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**Existence of bounded discrete steady state solutions of the
van Roosbroeck system with monotone Fermi–Dirac statistic
functions**

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Abstract If the statistic function is modified, the equations can be derived by a variational formulation or just using a generalized Einstein relation. In both cases a dissipative generalization of the Scharfetter-Gummel scheme [1], understood as a one-dimensional constant current approximation, is derived for strictly monotone coefficient functions in the elliptic operator $\nabla \cdot f(v)\nabla$, v chemical potential, while the hole density is defined by $p = \mathcal{F}(v) \leq e^v$. A closed form integration of the governing equation would simplify the practical use, but mean value theorem based results are sufficient to prove existence of bounded discrete steady state solutions on any boundary conforming Delaunay grid. These results hold for any piecewise, continuous, and monotone approximation of $f(v)$ and $\mathcal{F}(v)$.

1 Introduction

A short summary of the variational formulation is given to illustrate its consequences and to compare it with the phenomenologic derivation based on the generalized Einstein relation, which holds at equilibrium. The analytic equations and boundary conditions are stated. The next section discusses the generalization of the Scharfetter-Gummel scheme, its general properties and

the special cases, which are treated in such a way that they are high order consistent with the general equation. Finally, approximations are discussed that allow either analytic integration or fulfill the asymptotic relations in cases where analytic integration is replaced by a numerical one, which guarantees monotonicity of the function including the integration errors. The aim is a generalization of the Scharfetter-Gummel scheme to 'non-Boltzmann' distribution functions with an error defined by the approximation of the function and not by introducing stable averages like the 'discrete chain rule', which of course should be a qualitatively correct approximation and sufficiently correct with respect to the special functions and the argument differences involved. The applications in mind justify the basic assumptions for the chemical potential v and the distribution functions f, \mathcal{F} valid in the paper:

$$A_1 : -\infty < v_{min} < v < v_{max} < \infty, \quad (1)$$

$$A_2 : f(s) < f(t), \quad s < t, \quad 0 < f'(s) \leq f(s) \leq e^s, \quad (2)$$

$$A_3 : \mathcal{F}(s) < \mathcal{F}(t), \quad s < t, \quad 0 < \mathcal{F}'(s) \leq \mathcal{F}(s) \leq e^s. \quad (3)$$

To prove existence of discrete bounded steady state solutions current expressions and estimates are derived using the mean value theorem. Uniqueness of the thermodynamic equilibrium, dissipativity, and properties of the linearized problem are shown in complete analogy to the classical van Roosbroeck equations and Scharfetter-Gummel scheme.

2 Short summary of the variational formulation

The free energy functional F is the sum of the convex chemical part $\Phi(p)$ and the interaction part $\Psi(p)$:

$$F(p) = \Phi(p) + \Psi(p), \quad (4)$$

p denotes the density of holes. $F(p)$ is minimized under particle conservation (Neumann boundary conditions)

$$F'(p) = \varphi = v + w, \quad (5)$$

where φ is the grand chemical (quasi-Fermi) potential,

$$\Phi'(p) = v, \quad \Psi'(p) = w \quad (6)$$

are the chemical and the interaction potential. Φ^* denotes the conjugate function

$$p = (\Phi^*)'(v) = (\Phi^*)'(\varphi - w) = (\Phi')^{-1}(v), \quad (7)$$

Φ'^{-1} is the inverse function in case that $\Phi'(p)$ is monotone. Assuming

- a) conservation of mass in $\Omega \subset \mathbb{R}^d$,
- b) solutions along trajectories $t \mapsto n(t)$ satisfy the state equation with $\varphi(x)$,
- c) and the anti-gradient of φ is the driving force

yields

$$\frac{\partial p}{\partial t} + \nabla \cdot j_p = 0 \text{ in } \Omega, \quad \nu \cdot j_p = 0 \text{ on } \partial\Omega. \quad (8)$$

With b), c) and the chain rule (the constant diffusion coefficient, matrix is denoted by D), the particle current j_p of the holes is

$$-j_p = D(\Phi^*)''(\varphi - w)\nabla\varphi = D\frac{\partial p}{\partial v}\nabla\varphi. \quad (9)$$

Finally,

$$\begin{aligned} -j_p &= D(\Phi^*)''\nabla(v + w), \\ &= D\nabla(\Phi^*)'(v) + D(\Phi^*)''(v)\nabla w, \\ &= D\nabla p + D\frac{\partial p}{\partial v}\nabla w. \end{aligned}$$

Hence, in case of a variational formulation A_2 implies A_3 and the 'discrete chain rule' [2] is preserving the qualitative properties. In case the free energy functional is seen as a complete description, D provides the time scale, else it may include density dependent corrections accounting for the missing parts in the free energy functional. For the general setting (not restricted to Fermi-Dirac integrals only) and a rigorous treatment including phase separation problems compare, e.g., [3],[4], [5], [6],[7], [8], [9], [10] and cited literature. For relations with gradient structures, cf. [11].

When the equations are stated as a modification of the classical van Roosbroeck [12] equations (cf. [13]) the current expressions are

$$-j_{modclass} = \mu p \nabla \varphi_p,$$

$$-j_{var} = D\frac{\partial p}{\partial v}\nabla\varphi_p,$$

and therefore

$$\frac{\mu p}{D\frac{\partial p}{\partial v}} = 1,$$

$$\frac{\mu}{D} = \frac{\partial \ln p}{\partial v}.$$

Hence, the generalized Einstein relation, which holds at thermodynamic equilibrium due to the total current, equals zero. It is used for non-equilibrium states and relates the diffusion and drift current via the diffusion coefficient D and the mobility μ . Essentially it is a factor which can be attributed arbitrarily to drift and diffusion. The equations coincide if $\mu = D\frac{\partial p}{\partial v}/p$ is substituted.

If the densities are related to the chemical potential by exponential functions (Boltzmann statistics), the logarithmic derivative is equal to one and the Einstein relation is a constant, here one due to the scaling of the potentials.

The complete system reads in particle currents (electric charge densities, currents are multiplied by the charge per particle) and in more detail with respect to constants related to physics (density of states N_v and N_c , band edges of valence and conduction band E_v, E_c)

$$p/N_v = (\Phi^*)'(v_p) = (\Phi')^{-1}(v_p) = \mathcal{F}_i(v_p),$$

$v_p = \varphi_p - w + E_v$, while $\mathcal{F}_i(s)$ denotes the most relevant example, the Fermi-Dirac integral of index i . The index i typically depends on the space dimension, e.g., $i = 1/2$ for transport in \mathbb{R}^3 . Accordingly,

$$n/N_c = (\Phi^*)'(v_n) = (\Phi')^{-1}(v_n) = \mathcal{F}_i(v_n),$$

$v_n = -\varphi_n + w - E_c$, v_p and v_n are the chemical potentials for holes and electrons of the material. Here w , and φ_p and φ_n denote the electrostatic and quasi-Fermi potentials, which are continuous functions. All potential-like quantities are 'measured' in units of the thermal voltage $U_T := k_B T/q$, is the k_B Boltzmann constant, T is the temperature, and q is the elementary charge. Thus

$$-\nabla \cdot \varepsilon \nabla w = C - n + p, \quad (10)$$

$$\frac{\partial p}{\partial t} - \nabla \cdot D_p(\Phi^*)''\nabla\varphi_p = R(n, p)(1 - r(\varphi_p - \varphi_n)),$$

$$\frac{\partial n}{\partial t} + \nabla \cdot D_n(\Phi^*)''\nabla\varphi_n = R(n, p)(1 - r(\varphi_p - \varphi_n))$$

in the Lipschitzian domain $\Omega \subset \mathbb{R}^d$. For reasons of simplicity the boundary conditions are homogeneous Neumann for insulating parts and Dirichlet for contacts ($\Gamma_D = \cup_i \Gamma_{D_i}$ with positive surface measure), where $w_{applied_i}$ is added to the contact potentials ($w_i = w_i^* + w_{applied_i}$, $\varphi_{p,i} = w_{applied_i}$, $\varphi_{n,i} = w_{applied_i}$, $x_i \in \Gamma_{D_i}$).

Hence, the densities at contacts are those of the thermodynamic equilibrium. This is defined by the nonlinear Poisson equation

$$-\nabla \cdot \varepsilon \nabla w^* = C - n^* + p^* = C - \mathcal{F}(v_n^*) + \mathcal{F}(v_p^*) \quad (11)$$

with $\varphi_p^* = \varphi_n^* = 0$ and homogeneous Neumann boundary conditions. w^* , v_n^* and v_p^* denote the thermodynamic equilibrium solution. The recombination-generation expression $r(s)$ depends on the difference of the quasi-Fermi potentials. It is assumed: $r(s)$ is strictly monotone, $r(0) = 1$, $\lim_{s \rightarrow -\infty} r(s) = 0$, and $\lim_{s \rightarrow \infty} r(s) = \infty$, $R \geq 0$. This includes the classical Shockley-Read-Hall and Auger recombination-generation processes, but it is not anymore an expression of mass action law type. For the free energy expressions see, e.g., [4]. The discrete case fulfills analog discrete free energy relations in case it is applied to a variational formulation.

In the following the constants N_v , N_c are set to one, E_v , E_c to zero, re-substitution is not a problem, while $f_i(v_i) := D_i(\Phi^*)''(v_i)$, $i = p, n$ describes the transport as long as assumption (2) holds—it is not necessary to suppose the variational formulation in that respect. The properties of the discretization are studied for $\varphi = v + w$ (holes) and the other case follows by proper substitutions, while D or μ are included in f .

3 Generalized Scharfetter-Gummel scheme

The classical scheme discretizes all three parts of each continuity equation separately, providing local conservation of the total current (sum of displacement and charge density currents) as well as a dissipative approximations of the second order elliptic operator and the recombination-generation expressions. The second order operators of the classical equations can be integrated in closed form along an edge. Using the same assumption for the discrete electrostatic potential, $w_e = w_l + \frac{\delta w}{\delta x}(x - x_l)$ is a linear function along an edge e connecting x_l and x_r with boundary values w_l , w_r , v_l , v_r , and φ_l , φ_r . The indices are skipped in the following by using $\delta x := x_r - x_l$, $\delta \varphi := \varphi_r - \varphi_l$ etc.

The basic equation is the one-dimensional two-point boundary value problem

$$\frac{d}{dx} \left(f(v) \frac{d\varphi}{dx} \right) = 0, \quad x \in]x_l, x_r[\quad (12)$$

with boundary values φ_l , φ_r , $f(v(x_i)) = f(v_i)$, $i = l, r$. It is supposed that $f(v)$ is a rapidly varying coefficient function along an edge and density dependent parts of D (or μ) are included as long as assumption (2) holds. The subscripts a, b are used for arbitrary (sub)intervals, while l, r denote the integration interval of Equation (12). The

density is defined by $p = \mathcal{F}(v)$ and $f(v)$ can fulfill the relations imposed by the variational formulation or it may be modified in special models. Because the reaction terms depend on the difference of the quasi-Fermi potentials (up to positive pre-factors), the densities enter essentially via the right-hand side of the Poisson equation. Accordingly, the remaining part of the mobility is assumed to be slowly varying and its appropriate average is a constant pre-factor per edge in $f(v)$.

The first integration with an integration constant j , the edge current, yields

$$f(v) \frac{d\varphi}{dx} = f(v) \frac{d(v+w)}{dx} = -j, \quad (13)$$

hence

$$f(v) \frac{dv}{dx} \approx -j - f(v) \frac{\delta w}{\delta x}. \quad (14)$$

The approximation in (14) transforms (12) into a Cauchy problem with a special monotone dependence $f(v)$, which is neither changed by the constant $\delta w/\delta x$ nor by the constant j . Hence, for every Lipschitz continuous $f(v)$ and constant j the Cauchy problem with the initial value v_l has a unique solution $v(x, j)$. On the other hand, j has to be chosen such that the boundary value $v(x_r) = v_r$ is fulfilled. Testing (13) with φ' results in the dissipation expression

$$\int_{x_l}^{x_r} \varphi'^2 f(v) dx = -j(\varphi_r - \varphi_l).$$

The left hand side is nonnegative, hence j has to change sign with $\delta \varphi$. The thermodynamic equilibrium is defined by $\delta \varphi = 0$ for all edges in Ω , hence $\varphi = \text{const}$. Essentially one could allow such $w(x)$ that do not change the very implicit monotonicity of (13) and preserve the dissipativity of j and the uniqueness of the thermodynamic equilibrium.

For special $f(v)$ and $w(x)$ one can get special cases of (13) in form of a Bernoulli or Riccati equation, but separation of the variables in (14) and integration with respect to df was not successful up to now. Hence the aim is to give a construction for j and (14) that results in a j reproducing the dissipation of (14) and the unique thermodynamic equilibrium.

The second integration with respect to v and x yields an integral equation for j and finite differences in the potentials:

$$\int_{x_l}^{x_r} dx = \delta x \approx - \int_{v_l}^{v_r} \frac{dv}{\delta w/\delta x + j/f(v)}, \quad (15)$$

$$\int_{v_l}^{v_r} \frac{f(v) dv}{j/J + f(v)} = -\delta w, \quad (16)$$

or

$$\delta v - \int_{v_l}^{v_r} \frac{j/J dv}{j/J + f(v)} = -\delta w. \quad (17)$$

Hence, an implicit expression depending on v_l , v_r , δw , or $\delta\varphi$. While $J = \frac{\delta w}{\delta x}$ has the meaning of a drift current, $f_0 = -\frac{j}{J}$ is the pole of the integrand. Due to $\frac{f(v)}{f(v)-f_0} = 1 + \frac{f_0}{f(v)-f_0}$, the integrand is a monotone function for monotone $f(v)$ if $f_0 \notin [f(v_l), f(v_r)]$. The special cases $\delta\varphi = 0$ (hence $\delta w = -\delta v$, equilibrium due to (13)) and the vanishing drift current $\delta w = 0$ define the limiting cases in the discussion of the mapping properties of Equation (16). In the vanishing drift case a unique primitive of $f(v)$ defines j uniquely, see (15).

Interchanging all boundary values changes only the sign of j , compare (5), (12), and (14), hence it is sufficient to consider the case $v_l < v_r$.

Theorem 1 Equation (16) determines the current j uniquely if the value f_0 is chosen in dependence of δw , v_l , v_r ($\delta v > 0$ fixed) by the following rules:

- i) $0 < \delta w < \infty$ (meaning $0 < \delta w/\delta v < \infty$, $\delta\varphi > 0$): $f(v_r) < f_0 < \infty$,
 - ii) $-\delta v < \delta w < 0$ (meaning $-1 < \delta w/\delta v < 0$, $\delta\varphi > 0$): $-\infty < f_0 < 0$,
 - iii) $\delta w < -\delta v < 0$ (meaning $-\infty < \delta w/\delta v < -1$, $\delta\varphi < 0$): $0 < f_0 < f(v_l)$,
- j solves $I(f_0) := \int_{v_l}^{v_r} \frac{f(v)dv}{f(v)-f_0} = -\delta w$ and $\delta\varphi \cdot j \leq 0$.

Proof The rules and cases are cited in the following as i), ii), iii). By the mean value theorem and Assumption A_2

$$I(f_0) = \frac{\delta v f(\tilde{v})}{f(\tilde{v}) - f_0} = -\delta w \quad (18)$$

with exactly one $\tilde{v} \in]v_l, v_r[$ for a fixed f_0 . Further, it holds $\int_a^b f_1(s)ds > \int_a^b f_2(s)ds$ for $f_1 > f_2$ on a subset of $[a, b]$ of positive measure.

i) Due to the monotonicity of $f(v)$, the integrand is negative and strictly monotonously decreasing for $f(v) \in]0, f_0[$ for all $f_0 > f(v_r)$. For $f_0 \in]f(v_r), \infty[$, I is a monotonous mapping of $]f(v_r), \infty[$ onto $] -\infty, 0[$, hence there is exactly one f_0^* with $I(f_0^*) = -\delta w$.

ii) Now the integrand is a positive, strictly increasing function for $f(v) > 0$, hence (18) holds and, with respect to f_0 , it is a monotonous mapping of $] -\infty, 0[$ onto $]0, \delta v[$. Thus, (18) is fulfilled for exactly one $f_0^* \in] -\infty, 0[$.

iii) The integrand is now a positive, strictly decreasing function and the arguments apply again for the monotonous mapping $f_0 \in]0, f(v_l)[$ onto $] \delta v, \infty[$.

$j = 0$ implies $\delta v = -\delta w$ in (16), hence $\delta\varphi = 0$ according to (5). Due to the uniqueness for $\delta v \neq -\delta w$ and $j \neq 0$, the equilibrium is uniquely defined by $\delta\varphi = 0$.

For $\delta w \rightarrow \infty$ holds $f_0 \rightarrow f(v_r)$ and $\delta w \rightarrow -\infty$ gives $f_0 \rightarrow f(v_l)$. Hence, h with $h(\delta w) := -f_0 J = j$ is a monotone mapping from $] -\infty, \infty[$ onto $] -\infty, \infty[$ and it is bijective. To show $\delta\varphi \cdot j \leq 0$ one calculates the sign of $\delta\varphi f_0^*$ in each of the cases:

- i) $f_0^* > 0$, $\delta w > 0$, hence $j < 0$ and $\delta\varphi > 0$,
- ii) $f_0^* < 0$, $\delta w < 0$, hence $j < 0$ and $\delta\varphi > 0$,
- iii) $f_0^* > 0$, $\delta w < 0$, hence $j > 0$ and $\delta\varphi < 0$.

Remark 1 Choosing $f_0 \in]f(v_l), f(v_r)[$ and $\delta w \in] -\infty, \infty[$ gives $\delta\varphi \in] -\infty, \infty[$ and $f_0 > 0$, so that $\delta\varphi \cdot j \leq 0$ can not be true for all arguments.

4 Introduction of a subdivision on $[v_l, v_r]$ and approximation on the subintervals

A subdivision of $v_l = v_0 < v_1 < \dots < v_i < \dots < v_{k+1} = v_r$, $\delta v_i = v_{i+1} - v_i = \beta_i \delta v$ is introduced to get a computable approximation of the integral. β_i define the partitioning of the straight line from v_l to v_r in the φw -plane, hence the projections satisfy $\delta\varphi_i = \beta_i \delta\varphi$ and $\delta w_i = \beta_i \delta w$. Because $f_0 \notin [f(v_l), f(v_r)]$ and

$$\sum_{i=0}^k \int_{v_i}^{v_{i+1}} \frac{f(v)dv}{f(v) - f_0} = -\delta w, \quad (19)$$

there exists for each interval $[v_i, v_{i+1}]$ one $\tilde{v}_i \in [v_i, v_{i+1}]$ with $f_i := f(\tilde{v}_i)$ such that

$$\int_{v_i}^{v_{i+1}} \frac{f(v)dv}{f(v) - f_0} = \frac{f_i \delta v \beta_i}{f_i - f_0} = \frac{f_i \delta v_i}{f_i - f_0} \quad (20)$$

holds by the mean value theorem.

The only change to the previous section is the introduction of the decomposition of unity by β_i , given by the intervals δv_i , and $\zeta_i > 0$ with $\sum_{i=0}^k \zeta_i = 1$. Hence, f_0^* can be inserted that solves

$$\sum_{i=0}^k \frac{f_i \beta_i}{f_i - f_0^*} = -\frac{\delta w}{\delta v} \sum_{i=0}^k \zeta_i, \quad \frac{f_i \beta_i}{f_i - f_0^*} = -\frac{\delta w}{\delta v} \zeta_i, \quad (21)$$

because it is just a reformulation of $I(f_0^*)/\delta v$. ζ_i is the relative contribution of the partial integral i to the sum for a given f_0 . $\sum_{i=0}^k \zeta_i = 1$ holds for $f_0 = f_0^*$. The next step is to replace $f(v)$ by piecewise differentiable, monotone approximations $f_i(v)$,

$$\sum_{i=0}^k \int_{v_i}^{v_{i+1}} \frac{f_i(v)dv}{f_i(v) - f_0} = -\delta w, \quad (22)$$

f_0 identical for all i . The f_i are fulfilling the basic assumptions A_1 , A_2 (on each subinterval) and coincide with $f(v_i)$ at the collocation points v_i :

$$A_4 : f_0(v_0) = f(v_l), \dots, f_i(v_{i+1}) = f_{i+1}(v_{i+1}) \\ = f(v_{i+1}), \dots, f_k(v_{k+1}) = f(v_r). \quad (23)$$

Due to the construction, Theorem 1 holds for this approximation of $f(v)$. On each interval one can chose an approximation allowing integration in closed form.

5 Special cases

The main purpose of this section is to derive expressions for special cases that allow a sufficient overlap of the standard approximation of the integral equation. The reason is twofold: the influence of rounding errors is one aspect, the second one is sufficiently smooth function definitions that do not deteriorate the convergence of the global Newton method. Before special cases, like $v_r \approx v_l$, are treated, the verification of the discretization scheme in case of the exponential function is considered:

5.1 Boltzmann statistics

$$\begin{aligned} -\delta\varphi &= f_0 \int_{v_l}^{v_r} \frac{dv}{f(v) - f_0} = f_0 \int_{v_l}^{v_r} \frac{dv}{e^v - f_0} \\ &= (\ln(e^v - f_0) - v)|_{v_l}^{v_r} = \ln \frac{e^{v_r} - f_0}{e^{v_l} - f_0} - \delta v, \end{aligned}$$

$$(e^{v_l} - f_0)e^{-\delta w} = e^{v_r} - f_0,$$

$$\begin{aligned} f_0 &= \frac{e^{v_r} - e^{v_l - \delta w}}{1 - e^{-\delta w}} = -\frac{e^{v_r}}{e^{-\delta w} - 1} - \frac{e^{v_l}}{e^{\delta w} - 1} \\ &= \frac{e^{v_r}(1 - e^{\delta w}) + e^{v_l}(1 - e^{-\delta w})}{2(1 - \cosh(\delta w))} = -\frac{j\delta x}{\delta w}, \end{aligned}$$

where nominator and denominator vanish for $\delta w = 0$. For the current

$$j\delta x = e^{v_l} b(\delta w) - e^{v_r} b(-\delta w)$$

one gets back the Bernoulli functions and a smooth dependence of the parameters. The current j vanishes for

$$e^{\delta w} \frac{b(\delta w)}{b(-\delta w)} = e^{\delta\varphi},$$

$$\frac{\delta w(e^{-\delta w} - 1)}{e^{-\delta w}(e^{\delta w} - 1)(-\delta w)} = 1 = e^{\delta\varphi},$$

hence at the thermodynamic equilibrium.

5.2 Bounded logarithmic derivative

Here it is supposed that $f(v)$ has a logarithmic derivative fulfilling

$$0 < \varepsilon < f'(v)/f(v) \leq 1 \text{ for } v_{min} < v < v_{max}.$$

This is true for Fermi-Dirac integrals of index i , i real, $i \geq -1$, because $f(s) = \mathcal{F}_{-1}(s) \approx 1 - e^{-s}$ for large arguments.

Now the integral can be rewritten as

$$\begin{aligned} \int_{v_l}^{v_r} \frac{dv}{f(v) - f_0} &= \int_{v_l}^{v_r} \frac{ff'dv}{ff'(f(v) - f_0)} \\ &= \int_{f_l}^{f_r} \frac{fdf}{ff'(f(v) - f_0)} \\ &= \int_{f_l}^{f_r} \frac{df}{(\ln f)'f(v)(f(v) - f_0)} := K. \end{aligned}$$

Due to the generalized mean value theorem

$$\int_a^b f(x)g(x)dx = f(\xi) \int_a^b g(x)dx,$$

there exists at least one $\xi \in [a, b]$ if $f(x)$ is continuous and $g(x)$ does not change sign in $[a, b]$. Hence, K can be bounded by

$$L \leq K < \frac{1}{\varepsilon} L,$$

$$\begin{aligned} L &:= \int_{f_l}^{f_r} \frac{df}{f(v)(f(v) - f_0)}, \\ &= \frac{1}{f_0} \ln \frac{f_l(f_r - f_0)}{f_r(f_l - f_0)}, \quad 0 < f_l < f_r \end{aligned}$$

and $(f_r - f_0)/(f_l - f_0) > 0$ because $f_0 \notin [f_l, f_r]$. Denoting the mean value of one over the logarithmic derivative by $1/(\widetilde{\ln f(v)})'$ and due to $-\delta\varphi = f_0 K$ yields

$$K = \frac{1}{(\widetilde{\ln f(v)})'} L,$$

$$-\delta\varphi = \frac{1}{(\widetilde{\ln f(v)})'} \ln \frac{f_l(f_r - f_0)}{f_r(f_l - f_0)}.$$

Both sides vanish at equilibrium and $1/(\widetilde{\ln f(v)})' > 0$. Replacing the mean value by $1/c$ results in

$$e^{-\delta\varphi c} = \frac{f_l(f_r - f_0)}{f_r(f_l - f_0)},$$

$$e^{-\delta\varphi c} f_r(f_l - f_0) = f_l(f_r - f_0),$$

$$f_0 = \frac{(e^{-\delta\varphi c} - 1)f_r}{(e^{-\delta\varphi c} \frac{f_r}{f_l} - 1)}. \quad (24)$$

The nominator vanishes at the thermodynamic equilibrium, while f_0 moves to infinity for vanishing denominator, and $f_0 = f_r = f_l$ in case of $f_l = f_r$ ($\delta v = 0$) and $e^{-\delta\varphi c} = 1$. The qualitative properties are similar to that of the Boltzmann case. Inserting the known extreme values of the $f(v)/f'(v)$, $v \in [v_l, v_b]$ into Equation (24) improves the bounds for f_0 , and, hence, j .

5.3 The case $\delta w \approx 0$

The case of a finite j and $\delta w \approx 0$ (small drift contribution) simplifies the original equation: $-j \approx f(v)dv/dx$, hence $-j\delta x = F(v_r) - F(v_l)$, $F(v) = \int f(v)dv$ in case $\delta w = 0$. This case is consistent with an expansion of the denominator assuming $|f_0| \gg f(v_r)$, hence substitution of

$$\frac{1}{f(v) - f_0} = \frac{-1}{f_0} \frac{1}{1 - \frac{f(v)}{f_0}} = \frac{-1}{f_0} \sum_{i=0}^{\infty} \left(\frac{f(v)}{f_0} \right)^i$$

yields

$$\delta w f_0 = -j\delta x = \int_{v_l}^{v_r} f(v) \sum_{i=0}^{\infty} \left(\frac{f(v)}{f_0} \right)^i dv$$

if $|\delta w| \ll \min(|\delta v|, |\delta\varphi|)$ and $|\delta v| \approx |\delta\varphi|$. An additionally small $|\delta v|$ means a situation close to equilibrium and is considered below.

5.4 The case $\delta v \approx 0$

In case $\delta v \approx 0$ one can assume that all extrema of the densities are represented approximately by the grid. The case $\delta v \approx 0$ is just a reduction to the constant coefficient case and the one-dimensional equation $(f(v)\varphi)' = 0$ results in $-j\delta x = \bar{f}(v)\delta\varphi$, where $\bar{f}(v)$ is a suitable mean value of $f(v)$. In many situations one can assume that deviations from Boltzmann statistics are small for some v_B and $v_r < v_B$. (This case is handled in Section 10.1). Hence, $\delta v \approx 0$ implies $f_r - f_l \ll f_l$ and the interesting cases are

$$f_0 = f_l - \varepsilon, \quad f_0 = f_r + \varepsilon,$$

$$\delta f_l = f(v) - f_l > 0, \quad \delta f_r = f(v) - f_r < 0 \quad (25)$$

with $v \in [v_l, v_r]$ and $|\delta f_i/f_i| \ll 1$, $i = l, r$. The equality

$$\int_{v_l}^{v_r} \frac{f_0 dv}{f - f_0} = -\delta\varphi \quad (26)$$

is equivalent to

$$\begin{aligned} \int_{v_l}^{v_r} \frac{dv}{f/f_0 - 1} &= \int_{v_l}^{v_r} \frac{dv}{(1 + \delta f_r/f_r)/(1 + \varepsilon/f_r) - 1} \\ &= (f_r + \varepsilon) \int_{v_l}^{v_r} \frac{dv}{\delta f - \varepsilon}. \end{aligned} \quad (27)$$

The mean value theorem gives

$$\frac{f_r \frac{\delta v}{\delta\varphi} + \delta f_r(v_l)}{1 - \frac{\delta v}{\delta\varphi}} < \varepsilon < \frac{f_r \frac{\delta v}{\delta\varphi}}{1 - \frac{\delta v}{\delta\varphi}}. \quad (28)$$

These bounds and Equation (27) result in a case handled in Section 10.3, a symmetric expansion of the integral with respect to the difference of the bounds should be used. The situation $f_0 = f_l - \varepsilon < 0$ can be handled similarly.

The other option is to evaluate numerical integration formulas analytically and to bootstrap via different formulas. The starting point is the simplest version of the trapezoidal rule,

$$\begin{aligned} f_0 \left(\frac{1}{f_l - f_0} + \frac{1}{f_r - f_0} \right) \frac{\delta v}{2} &\approx -\delta\varphi, \\ f_0^2(\delta\varphi - \delta v) + f_0 \frac{f_l + f_r}{2}(\delta v - 2\delta\varphi) + \delta\varphi f_l f_r &= 0. \end{aligned} \quad (29)$$

The first order approximation ($\bar{f} = (f_l + f_r)/2$, $\delta f = (f_r - f_l)$) is

$$f_{0,1} = \frac{\delta\varphi(\bar{f}^2 - (\delta f/2)^2)}{\bar{f}(2\delta\varphi - \delta v)} \quad (30)$$

and the second order approximation reads

$$f_{0,2\pm} = \frac{-2\delta\varphi\bar{f} + \bar{f}\delta v \pm \sqrt{\delta f^2 \delta\varphi(\delta\varphi - \delta v) + \bar{f}^2 \delta v^2}}{2(\delta\varphi - \delta v)}. \quad (31)$$

Here the sign is defined by the cases (*i, ii, iii*). During computations the correctness of both formulas with respect to f_l, f_r can be easily checked. If at least (31) is correct, the third order equation resulting from Equation (27) using the trapezoidal rule with two (or more) intervals can be solved by Newton's method without any transformation of the formula using $f_{0,2\pm}$ as initial guess.

The numerical integration is of general interest. The 'expansion-like' expressions show different forms of the deviation of the pole from the mean value \bar{f} , hence error control is an issue for expansions and numerical integration.

5.5 The equilibrium

The equilibrium and the computation of the related derivatives is based on the expansion of the integral equation for sufficiently small, scaled currents f_0 . It yields

$$\int_{v_l}^{v_r} \sum_{i=0}^{\infty} \left(\frac{f_0}{f(v)} \right)^i dv = -\delta w, \quad (32)$$

hence using monotonicity and $0 \leq |f_0| < f(v_l) < f(v_r)$ results in a convergent power series of the integrand and the zero-order term is reproducing the equilibrium condition. The original integral equation can result in large rounding errors for the close to equilibrium cases. Subtracting the equilibrium condition or the zero order term in (32) yields

$$\int_{v_l}^{v_r} \sum_{i=1}^{\infty} \left(\frac{f_0}{f(v)} \right)^i dv = \sum_{i=1}^{\infty} f_0^i \int_{v_l}^{v_r} \frac{dv}{f^i(v)} = -\delta\varphi. \quad (33)$$

This is the defining nonlinear equation for f_0 , which is truncated accordingly to the precision needed. Equation (33) can be evaluated easily: the integrals are independent of f_0 and can be precomputed for all approximation intervals (including the sums, if the data is ordered with respect to the start intervals v_l , which is an advantage with respect to data locality anyway). Hence at most start and end interval have to be evaluated and summed. Very close to equilibrium it is sufficient to keep the first order term, hence

$$j \approx \frac{\delta w}{\delta x} \frac{1}{\int_{v_l}^{v_r} \frac{dv}{f(v)}} \delta\varphi.$$

Due to $\delta\varphi \approx 0$ it holds $-\delta w = \delta v - \delta\varphi$ with $\delta v > 0$ holds, hence

$$j \approx \frac{-1}{\left(\frac{1}{f(v)} \right)} \frac{\delta\varphi}{\delta x}. \quad (34)$$

The derivative with respect to δw vanishes for $\delta\varphi = 0$.

The chosen approximations can be evaluated up to four terms without much effort. Because $f_0 < cf(v_l)$ for sufficiently small c ($c < 1/1000$), monotonicity of the expansion is guaranteed for $v \in [v_l, v_r]$ and the remaining term is of order 10^{-15} . No problems in solving that equation by two steps of an undamped Newton's method are expected if the solution of the truncated linear equation is used as an initial guess. For $\delta v \approx 0$ an expansion at \bar{v} simplifies the problem further, see above.

6 Discretization and finite volume notation

The basic assumptions of the finite volume discretization are:

- Gauss' theorem holds,
- boundary conforming Delaunay meshes [14], [15] cover the bounded polyhedral domain $\Omega = \cup_l \mathbf{E}_l^N$,

where \mathbf{E}_l^N denotes l th N -dimensional simplex. The notation follows [16] and aims the similarity with the analytic

one, hence G stands for 'Gradient' ∇ , G^T for $\nabla \cdot$, and $-\nabla \cdot \varepsilon \nabla$ 'translates' into $G^T[\varepsilon]G$.

G includes the geometric weights $[\gamma]$ and contributions of boundary conditions while \tilde{G} is a difference matrix. \tilde{G} maps a vector \mathbf{u} defined on the nodes of \mathbf{E}_l^N as edge differences onto the edges of \mathbf{E}_l^N , and \tilde{G}^T maps the differences with different signs back to the nodes of \mathbf{E}_l^N . The advantage is an explicit product of first order differences and 'integration by parts' is as simple as in the analytic case. The summation order does not matter and summing over all simplices or only one edge is not indicated but is clear from the context.

The integration over the intersection of each simplex and the Voronoi volumes associated with its nodes results in the weight $[V]$, $V_i > 0$, while density contributions are summed per Voronoi volume intersection and simplex, because in case of hetero structures (not dealt with in detail here) an explicit dependence of the material of each simplex has to be taken into account and can not be factored into a global diagonal matrix as in the Boltzmann case. Using $[\]$ to denote diagonal matrices gives

$$G^T[\varepsilon]G\mathbf{w} = [V](\mathbf{C} - \mathbf{n} + \mathbf{p}). \quad (35)$$

The nonlinear Poisson equation remains unchanged up to the definition of n and p . The continuity equations have to be expressed by the implicitly defined edge currents. Equation (16), the cases (*i, ii, iii*), and the approximation used due to the boundary values result in

$$\tilde{G}^T[\gamma]\mathbf{j}(\mathbf{v}_p, \tilde{G}\varphi_p) = [V][R([n], [p])](\mathbf{1} - \mathbf{r}([\varphi_p - \varphi_n])), \quad (36)$$

$$-\tilde{G}^T[\gamma]\mathbf{j}(\mathbf{v}_n, \tilde{G}\varphi_n) = [V][R([n], [p])](\mathbf{1} - \mathbf{r}([\varphi_p - \varphi_n])). \quad (37)$$

Because the mean value theorem based currents include a factor $1/\delta x$ the weights that are used in explicit form only in the continuity equations differ from those introduced in [16] by a factor δx . Using the standard expression for the current resulting from

$$\int_{v_l}^{v_r} \frac{f(v)dv}{f(v) - f_0} = -\delta w, \quad (38)$$

$$f_0\delta v = -(f(\tilde{v}) - f_0)\delta w,$$

hence

$$-j = \frac{f(\tilde{v})}{\delta x} \delta\varphi, \quad (39)$$

and remembering the negative definite Equation (12) for the edge problem yields the final form of Equation (36) for the proofs

$$\tilde{G}^T [\gamma] \left[\frac{f(\tilde{v}_p)}{\delta x} \right] \tilde{G} \varphi_{\mathbf{p}} = [V][R([n], [p])](\mathbf{1} - \mathbf{r}(\varphi_{\mathbf{p}} - \varphi_{\mathbf{n}})), \quad (40)$$

where $[f(\tilde{v}_p)]$ denotes the intermediate value per edge solving Equation (38). Assuming a boundary conforming Delaunay grid and $f(\tilde{v}_p) > 0$ guarantee a weakly diagonally dominant S-matrix. The strict monotonicity and the mean value estimates are sufficient to prove existence of steady state solutions for that system.

Remark 2 Due to the assumptions, $j = 0$ iff $\delta\varphi = 0$, hence $\varphi = \text{const}$.

7 Existence of bounded steady state solutions

The 'physics' related constants are omitted because they don't influence the qualitative behavior of Equations (35), (36), (37), (16). Let

$$V_i g_i(w_i, \varphi_{p,i}, \varphi_{n,i}) := \{[V](\mathbf{C} - \mathbf{n} + \mathbf{p})\}_i = \quad (41)$$

$$V_i(C_i - \mathcal{F}(-\varphi_{n,i} + w_i) + \mathcal{F}(\varphi_{p,i} - w_i)), \quad i \in [1, M],$$

be the i th component of the right-hand side of Equation (35) and M the number of nodes in the discretization. Because of A_3 $w_i \mapsto g_i(w_i, \varphi_{p,i}, \varphi_{n,i})$ is a strictly monotone mapping from \mathbb{R} onto $\mathbb{R} \forall i$. Hence, $g_i(\cdot, \varphi_{p,i}, \varphi_{n,i}) = 0$ has a unique solution w_i for given $\varphi_{p,i}, \varphi_{n,i}$. To construct upper and lower bounds for w the monotone increasing function $h(s) := \mathcal{F}(s) - \mathcal{F}(-s)$ is used. Let $\check{C} = \min(\mathbf{C})$, $\hat{C} = \max(\mathbf{C})$ denote the minimum and maximum of the doping $\forall i$, hence $\check{w}^* \leq h^{-1}(\check{C}) \leq w^* \leq h^{-1}(\hat{C}) \leq \hat{w}^*$ are the minimum, maximum of the built-in potential.

Assuming that the quasi-Fermi potentials are bounded by the Dirichlet data

$$w = \min(0, w_{\text{applied}}), \quad \bar{w} = \max(0, w_{\text{applied}}), \quad (42)$$

which are the bounds for the applied voltages, one has

$$\check{\varphi}_p = w, \quad \hat{\varphi}_p = \bar{w}, \quad \check{\varphi}_n = w, \quad \hat{\varphi}_n = \bar{w}, \quad (43)$$

hence

$$\check{\varphi}_p \leq \varphi_p \leq \hat{\varphi}_p, \quad \check{\varphi}_n \leq \varphi_n \leq \hat{\varphi}_n. \quad (44)$$

Now bounds for w can be constructed using the right hand side of the Poisson equation for nonequilibrium states: let i be the vertex where \hat{C} is realized, hence the right hand side of

$$\mathcal{F}(-\varphi_{n,i} + w_i) = \hat{C} + \mathcal{F}(\varphi_{p,i} - w_i) \quad (45)$$

is maximized for

$$\mathcal{F}(s) \leq \hat{C} + \mathcal{F}(\hat{\varphi}_p - w - \check{w}^*), \quad (46)$$

$$s = \mathcal{F}^{-1}(\hat{C} + \mathcal{F}(\hat{\varphi}_p - w - \check{w}^*)), \quad (47)$$

$$\begin{aligned} \hat{w} &\leq \mathcal{F}^{-1}(\hat{C} + \mathcal{F}(\hat{\varphi}_p - w - \check{w}^*)) + \hat{\varphi}_p \\ &= \mathcal{F}^{-1}(\hat{C} + \mathcal{F}(\bar{w} - w - \check{w}^*)) + \bar{w}. \end{aligned} \quad (48)$$

The lower bound \check{w} is derived similarly,

$$\check{w} \geq -\mathcal{F}^{-1}(|\check{C}| + \mathcal{F}(-w + \hat{w} + \hat{w}^*)) + w. \quad (49)$$

Theorem 2 Let $\varphi_{\mathbf{p}}, \varphi_{\mathbf{n}}$ be given vectors with $\check{w} \leq \varphi_{p,i} \leq \hat{w}$, $\check{w} \leq \varphi_{n,i} \leq \hat{w}$. Then \mathbf{w} is the unique solution of Equation (35) and fulfills the bounds $\check{w} \leq w_i \leq \hat{w}$.

Proof Existence: $G^T[\varepsilon]G$ is a weakly diagonally dominant M-matrix and $\partial(\mathcal{F}(-\varphi_{n,j} + w_j) - \mathcal{F}(\varphi_{p,j} - w_j))/\partial w_j := g_{w,j} > 0$ holds $\forall j \in [1, M]$, hence a unique positive inverse of $G^T[\varepsilon]G + [V][g_w]$ exists for any \mathbf{w} fulfilling the bounds. Hence, a damped Newton's method can be used to construct a unique \mathbf{w} fulfilling the equation and the boundary conditions.

Bounds: assume $w_i > \hat{w}$ for some i , $x_i \notin \Gamma_D$, hence

$$\begin{aligned} (\mathbf{w} - \hat{w})^{+T} G^T[\varepsilon]G\mathbf{w} &= \\ (\mathbf{w} - \hat{w})^{+T} [V](\mathbf{C} - \mathcal{F}(-\varphi_{n,i} + w_i) + \mathcal{F}(\varphi_{p,i} - w_i)). \end{aligned}$$

$(\mathbf{w} - \hat{w})^{+T} G^T[\varepsilon]G\mathbf{w} > 0$ but $\mathbf{C} - \mathcal{F}(-\varphi_{n,i} + w_i) + \mathcal{F}(\varphi_{p,i} - w_i) < 0 \forall i$ with $w_i > \hat{w}$, hence a contradiction. The lower bound follows by testing with $(\mathbf{w} - \check{w})^{-T}$.

These bounds for \mathbf{w} provide bounds on $\varphi_{\mathbf{p}}, \varphi_{\mathbf{n}}$, Equation (44). The next step is to verify these bounds.

Theorem 3 Let $\mathbf{w}(\varphi_{\mathbf{p}}^0, \varphi_{\mathbf{n}}^0)$, $\varphi_{\mathbf{p}}^0, \varphi_{\mathbf{n}}^0$ be solutions of Equations (36), (50), the analog equation for $\varphi_{\mathbf{n}}$ with frozen coefficients and $\varphi_{\mathbf{p}}$ the solution of

$$\begin{aligned} \tilde{G}^T [\gamma] \left[\frac{f(\tilde{v}_p)}{\delta x} \right] \tilde{G} \varphi_{\mathbf{p}} &= \\ [V][R([n^0], [p^0])](\mathbf{1} - \mathbf{r}(\varphi_{\mathbf{p}} - \varphi_{\mathbf{n}}^0)), \end{aligned} \quad (50)$$

$\mathbf{v}_{\mathbf{p}}^0 = \varphi_{\mathbf{p}}^0 - \mathbf{w}$, $\mathbf{p}^0 = \mathbf{p}(\mathbf{v}_{\mathbf{p}}^0)$, $\mathbf{v}_{\mathbf{n}}^0 = \mathbf{w} - \varphi_{\mathbf{n}}^0$, $\mathbf{n}^0 = \mathbf{n}(\mathbf{v}_{\mathbf{n}}^0)$, but $f(\tilde{v}_{p_i})$ is the solution of Equations (38) for all edges i with frozen coefficients. The initial guesses $\varphi_{\mathbf{p}}^0, \varphi_{\mathbf{n}}^0$ are constructed such that they are bounded by the Dirichlet values.

Proof Assume $v_{p_i} > \bar{w}$ for some interior vertices. Testing with $(\mathbf{v}_{\mathbf{p}} - \bar{w})^{+T}$ results in

$$(\mathbf{v}_{\mathbf{p}} - \bar{w})^{+T} \tilde{G}^T [\gamma] \left[\frac{f(\tilde{v}_p)}{\delta x} \right] \tilde{G} \mathbf{v}_{\mathbf{p}} > 0$$

and

$$(\mathbf{v}_{\mathbf{p}} - \bar{w})^{+T} [V][R([n^0], [p^0])](\mathbf{1} - \mathbf{r}(\varphi_{\mathbf{p}} - \varphi_{\mathbf{n}}^0)) < 0$$

because $(v_{p_i} - \varphi_{n_i}^0) > 0$ for $(\mathbf{v}_p - \bar{w})^{+T} > 0$, hence $r(v_{p_i} - \varphi_{n_i}^0) > 1$, a contradiction.

Assuming now $(\mathbf{v}_p - w)^{-T} < 0$ for some interior vertices does not change the sign of the left-hand side, but $(v_{p_i} - \varphi_{p_i}^0) < 0$ for all vertices where $(\mathbf{v}_p - w)^{-T} < 0$, hence $r(v_{p_i} - \varphi_{n_i}^0) < 1$, hence

$$(\mathbf{v}_p - w)^{-T} [V][R([n^0], [p^0])](\mathbf{1} - \mathbf{r}(\varphi_p - \varphi_n^0)) < 0$$

yields a contradiction again. Solutions \mathbf{v}_p have to fulfill the bounds. The same holds for \mathbf{v}_n due to the sign changes of φ_n , in the recombination term, and in the equation.

Theorem 4 *On any connected, boundary conforming Delaunay mesh with M vertices the problem (35), (36), and (37) with positive Dirichlet boundary measure has at least one solution. It fulfills the bounds (42), (44), (48), and (49).*

Proof Because the Gummel map of solving the nonlinear Poisson equation (35) and the continuity equations is continuous, differentiable, and maps the convex set of the $3M$ tensorated intervals of the bounds onto itself, Brouwer's fixed point theorem guarantees at least one fixed point [17, p. 23].

The uniqueness of the solution for small applied voltages can be shown by repeating the steps in the corresponding section [16]. The decoupling of the Jacobian of the quasi-Fermi potentials with respect to the electrostatic potential at the thermodynamic equilibrium follows directly from Equation (39) or the dissipativity of the current relation.

8 Global Newton's method

The nonlinear equation

$$\tilde{I}(f_0, \delta w, v_l, v_r) = I(f_0, v_l, v_r) + \delta w = 0, \quad (51)$$

$$f_0 = \frac{-j}{J} = \frac{-j\delta x}{\delta w}, \quad (52)$$

$$I(f_0, v_l, v_r) = \int_{v_l}^{v_r} \frac{f(v)dv}{f(v) - f_0} := \int_{v_l}^{v_r} i(f_0, v)dv \quad (53)$$

is solved by a local Newton's method, hence the derivative $\frac{\partial I}{\partial f_0}$ is known. $\frac{\partial I}{\partial v_n} = i(f_0, v_n)$ can be computed on the fly after the last function evaluation of the local Newton's method. Differentiation of Equation (51) and application of the chain rule results in all needed derivatives to assemble the Jacobian:

$$\frac{\partial I}{\partial v_n} = -\frac{\partial I}{\partial f_0} \frac{\partial f_0}{\partial j} \frac{\partial j}{\partial v_n}, \quad (54)$$

$$\frac{\partial j}{\partial v_n} = -i(f_0, v_n) \left/ \left(\frac{\partial I}{\partial f_0} \frac{\partial f_0}{\partial j} \right) \right., \quad n = l, r, \quad (55)$$

while the derivative with respect to δw reads as

$$\frac{\partial I}{\partial f_0} \frac{\partial f_0}{\partial \delta w} + 1 = -\frac{\partial I}{\partial f_0} \frac{\partial f_0}{\partial j} \frac{\partial j}{\partial \delta w}, \quad (56)$$

$$\frac{\partial j}{\partial \delta w} = -\left(\frac{\partial I}{\partial f_0} \frac{\partial f_0}{\partial \delta w} + 1 \right) \left/ \left(\frac{\partial I}{\partial f_0} \frac{\partial f_0}{\partial j} \right) \right., \quad (57)$$

Using $\frac{\partial f_0}{\partial \delta w} = \frac{j\delta x}{(\delta w)^2} = -\frac{f_0}{\delta w}$, $\frac{\partial f_0}{\partial j} = \frac{-1}{J}$ completes the post-processing of the local Newton's method data. Transformation of the expression to the combination of potentials used is possible, as well.

9 Properties of the Jacobian

Knowing the solution f_0 of the integral equation (38) and the existence of an intermediate value \tilde{v} (see Equation (39)), is sufficient to derive the qualitative properties of the Jacobian. It is sufficient to show this for one edge. Further, Equation (39) provides the simplest way to derive a new initial guess for solving the integral equation.

Theorem 5 *The Jacobian with respect to the electrostatic potential w_l, w_r is a symmetric negative semidefinite matrix for each edge. Because one assumes Δw_i , the initial guess ($i = 0$), and each solution of Newton's method at step i to fulfill homogeneous Dirichlet boundary conditions, the global matrix is symmetric negative definite.*

Proof Using equation (56) and differentiation of equation (18) with respect to f_0 results in

$$\frac{\partial I}{\partial f_0} = \frac{I}{f(\tilde{v}) - f_0} = -\frac{\delta w}{f(\tilde{v}) - f_0},$$

hence

$$\left(\frac{\partial j}{\partial w_l}, \frac{\partial j}{\partial w_r} \right) = -\tilde{G} \frac{f(\tilde{v})}{\delta x}, \quad \tilde{G} = (-1, 1),$$

hence $\tilde{G}^T \gamma \tilde{G} \frac{f(\tilde{v})}{\delta x}$ reads as

$$A_{v_p, w_{edge}} = \begin{pmatrix} a & -a \\ -a & a \end{pmatrix}, \quad a := -\gamma \frac{f(\tilde{v})}{\delta x} < 0.$$

Because the domain is assumed to be connected or each subdomain has a nonvanishing Dirichlet measure, related columns have a positive row sum.

Theorem 6 *Using the above assumptions of Theorem 4 on the grid and the boundary conditions, the Jacobian with respect to the chemical potential of the holes v_l and v_r is a weakly diagonally dominant M -matrix.*

Proof Direct calculation yields for one edge

$$b_l := \frac{\partial I}{\partial v_l} = -\frac{(f(\tilde{v}) - f_0)f(v_l)\gamma}{(f(v_l) - f_0)\delta x} < 0,$$

$$b_r := \frac{\partial I}{\partial v_r} = \frac{(f(\tilde{v}) - f_0)f(v_r)\gamma}{(f(v_r) - f_0)\delta x} > 0,$$

hence

$$A_{v_p, v_{pedge}} = \tilde{G}^T(b_l, b_r) = \begin{pmatrix} -b_l & -b_r \\ b_l & b_r \end{pmatrix}.$$

The other derivatives are diagonal matrices of the form $V\mathcal{F}'$, $V(R'(1-r) - Rr')$.

Remark 3 The use of high order or less local discretizations may result in a loss of definiteness of the Jacobi matrices $A_{v_p, w_{edge}}$, $A_{v_n, w_{edge}}$, which are well defined elliptic operators in the analytic case, and a coupling of the continuity and the electrostatic potential equation in the thermodynamic equilibrium, compare Equation (34).

If using discretization schemes that are not unconditionally stable, estimating the smallness conditions for guaranteed definiteness of these matrices results in a characterization of the 'safe to apply area' of these discretizations. With respect to the properties of the Schur complement of $A_{w, w}$ lost definiteness is equivalent to negative densities.

Schemes that result in coupled, linearized continuity equations and the electrostatic potential equation in the thermodynamic equilibrium can realize multiple thermodynamic equilibrium solutions or spurious bifurcation very close to the equilibrium.

10 Approximation of special functions

As the Fermi-Dirac integrals show, for typical functions $f(v)$, $\mathcal{F}(v)$ one should expect at least one intermediate region between two asymptotic branches. Here the situation is considered where for $\lim_{v \rightarrow -\infty}$ an exponential behavior and for $\lim_{v \rightarrow \infty}$ rational powers dominate. If one is interested in using analytic integration one faces restrictions for $f(v)$. On the other hand, the benefit is an approximation of the transport up to rounding errors.

10.1 Extension of the Blakemore approximation

The Blakemore approximation [18] is easily generalized and covers the left asymptotic, hence one looks in general for functions f_{Bg} of the form

$$f_{Bg}(x) = \frac{P_n(x)}{P_m(x) + e^{-\frac{Q_k(x)}{Q_l(x)}}} \quad (58)$$

or similar ones, where P_i , Q_i denote polynomials of degree i . One needs $\lim_{x \rightarrow -\infty}$ of $\frac{Q_k(x)}{Q_l(x)} = -x$ and $\frac{P_n(x)}{P_m(x)} = 1$, hence $k = l + 1$, $m = n$ follows.

Checking the integral tables [19] restricts (58) to

$$f_{B_3}(x) = \frac{1/c}{b/c + e^{-ax}} = \frac{1}{b + ce^{-ax}}. \quad (59)$$

With $a = 1$, $c = 1$ one can extend the asymptotic expression from the leftmost approximation interval. Unfortunately this is only a three parameter approximation, hence one can not have a Hermite spline approximation. On the other hand, it is easy to prove: for functions with a decaying, positive logarithmic derivative a unique solution exists for the parameters a , b , c if $f(v_a)$, $f'(v_a)$, (or $f'(v_b)$) and $f(v_b)$ are specified.

10.2 Nonlinear equations for the edge currents

The Blakemore approximation Equation (59) on intervals yields

$$\hat{b} = b - \frac{1}{f_0}, \quad f_B(v) = b + ce^{-av}$$

with f_B being the nominator of f_{B_3} (the interval indices and sums are omitted, all functions are continuous but not necessarily the integrals—due to discontinuous individual coefficients as weights, hence here the formulas are written in differences per interval)

$$\begin{aligned} I_{B_3} &:= \int \frac{f(v)dv}{f(v) - f_0} \approx \frac{-1}{f_0} \int \frac{dv}{\frac{1}{f_0} + f_B(v)} = -\delta w, \\ &= \frac{-1}{f_0} \left(\frac{av}{\hat{a}\hat{b}} - \frac{1}{-\hat{a}\hat{b}} \ln(\hat{b} + ce^{-av}) \right) \Big|_{v_a}^{v_b} \\ &= \frac{-1}{f_0 \hat{a}\hat{b}} \left(\ln e^{av} + \ln(\hat{b} + ce^{-av}) \right) \Big|_{v_a}^{v_b} \\ &= \frac{-1}{af_0 \hat{b}} \ln(\hat{b}e^{av} + c) \Big|_{v_a}^{v_b} = \frac{-1}{af_0 \hat{b}} \ln \left(\frac{\hat{b}e^{av_b} + c}{\hat{b}e^{av_a} + c} \right). \quad (60) \end{aligned}$$

Using $I_{B_3} = -\zeta_i \delta w$ for multiple intervals i each contribution to the sum over the piecewise approximation can be transformed into a Bernoulli function $b(s) = s/(e^s - 1)$:

$$e^{\zeta \delta w f_0 a \hat{b}} = \frac{\hat{b}e^{av_b} + c}{\hat{b}e^{av_a} + c}.$$

Using $z := \zeta \delta w f_0 a$,

$$e^{z\hat{b}} - 1 = \frac{-\hat{b}}{c} \left(e^{av_a} e^{z\hat{b}} - e^{av_b} \right),$$

$$z = \frac{z\hat{b}}{c} \left(\frac{-e^{av_a} e^{z\hat{b}}}{e^{z\hat{b}} - 1} + \frac{e^{av_b}}{e^{z\hat{b}} - 1} \right),$$

$$zc = b(z\hat{b})e^{av_b} - b(-z\hat{b})e^{av_a},$$

and $z\hat{b} = (\zeta\delta w f_0 a)(b - \frac{1}{f_0}) = j\zeta\delta x ab - \zeta\delta wa$ yields

$$-j\zeta\delta x ac = b(-z\hat{b})e^{avb} - b(z\hat{b})e^{ava}. \quad (61)$$

This is a set of fixed point equations for $\zeta_i j$ and

$$\sum_{i=n}^m \zeta_i = 1 \quad (62)$$

determines the Lagrange parameter j . The start and end interval of the integration are denoted by n and m . This dependency of the decomposition is not present in the sum (or the related product) in Equation (60). Equation (61) is very well suited to solve the problem for $\delta v \approx 0$, $v_r < v_B$, and one interval. Due to $b'(s) + b'(-s) = -1$, the fixed point equation converges for $|b/c e^{av} (1 + a|\delta v|/2)| < 1$, while the derivative with respect to j of the Newton's method related function of Equation (61) is negative, due to $b'(s) < 0$ for finite potentials. Hence the implicit function theorem results in one solution.

All approximation parameters can be expressed by the approximated function, a detailed discussion is omitted. For $a = 1$, $b = 0$, $c = 1$, and one interval ($\zeta = 1$) the Equation (61) reproduces the classic Scharfetter-Gummel scheme. The Blakemore type approximations are well suited to represent the close to exponential branch (and the saturation in case of the Fermi-Dirac integral of index -1).

10.3 Padé spline approximation

The right asymptotic requires a Padé type approximation due to $\lim_{x \rightarrow \infty} F_i(x) = x^{i+1}$, $F_i(x)$ Fermi-Dirac integral of index i . In case $i = j/k > -1$ one would look for approximations of the form

$$f_P(x) = \frac{P_n(x)}{Q_m(x)} \quad (63)$$

with

$$P_n(x) = \sum_i p_i x^i + p_{n_i(j)} x^{n_i(j)}, \quad (64)$$

$$Q_m(x) = \sum_i q_i x^i + q_{n_i(k)} x^{n_i(k)}, \quad (65)$$

and $n_i(j)$ denotes selected multiples of j to force the approximation of the asymptotic part. The intermediate range is addressed by the small powers x^i . In case of analytic integration the choice is

$$P_{1,2}(x) = \frac{a_0 + a_1 x}{b_0 + b_1 x + b_2 x^2}, \quad a_0 = 1,$$

which, by chance, has the wanted asymptotic for $f(x) = F'_{1/2}(x)$. This is essential for transport in \mathbb{R}^3 and does

not require the computation of a f_0 -dependent partial fraction decomposition. Specifying function and first derivative at v_a and v_b results in a Hermite spline that provides a convex/concave approximation of convex/concave functions $f(v)$, respectively.

It holds

$$\begin{aligned} I - (x_{i+1} - x_i) &= \int_{x_i}^{x_{i+1}} \frac{f_0 dx}{f(x) - f_0} \\ &\approx \int_{x_i}^{x_{i+1}} \frac{f_0(b_0 + b_1 x + b_2 x^2) dx}{a_0 + a_1 x - f_0(b_0 + b_1 x + b_2 x^2)} \\ &= - \int_{x_i}^{x_{i+1}} \frac{(b_0 + b_1 x + b_2 x^2) dx}{b_0 - a_0/f_0 + (b_1 - a_1/f_0)x + b_2 x^2} := \tilde{I}(f_0). \end{aligned}$$

The denominator notation in the last line is changed to

$$p(x) := c_2 x^2 + c_1 x + c_0, \quad \Delta = 4c_2 c_0 - c_1^2,$$

$$c_0 = b_0 - a_0/f_0, \quad c_1 = b_1 - a_1/f_0, \quad c_2 = b_2,$$

where Δ is the discriminant. Under the assumption $\Delta \neq 0$, hence excluding $\int \frac{dx}{(x-x_0)^2}$, the elementary integrals are ($\Delta > 0$, $\Delta < 0$):

$$\tilde{I}_0 := \int \frac{dx}{c_2 x^2 + c_1 x + c_0} = \begin{cases} \frac{2}{\sqrt{\Delta}} \arctan \frac{2c_2 x + c_1}{\sqrt{\Delta}}, \\ \frac{1}{\sqrt{-\Delta}} \ln \left| \frac{2c_2 x + c_1 - \sqrt{-\Delta}}{2c_2 x + c_1 + \sqrt{-\Delta}} \right|. \end{cases}$$

$$\int \frac{x dx}{p(x)} = \frac{1}{2c_2} \ln |p(x)| - \frac{c_1}{2c_2} \tilde{I}_0,$$

$$\int \frac{x^2 dx}{p(x)} = \frac{x}{c_2} - \frac{c_1}{2c_2^2} \ln |p(x)| + \frac{c_1^2 - 2c_2 c_0}{2c_2^2} \tilde{I}_0,$$

hence

$$\begin{aligned} I &= \left(1 - \frac{b_2}{c_2}\right)x - \left(\frac{b_1}{2c_2} - \frac{c_1 b_2}{2c_2^2}\right) \ln |p(x)| - \\ &\quad \left(b_0 - \frac{c_1}{2c_2} b_1 + \frac{c_1^2 - 2c_2 c_0}{2c_2^2} b_2\right) \tilde{I}_0, \end{aligned} \quad (66)$$

where $c_2 = b_2$, hence in the coefficients of the spline (up to p , \tilde{I}_0)

$$I = -\frac{1}{2b_2} (a_1/f_0 \ln |p(x)| + (2b_2 a_0 - b_1 a_1 + a_1^2/f_0) \tilde{I}_0 / f_0).$$

To handle the cases $\delta v \approx 0$, $v_B < v_l$, and $\Delta \rightarrow 0$ for $f_0 \rightarrow f_0^*$, an expansion at x_i (or x_{i+1}, \dots) with respect to Δ using $r = 2c_2 x + c_1$, $d = \sqrt{\pm \Delta}$ and the derivatives r' , d' , $r = r(x, f_0)$, $d = d(f_0)$ yields

$$\left(\frac{2}{d} \arctan \frac{r}{d}\right)' = \frac{-2d'}{d^2} \arctan \frac{r}{d} + \frac{2}{d} \frac{d^2}{d^2 + r^2} \left(\frac{r'd - rd'}{d^2}\right),$$

$$\left(\frac{1}{d} \ln \left|\frac{r-d}{r+d}\right|\right)' = \frac{-d'}{d^2} \ln \left|\frac{r-d}{r+d}\right| + \left(\frac{1}{d} \cdot \left|\frac{2(r'd - d'r)}{(r+d)(r-d)}\right|\right).$$

$|\cdot|'$ does not cause any problems for arguments close to 1.

Hence, for prefactors independent of d (or common in both integrals) and $d \rightarrow 0$ ($|\frac{d}{r}| \ll 1$) holds

$$\begin{aligned} \frac{2}{d} \left(\arctan \frac{r_l + (r_r - r_l)}{d} - \arctan \frac{r_l}{d} \right) &\approx \\ \frac{2}{d} \frac{d^2}{d^2 + r_l^2} \frac{r_r - r_l}{d} &= \frac{2(r_r - r_l)}{d^2 + r_l^2}, \\ \frac{1}{d} \ln \left| \frac{r_r - d}{r_r + d} \cdot \frac{r_l + d}{r_l - d} \right| &= \frac{1}{d} \ln \left| \frac{1 + (r_r - r_l)/(r_l - d)}{1 + (r_r - r_l)/(r_l + d)} \right| \approx \\ \frac{1}{d} \ln 1 + \frac{r_r - r_l}{r_l - d} - \frac{r_r - r_l}{r_l + d} &\approx \frac{2(r_r - r_l)}{r_l^2 - d^2}. \end{aligned}$$

The integrals are continuous for $d \rightarrow 0$, $r_l > 0$, and $\frac{-c_1}{2c_2} \notin [x_i, x_{i+1}]$.

Figure 1 shows the relative error of both approximations. One could try to glue Equation (58) and (63) together. That would not be helpful for this application: in case of analytic integration the constraints are very large and numerical integration would be based on sets of precomputed values anyway.

10.4 Numerical solution

Theorem 1 provides the basis for the numerical solution. The first step is to deduce the sign and size relation of δv and δw , hence to select the actual case *i*), *ii*), or *iii*). The discussion of the special cases, rough numerical integration, the edge current of the last global step of Newton's method or a predictor, ... or those cases, where Equation (24) can be used, provide an initial guess for f_0 together with bounds. Hence, with two (in some cases three) function evaluations one sign change of $h(f_0) := I(f_0) + \delta w = 0$ can be constructed, starting with the initial guess. Some care is necessary to handle the rapid and slow variation of h , depending on the distance $|f_{0,k} - f_0|$ with the iteration index k . It is useful to keep a short history of left and right arguments and function values for computing the new estimate and save switching decision to Newton's method, if h and h' are consistent with the history. The case small $|\delta v|$ can typically be restricted to approximation of data using one interval only.

Figure 2 compares edge currents for the classical Scharfetter-Gummel scheme, an approximation of $F_{1/2}$ with relative errors smaller 1%, and the classical Blake-more approximation with arguments $(\varphi_l, \varphi_r, w_l)$ in the cube $[-5, 5]^3$. As expected, overestimated saturation effects show up in the classical Blakemore approximation.

11 Discussion and summary

Mean value theorem based arguments are sufficient to show essential stability properties for discrete drift-dif-

fusion problems and a general construction principle of spatial discretizations together with boundary conforming Delaunay grids. The proposed construction results in a unique, dissipative solution of an integral equation defining the edge current and reproducing the dissipation of the one dimensional problem up approximation errors of the governing function, which can be made smaller than the typical errors in the data of the problem. This generalized Scharfetter-Gummel scheme is compatible with the thermodynamic equilibrium and the characteristic structure of the Jacobian of the analytic problem. A detailed discussion for distribution functions of special interest in different semiconductor device applications supplements the general facts. The short hint to variational formulations should help to understand the implications of the variational formulation for the structure of special models. On the other hand, the assumption that the velocity is the gradient of a potential can be relaxed by either introducing a potential on a local scale or proper discretizations of a constant velocity onto edges.

If the strict monotonicity of the density with respect to the chemical potential is lost, the so called charge-neutral approximation does not exist for sufficiently large doping values and, for instance, large applied voltages at gate boundaries. Before that happens one is entering the problems associated with phase separation and degenerate diffusion in case of a variational formulation. If $f(v)$ is not anymore strictly monotone, the Cauchy problem may have more than one solution for the given boundary data. Dissipativity would still be a selection criterion. Formally, the integration can be performed by the same technique: for instance one mirrors $f(v)$ at its maximum at $v_m \in [v_l, v_r]$, hence it is a monotone function and a correction of the known difference of the integral is possible using $(f(v_m) - f(\infty))(v_r - v_m)$. The essential problem is to prove bounds for the solution of the analytic problem away from $\min(\mathcal{F}(v))$, $\max(\mathcal{F}(v))$ or to study the consequences of degenerate diffusion together with the interaction potential defined by the Poisson equation.

The intuition based on physics would suggest two (or more) types of particles, each described by monotone functions (or convex free energy functionals) and one or more reactions, that relate the densities in the proper way.

For models of organic (amorphous) semiconductors, like EGDM [20], it would be interesting to find states close to degenerate diffusion either by numerical solution of the complete set of model equations or experimentally. To some extent (solution methods are expected to deteriorate) model changes with respect to $f(v)$, $\mathcal{F}(v)$ are reduced to changing approximating functions.

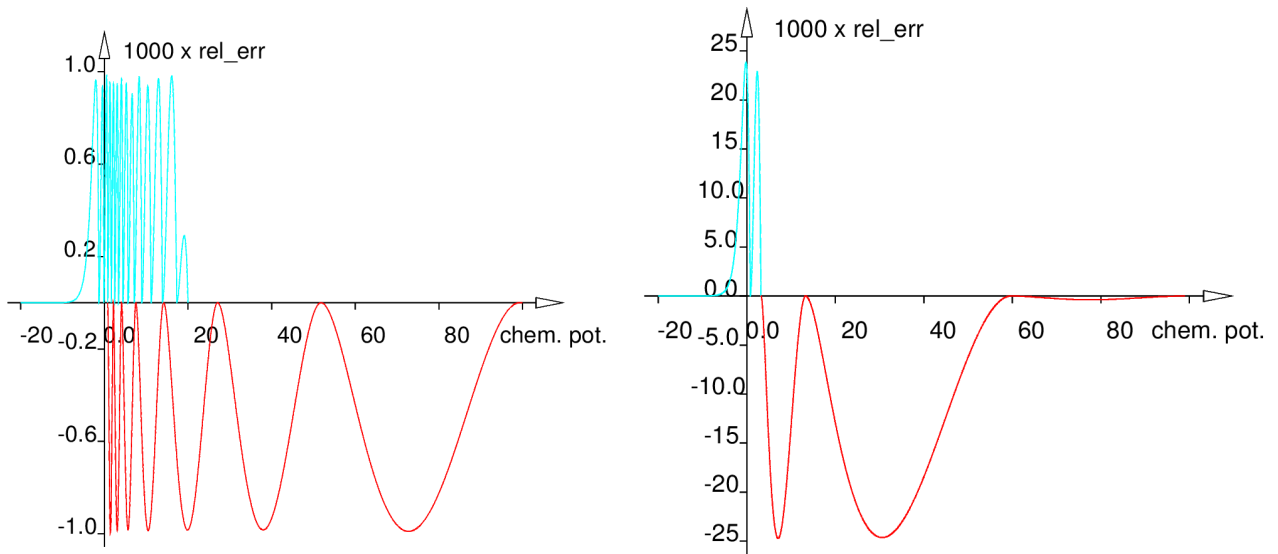


Fig. 1 Typical approximation properties of a Blakemore type approximation with three parameters (blue) and Padé splines ($F_{1/2}(v)$) with relative errors $1/1000$ and $2.5/100$, larger errors violate the monotonicity of the approximation).

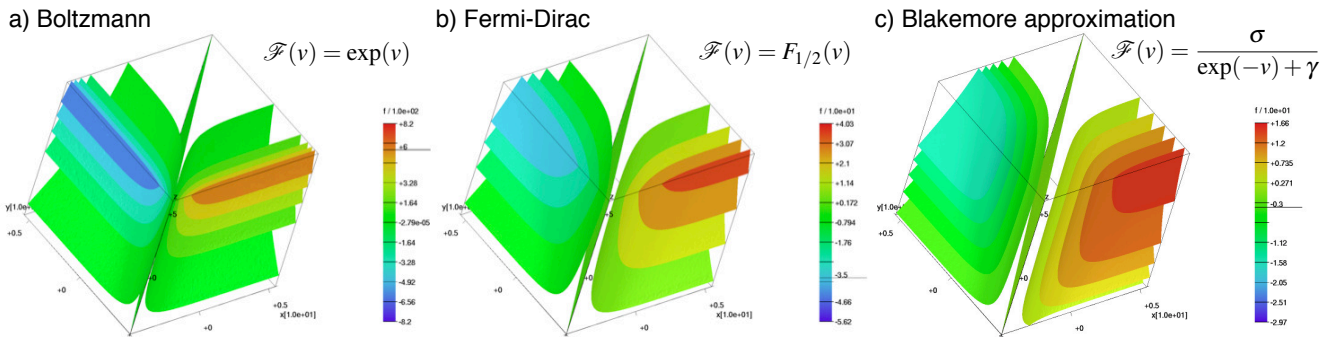


Fig. 2 Influence of the distribution function on the edge current: shown are isosurfaces of the current for 10^6 random argument triples (in U_T) for the Boltzmann case (l.), the Fermi-Dirac integral $F_{1/2}$ (m.), and the original Blakemore approximation ($\sigma = 1$, $\gamma = 0.27$, r.). The amplitude varies by one order of magnitude. x, y, z correspond to $\varphi_a, \varphi_b, w_a$; $w_b = 0$. The correction terms for nonvanishing drift break the symmetry with respect to interchanging φ_a and φ_b , present in the Boltzmann case.

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