system with strong forcing

We complete this section by writing back system (3.23) in terms of the electric field E

$$\eta\rho_t + \text{div}\, j = 0 \tag{3.30.1}$$

$$\begin{aligned} j = -\tau\eta\,E\rho - \varepsilon\,\tau\left(\nabla_x(\rho(\theta + 2(\eta\tau)^2\,E_{\otimes}E))\right) + \varepsilon\tau^2\,\eta E\;\text{div}\,(\tau\eta\,E\rho) \\ + \varepsilon\tau^2\,\rho\,\frac{\gamma}{\eta^d}\;\;(-\tau\,\eta\,\rho\,E + \omega) \end{aligned} \tag{3.30.2}$$

$$E = -\nabla\phi, \qquad \text{div }(\nabla\phi) = \frac{\gamma}{\eta^d}(\;\rho - C(x)\;), \tag{3.30.3}$$

$$\text{div }\omega = 0 \qquad \text{and} \qquad \text{curl }\omega = \text{curl }(\tau\eta\rho E). \tag{3.30.4}$$

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

$$\begin{aligned} \eta\rho_t - \text{div}\,(\tau\eta E\rho) + \frac{\delta}{\eta}\,\text{div}\Big\{ -\tau\nabla_x(\rho(2\tau^2\eta^2 E_{\otimes}E + \theta)) \\ + \tau^2\eta E\,\text{div }(\tau\eta E\rho) + \tau^2\eta\,\rho\,\frac{\gamma}{\eta^d}(-\tau\,\eta\,\rho\,E + \omega)\Big\}, \end{aligned} \tag{3.31.1}$$

$$\text{div } \omega = 0 \qquad \text{and} \qquad \text{curl } \omega = \text{curl } (\tau\eta\rho E), \tag{3.31.2}$$

$$E = -\nabla\phi, \quad \text{div } (\epsilon\nabla\phi) = \gamma(\frac{1}{\eta^d}\rho - C(x)). \tag{3.31.3}$$

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

$$\rho_t + \text{div}\, j = 0$$

$$j = \left\{ -\tau\nabla\rho \left(\tau^2 \frac{e^2}{m^2}\, E_{\otimes}E + \theta\right)\right\} - \frac{\tau e}{m}\, E\rho + \tau\, \frac{e\tau}{m}\, E\, \rho\text{div}(\frac{e\tau}{m}E) - \frac{e\tau^2}{m}\frac{e}{\epsilon}\,\rho\left(\frac{\tau e}{m}\rho E - \omega\right)$$

$$\text{div } \omega = 0 \qquad \text{and} \qquad \text{curl } \omega = \text{curl } (\frac{e\tau}{m}\rho E) = \frac{e\tau}{m}\, E \otimes \nabla\rho,$$

$$E = -\nabla\phi, \qquad \text{div } (\epsilon\nabla\phi) = e(\rho - C(x)).$$

See that $\frac{e\tau}{m} = \mu$ is the mobility coefficient in the case of the drift–diffusion equation for a low electric field scaling. Thus the dimensionalized equations (1.8) hold.

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 n^{th} order moment of F by

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

the n^{th} order moment of the kinetic equation (2.11) yields (where $u = -\eta\,\tau\, E = \eta\,\tau\nabla\phi$)

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

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

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. Balancing terms of order ε^{-1} in the moment equation of order $(N+1)$, we obtain our first approximation. By (4.2),

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

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 equation (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 in 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 equation (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

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

From (3.12), $(N+1)\, u_{\otimes} m_P^{(N)} = m_P^{(N+1)} - m_M^{(N+1)}$, then (4.6) gives

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

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 $(N+1)^{th}$ moment

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

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

Hence, the $(N+1)^{th}$ moment is given by

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

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

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

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

See that, by Lemma 3, $-u_t$ 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 C–E expansion, i.e. system ((3.21).

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 non-degeneracy 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 somehow 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 of 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.

We first 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. Since 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.

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.

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].

Here we shall use an approximate procedure which will yield qualitatively correct conditions. This procedure which was first used by Maxwell [M] for the gas dynamics Boltzmann equation, became popular in neutron transport because of the work of Marshak [D]. Essentially the procedure is based on the remark that there is a boundary layer, whose thickness is of the order of a mean free-path, where the Chapman-Enskog or similar expansions (to be called outer expansions) do not hold. The idea is then to equate some moments evaluated at the wall to the corresponding moments evaluated with the outer expansion, assuming that the molecules arriving there have a distribution dictated by the outer expansion (since they had their last collision a mean free-path away) and the molecules leaving the wall have the distribution dictated by the boundary conditions. One must remark that we cannot do this for all moments because we obtain twice as much boundary conditions as we need. Practice shows that the best way is to take moments which are odd in the normal component. The resulting boundary conditions will be qualitatively but not numerically accurate; to improve upon them one must study the aforementioned boundary layer.

Here we shall restrict ourselves to the leading order closure, equation (1.8), or, equivalently, (3.30). Let us start from the "Dirichlet" boundary condition (5.4). We remark that these boundary conditions have an exact consequence, *i.e.* the usual Dirichlet boundary condition for ρ, as we checked above. Thus we might be tempted to use this exact boundary condition instead of the approximate boundary condition delivered by the Marshak procedure. This idea would not lead to a correct estimate of the solution, because our moment equations only hold outside a boundary layer and thus it makes no sense to obtain their solutions from an exact boundary condition imposed at points where they do not hold.

Since we want to equate the particle flows in normal direction when computed according to the outer expansion and to the boundary conditions, we have:

$$\left(C(x) - \int_{v\cdot n>0} F_+\, dv\right)\; \frac{\int_{v\cdot n<0} P(\nabla\phi, v) v\cdot n\, dv}{\int_{v\cdot n<0} P(\nabla\phi, v) dv} + \int_{v\cdot n>0} v\cdot n F_+\, dv = j\cdot n \tag{5.7}$$

where j is given by equation (4.28), while P and F_+ is the restriction to $v \cdot n > 0$ of F_1, the second order approximation to F, as computed from equation (4.10) (with $F_0 = \rho P$).

It is expedient to rewrite the above condition in terms of the density $\rho = \rho^{(0)}$ and the normal current $j \cdot n = \rho^{(1)} \cdot n$ and the contributions to these moments from positive and negative values of $v \cdot n$. We obtain, after multiplying by ρ_{0-}:

$$(C(x) - \rho_+) j_{0-} \cdot n = j_- \cdot n \rho_{0-} \tag{5.8}$$

where j_0 is the contribution to the current from the zeroth order approximation. We remark that if we accept this approximation then j_0 coincides with $j_- = \langle vF_- \rangle$ and since it cannot be zero (because the field is high and not tangential to the boundary), we obtain the usual Dirichlet boundary conditions for ρ, even from the Marshak procedure. This had to be expected because the effect of boundary layers is negligible when the first order terms are.

If we go to the next order then j decomposes into $j_0 + \varepsilon j_1$ and, although ρ does not decompose, because of the condition we imposed, we must expect, generally speaking, ρ_- to decompose into $\rho_{0-} + \varepsilon \rho_{1-}$.

Eq. (5.8) then becomes:

$$(C(x) - \rho) j_{0-} \cdot n = \varepsilon \rho_{0-} j_{1-} \cdot n - \varepsilon \rho_{1-} j_{0-} \cdot n + o(\varepsilon^2). \tag{5.9}$$

Hence we can no longer delay the solution of equation (3.1), which was given by Trugman and Taylor [TT] and Frosali, Van der Mee and Paveri Fontana [FV], and discussed by Poupaud [P2] for higher dimensions, all for given electric fields.

In keeping with the idea of high fields and hence with the fact that the electron temperature is much higher than that of the lattice, we shall assume a zero temperature for the lattice and replace the Maxwellian M in equation (3.1) by $\delta(v)$. Then the ground state solution is given by

$$P = \frac{1}{|u|} \delta(v_\perp) H(-v_\parallel) \exp\left(\frac{v_\parallel}{|u|}\right) \tag{5.10}$$

where v has been decomposed into a vector $v_\perp \in R^2$ (perpendicular to u) and a scalar $v_\parallel$ along u, with $u = -\frac{\bar{\tau}}{\theta^{1/2}} \frac{e}{m} E$, E the electric field.

In order to find F_1 we must solve

$$\begin{aligned} \eta \nabla_x \phi \cdot \nabla_v F_1 + \frac{F_1}{\tau} &= - v \cdot \nabla_x (\rho P) + P \langle v \cdot \nabla_x (\rho P) \rangle \\ &\quad + \frac{\gamma}{\eta^d} \rho D_{\nabla \phi} P \left(\langle \rho v P \rangle + \omega \right) \end{aligned} \tag{5.11}$$

where $\operatorname{div} \omega = 0$ and $\operatorname{curl} \omega = \operatorname{curl} \langle \rho v P \rangle$ with boundary conditions $\omega\big|_{\partial\Omega} = \partial_t \nabla \phi - \langle \rho v P \rangle\big|_{\partial\Omega} = \nabla \phi_t - j_0\big|_{\partial\Omega}$.

For a given field, equation (5.11) can be solved in closed form by a straightforward, albeit tedious calculation, into which we refrain from entering here. Once F_1 is found, it is an easy matter to compute j_1 and ρ_{1-} using the recursion relations. Equation (5.9) then delivers the boundary conditions for the first order correction. We remark that, given the form of equation (5.9) the corrections to charge neutrality at the boundary will be related to the density gradient. At this point it becomes imperative to solve the macroscopic system (1.8) that give densities for strong forcing models with the corresponding boundary data derived from (5.9) (see below).

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 from (5.9) for the macroscopic system (1.8) 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 satisfy

$$j \cdot n = 0 \qquad \text{and} \qquad E \cdot n = -\nabla\Phi \cdot n = 0 \quad \text{on } \Gamma_{\mathcal{N}} \tag{5.12.1}$$

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

$$\omega \cdot n = (E_t + j_0) \cdot n = 0 \quad \text{on } \Gamma_{\mathcal{N}} \tag{5.12.2}$$

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.

Since the right hand side of (5.9) is of order ε and $j_-^{(0)} \cdot n$ or order one at contacts under high fields, then (5.9) yields neutral space charge condition at these contacts with a correction of order ε, that is, for a given doping profile function $C(x)$,

$$\rho = C(x) - \varepsilon \frac{j_{1-} \cdot n \rho_{0-}}{j_{0-} \cdot n} \qquad \text{and} \qquad \Phi = \text{constant} \quad \text{on } \Gamma_{\mathcal{D}}, \tag{5.12.3}$$

where j_{1-}, j_{0-} and ρ_{0-} are given by the kinetic computation on the left side of the boundary layer. Then the condition for ω can be computed as

$$\omega \cdot s = (E_t + j_0) \cdot s = (\nabla\Phi_t + \mu\rho E) \cdot s = (\nabla\Phi \cdot s)_t - \mu\rho\nabla\Phi \cdot s = 0 \quad \text{on } \Gamma_{\mathcal{D}}. \tag{5.12.4}$$

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