

A MIXED SPECTRAL-DIFFERENCE METHOD FOR THE STEADY STATE BOLTZMANN–POISSON SYSTEM*

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Abstract. The approximate solution of the Boltzmann transport equation via Galerkin-type series expansion methods leads to a system of conservation laws in space and time for the expansion coefficients. In this paper, we derive discretization methods for these equations in the mean field approximation, which are based on the entropy principles of the underlying Boltzmann equation, and discuss the performance of these discretizations and the series expansion approach in nonequilibrium regimes.

Key words. Boltzmann equation, Galerkin methods, finite differences

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1. Introduction. This paper is concerned with the numerical solution of the steady state Boltzmann–Poisson system, describing the transport of an ensemble of electrons or holes in a crystal interacting with a phonon background under the mean field approximation. The Boltzmann–Poisson system in steady state is given by (see [14])

$$(1) \quad (a) \quad \nabla_x \cdot [\nabla_k \varepsilon(k) f] - q \nabla_k \cdot [\nabla_x V(x) f] + \frac{1}{\lambda} Q(f) = 0,$$

$$(b) \quad -\sigma \Delta_x V + q[D^{dop}(x) - \rho] = 0, \quad \rho(x) := \int f(x, k) dk,$$

where the phase space density function $f(x, k)$ is a function of position $x \in R_x^d$ ($d = 1, 2, \text{ or } 3$) and wave vector $k \in R_k^3$. The function $\varepsilon(k)$ describes the energy band under consideration. So $\nabla_k \varepsilon$ denotes the velocity with which a particle (electron or hole) with wave vector k travels. (If more than one energy band is considered, one density function f per band would have to be computed.) The Boltzmann equation (1) arises from a many body problem under the mean field approximation. So the function $V(x)$ denotes the mean field potential and q denotes the charge of the particle ($q = -1$ for electrons, $q = 1$ for holes). $\rho(x)$, as defined in (1)(b), denotes the density of particles in physical space and σ stands for the dielectricity constant of the material. The function $D^{dop}(x)$ in (1)(b) models the doping concentration, the background density of ions due to the implantation of donor and acceptor atoms into the crystal. Equation (1) has already been brought into a scaled dimensionless form, where the parameter λ denotes scaled mean-free path, i.e., the average distance a particle travels before it undergoes a collision event. (See [14, Chap. 1] for details of the scaling.) Finally, collisions of electrons or holes with the phonon background (the vibrations of the crystal lattice)

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are modeled by the integral operator Q in (1)(a). For the semiconductor Boltzmann–Poisson problem, Q is of the form

$$(2) \quad Q[f](x, k) = \int_{R_k^3} S(k, k') [f(x, k) e^{\varepsilon(k)} - f(x, k') e^{\varepsilon(k')}] dk',$$

where $S(k, k')$ denotes the scaled scattering cross section. Because of the principle of detailed balance [3], the scattering cross section S is a symmetric function ($S(k, k') = S(k', k)$), which guarantees that the charge ρ is conserved by the collision operator Q . Moreover, the above form of the collision operator guarantees that the Maxwellians of the form $f(x, k) = c(x) e^{-\varepsilon(k)}$ are in the kernel of Q . The collision operator Q models the generation and annihilation of phonons, resulting in a specified gain or loss of energy of the particles. Consequently, the function S is a distribution of the form

$$(3) \quad S(k, k') = \sum_{\nu=-1}^1 s_\nu(k, k') \delta(\varepsilon(k) - \varepsilon(k') + \nu\omega),$$

where ω is the amount of energy gained or lost due to the collisions. Because of the symmetry of the scattering cross section,

$$s_\nu(k, k') = s_{-\nu}(k', k)$$

has to hold. The assumption of a linear collision operator of the form (2) implies that we neglect electron–electron interactions. The steady state Boltzmann–Poisson system (1) is subject to a mixed set of Dirichlet and Neumann boundary conditions which will be discussed in the context of the discretization in section 3.

The outline of this paper is as follows. We will discretize the Boltzmann equation (1)(a) by a spectral Galerkin method in the wave vector direction, obtaining a system of conservation laws in x , which is solved by a difference method. This difference method is the actual topic of this paper. The spectral Galerkin method is chosen such as to preserve the entropy properties of the Boltzmann equation. So in section 2 we briefly review the general concepts involved in entropy based series expansion methods for the Boltzmann equation. In section 3, we derive the actual difference scheme which, in more than one spatial dimension, is based on a staggered grid approach. The resulting difference equations are nonlinear due to the coupling to the Poisson equation (1)(b). In section 4, we prove the stability of the linearization of these equations. Section 5 is devoted to the actual implementation of the method in one spatial dimension and to a numerical test example. The example consists of a standard $n^+ - n - n^+$ semiconductor diode with a $50nm$ channel. We demonstrate that in this example the solution to the Boltzmann equation exhibits truly kinetic features, which cannot be modeled by fluid dynamical approximations.

2. Entropy based Galerkin methods. This paper is concerned with the spatial discretization of first order systems of partial differential equations in physical (x -) space, which arise from employing a certain type of series expansion method for the Boltzmann equation (1) in the wave vector direction. Series expansion methods for the Boltzmann–Poisson system in the context of modeling semiconductor devices were first used effectively in [8]. The expansion methods considered in this paper make use of the entropy property of the Boltzmann equation. In this section, we briefly present the use of such entropy principles in a somewhat more general framework than is actually used in this paper. It is generally more convenient to consider entropy principles

for the case of the time dependent Boltzmann equation in the absence of boundary conditions ($x \in R_x^d$, $k \in R_k^3$), which we will do in this section. So the following is a brief review of general concepts described in detail in [7] or [11]. It should be pointed out here that, for the purpose of this paper, we approach the subject from a somewhat different angle. The entropy concept is usually relevant for the transient kinetic problem in the absence of boundary conditions. As a matter of fact, it does not hold in the form described here in the presence of boundary conditions. (See [5].) However, when discretizing the steady state Boltzmann equation with boundary conditions, one still has to deal with a rather stiff system of partial differential equations due to rapid potential variation; i.e., the same problems which make the discretization of the drift-diffusion or the energy transport system non-trivial arise again. The subject of this paper is the development of discretization methods for these systems, and we will only make use of the structure of the free-space operator induced by the free-space entropy property.

Generally, an entropy is given by a function $H(f, x, k)$, satisfying the following properties.

P1. The entropy is dissipated by the collision operator, so

$$\int_{R_x^d \times R_k^3} \partial_f H(f, x, k) Q[f](x, k) dx dk > 0$$

holds.

P2. The entropy is preserved by the free streaming operator, so

$$\int_{R_x^d \times R_k^3} \partial_f H(f, x, k) [\nabla_x \cdot (\nabla_k \varepsilon(k) f) - q \nabla_k \cdot (\nabla_x V(x) f)] dx dk = 0$$

holds.

P3. For fixed x and k the function H is a strictly convex function of the variable f and the functional

$$(4) \quad \eta(f) = \int_{R_x^d \times R_k^3} H(f(x, k), x, k) dx dk$$

is a convex functional of f .

The above properties guarantee that, for the time dependent Boltzmann equation

$$(5) \quad \partial_t f + \nabla_x \cdot [\nabla_k \varepsilon(k) f] - q \nabla_k \cdot [\nabla_x V(x) f] + \frac{1}{\lambda} Q(f) = 0,$$

the functional η is nonincreasing in time. This can be easily verified by integrating (5) against $\partial_f H(f, x, k)$ over $R_x^d \times R_k^3$. However, since this paper is concerned with the steady state problem, we will use the structure induced by the entropy functional for a stability estimate for the steady state problem. Entropy based Galerkin methods are truncated series expansions of the solution f of (1) which preserve this structure. To this end, we introduce the inverse of $\partial_f H$ with respect to the variable f by

$$g = \partial_f H(f, x, k) \iff f = \mu(g, x, k),$$

which exists since $\partial_f H$ is a monotone function of f . To obtain an approximation which preserves the entropy property, we apply a Galerkin procedure to the Boltzmann

equation (5) in the entropy variable g . Thus, after choosing some basis functions $\{\phi_m(k), m = 0, 1, \dots, M\}$, we set

$$g(x, k, t) = \sum_{n=0}^M f_n(x, t)\phi_n(k), \quad f(x, k, t) = \mu \left(\sum_{n=0}^M f_n(x, t)\phi_n(k), x, k \right)$$

and integrate the Boltzmann equation for the entropy variable g , which is of the form

$$\partial_t \mu(g, x, k) + \nabla_x \cdot [\nabla_k \varepsilon(k)\mu(g, x, k)] - q \nabla_k \cdot [\nabla_x V(x)\mu(g, x, k)] + \frac{1}{\lambda} Q(\mu(g, x, k)) = 0$$

against each of the basis functions with respect to the wave vector k . This yields a first order system of partial differential equations of the form

$$(6) \text{ (a) } \quad \partial_t G(F) + \sum_{j=1}^d [\partial_{x_j} A^j(F) - q(\partial_{x_j} V) B^j(F)] + \frac{1}{\lambda} C(F) = 0, \quad F = (f_0, \dots, f_M)^T,$$

$$(b) \quad G_m(F, x) = \int \phi_m(k) f(x, k, t) dk, \quad A_m^j(F, x) = \int \phi_m(k) (\partial_{k_j} \varepsilon(k)) f(x, k, t) dk,$$

$$(c) \quad B_m^j(F, x) = \int \phi_m(k) \partial_{k_j} f(x, k, t) dk, \quad C_m(F, x) = \int \phi_m(k) Q[f](x, k, t) dk,$$

which, by virtue of construction, automatically satisfies the entropy estimate

$$\partial_t \eta(F) \leq 0, \quad \eta(F) = \int F^T(x, t) G(F, x) dx,$$

where, for simplicity, we denote the entropy function $\eta(F)$ of the coefficient vector F with the same symbol as the entropy $\eta(f)$ in (4) evaluated at the corresponding linear combination of the basis functions. The existence of the above estimate automatically guarantees that the generally nonlinear first order system (6) is hyperbolic [11]. The actual form of the system is determined by the choice of basis function ϕ_m and the form of the entropy function H .

Choice of entropies. The classical physical entropy, which arises in the kinetic description of fluids, where the collision operator Q models particle-particle interactions and is nonlinear, is given by the natural logarithm $\partial_f H = \ln f$, $H = f(\ln f - 1)$. Since we are dealing with a greatly simplified linear operator, and also are considering a plasma driven by the field $\nabla_x V$, there is a much larger degree of freedom in the choice of entropy. A straightforward calculation gives

$$(7) \quad \int \partial_f H(f, x, k) Q[f](x, k) dk \\ = \frac{1}{2} \int_{R_k^3 \times R_k^3} S(k, k') [\partial_f H(f, x, k) - \partial_f H(f', x, k')] [f e^\varepsilon - f' e^{\varepsilon'}] dk dk',$$

where the prime denotes evaluation of the corresponding function at k' . Thus, any entropy H whose derivative is a nondecreasing function of $f e^\varepsilon$ (meaning $\partial_f H(f, x, k) = h_1(f e^{\varepsilon(k)}, x)$ with $\partial_u h_1(u, x) \geq 0$) will satisfy the first requirement on the entropy

since the term $[h_1(f e^{\varepsilon(k)}, x) - h_1(f' e^{\varepsilon(k')}, x)][f(x, k) e^{\varepsilon(k)} - f(x, k') e^{\varepsilon(k')}]$ in the integrand of (7) will always be nonnegative. To satisfy the second requirement, namely, that the entropy is preserved by the free streaming operator, we note that

$$(8) \quad \begin{aligned} & \partial_f H(f, x, k) [\nabla_x \cdot (\nabla_k \varepsilon(k) f) - q \nabla_k \cdot (\nabla_x V(x) f)] \\ &= [\nabla_x \cdot (\nabla_k \varepsilon(k) H) - q \nabla_k \cdot (\nabla_x V(x) H)] - [\nabla_k \varepsilon \cdot \nabla_2 H - q \nabla_x V(x) \cdot \nabla_3 H] \end{aligned}$$

holds, where ∇_2, ∇_3 denote the derivatives with respect to the second and third variables of $H(f, x, k)$. The integral over the whole phase space of the first term on the right-hand side of (8) is zero since it represents a total derivative. So the second condition on the entropy H is satisfied if the second term on the right-hand side of (8) vanishes. The general solution of $[\nabla_k \varepsilon \cdot \nabla_2 - q \nabla_x V(x) \cdot \nabla_3] H(f, x, k) = 0$ is given by all functions of the total energy $\varepsilon(k) + qV(x)$. So $H(f, x, k)$, and therefore also $\partial_f H(f, x, k)$, should depend on x and k only through the total energy $\varepsilon(k) + qV(x)$. Combining this with the first requirement $\partial_f H(f, x, k) = h_1(f e^{\varepsilon(k)}, x)$, we see that any function H satisfying

$$\partial_f H(f, x, k) = h(f \exp(\varepsilon(k) + qV(x)), \quad h'(u) \geq 0,$$

can be chosen as an entropy for the Boltzmann equation. The physical entropy, the logarithm, now corresponds to the choice

$$h(u) = \ln u, \quad H(f, x, k) = f [\ln f - 1 + \varepsilon(k) + qV(x)], \quad \mu(g, x, k) = \exp[g - \varepsilon(k) - qV(x)].$$

If this entropy is used with the basis functions $1, k, \varepsilon(k)$, we obtain the classical hydrodynamic model for semiconductors. If more terms are used in the Galerkin approximation (6), we face the problem that, because of the exponential function μ , the involved integrals will in general become infinite. This problem can be remedied by using special restricted sets of basis functions developed by Levermore [11]. However, we face the additional problem that we have to evaluate the quite complicated integrals of the collision operator Q . In the Levermore approach, as well as in the hydrodynamic models, the collision operator is usually replaced by some form of BGK approximation with fitted relaxation times. Indeed, the Galerkin approach (6) can be philosophically viewed in two different ways. One is to regard (6) as deriving extensions of the Euler equations. The other one is to regard (6) as an actual numerical method for the Boltzmann equation. The difference is that in the first approach only relatively few terms are taken which have some physical interpretation. In the second approach, arbitrarily many terms in the expansion (6) have to be generated automatically, and the physical interpretation of the high order terms is not important. In this paper, we follow the second approach. This means that we use the simplest possible entropy, namely a quadratic function.

$$(9) \quad \eta(u) = u, \quad H(f, x, k) = \frac{1}{2} f^2 \exp[\varepsilon(k) + qV(x)], \quad \mu(g, x, k) = g \exp[-\varepsilon(k) - qV(x)].$$

This choice makes the Galerkin equations (6) linear, as long as we do not couple the Boltzmann equation to the Poisson equation (1)(b), and the entropy estimate becomes an L^2 estimate with the weight function $\exp[\varepsilon + qV]$. Methods based on these basis functions have been analyzed and implemented in [17], [18], and suitable time

discretization methods have been developed in [15]. All of this work was concerned with the linear time dependent Boltzmann equation for a given potential V . In this paper, we treat the steady state Boltzmann–Poisson problem instead, using the same linear entropy. So the role of the entropy will not be to provide an a priori estimate on the time dependent solution. Instead, we will make use of the effect of the entropy on the structure of the involved nonlinear operators. The convergence of Galerkin methods using the linear entropy in the linear case (i.e., for a given potential) has been analyzed in [16], [18].

3. Difference schemes. In this section, we present the spatial discretization of the Galerkin equations arising from (6) together with the Poisson equation (1)(b). When designing the spatial discretization one is confronted with two somewhat contradictory priorities. On one hand, the discretization should reflect the entropy preservation property of the free streaming operator; that is, a discrete equivalent of P3 in section 2 should hold. In the case of the quadratic entropy used in this paper, this means that the spatially discretized free streaming operator should be antisymmetric with respect to the weight function e^{qV} . This results in obviously desirable stability properties of the discretization. On the other hand, we wish to locally conserve charge. Building the zero order moment of the Boltzmann equation (1)(a) with respect to the wave vector k yields the continuity equation

$$(10) \quad \nabla_x \cdot \langle \nabla_k \varepsilon \rangle = 0, \quad \langle \nabla_k \varepsilon \rangle := \int \nabla_k \varepsilon(k) f(x, k) dk.$$

This continuity equation should hold locally; that is, we should be able to apply a discrete version of Gauss’s theorem locally over any submesh. In the context of a finite element discretization in the spatial direction, the first priority would suggest a straightforward finite element discretization using a weighted scalar product, which would automatically not be locally conservative. A similar problem exists when using difference schemes. Our approach is the following: We will split the balance equations (6)(a) into those governing the even and odd order moments of the kinetic density function f . The difference scheme for the even order moment equations will be designed in such a way that it locally conserves the appropriate momenta. The difference scheme for the odd order moment equations will then be chosen such that the whole scheme has the appropriate entropy properties outlined in the previous section. This represents a compromise between the two priorities of local conservation and entropy dissipation. This compromise is acceptable, since the collisions modeled by the operator Q are nonelastic and the odd order moments are not conserved anyway. In the steady state case, the odd order moments have to be viewed rather as constitutive relations.

First we observe that the free streaming operator L , defined by

$$L[f] = \nabla_x \cdot [\nabla_k \varepsilon(k) f] - q \nabla_k \cdot [\nabla_x V(x) f],$$

induces a natural decomposition of the function space for f . If the band energy $\varepsilon(k)$ is an even function of the wave vector k (which always can be assumed), the operator L maps even functions of k into odd functions and vice versa. So we split the density function f , as well as the Boltzmann equation, into its even and odd parts

$$(11) \quad (a) \quad f = f^e + f^o, \quad f^e(x, k) = f^e(x, -k), \quad f^o(x, k) = -f^o(x, -k),$$

$$(b) \quad L[f^o] + Q^e[f^e + f^o] = 0, \quad (c) \quad L[f^e] + Q^o[f^e + f^o] = 0,$$

where Q^e, Q^o denote the even and odd parts of the collision operator. Next we observe that the important conservation laws (for charge and energy) are given by the even part of the Boltzmann equation. Since the given collision operator does not preserve momentum anyway, the moments of the odd part of the Boltzmann equation gives rise to constitutive relations rather than conservation laws. Consequently, we will discretize (11)(b) conservatively and choose the discretization of (11)(c) to satisfy the entropy conservation property P2 of the operator L . After splitting into even and odd parts, the entropy property of the free streaming operator L reads

$$(12) \quad \int_{R_x^3 \times R_k^3} e^{\varepsilon+V} f^e L[f^o] dx dk + \int_{R_x^3 \times R_k^3} e^{\varepsilon+V} f^o L[f^e] dx dk = 0.$$

We will use (12) as a weak definition of $L[f^e]$ in terms of $L[f^o]$. Moreover, we can also assume that in general the scattering cross section $S(k, k')$ (3) is an even function of its arguments. This implies that the collision operator Q maps even functions of k into even functions and odd functions into odd functions, giving

$$Q^e[f^e + f^o] = Q[f^e], \quad Q^o[f^e + f^o] = Q[f^o].$$

In keeping with the spirit of the entropy based Galerkin approach outlined in the previous section, we expand f^e and f^o into

$$f^e(x, k) = \sum_{n=0}^{N_e} f_n^e(x) e^{-\varepsilon} \phi_n^e(k), \quad f^o(x, k) = \sum_{n=0}^{N_o} f_n^o(x) e^{-\varepsilon} \phi_n^o(k),$$

where we have absorbed the factor e^{-qV} in (9) into the coefficients $f_n^{e,o}$ for notational convenience. Integrating (11)(b) against the even basis functions ϕ_m^e and (11)(c) against the odd basis functions ϕ_m^o yields the system

$$(13) \quad \begin{aligned} \text{(a)} \quad & \sum_{\nu=1}^d [A_{\nu}^{eo} \partial_{x_{\nu}} F^o - q(\partial_{x_{\nu}} V) B_{\nu}^{eo} F^o] + \frac{1}{\lambda} C^e F^e = 0, \\ \text{(b)} \quad & \sum_{\nu=1}^d [A_{\nu}^{oe} \partial_{x_{\nu}} F^e - q(\partial_{x_{\nu}} V) B_{\nu}^{oe} F^e] + \frac{1}{\lambda} C^o F^o = 0, \end{aligned}$$

where $F^{e,o}(x)$ denotes the coefficient vector $(f_0^{e,o}, \dots, f_{N_{e,o}}^{e,o})$ and the matrices are defined in the obvious way by

$$(14) \quad \begin{aligned} \text{(a)} \quad & A_{\nu}^{eo}(m, n) = \int [\phi_m^e(\partial_{k_{\nu}} \varepsilon) e^{-\varepsilon} \phi_n^o] dk, \quad A_{\nu}^{oe}(m, n) = \int [\phi_m^o(\partial_{k_{\nu}} \varepsilon) e^{-\varepsilon} \phi_n^e] dk, \\ \text{(b)} \quad & B_{\nu}^{eo}(m, n) = \int \phi_m^e \partial_{k_{\nu}} [e^{-\varepsilon} \phi_n^o] dk, \quad B_{\nu}^{oe}(m, n) = \int \phi_m^o \partial_{k_{\nu}} [e^{-\varepsilon} \phi_n^e] dk, \\ \text{(c)} \quad & C^e(m, n) = \int \phi_m^e Q[e^{-\varepsilon} \phi_n^e] dk, \quad C^o(m, n) = \int \phi_m^o Q[e^{-\varepsilon} \phi_n^o] dk. \end{aligned}$$

As mentioned, we will discretize the even part (13)(a) by a conservative difference method and the odd part (13)(b) in its weak form defined by the relation (12). A simple calculation gives that the relations

$$(15) \quad B_{\nu}^{eo} + (B_{\nu}^{oe})^T + A_{\nu}^{eo} = 0, \quad \nu = 1, \dots, d,$$

hold. Furthermore, because of the symmetry of the scattering cross section S , the odd collision operator is given by

$$C^o(m, n) = \int \phi_m^o \sigma(k) \phi_n^o dk, \quad \sigma(k) = \int S(k, k') dk'.$$

Therefore the matrix C^o , corresponding to the odd part of the collision operator, is invertible as a consequence of the fact that the kernel of Q contains only even functions. This suggests eliminating F^o locally by inverting C^o in (13)(b) and inserting the resulting expression into (13)(a). To discretize (13) in the spatial direction, we will need difference operators which are conservative and satisfy a discrete version of Gauss's theorem. This is nontrivial in more than one spatial dimension if a general nonrectangular mesh is used, unless they do not act on the same grids. We therefore assume two separate grids for F^e and F^o and difference operators acting between them. We define the meshes

$$M^e = \{\mathbf{x}_j, j = 0, \dots, J_e\}, \quad M^o = \{\mathbf{y}_j, j = 0, \dots, J_o\}$$

and difference operators D_ν^{eo}, D_ν^{oe} , both approximating ∂_{x_ν} , acting between them

$$(D_\nu^{eo} u^o)(\mathbf{x}_j) = \sum_{s=0}^{J_o} d_\nu^{eo}(j, s) u^o(\mathbf{y}_s), \quad (D_\nu^{oe} u^e)(\mathbf{y}_j) = \sum_{s=0}^{J_e} d_\nu^{oe}(j, s) u^e(\mathbf{x}_s)$$

for grid functions u^e, u^o defined on the respective meshes. Using appropriate discrete integration operators I_e, I_o , the discrete integration by parts formula we assume takes the form

$$(16) \quad (a) \quad I_e[(u^e)^T (D_\nu^{eo} u^o)] = -I_o[(u^o)^T (D_\nu^{oe} u^e)] + b^e (u^e)^T b^o (u^o), \quad \nu = 1, \dots, d,$$

$$(b) \quad I_e[u^e] = \sum_{s=0}^{J_e} \gamma_e(s) u^e(\mathbf{x}_s), \quad I_o[u^o] = \sum_{s=0}^{J_o} \gamma_o(s) u^o(\mathbf{y}_s)$$

for vector grid functions u^e, u^o with appropriate integration weights γ_e, γ_o . The boundary operators b^e, b^o correspond to evaluation of the grid function at the boundary points of the respective meshes M^e, M^o . There is one minor problem caused by the introduction of the dual meshes M^e, M^o , which is that the free streaming operator L contains derivatives of the density function as well as zero order terms, which couples the meshes. This is remedied by using an interpolation formula which is in some sense generic for the free streaming operator. In order to write the term $q(\partial_{x_\nu} V)(\partial_{k_\nu} f)$ solely in terms of spatial derivatives of f , we replace it by $\partial_{x_\nu} [qV \partial_{k_\nu} f] - qV \partial_{x_\nu} \partial_{k_\nu} f$. Thus (13)(a) is discretized by

$$(17) \quad L^{eo} F^o + \frac{1}{\lambda} C^e F^e = 0, \quad L^{eo} F^o = \sum_{\nu=1}^d [D_\nu^{eo} (A_\nu^{eo} F^o - qV B_\nu^{eo} F^o) + qV B_\nu^{eo} D_\nu^{eo} F^o].$$

The odd part (13)(b) of the Boltzmann equation is now discretized using the dual operator to L^{eo} as defined by (12). This gives

$$(18) \quad (a) \quad L^{oe} F^e + \frac{1}{\lambda} C^o F^o = 0,$$

$$(b) \quad L^{oe} F^e = \sum_{\nu=1}^d e^{-qV} [(A_\nu^{eo} - qV B_\nu^{eo})^T D_\nu^{oe} (e^{qV} F^e) + (B_\nu^{eo})^T D_\nu^{oe} (qV e^{qV} F^e)].$$

This represents a consistent discretization of (13)(b) because of the relation (15) for the coefficient matrices, as can be easily verified. By virtue of construction, the

discrete system (17), (18) now has the desired symmetry properties and accurately represents a discrete version of the conservation law (10). We summarize these statements in the following proposition.

PROPOSITION 1. *The discretized operators L^{eo}, L^{oe} in (17), (18) satisfy the equality*

$$(19) \quad I_e[e^{qV}(F^e)^T L^{eo} F^o] + I_o[e^{qV}(F^o)^T L^{oe} F^e]$$

$$= \sum_{\nu=1}^d b^\nu(e^{qV} F^e)^T b^\nu(A_\nu^{eo} F^o - qV B_\nu^{eo} F^o) + b^\nu(qV e^{qV} F^e) b^\nu(B_\nu^{eo} D_\nu^{eo} F^o)$$

for any choice of grid functions F^e, F^o, V . Furthermore, the discrete conservation law

$$(20) \quad I_e[e^T L^{eo} F^o] = \sum_{\nu=1}^d b^\nu(\mathbf{e})^T b^\nu(A_\nu^{eo} F^o)$$

holds, where \mathbf{e} denotes the first unit vector in R^{N_e} .

Proof. Equation (19) holds by virtue of construction, using the discrete integration by parts formulae (16). Equation (20) is obtained from (19) by setting $F^e = \mathbf{e}$ and observing that because of (14)(b) the first row of B_ν^{eo} vanishes. \square

We now turn to coupling (17), (18) to the Poisson equation (1)(b). Using the obvious discretization induced by the difference operators D_ν^{eo}, D_ν^{oe} , the discretization of the Poisson equation reads

$$-\sigma \sum_{\nu=1}^d D_\nu^{eo} D_\nu^{oe} V^e + q[D^{dop} - \rho^T F^e] = 0, \quad \rho^T = (\rho_1, \dots, \rho_{N_e}), \quad \rho_n = \int e^{-\varepsilon} \phi_n^e dk.$$

Therefore, if the even coefficient vector F^e is only defined on the mesh M^e , so is the potential. The discretization of the Boltzmann equation (17), (18) requires, however, the potential on both meshes M^e and M^o , and therefore some interpolation formula is needed which computes the potential V on the mesh M^o from V^e . So, in summary, the discretized Boltzmann–Poisson system is given by

$$(21) \quad (a) \quad L^{eo}(F^e, F^o) + \frac{1}{\lambda} C^e F^e = 0, \quad (b) \quad L^{oe}(F^e) + \frac{1}{\lambda} C^o F^o = 0,$$

$$(c) \quad -\sigma \sum_{\nu=1}^d D_\nu^{eo} D_\nu^{oe} V^e + q[D^{dop} - \rho^T F^e] = 0, \quad V^o = S(V^e),$$

$$(d) \quad L^{eo}(F^e, F^o) = \sum_{\nu=1}^d [D_\nu^{eo}(A_\nu^{eo} F^o - qV^o B_\nu^{eo} F^o) + qV^e B_\nu^{eo} D_\nu^{eo} F^o],$$

$$(e) \quad L^{oe}(F^e) = \sum_{\nu=1}^d e^{-qV^o} [(A_\nu^{eo} - qV B_\nu^{eo})^T D_\nu^{oe}(e^{qV^e} F^e) + (B_\nu^{eo})^T D_\nu^{oe}(qV^e e^{qV^e} F^e)],$$

where V^o is somehow interpolated from V^e using the interpolation operator S . Notice that L^{eo} and L^{oe} are now nonlinear operators because the potentials V^e, V^o are given

in terms of F^e through the solution of the Poisson equation (21)(c). In principle, any interpolation formula could be used which is of a high enough order as to keep the total order of accuracy of (17), (18), and the choice of interpolation formula cannot be discussed further without being more specific about the structure of the mesh and the form of the difference operators. In practice, we will take the following approach: The Galerkin approximation to the Boltzmann–Poisson system will reduce to the drift-diffusion system if only the basis functions $1, k_1, k_2, k_3$ are used with $N_e = 0$, $N_o = 2$. In this case, the matrices B_{ν}^{eo} and C^e vanish and the matrices A_{ν}^{eo} will form the rows of a multiple of the identity matrix; i.e., there will be no mixed derivatives appearing in the equations. Given a certain mesh structure and a set of difference operators, we will choose the interpolation formula to compute V^o in such a way that the resulting scheme reduces to the well-known Scharfetter–Gummel scheme on this mesh.

Boundary conditions. For practical applications, the boundary will be decomposed in two types of boundary segments, namely insulating parts at which the particle fluxes normal to the boundary vanish and parts at which particles are injected according to a Maxwellian distribution in such a way that charge neutrality in the Poisson equation is preserved (meaning $\rho = D$ in (1)(b)). The insulation property simply translates into the odd component of the density function being equal to zero. The injection of particles results in a quite complicated mixed boundary condition involving the diagonalization of the matrices $A_{\nu}^{eo}, A_{\nu}^{oe}$. (See [15] for more details.) For the solution of the transient problem, it is quite essential to capture the precise structure of the boundary conditions in order to avoid artificial reflections. For the steady state problem, it turns out the structure of the boundary conditions has actually relatively little impact on the solution as long as charge neutrality is guaranteed. As mentioned before, we will actually eliminate the odd component vector F^o for the practical implementation of the scheme and solve (21) in the form

$$\lambda L^{eo}(F^e, -\lambda(C^o)^{-1}L^{oe}(F^e)) + C^e F^e = 0.$$

In this formulation, dealing with the mixed boundary condition resulting from the particle injection is actually quite cumbersome. We therefore use the simplified set of boundary conditions

$$(22) \quad (a) \quad b^e(F^e) = D^{dop} \mathbf{e}, \quad V^e = V_b^e \quad \text{for } \mathbf{x}_j \in \partial M_{Dir}^e,$$

$$(b) \quad b^o(F^o) = 0, \quad b^o(D^{eo}V^e) = 0 \quad \text{for } \mathbf{y}_j \in \partial M_{Neu}^o,$$

where the subscripts *Dir*, *Neu* denote the union of Dirichlet and Neumann segments of the boundary and b^e, b^o are the boundary operators in (16). Note that b^o is actually the discretization of the outward normal component of a vector. Also, (22)(a) tacitly assumes that $\phi_0^e = 1$ holds and that the basis functions form an orthonormal system, which implies that the physical space density ρ is actually given by F_0^e and therefore Maxwellians of the form $e^{-\varepsilon}$ correspond to the first unit vector \mathbf{e} .

4. Stability of the linearization. In this section, we prove that the linearization of the scheme defined in the previous section around the equilibrium solution is stable. This implies, among other things, that close to equilibrium Newton’s method will be locally quadratically convergent when applied to the nonlinear system (21). To this end, we first reformulate (21) slightly by essentially writing it as a correction to a discretization of the drift-diffusion–Poisson equations. We assume that the Galerkin

approximation (13) to the Boltzmann equation contains the balance equations for charge and momentum, i.e., that the functions $1, k$ are contained in the set of basis functions. So we set

$$\phi_0^e = 1, \quad \phi_n^o = k_n, \quad n = 1, \dots, d.$$

Next we split the system (21) into the balance equations for charge and momentum and the rest by setting

$$F^e = \begin{pmatrix} F_0^e \\ F_1^e \end{pmatrix}, \quad F^o = \begin{pmatrix} F_0^o \\ F_1^o \end{pmatrix}, \quad L^{eo} = \begin{pmatrix} L_0^{eo} \\ L_1^{eo} \end{pmatrix}, \quad L^{oe} = \begin{pmatrix} L_0^{oe} \\ L_1^{oe} \end{pmatrix},$$

where F_0^e and L_0^{eo} denote the first component of F^e, L^{eo} and F_1^e and L_1^{eo} denote the other N_e components. In the same way, F_0^o, L_0^{oe} denote the first d components of F^o, L^{oe} and F_1^o, L_1^{oe} denote the other $N_o + 1 - d$ components. Accordingly, we partition the matrices $A_\nu^{eo}, B_\nu^{eo}, C^e$, and C^o into

$$A_\nu^{eo} = \begin{pmatrix} A_\nu^{00} & A_\nu^{01} \\ A_\nu^{10} & A_\nu^{11} \end{pmatrix}, \quad B_\nu^{eo} = \begin{pmatrix} 0 & 0 \\ B_\nu^{10} & B_\nu^{11} \end{pmatrix},$$

$$C^e = \begin{pmatrix} 0 & 0 \\ 0 & C_e^{11} \end{pmatrix}, \quad C^o = \begin{pmatrix} C_o^{00} & C_o^{01} \\ C_o^{10} & C_o^{11} \end{pmatrix}.$$

Note that the first row of B^{eo} and the first row and column of C^e vanish because of the conservation properties. In this partition, the system (21) now becomes

$$(23) \quad (a) \quad L_0^{eo}(F_0^o, F_1^o) = 0, \quad (b) \quad L_0^{oe}(F_0^e, F_1^e) + \frac{1}{\lambda}[C_o^{00}F_0^o + C_o^{01}F_1^o] = 0,$$

$$(c) \quad -\sigma \sum_{\nu=1}^d D_\nu^{eo} D_\nu^{oe} V^e + q[D^{dop} - F_0^e] = 0, \quad V^o = S(V^e),$$

$$(d) \quad b^e(F_0^e) = D^{dop}, \quad b^e(V^e) = V_b^e, \quad \mathbf{x}_j \in \partial M_{Dir}^e,$$

$$b^o(F_0^o) = 0, \quad b^o(D^{eo}V^e) = 0 \quad \mathbf{y}_j \in \partial M_{Neu}^o,$$

(24)

$$(a) \quad L_1^{eo}(F_0^e, F_1^e, F_0^o, F_1^o) + \frac{1}{\lambda} C_e^{11} F_1^e = 0, \quad (b) \quad L_1^{oe}(F_0^e, F_1^e) + \frac{1}{\lambda}[C_o^{10}F_0^o + C_o^{11}F_1^o] = 0,$$

$$(c) \quad b^e(F_1^e) = 0, \quad \mathbf{x}_j \in \partial M_{Dir}^e, \quad b^o(F_1^o) = 0, \quad \mathbf{y}_j \in \partial M_{Neu}^o,$$

where the involved operators are given by

$$(25) \quad (a) \quad L_0^{eo}(F_0^o, F_1^o) = \sum_{\nu=1}^d D_\nu^{eo} (A_\nu^{00} F_0^o + A_\nu^{01} F_1^o),$$

$$(b) \quad L_0^{oe}(F_0^e, F_1^e)$$

$$= \sum_{\nu=1}^d e^{-qV^o} [(A_\nu^{00})^T D_\nu^{oe}(e^{qV^e} F_0^e) + (A_\nu^{10} - qV B_\nu^{10})^T D_\nu^{oe}(e^{qV^e} F_1^e) + (B_\nu^{10})^T D_\nu^{oe}(qV^e e^{qV^e} F_1^e)],$$

$$(c) \quad L_1^{eo}(F_0^e, F_1^e, F_0^o, F_1^o)$$

$$= \sum_{\nu=1}^d [D_\nu^{eo}(A_\nu^{10} F_0^o + A_\nu^{11} F_1^o - qV^o B_\nu^{10} F_0^o - qV^o B_\nu^{11} F_1^o) + qV^e B_\nu^{10} D_\nu^{eo} F_0^o + qV^e B_\nu^{11} D_\nu^{eo} F_1^o],$$

$$(d) \quad L_1^{oe}(F_0^e, F_1^e)$$

$$= \sum_{\nu=1}^d e^{-qV^o} [(A_\nu^{01})^T D_\nu^{oe}(e^{qV^e} F_0^e) (A_\nu^{11} - qV B_\nu^{11})^T D_\nu^{oe}(e^{qV^e} F_1^e) + (B_\nu^{11})^T D_\nu^{oe}(qV^e e^{qV^e} F_1^e)].$$

We write the system (23), (24) as a nonlinear equation for F_1^e and F_1^o , where the remaining variables are given implicitly by (23). So write (24) as

$$(26) \quad (a) \quad K^e(F_1^e, F_1^o) = 0, \quad K^o(F_1^e, F_1^o) = 0,$$

$$(b) \quad K^e(F_1^e, F_1^o) = L_1^{eo}(F_1^e, F_1^o, F_0^o, F_1^o) + \frac{1}{\lambda} C_e^{11} F_1^e,$$

$$(c) \quad K^o(F_1^e, F_1^o) = L_1^{oe}(F_0^e, F_1^e) + \frac{1}{\lambda} [C_o^{10} F_0^o + C_o^{11} F_1^o]$$

with V^e, V^o, F_0^o, F_0^e given in terms of F_1^e, F_1^o as the solution of the equations (23). So, in order to evaluate K^e, K^o a drift-diffusion-Poisson problem has to be solved where F_1^e, F_1^o appear as source terms. We will show that the linearization of (26) is stable around the equilibrium solution. The equilibrium solution is given by a Maxwellian in the wave vector direction multiplied by the function e^{iqV} , where the potential V is such that it satisfies the resulting nonlinear Poisson equation (1). We first confirm that this solution is an exact solution of our difference scheme by proving the following theorem.

THEOREM 1. *If the boundary potential V_b^e in (23)(b) is given by $V_b^e = -\frac{1}{q} \ln D^{dop}$, and the corresponding discrete Poisson problem*

$$-\sigma \sum_{\nu=1}^d D_\nu^{eo} D_\nu^{oe} V^e + q[D^{dop} - e^{-qV^e}] = 0$$

has a solution, the system

$$K^e(F_1^e, F_1^o) = 0, \quad K^o(F_1^e, F_1^o) = 0$$

has a solution $F_1^e = 0, F_1^o = 0$.

The proof is deferred to the appendix.

If we now consider the linearization around this equilibrium solution, we have the following theorem.

THEOREM 2. *Let $\delta F_1^e, \delta F_1^o$ be the solution of the linearized problem*

$$(27) \quad (a) \quad dK^e(0,0)(\delta F_1^e, \delta F_1^o) = R_1^e, \quad dK^o(0,0)(\delta F_1^e, \delta F_1^o) = R_1^o,$$

$$(b) \quad b^e(\delta F_1^e) = 0, \quad \mathbf{x}_j \in \partial M_{Dir}^e, \quad b^o(\delta F_1^o) = 0, \quad \mathbf{y}_j \in \partial M_{Neu}^o.$$

Then there exists a constant c , dependent only on the collision matrices C^e, C^o , such that $\delta F_1^e, \delta F_1^o$ satisfy $\|(\delta F_1^e, \delta F_1^o)\| \leq c\lambda\|(R_1^e, R_1^o)\|$, where the norm is defined by

$$\|(\delta F_1^e, \delta F_1^o)\| = I_e[e^{qV^e}|\delta F_1^e|^2] + I_o[e^{qV^o}|\delta F_1^o|^2],$$

and V^e, V^o are the potentials corresponding to the equilibrium solution.

The proof is deferred to the appendix.

Two remarks should be made at this point. First, while the reformulation and partitioning of the problem seems like a formality at first sight, it does have a practical implication. The stability result of Theorem 2 guarantees, among other things, that the solution can be computed by a locally quadratically convergent Newton method of the form

$$dK^e(F_1^e, F_1^o)(\delta F_1^e, \delta F_1^o) = -K^e(F_1^e, F_1^o), \quad dK^o(F_1^e, F_1^o)(\delta F_1^e, \delta F_1^o) = -K^o(F_1^e, F_1^o).$$

However, to compute the right-hand side of the linearized equations, we have to evaluate the terms K^e, K^o , which involves solving the nonlinear problem (23) exactly, which corresponds to solving a nonlinear drift-diffusion–Poisson problem at each Newton step. While this is not really necessary in practice, the convergence of Newton’s method can be improved dramatically if a few extra iterations are performed on the low-dimensional system (23) within each Newton step. Second, the above formulation tacitly assumes that K^e, K^o can be evaluated, that is, that the drift-diffusion–Poisson system can be solved by the discretization (23) for any source terms arising from F_1^e, F_1^o . This is the main reason why the interpolation operator S in (21) is chosen such that the resulting scheme reduces to the Scharfetter–Gummel scheme on the given mesh, which is a well tested and incredibly robust discretization. (See [19] for an overview.)

5. Implementation and numerical test example. In this section we present a numerical test example in one spatial dimension and outline how to actually compute the coefficient matrices C^e, C^o , corresponding to the collision operator. The computation of these matrices is not completely trivial because of the presence of the δ -functions in the integral kernel (3). (See [12], [13].) In one spatial dimension, the choice of meshes M^e and M^o and the choice of the corresponding difference operators D_1^{eo}, D_1^{oe} is quite obvious. We define the grids by

$$M^e = \{\mathbf{x}_0 < \dots < \mathbf{x}_J\}, \quad M^o = \left\{ \mathbf{y}_j : \mathbf{y}_j = \frac{1}{2}(\mathbf{x}_j + \mathbf{x}_{j+1}), j = 0, \dots, J-1 \right\}$$

and the difference operators by

$$(D^{oe}u^e)(\mathbf{y}_j) = \frac{u^e(\mathbf{x}_{j+1}) - u^e(\mathbf{x}_j)}{\mathbf{x}_{j+1} - \mathbf{x}_j}, \quad (D^{eo}u^o)(\mathbf{x}_j) = \frac{u^o(\mathbf{y}_j) - u^o(\mathbf{y}_{j-1})}{\mathbf{y}_j - \mathbf{y}_{j-1}}.$$

If we define the discrete integral operators I_e, I_o by

$$I_e(u^e) = \sum_{j=1}^{J-1} (\mathbf{y}_j - \mathbf{y}_{j-1}) u^e(\mathbf{x}_j), \quad I_o(u^o) = \sum_{j=0}^{J-1} (\mathbf{x}_{j+1} - \mathbf{x}_j) u^o(\mathbf{y}_j),$$

then the discrete integration by parts formula (16) holds with the boundary terms b^e, b^o given by

$$b^e(u^e) = \begin{pmatrix} -u^e(\mathbf{x}_0) \\ u^e(\mathbf{x}_J) \end{pmatrix}, \quad b^o(u^o) = \begin{pmatrix} -u^o(\mathbf{y}_0) \\ u^o(\mathbf{y}_{J-1}) \end{pmatrix}.$$

In order for the scheme to reduce to the exponentially fitted Scharfetter–Gummel scheme in one dimension, the interpolation operator S for the potential V^o is chosen such that e^{qV} is expressed as $\frac{d}{dV} e^{qV}$. So S is chosen as

$$S(V^e)(\mathbf{y}_j) = \frac{1}{q} \ln \left(\frac{\exp[qV(\mathbf{x}_{j+1})] - \exp[qV(\mathbf{x}_j)]}{qV(\mathbf{x}_{j+1}) - qV(\mathbf{x}_j)} \right).$$

For a general band energy function $\varepsilon(k)$, the matrices A^{eo}, B^{eo}, C^e, C^o will have to be computed numerically. This can be done at a considerable computational expense, since it has to be done only once for a given set of basis functions. In particular, the collision matrices C^e, C^o have to be computed exercising some care so that the conservation and dissipation properties are not destroyed by the involved numerical integration. Generally, we have to compute integrals of the form $\int \phi_m(k) Q[e^{-\varepsilon} \phi_n(k)] dk$, where ϕ_m, ϕ_n denote either the even or the odd basis functions. Using the symmetry of the collision operator, we will compute the matrix elements of the collision operator as

$$C(m, n)$$

$$= \frac{1}{2} \sum_{\nu=-1}^1 \int_{R_k^3 \times R_{k'}^3} s_\nu(k, k') \delta(\varepsilon(k) - \varepsilon(k') + \nu\omega) [\phi_m(k) - \phi_m(k')] [\phi_n(k) - \phi_n(k')] dk dk'$$

and use numerical integration formulas for the integral in this form. Note that, in this form, it is apparent that the matrix C will be symmetric and that, if either ϕ_m or ϕ_n are constants, the matrix element will be zero, corresponding to conservation of charge and the Maxwellian kernel. Thus, we just have to make sure that numerical integration is applied in the same way in the k and k' variables to preserve these properties. The presence of the δ -functions in the integration kernel suggests writing the wave vector k in polar coordinates $k = r(\cos \alpha, \sin \alpha \sin \beta, \sin \alpha \cos \beta)$ giving

$$C(m, n)$$

$$= \frac{1}{2} \sum_{\nu=-1}^1 \int s_\nu \delta(\varepsilon - \varepsilon' + \nu\omega) [\phi_m - \phi'_m] [\phi_n - \phi'_n] r^2 \sin(\alpha) (r')^2 \sin(\alpha') dr d\alpha d\beta dr' d\alpha' d\beta',$$

where the $'$ denotes evaluation at r', α', β' . We now choose as basis functions spherical harmonic functions in the angular directions and polynomials in the radial direction $r = |k|$,

$$\phi_m(r, \alpha, \beta) = P_{m_1}(r) \Gamma_{m_2}(\alpha, \beta), \quad m = (m_1, m_2).$$

To take care of the δ -function in the integral kernel, we change variables in the integral from r to ε . Thus, we need to invert the band energy function ε as a function of the radius r for fixed angles α, β :

$$(28) \quad \varepsilon(r, \alpha, \beta) = u \quad \iff \quad r = g(\varepsilon, \alpha, \beta).$$

In the transformed variables, the integration with respect to ε' can now be carried out exactly using the δ function. So the matrix element $C(m, n)$ now becomes

$$(29) \quad C(m, n) = \frac{1}{2} \sum_{\nu=-1}^1 \int_0^\infty d\varepsilon \int d\alpha d\beta d\alpha' d\beta' [g^2(g')^2 \frac{dg}{d\varepsilon} \frac{dg'}{d\varepsilon'} \sin(\beta) \sin(\beta')] \\ \times \theta(\varepsilon + \nu\omega) s_\nu [P_{m_1} \Gamma_{m_2} - P'_{m_1} \Gamma'_{m_2}] [P_{n_1} \Gamma_{n_2} - P'_{n_1} \Gamma'_{n_2}],$$

where the $'$ now denotes evaluation at $r = g(\varepsilon + \nu\omega, \alpha', \beta')$ and α', β' , and θ is the Heaviside function. The structure of the scattering cross sections s_ν is usually sufficiently simple, such that the integrals with respect to the angular variables can be carried out exactly, leaving only the one-dimensional integral with respect to the energy to be evaluated numerically. The procedure outlined above is applicable in principle to an arbitrary band structure. It becomes significantly simpler if the band energy is actually radially symmetric, i.e., $\varepsilon = \varepsilon(|k|)$, since in this case the inverse band energy function g depends only on the energy. A popular choice is the dispersion relation due to Kane which is of the form (see [9])

$$\varepsilon(k) = \frac{|k|^2}{1 + \sqrt{1 + \kappa|k|^2}}.$$

We should point out that, if the band energy is actually not radially symmetric, the solution will actually depend on how the sample is aligned with the crystal direction, which might pose a considerable technological problem.

We now present results of a numerical test on the standard $n^+ - n - n^+$ silicon diode with a channel of $50nm$ length. This means that the doping concentration D^{dop} in (1) is given by a step function of the form

$$D^{dop}(x) = \begin{pmatrix} 10^{24}m^{-3} & 0 < x < 50nm \\ 10^{21}m^{-3} & 50nm < x < 100nm \\ 10^{24}m^{-3} & 100nm < x < 150nm \end{pmatrix}.$$

For the sake of simplicity, we restrict ourselves to parabolic band structures. So (in scaled variables) $\varepsilon(k) = \frac{|k|^2}{2}$ holds, which makes the computation of the inverse function $g(\varepsilon, \alpha, \beta)$ in (28) trivial. ($g(\varepsilon, \alpha, \beta) = \sqrt{2\varepsilon}$ holds and all integrations in (29) can be carried out exactly.) Also, since the problem in one spatial dimension admits solutions which are cylindrically symmetric around the k_1 direction (i.e., $f(x, k) = f(x_1, k_1, k_2^2 + k_3^2)$), we choose only spherical harmonics with this symmetry as basis functions. For scattering cross sections we choose Fermi's golden rule formula

(30)

$$(a) \quad Q[f](x, k) = \frac{\hbar 2V_L F(\xi)^2 \pi}{\Omega} \sum_{\nu=\pm 1} \left(N_\xi + \frac{1+\nu}{2} \right) \delta(\varepsilon(k) - \varepsilon(k') + \nu\hbar\omega) f(x, k') dk' - \frac{f(x, k)}{\tau(k)},$$

$$(b) \quad \frac{1}{\tau(k)} = \frac{2V_L F(\xi)^2 m_*^{3/2}}{\hbar^2 \Omega} 4\pi^2 \sum_{\nu=\pm 1} \left(N_\xi + \frac{1+\nu}{2} \right) \sqrt{2(\varepsilon(k) - \nu \hbar \omega)^+},$$

$$(c) \quad \varepsilon(k) = \frac{\hbar^2 |k|^2}{2m_*}, \quad \Omega = \ln \left(\frac{N_\xi + 1}{N_\xi} \right),$$

where $F(\xi)$ denotes the frequency of the lattice state with momentum ξ and N_ξ denotes its occupation number. V_L denotes the volume of one lattice cell. $F(\xi)$ is given according to the formula

$$F(\xi) = \sqrt{\frac{q^2 \hbar \omega}{2V_L |\xi|^2 \varepsilon_0} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s} \right)}.$$

The constants are given by the following expressions:

Symbol	Value	Unit	Meaning
q	$1.602 * 10^{-19}$	C	electron charge
\hbar	$6.626196 * 10^{-34}$	kgm^2/sec	Planck constant
m_*	$0.063 * 0.109 * 10^{-31}$	kg	effective electron mass
$\hbar \omega$	0.036	eV	emission/absorption energy
ε_0	$8.85 * 10^{-12}$	$\frac{C}{Vm}$	dielectricity constant (vacuum)
ε_∞	10.92	1	
ε_s	12.9	1	

We take into account only one single phonon momentum vector (corresponding to a δ - function collision potential; see [2], [4], [10]), which is evaluated at equilibrium, meaning $|\xi|^2 = m_* K T$ holds at room temperature. This gives, for an occupation number N_ξ corresponding to room temperature, numerical values of

$$\frac{\hbar 2V_L F(\xi)^2 \pi}{\Omega} N_\xi = 5.9356e * 10^5 \frac{m^3}{sec^2}, \quad \frac{2V_L F(\xi)^2 m_*^{3/2}}{\hbar^2 \Omega} N_\xi 4\pi^2 = 9.6044 * 10^{23} \frac{1}{m\sqrt{kg}}$$

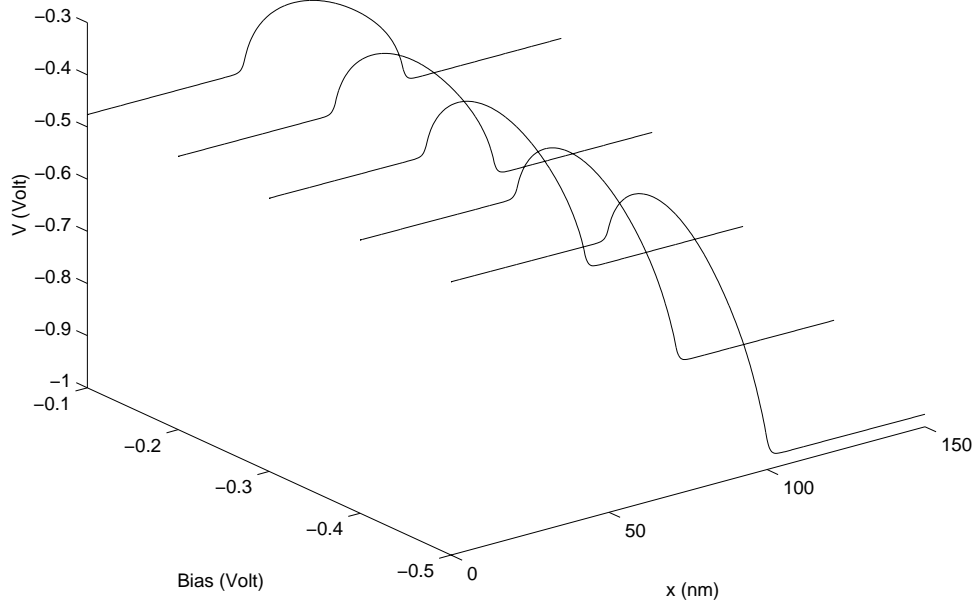
for the constants necessary to evaluate (30). Finally, choosing computational units of $10^{-7}m$ for x and $10^7 m^{-1}$ for k , this gives a value of $\lambda = 0.3974$ for the dimensionless parameter λ in (1) with a scaled band energy $\varepsilon = \frac{|k|^2}{2}$.

The results below were obtained by varying the applied bias (the difference of the boundary potential V_b^e between the right and the left endpoint) from $-0.1V$ to $-0.5V$. A uniform mesh with 151 gridpoints and 128 expansion terms (16 in the energy direction and 8 in the angular direction) was used. The obtained figures did not change significantly when either doubling the number of expansion terms or halving the mesh size.

Figures 1–4 depict the potential as well as the physical densities for electrons, electron velocity, and electron energy as functions of the spatial variable x . Figure 1 shows the potential distribution $V(x)$. Figure 2 shows the electron density $\langle 1 \rangle(x) = \int f(x, k) dk = \rho^T F^e$. Figure 3 shows the velocity distribution $u(x) = \frac{\langle \partial_{k_1} \varepsilon \rangle(x)}{\langle 1 \rangle(x)}$ with $\langle \partial_{k_1} \varepsilon \rangle = \int \partial_{k_1} \varepsilon(k) f(x, k) dk$. Figure 4 shows the corresponding energy densities given by $w(x) = \frac{\langle \varepsilon \rangle(x)}{\langle 1 \rangle(x)}$.

Figures 5–8 depict the kinetic density $f(x, k)$ for the bias value of $0.4V$ for various values of x . Using spherical harmonic basis functions $\phi_m(k)$ gives the kinetic density function f in spherical coordinates as $f = f^{sph}(x, r, \cos(\alpha), \beta)$ with

FIGURE 1: Potential

FIG. 1. *Potential.*

$k = (r \cos(\alpha), r \sin(\alpha) \sin(\beta), r \sin(\alpha) \cos(\beta))$, $\alpha \in [0, \pi]$, $\beta \in [-\pi, \pi]$. It is, however, more instructive to look at the kinetic density $f = f^{car}$ in Cartesian coordinates. In the case of one spatial dimension, the kinetic energy density will be cylindrically symmetrical around the k_1 -axis. So $f^{car}(x, k) = f(x, k_1, \sqrt{k_2^2 + k_3^2})$ and $f^{sph}(x, k) = f(x, r, \cos(\alpha))$ hold. f^{car} and f^{sph} are related through $f^{car}(x, r \cos(\alpha), r \sin(\alpha)) = r^2 f^{sph}(x, r, \cos(\alpha))$, where the factor r^2 arises from the infinitesimal volume element due to the coordinate transformation. So Figures 5–8 show the function $r^2 f^{sph}(x, r, \cos(\alpha))$ for fixed values of x as a function of $k_1 = r \cos(\alpha)$ and $\sqrt{k_2^2 + k_3^2} = r \sin(\alpha)$, which is the density against which any function of Cartesian coordinates has to be integrated to compute expectations.

The purpose of these computations is to investigate how far away from the fluid dynamic regime we are. (For such a short channel and the given applied bias, we expect to see some distinctly nonequilibrium phenomena.) Figure 5 shows the distribution to the left of the channel. It is essentially given by a forward and a backward traveling Maxwellian of roughly the same amplitude. Figures 6 and 7 show the distribution at the beginning and the end of the channel. First we notice that the wave has developed a second peak in the forward as well as in the backward traveling component. Moreover, it has become definitely asymmetric in the k_1 direction at the end of the channel (in Figure 7). After the electron has left the channel in Figure 8, remnants of the second peak are still visible, but the solution has become symmetric in k_1 again. Figure 5 could have been produced by a hydrodynamic model or even by drift-diffusion equations, considering the low values of the group velocity in Figure 3 at this point. The second peak in Figure 8 (after leaving the channel) could have

FIGURE 2: Particle Density

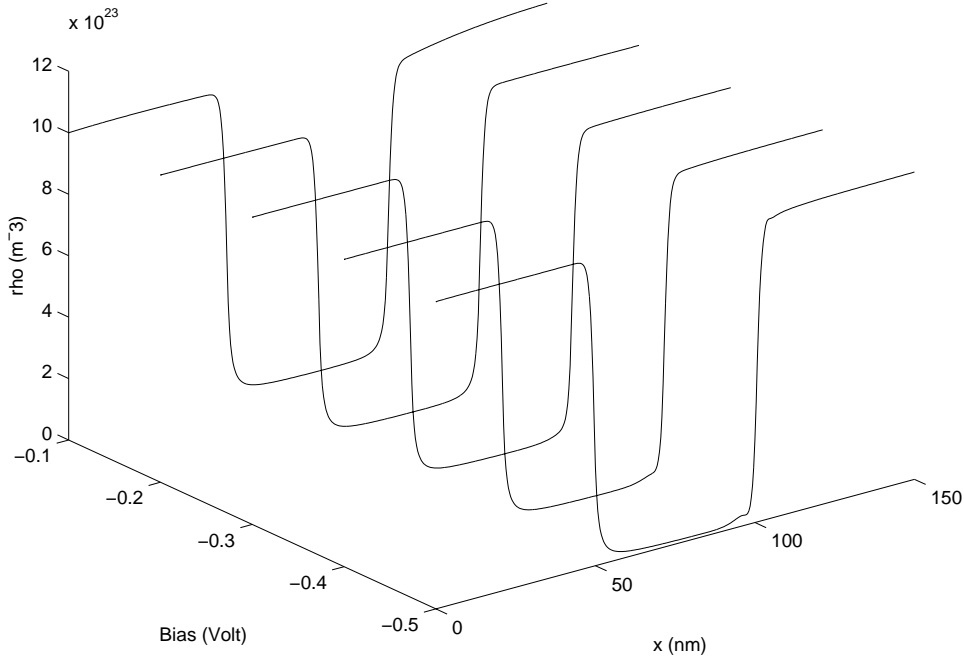
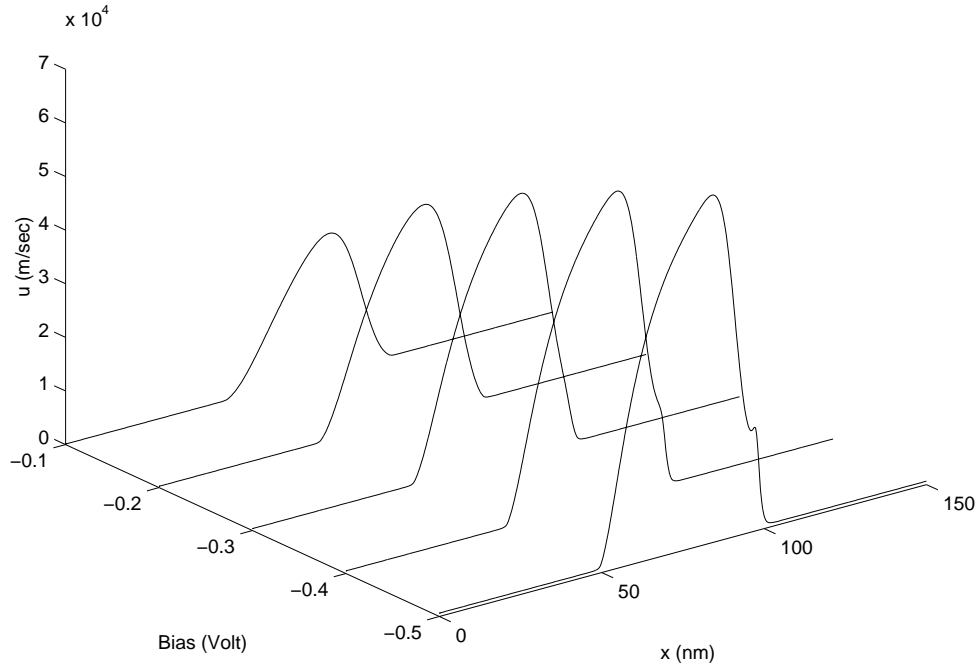


FIG. 2. Particle density.

been produced by a SHE-model. However, the strongly asymmetric distribution at the channel end (Figure 7) is a truly kinetic phenomenon and could not have been produced by either of the above approximations.

Concluding remarks. We conclude this section with some remarks concerning future work and the extension of this approach to two spatial dimensions. First, going to two spatial dimensions means a dramatic increase in the computational cost, since in addition to the added spatial dimension the cylindrical symmetry of the density function is lost. In the two-dimensional case, the density has to be taken of the form $f(x, k) = f(x_1, x_2, k_1, k_2, |k_3|)$, thus going effectively from a three- to a five-dimensional problem. The computations above were carried out using 16 expansion terms in the energy direction and 8 terms in the angular directions, so a system of 128 one-dimensional conservation laws was solved. Roughly estimating the cost in the two-dimensional case, allowing for a little less resolution and still exploiting the symmetry in the k_3 direction, this would translate into solving anywhere between 256 and 1024 two-dimensional conservation laws. On the other hand, we do not expect it to be necessary to solve the full kinetic problem in the whole device; i.e., for the simulation of a transistor this amount of resolution would only be necessary in a rather narrow region around the channel. Indeed, the promise of the expansion approach in two spatial dimensions is that it allows for a model hierarchy ranging from a Scharfetter–Gummel solution of the drift-diffusion equation (i.e., taking only three terms) to the full Boltzmann solution. Taking this into account, we estimate that a two-dimensional solution would involve around half a million variables. This raises, of course, the issue of the iterative solution of the involved linear system. In the one-

FIGURE 3: Velocity

FIG. 3. *Velocity.*

dimensional case, a direct solution of the linear system was combined with a standard Gummel iteration procedure for the coupling to Poisson's equation. (See [19].) One possibility is to precondition the system by a solution of the drift-diffusion equations (i.e., by the equations corresponding to the first three terms only). This would result in a pseudo time marching algorithm where the diffusive part of the operator is discretized implicitly in time and the hyperbolic part explicitly, as first proposed in [17] for the solution of the transient problem.

Finally, we would like to comment on the differences in the approaches to solving the steady state problem and the transient Boltzmann equation. There have been several approaches to deterministic solutions of the transient Boltzmann equation using methods designed for hyperbolic conservation laws. (See [1], [6], and references therein.) The transient solution (as well as the conservation law resulting from its Galerkin approximation in the wave vector direction) will exhibit a variety of hyperbolic and dispersive transient phenomena which would be unduly damped by the pseudo time marching algorithm suggested above. (See [15].) On the other hand, because of this fact, a pseudo time marching algorithm, based on the discretization presented here, will arrive at the correct steady state much faster, albeit with the wrong transient response, than a method designed for hyperbolic equations. So the method presented in this paper is really designed for the computation of steady states and for accurate deterministic simulations of the transient behavior it is probably preferable to use methods which take into account the hyperbolic and dispersive nature of the transient problem as given in [6] and [15].

FIGURE 4: Energy Density

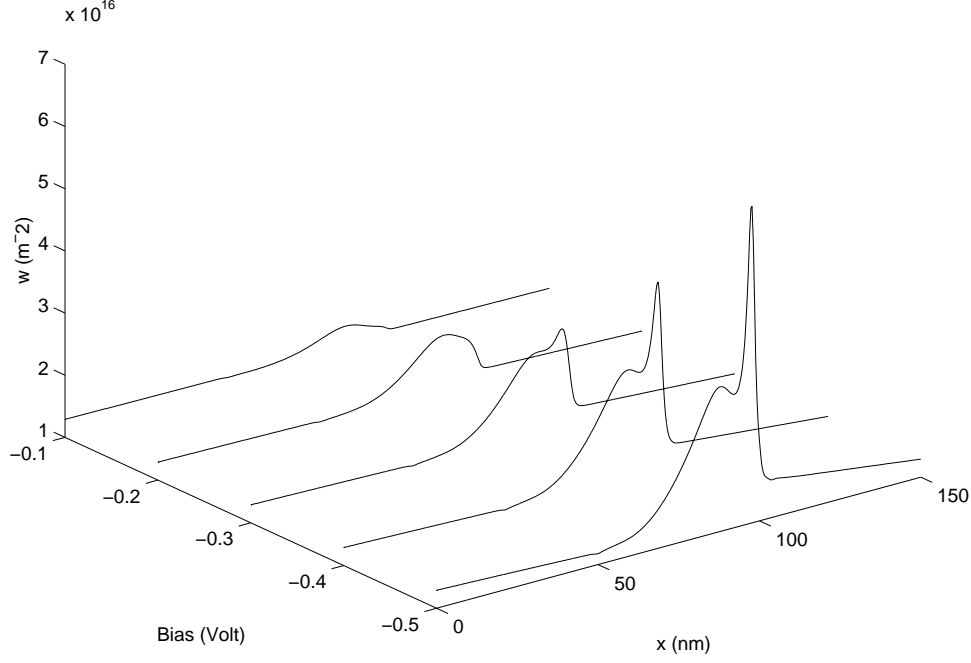


FIG. 4. Energy density.

6. Appendix.

Proof of Theorem 1. Setting $F_1^e = 0$, $F_1^o = 0$ in (26) gives the equations

$$\sum_{\nu=1}^d [D_{\nu}^{eo} (A_{\nu}^{10} F_0^o - qV^o B_{\nu}^{10} F_0^o) + qV^e B_{\nu}^{10} D_{\nu}^{eo} F_0^o] = 0,$$

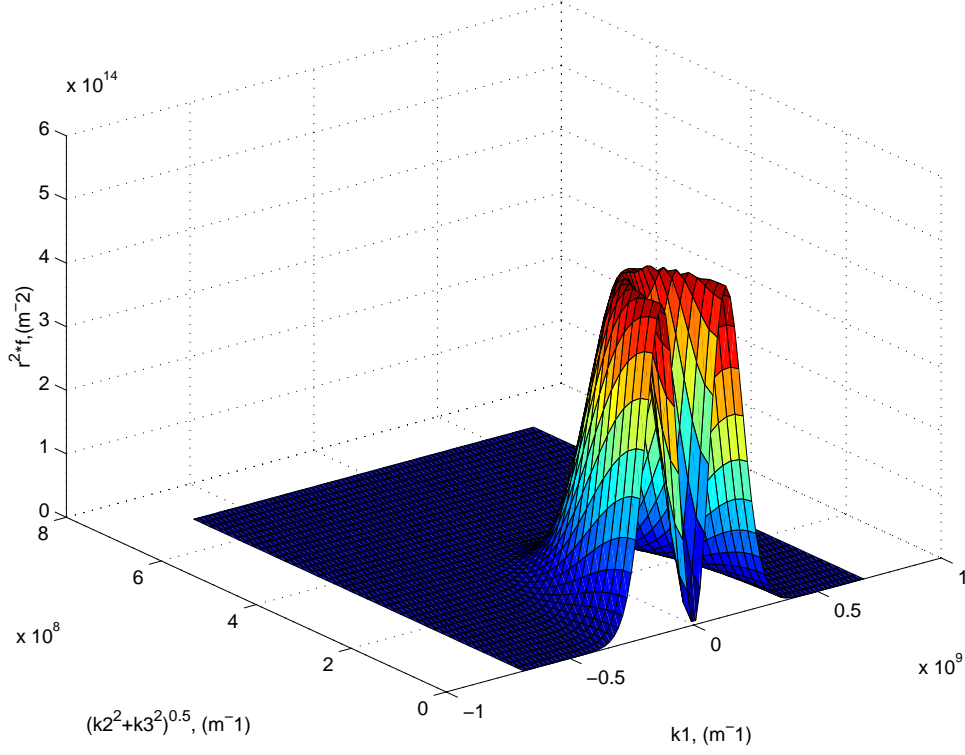
$$\sum_{\nu=1}^d e^{-qV^o} [(A_{\nu}^{01})^T D_{\nu}^{oe} (e^{qV^e} F_0^e)] + \frac{1}{\lambda} C_o^{10} F_0^o = 0,$$

which depend only on F_0^o and discrete derivatives of $e^{qV^e} F_0^e$. For $F_1^e = 0$, $F_1^o = 0$ these terms are given by (23) as the solution of

$$\sum_{\nu=1}^d D_{\nu}^{eo} (A_{\nu}^{00} F_0^o) = 0,$$

$$\sum_{\nu=1}^d e^{-qV^o} [(A_{\nu}^{00})^T D_{\nu}^{oe} (e^{qV^e} F_0^e)] + \frac{1}{\lambda} C_o^{00} F_0^o = 0,$$

$$-\sigma \sum_{\nu=1}^d D_{\nu}^{eo} D_{\nu}^{oe} V^e + q[D^{dop} - F_0^e] = 0,$$

FIGURE 5: $r^2 * f$, Bias=-0.4V, x=30.0752nmFIG. 5. $r^2 * f$: Bias = -0.4V, $x = 30.0752nm$.

and setting $F_0^o = 0$ and $F_0^e = e^{-qV}$ satisfies all of the above equations and the boundary conditions, except for the Poisson equation. Therefore V^e has to be chosen as the solution of

$$-\sigma \sum_{\nu=1}^d D_{\nu}^{eo} D_{\nu}^{oe} V^e + q[D^{dop} - e^{-qV^e}] = 0$$

together with the corresponding boundary conditions (23)(d) which corresponds to the equilibrium solution. \square

Proof of Theorem 2. The linearized problem (27) is given by the equations

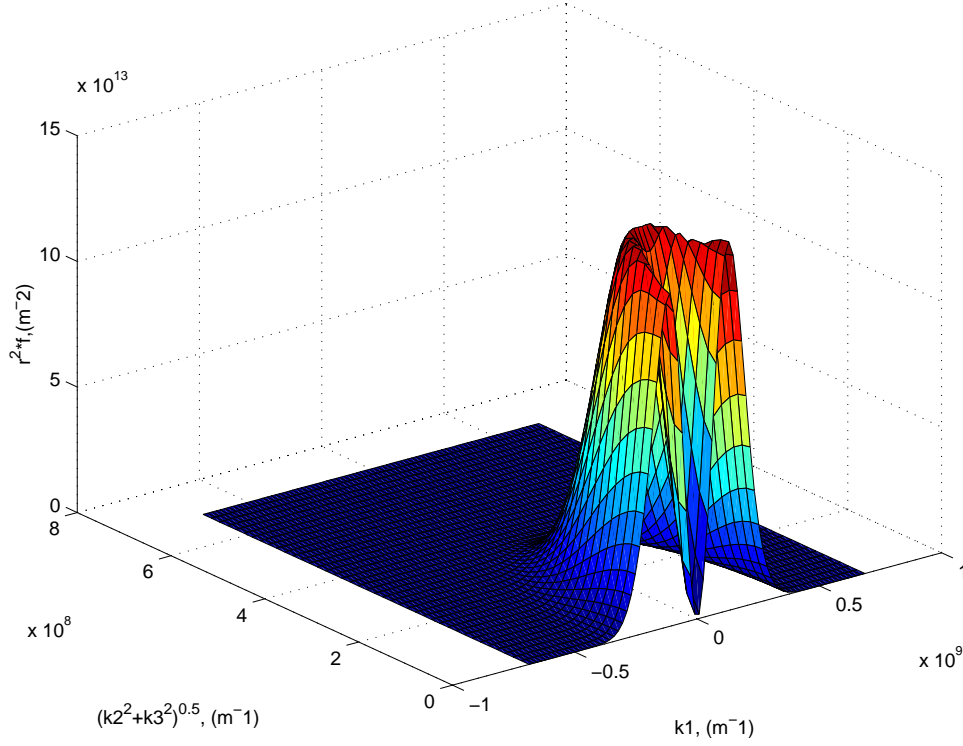
$$(31) \quad (a) \quad dL_1^{eo}(F_0^e, 0, 0, 0)(\delta F_0^e, \delta F_1^e, \delta F_0^o, \delta F_1^o) + \frac{1}{\lambda} C_e^{11} \delta F_1^e = R_1^e,$$

$$(b) \quad dL_1^{oe}(F_0^e, 0)(\delta F_0^e, \delta F_1^e) + \frac{1}{\lambda} [C_o^{10} \delta F_0^o + C_o^{11} \delta F_1^o] = R_1^o,$$

where the terms $\delta F_0^e, \delta F_0^o, \delta V^e, \delta V^o$ are given in terms of $\delta F_1^e, \delta F_1^o$ by linearizing the drift-diffusion-Poisson system (23):

$$(32) \quad (a) \quad dL_0^{eo}(0, 0)(\delta F_0^o, \delta F_1^o) = 0,$$

$$(b) \quad dL_0^{oe}(F_0^e, 0)(\delta F_0^e, \delta F_1^e) + \frac{1}{\lambda} [C_o^{00} \delta F_0^o + C_o^{01} \delta F_1^o] = 0,$$

FIGURE 6: $r^2 * f$, Bias=-0.4V, x=50nmFIG. 6. $r^2 * f$: Bias = -0.4V, $x = 50nm$.

$$(c) \quad -\sigma \sum_{\nu=1}^d D_{\nu}^{eo} D_{\nu}^{oe} \delta V^e + q[D^{dop} - \delta F_0^e] = 0$$

together with homogeneous boundary conditions of the form (23)(d). Combining (31)(a-b) with (32)(a-b) we obtain the linearized system for the full equations

$$(33) \quad (a) \quad dL^{eo}(F^e, 0)(\delta F^e, \delta F^o) + \frac{1}{\lambda} C^e \delta F^e = R^e,$$

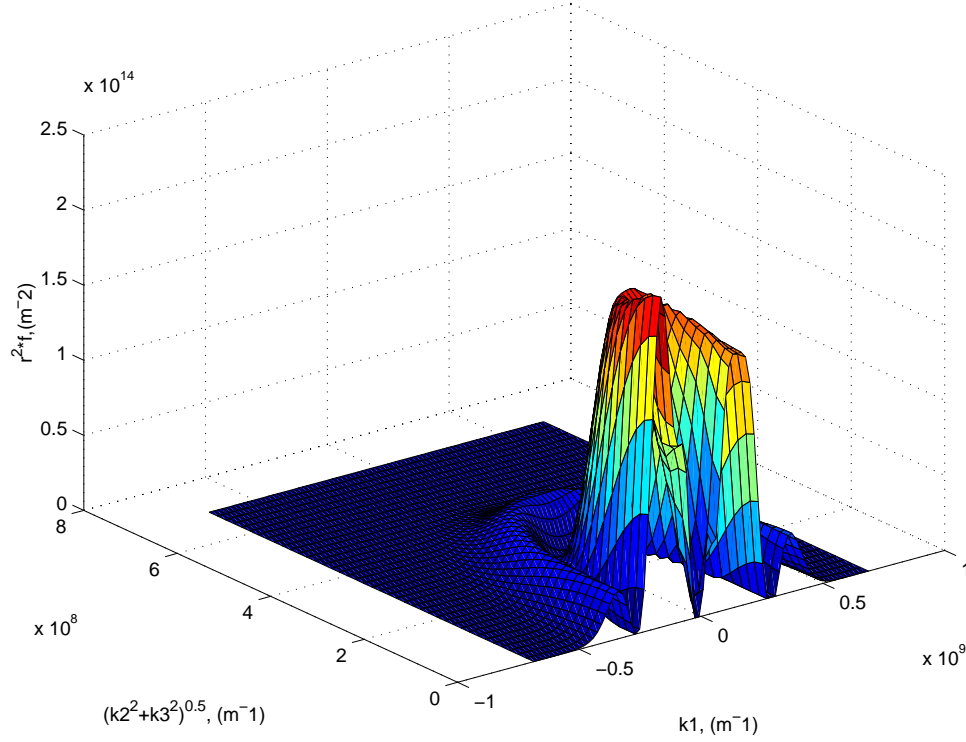
$$(b) \quad dL^{oe}(F^e)(\delta F^e) + \frac{1}{\lambda} C^o \delta F^o = R^o,$$

with

$$\delta F^e = \begin{pmatrix} \delta F_0^e \\ \delta F_1^e \end{pmatrix}, \quad \delta F^o = \begin{pmatrix} \delta F_0^o \\ \delta F_1^o \end{pmatrix}, \quad F^e = \begin{pmatrix} F_0^e \\ 0 \end{pmatrix},$$

$$R^e = \begin{pmatrix} 0 \\ R_1^e \end{pmatrix}, \quad R^o = \begin{pmatrix} 0 \\ R_1^o \end{pmatrix}.$$

So we basically obtain the same linearized system as if we had linearized (21) directly, except for the crucial fact that the first component of R^e and the first three components of R^o are zero. Now, by virtue of construction of the discrete operators L^{eo}, L^{oe}

FIGURE 7: $r^2 * f$, Bias = -0.4V, x = 100nmFIG. 7. $r^2 * f$: Bias = -0.4V, $x = 100nm$.

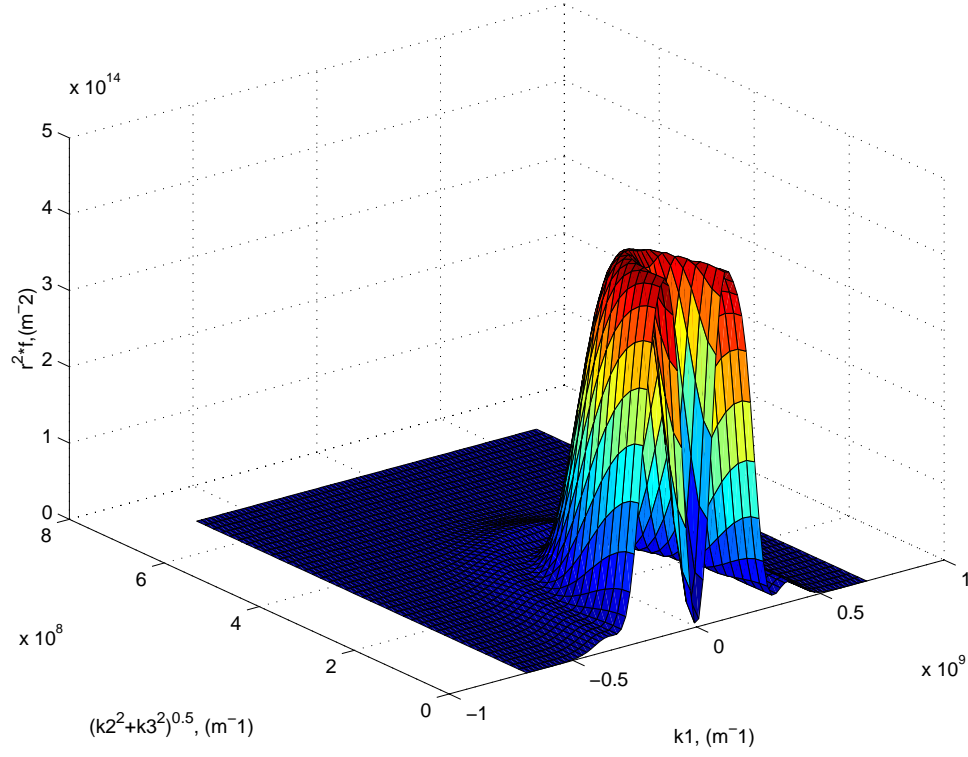
(see Proposition 1) and because of the structure of the boundary conditions, we have that

$$(34) \quad I_e[h^e(F^e)^T L^{eo}(F^e, F^o)] + I_o[h^o(F^e, F^o)^T L^{oe}(F^e)] = 0$$

holds for any choice of F^e, F^o , where I_e, I_o denote the discrete integral operators defined in (16) and the entropies h^e, h^o are given by $h^e(F^e) = e^{qV^e} F^e$, $h^o(F^e, F^o) = e^{qV^o} F^o$ and, of course, the potentials V^e, V^o depend on F^e through the Poisson equation. Differentiating (34) twice functionally with respect to all of its arguments yields

$$\begin{aligned} & I_e[(d^2 h^e(F^e)(\delta F^e)^2)^T L^{eo}(F^e, F^o)] \\ & + 2I_e[(dh^e(F^e)(\delta F^e))^T (dL^{eo}(F^e, F^o)(\delta F^e, \delta F^o))] \\ & + I_e[h^e(F^e)(d^2 L^{eo}(F^e, F^o)^T (\delta F^e, \delta F^o)^2)] \\ & + I_o[(d^2 h^o(F^e, F^o)(\delta F^e, \delta F^o)^2)^T L^{oe}(F^e)] \\ & + 2I_o[(dh^o(F^e, F^o)(\delta F^e, \delta F^o))^T (dL^{oe}(F^e)(\delta F^e))] \\ & + I_o[h^o(F^e, F^o)(d^2 L^{oe}(F^e)^T (\delta F^e)^2)] = 0. \end{aligned}$$

Inserting the equilibrium solution $F^o = 0$, $F^e = e^{-qV^e} \mathbf{e}$ into the above equations, we

FIGURE 8: $r^2 * f$, Bias = -0.4V, x = 120.3008nmFIG. 8. $r^2 * f$: Bias = -0.4V, $x = 120.3008nm$.

see that

$$L^{eo}(F^e, F^o) = 0, \quad L^{oe}(F^e) = 0, \quad h^o(F^e, F^o) = 0, \quad h^e(F^e) = \mathbf{e}$$

holds, which eliminates three of the six terms in the above relations. Thus, we obtain

$$(35) \quad \begin{aligned} & 2I_e[(dh^e(F^e)(\delta F^e))^T(dL^{eo}(F^e, F^o)(\delta F^e, \delta F^o))] \\ & + I_e[h^e(F^e)(d^2L^{eo}(F^e, F^o)^T(\delta F^e, \delta F^o)^2)] \\ & + 2I_o[(dh^o(F^e, F^o)(\delta F^e, \delta F^o))^T(dL^{oe}(F^e)(\delta F^e))] = 0, \end{aligned}$$

where in the second term of (35) only the first component of L^{eo} is left because of the form of h^e . However, from (25) it can be seen that L_0^{eo} is a pure divergence operator, and therefore, because of the structure of the boundary conditions, the discrete integral over L_0^{eo} vanishes for all arguments. Therefore the same is true for its second functional derivative, and we obtain the formula

$$\begin{aligned} & 2I_e[(dh^e(F^e)(\delta F^e))^T(dL^{eo}(F^e, F^o)(\delta F^e, \delta F^o))] \\ & + 2I_o[(dh^o(F^e, F^o)(\delta F^e, \delta F^o))^T(dL^{oe}(F^e)(\delta F^e))] = 0 \end{aligned}$$

which we use to estimate the linearized equations (33). Multiplying (33)(a) by $(dh^e(F^e)(\delta F^e))^T$ and (33)(b) by $(dh^o(F^e, 0)(\delta F^e, \delta F^o))^T$, and applying the discrete integral operators I_e, I_o , we obtain

$$(36) \quad I_e[(dh^e(F^e)(\delta F^e))^T C^e \delta F^e] + I_o[(dh^o(F^e, 0)(\delta F^e, \delta F^o))^T C^o \delta F^o] \\ = \lambda I_e[(dh^e(F^e)(\delta F^e))^T R^e] + \lambda I_o[(dh^o(F^e, 0)(\delta F^e, \delta F^o))^T R^o].$$

Computing the first Frechet derivatives of h^e, h^o at the equilibrium solution gives

$$dh^e(F^e)(\delta F^e) = q\delta V^e \mathbf{e} + e^{qV^e} \delta F^e, \quad dh^o(F^e, 0)(\delta F^o, \delta V^o) = e^{qV^o} \delta F^o,$$

with $\delta V^e, \delta V^o$ the solutions of the linearized Poisson equation with homogeneous boundary conditions. Inserting this into (36), and using the fact that the first row and column of C^e vanishes, and that the first component of R^e, R^o is also zero, we get

$$I_e[e^{qV^e} (\delta F_1^e)^T C_e^{11} \delta F_1^e] + I_o[e^{qV^o} (\delta F^o)^T C^o \delta F^o] \\ = \lambda I_e[e^{qV^e} (\delta F_1^e)^T R_1^e] + \lambda I_o[e^{qV^o} (\delta F_1^o)^T R_1^o].$$

Now the matrices C_e^{11} and C^o are strictly positive definite. Using the Cauchy–Schwarz inequality gives the result. \square

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