

# Comparison of thermodynamically consistent charge carrier flux discretizations for Fermi–Dirac and Gauss–Fermi statistics

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**Abstract** We compare three thermodynamically consistent Scharfetter–Gummel schemes for different distribution functions for the carrier densities, including the Fermi–Dirac integral of order 1/2 and the Gauss–Fermi integral. The most accurate (but unfortunately also most costly) generalized Scharfetter–Gummel scheme requires the solution of an integral equation. Since one cannot solve this integral equation analytically, several modified Scharfetter–Gummel schemes have been proposed, yielding *explicit* flux approximations to the *implicit* generalized flux. The two state-of-the-art modified fluxes used in device simulation software are the diffusion-enhanced flux and the inverse activity coefficient averaging flux. We would like to study which of these two modified schemes approximates the implicit flux better. To achieve this, we propose a new method to solve the integral equation numerically based on Gauss quadrature and Newton’s method. This numerical procedure provides a highly accurate reference flux, enabling us to compare the quality of the two modified Scharfetter–Gummel schemes. We extend previous results (Farrell in *J Comput Phys* 346:497–513, 2017a) showing that the diffusion-enhanced ansatz leads to considerably lower flux errors for the Blakemore approximation to the physically more relevant Fermi–Dirac and Gauss–Fermi statistics.

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## 1 Introduction

The classical Scharfetter–Gummel scheme in combination with a Voronoi finite volume method provides a discrete approximation to drift-diffusion currents in non-degenerate semiconductors (Boltzmann regime). The scheme is consistent with the thermodynamic equilibrium in the sense that the (full) zero-bias solution coincides with the unique thermodynamic equilibrium. This consistency helps to avoid unphysical steady state dissipation, see Bessemoulin-Chatard (2012). Furthermore, the consistent discretization of dissipative effects is crucial when coupling the semiconductor equations to heat transport models. Among all discretization schemes this finite volume method is the most established one for simulating the current flow in opto-electronic devices.

However, the classical Scharfetter–Gummel scheme is only consistent when one is justified in using the Boltzmann approximation. Non-Boltzmann distribution functions describing degenerate semiconductors are required for organic semiconductors, highly doped materials and semiconductor devices operated at cryogenic temperatures as shown e.g. by Kantner and Koprucki (2016). Strong degeneracy effects make it mandatory to employ Fermi–Dirac statistics. Therefore, it is crucial to develop generalizations of the Scharfetter–Gummel scheme beyond the Boltzmann approximation. A number of schemes for degenerate semiconductors proposed in the literature Purbo et al. (1989), Jünger (1995), Stodtmann et al. (2012) are not thermodynamically consistent.

Bessemoulin-Chatard (2012), Koprucki et al. (2015), and Fuhrmann (2015) proposed modified Scharfetter–Gummel schemes which are thermodynamically consistent. Based on Eymard et al. (2006), Koprucki and Gärtner (2013) introduced (an accurate but costly) thermodynamically consistent generalized Scharfetter–Gummel scheme which requires the solution of an integral equation summarized in Sect. 4.

The focus of the present paper is on the Fermi–Dirac integral of order  $1/2$  as well as the Gauss–Fermi integral. Furthermore, in Sect. 5 we present a new algorithm to solve the integral equation proposed in Koprucki and Gärtner (2013) based on Gauss quadrature and Newton’s method. Using this numerical flux as reference, we compare the performance of the two modified Scharfetter–Gummel schemes in Sect. 6.

We point out that even though in this paper we discuss only *local* flux corrections, Farrell et al. (2017a) previously also confirmed the beneficial influence of the modified Scharfetter–Gummel fluxes on the *global* solution of the fully coupled van Roosbroeck system via a p-i-n benchmark. However, this simulation was restricted to the Blakemore distribution function (an approximation of the Fermi–Dirac integral). Here we perform a thorough comparison for the physically more accurate and computationally more challenging Fermi–Dirac and Gauss–Fermi integrals. Nevertheless, the local errors behave in both settings very similarly which leads us to expect that the local improvement has a similar influence on device simulations using the fully coupled van Roosbroeck system.

## 2 Van Roosbroeck system and distribution functions

We consider the stationary van Roosbroeck system of charge transport in semiconductors using standard notation from Farrell et al. (2017a) ( $\psi$ : electrostatic potential,  $\varphi_n, \varphi_p$ : quasi-Fermi potentials,  $\eta_n, \eta_p$ : chemical potentials):

$$-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla \psi) = q(p - n + C), \tag{1a}$$

$$\nabla \cdot \mathbf{j}_n = qR, \quad \mathbf{j}_n = -q\mu_n n \nabla \varphi_n, \tag{1b}$$

$$\nabla \cdot \mathbf{j}_p = -qR, \quad \mathbf{j}_p = -q\mu_p p \nabla \varphi_p \tag{1c}$$

where  $\mu_n$  and  $\mu_p$  denote the electron and hole mobilities,  $C$  the doping,  $R$  the recombination rate and  $\varepsilon_0, \varepsilon_r$  the vacuum and relative permittivity. The electron and hole densities are defined by

$$n = N_c \mathcal{F}(\eta_n), \eta_n = \frac{q(\psi - \varphi_n) - E_c}{k_B T}, \tag{2a}$$

$$p = N_v \mathcal{F}(\eta_p), \eta_p = \frac{q(\varphi_p - \psi) + E_v}{k_B T}. \tag{2b}$$

Here the effective densities of states for electrons in the conduction band  $N_c$  and holes in the valence band  $N_v$  as well as the corresponding band-edge energies  $E_c$  and  $E_v$  are constant material parameters. The temperature  $T$  is also assumed to be constant; in general it can be space or even time dependent. The Boltzmann constant is denoted with  $k_B$ .

Distribution functions describe how potentials and charge carriers are related. For inorganic, 3D bulk semiconductors with parabolic bands this relation is given by the Fermi–Dirac integral of order 1/2,

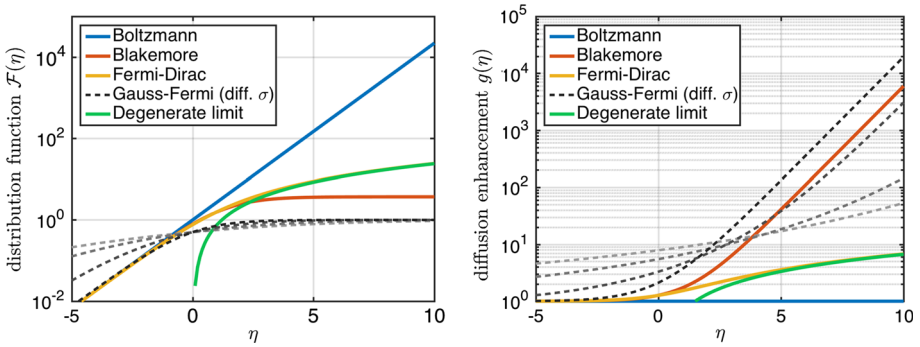
$$\mathcal{F}(\eta) = F_{1/2}(\eta) := \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\xi^{1/2}}{\exp(\xi - \eta) + 1} d\xi, \tag{3}$$

which can be approximated by a Blakemore ( $\mathcal{F}(\eta) = (\exp(-\eta) + \gamma)^{-1}$  with  $\gamma = 0.27$ ) or Boltzmann ( $\mathcal{F}(\eta) = \exp(\eta)$ ) distribution in the low density limit. For large arguments,  $F_{1/2}(\eta)$  can be approximated by the degenerate limit  $\frac{4}{3\sqrt{\pi}} \eta^{3/2}$ . For organic semiconductors the Gauss–Fermi integral, a term coined by Paasch and Scheinert (2010),

$$\mathcal{F}(\eta) = \mathcal{G}(\eta; \sigma) := \frac{1}{\sqrt{2\pi\sigma}} \int_{-\infty}^\infty \frac{\exp(-\frac{\zeta^2}{2\sigma^2})}{\exp(\zeta - \eta) + 1} d\zeta, \tag{4}$$

describes the relationship between potentials and carrier densities. The variance  $\sigma$  measures the disorder of the energy levels. The Gauss–Fermi integral reduces to a Blakemore distribution function (with  $\gamma = 1$ ) for vanishing disorder  $\sigma$ , corresponding to a  $\delta$ -shaped density of states, describing a single transport level. All relevant functions are depicted in Fig. 1.

In the following we restrict our considerations to the continuity equation for electrons, partially omitting the index  $n$ . The electron current can be rewritten in drift-diffusion form,



**Fig. 1** Distribution functions and their corresponding diffusion enhancement (6)

$$\mathbf{j}_n = -q\mu_n n \nabla \psi + qD_n \nabla n. \tag{5}$$

The diffusion coefficient  $D_n$  is linked to the carrier mobilities by a generalized Einstein relation  $\frac{D_n}{\mu_n} = \frac{k_B T}{q} g(\eta_n)$ , where the *diffusion enhancement* is given by

$$g(\eta) = \frac{\mathcal{F}(\eta)}{\mathcal{F}'(\eta)} = \frac{1}{(\log \mathcal{F}(\eta))'}. \tag{6}$$

For the Boltzmann distribution, we have  $g \equiv 1$ . Therefore,  $g$  is a measure of the degeneracy (i.e. the deviation from the Boltzmann regime), see Fig. 1.

### 3 Finite volume discretization and thermodynamic consistency

We partition the domain  $\Omega$  into control volumes (Voronoi cells)  $\omega_K$  such that  $\Omega = \bigcup_{K=1}^N \omega_K$ . With each control volume we associate a node  $\mathbf{x}_K \in \omega_K$ . Via the divergence theorem we obtain after integration over each control volume a discrete version of the continuity equation (1b). Consistent with the continuous van Roosbroeck system, this *finite volume* discretization describes the change of the carrier density within a control volume. The corresponding numerical flux  $j$  describing the flow between neighboring control volumes can be expressed as a function, depending nonlinearly on the values  $\psi_K, \psi_L, \eta_K, \eta_L$  such that

$$j(\psi_K, \psi_L, \eta_K, \eta_L) \approx \frac{1}{|\partial\omega_K \cap \partial\omega_L|} \int_{\partial\omega_K \cap \partial\omega_L} \mathbf{j} \cdot \mathbf{n} \, dS.$$

Here a function with subindex, e.g.  $K$ , denotes evaluation of the function at the node  $\mathbf{x}_K$ . Farrell et al. (2017b) give more details on the derivation of this scheme.

We require our numerical current approximation to satisfy *thermodynamic consistency*, a property which holds at the continuous level: constant quasi Fermi potentials lead to vanishing currents. Thus, setting any discrete numerical flux between two adjacent discretization nodes  $\mathbf{x}_K$  and  $\mathbf{x}_L$  to zero

$$j = j(\eta_L, \eta_K, \psi_L, \psi_K) = 0$$

shall imply

$$\frac{\psi_L - \psi_K}{U_T} =: \delta\psi_{KL} \stackrel{!}{=} \delta\eta_{KL} := \eta_L - \eta_K \tag{7}$$

where  $U_T = k_B T/q$  denotes the thermal voltage.

### 4 Generalized Scharfetter–Gummel schemes

If one assumes that the (unknown) flux  $j$  between two cells is constant, it fulfills the integral equation, studied by Eymard et al. (2006), Koprucki and Gärtner (2013),

$$\int_{\eta_K}^{\eta_L} \left( \frac{j_n/j_0}{\mathcal{F}(\eta)} + \frac{\psi_L - \psi_K}{U_T} \right)^{-1} d\eta = 1, \quad j_0 = q\mu_n N_c \frac{U_T}{h_{KL}} \tag{8}$$

where the integration limits are given by  $\eta_K = \eta_n(\psi_K, \varphi_K)$  and  $\eta_L = \eta_n(\psi_L, \varphi_L)$ . The distance between both nodes associated with each cell is denoted with  $h_{KL}$ . Gärtner (2015) showed that for strictly monotonously increasing  $\mathcal{F}(\eta)$  this equation has always a unique solution. We will refer to it as the *generalized Scharfetter–Gummel flux*.

For the Boltzmann approximation we recover from (8) the classical scheme by Scharfetter and Gummel (1969),

$$j_{sg} = B(\delta\psi_{KL})e^{\eta_L} - B(-\delta\psi_{KL})e^{\eta_K}, \tag{9}$$

for the non-dimensionalized edge current  $j_{sg} = j_n/j_0$  and the Bernoulli function  $B(x) := x/(e^x - 1)$ . Koprucki and Gärtner (2013) showed that the Blakemore approximation  $\mathcal{F}(\eta) = \frac{1}{e^{-\eta+\gamma}}$  yields for (8) a fixed point equation

$$j_b = B(\gamma j_b + \delta\psi_{KL})e^{\eta_L} - B(-[\gamma j_b + \delta\psi_{KL}])e^{\eta_K} \tag{10}$$

for the non-dimensionalized edge current  $j_b = j_n/j_0$ . The right-hand side is a Scharfetter–Gummel expression where the argument of the Bernoulli function is shifted by  $\gamma j_b$ . Hence, for  $\gamma = 0$  the generalized flux  $j_b$  reduces to the classical Scharfetter–Gummel scheme (9) since the Blakemore function reduces to the Boltzmann function.

### 5 Solving for the generalized Scharfetter–Gummel flux numerically

For general distribution functions like (3) and (4), we cannot find closed expressions for the unknown current as a solution to (8). For this reason one may employ physically motivated approximate flux solutions. These *modified Scharfetter–Gummel schemes* we discuss in Sect. 6. To obtain more accurate flux approximations, we solve the generalized Scharfetter–Gummel scheme (8) numerically. The implementation is challenging due to two reasons: First one needs to approximate the integral accurately and then solve a nonlinear equation. We use Gauss-Legendre quadrature to approximate the integral. Not only is this highly efficient for smooth integrands but also the quadrature excludes the boundary nodes thus preventing the integrand from coming too close to a pole. Gärtner (2015) showed that no pole can appear within the integration limits. However, it might come very close to the

domain of integration. Denoting the integrand in (8) with  $G(\eta_j; \delta\psi_{KL}, j)$  for  $j = j_n/j_0$ , we can approximate (8) by

$$H(j) := \sum_{i=1}^N w_i G(\eta_i; \delta\psi_{KL}, j) - 1 = 0, \tag{11}$$

where  $w_i$  are the integration weights and  $\eta_i$  the quadrature nodes.

We solve the nonlinear equation for the flux  $j$  via Newton’s method, using the diffusion-enhanced Scharfetter–Gummel flux (13) as a starting guess. This choice is very crucial as already small perturbations may result in divergence. We treat pure drift and pure diffusive currents separately. For small drift and small diffusion we use the low-order series expansion of the unknown current derived by Farrell et al. (2017a) to avoid numerical difficulties. In Fig. 2, isosurfaces of the generalized Scharfetter–Gummel current using this method are shown for Fermi–Dirac and Gauss–Fermi statistics.

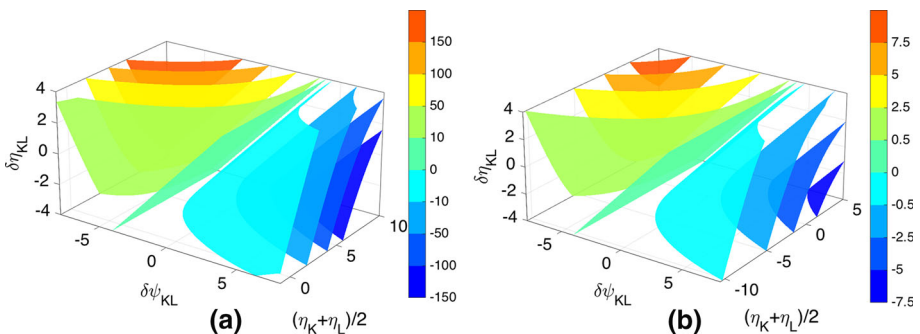
To verify the accuracy of our method, we tested how fast the current converges. We observed exponential convergence with respect to the number of quadrature nodes. For this quality assessment we used the Blakemore distribution function because in this case the solution to (8) can also be obtained via the fixed point equation (10). This analysis showed that usually  $N = 16$  quadrature nodes are sufficient to resolve the integral equation (8) highly accurately.

## 6 Error analysis for modified Scharfetter–Gummel fluxes

Since solving an integral equation for each pair of neighboring discretization points  $\mathbf{x}_K, \mathbf{x}_L$  appears to be too expensive in general, we present two modified schemes as approximate solutions to (8). They keep the beneficial Scharfetter–Gummel structure and are thermodynamically consistent. Farrell et al. (2017a, b) presents more details and physical motivations.

### 6.1 Diffusion enhanced Scharfetter–Gummel scheme

Bessemoulin-Chatard (2012), Koprucki et al. (2015) suggest a logarithmic average of the diffusion enhancement  $g(\eta) = \frac{1}{(\ln \mathcal{F}(\eta))' = \mathcal{F}(\eta)/\mathcal{F}'(\eta) \geq 1}$  given by



**Fig. 2** Isosurfaces of the generalized Scharfetter–Gummel flux (8) computed via (11). The plane  $\delta\psi_{KL} - \delta\eta_{KL} = 0$  in the middle of both figures corresponds to the thermodynamic consistency (7), where the current vanishes thus separating negative and positive currents. **a** Fermi–Dirac. **b** Gauss–Fermi ( $\sigma = 5$ )

$$g_{KL} = \frac{\eta_L - \eta_K}{\log \mathcal{F}(\eta_L) - \log \mathcal{F}(\eta_K)}, \tag{12}$$

leading to the current approximation

$$j_d = g_{KL} \left[ B \left( \frac{\delta\psi_{KL}}{g_{KL}} \right) \mathcal{F}(\eta_L) - B \left( -\frac{\delta\psi_{KL}}{g_{KL}} \right) \mathcal{F}(\eta_K) \right]. \tag{13}$$

### 6.2 Inverse activity coefficients

In addition to the diffusion enhancement  $g(\eta)$  another measure for the degeneracy is given by the inverse  $\beta(\eta) = \mathcal{F}(\eta)/e^\eta$  of the activity coefficient, also known as degeneracy factor. For the Boltzmann distribution the factor  $\beta(\eta)$  becomes one. For non-exponential distribution functions it is less than one. Fuhrmann (2015) derived the scheme

$$j_a = -\bar{\beta}_{KL} \left( B(-\delta\psi_{KL})e^{\eta_K} - B(\delta\psi_{KL})e^{\eta_L} \right), \tag{14}$$

where  $\bar{\beta}_{KL}$  denotes either an arithmetic or a geometric average between  $\beta(\eta_K)$  and  $\beta(\eta_L)$ .

### 6.3 Error estimates and comparison

Finally, we compare the performance of both modified Scharfetter–Gummel schemes. For general distribution functions Farrell et al. (2017a) derived error estimates between the modified fluxes [(13) and (14)] and the generalized Scharfetter–Gummel flux (8):

$$err_a(\bar{\eta}_{KL}, \delta\eta_{KL}, \delta\psi_{KL}) := |j_a - j| \leq \frac{1}{2} \mathcal{F}(\bar{\eta}_{KL}) |\delta\psi_{KL} \delta\eta_{KL}|, \tag{15}$$

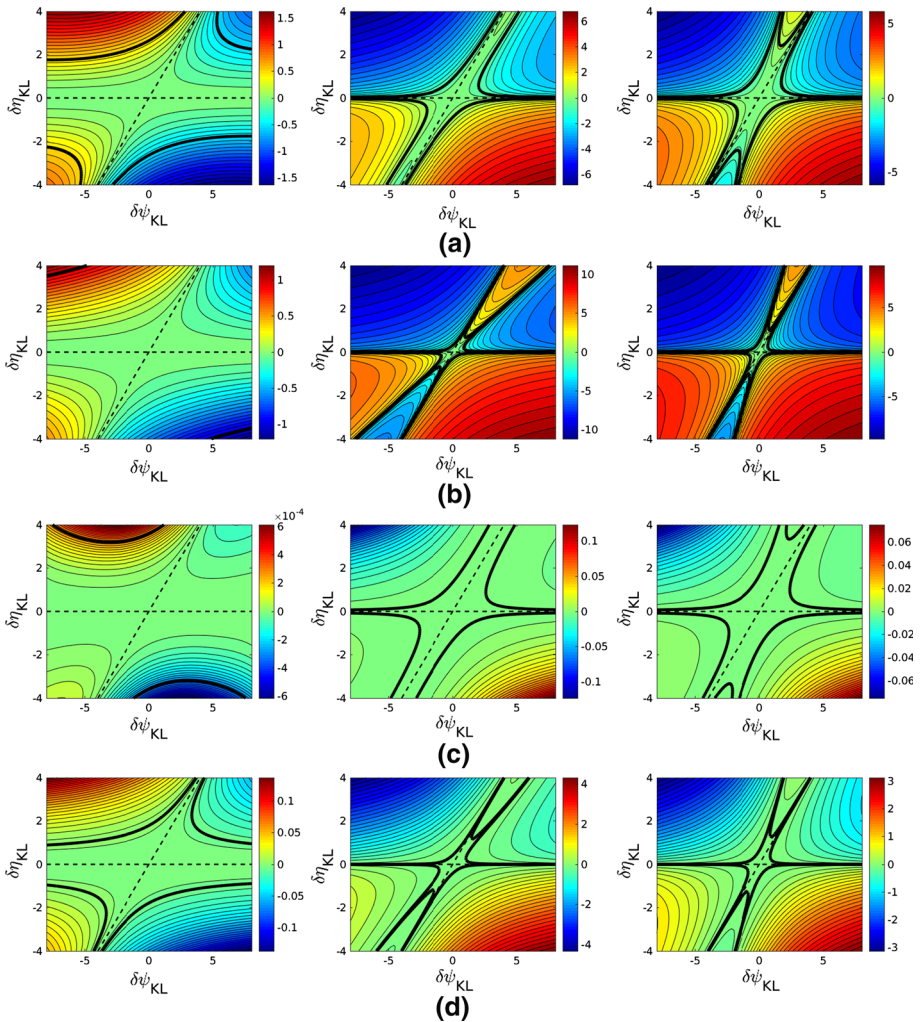
$$err_d(\bar{\eta}_{KL}, \delta\eta_{KL}, \delta\psi_{KL}) := |j_d - j| \leq \frac{1}{2} \frac{\mathcal{F}(\bar{\eta}_{KL})}{g(\bar{\eta}_{KL})} |\delta\psi_{KL} \delta\eta_{KL}|. \tag{16}$$

In these estimates  $\bar{\eta}_{KL}$  denotes the arithmetic average

$$\bar{\eta}_{KL} := \frac{\eta_L + \eta_K}{2}$$

and higher order terms have been neglected. The bound for the diffusion-enhanced scheme (unlike for the inverse activity scheme) additionally depends on the inverse of the diffusion enhancement. Hence, if  $g(\bar{\eta}_{KL})$  becomes large (strong degeneracy) the a priori error is considerably lower. Kantner and Koprucki (2016) showed that high values of  $g$  can appear in devices operating at cryogenic temperatures.

Figure 3 depicts the errors in terms of  $\delta\eta_{KL}$  and  $\delta\psi_{KL}$  for fixed averages  $\bar{\eta}_{KL}$  (guaranteeing a diffusion enhancement significantly larger than one) and different distribution functions. The errors vanish along the dashed lines indicating  $\eta_K = \eta_L$  (pure drift current) as well as  $\delta\psi_{KL} = \delta\eta_{KL}$  due to the consistency with the thermodynamic equilibrium. As predicted by the error estimates (15) and (16), the comparison in Fig. 3 reveals that the error of diffusion-enhanced scheme (13) is considerably smaller than the error of the inverse activity scheme (14), in particular when the degeneracy becomes strong.



**Fig. 3** Logarithmic absolute errors between the generalized Scharfetter–Gummel and modified schemes depending on the potential differences  $\delta\psi_{KL}$  and  $\delta\eta_{KL}$  for a fixed value of  $\bar{\eta}_{KL}$ , cp. (15) and (16). Each row corresponds to a different distribution function and each column corresponds to a different flux approximation: diffusion enhanced scheme (left), the arithmetically averaged inverse activity scheme (middle) and the geometrically averaged one (right). The dashed lines show where generalized and modified schemes agree exactly. The bold black lines highlight the same contour level in each row. **a** Fermi–Dirac integral  $F_{1/2}$ ,  $\bar{\eta}_{KL} = 5$ : diffusion enhancement  $g(5) \approx 3.58$ . **b** Degenerate limit  $\frac{4}{3\sqrt{\pi}}\eta^{3/2}$ ,  $\bar{\eta}_{KL} = 60$ : diffusion enhancement  $g(60) = 40$ . **c** Gauss–Fermi  $\mathcal{G}(\eta; \sigma = 5)$ ,  $\bar{\eta}_{KL} = -15$ : diffusion enhancement  $g(-15) \approx 1.74$ . **d** Gauss–Fermi  $\mathcal{G}(\eta; \sigma = 5)$ ,  $\bar{\eta}_{KL} = 0$ : diffusion enhancement  $g(0) \approx 6.65$

## 7 Conclusion

This paper extends previous error analysis for thermodynamically consistent fluxes by Farrell et al. (2017a). The authors focused on general analytical results illustrating them using the Blakemore distribution function. The authors showed that the diffusion-enhanced



scheme is superior to the inverse activities scheme when the diffusion enhancement is large, i.e. degeneracy effects are strong. In the present paper, we confirm that this holds true for a larger class of distribution functions, in particular the Fermi–Dirac integral of order 1/2, the Gauss–Fermi integral and the degenerate limit  $\mathcal{F}(\eta) = \frac{4}{3\sqrt{\pi}}\eta^{3/2}$  which becomes important at cryogenic temperatures.

The comparison is based on studying the difference between modified fluxes and the more accurate generalized Scharfetter–Gummel flux. To obtain the generalized flux, we had to numerically solve an integral equation. For this reason, we devised an algorithm based on Gauss quadrature and Newton’s method. The exponential convergence with respect to the number of quadrature nodes makes the numerical implementation of the generalized flux an interesting alternative to the existing modified Scharfetter–Gummel schemes.

Farrell et al. (2017a) analyzed the beneficial influence of the diffusion-enhanced flux on the solution of the fully coupled van Roosbroeck system via a p-i-n benchmark. This simulation was restricted to the Blakemore distribution function. However, since the error plots in Fig. 3 for the Fermi–Dirac and Gauss–Fermi distribution function as well as the degenerate limit are comparable, it is reasonable to expect similar performance gains for opto-electronic device simulations using the fully coupled van Roosbroeck system. Important applications include devices operating at cryogenic temperatures such as single-photon sources, highly-doped semiconductors as well as organic semiconductors.

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