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Abstract

Electro-thermal transport phenomena in semiconductors are described by the non-isothermal drift-diffusion system. The equations take a remarkably simple form when assuming the Kelvin formula for the thermopower. We present a novel, non-isothermal generalization of the Scharfetter–Gummel finite volume discretization for degenerate semiconductors obeying Fermi–Dirac statistics, which preserves numerous structural properties of the continuous model on the discrete level. The approach is demonstrated by 2D simulations of a heterojunction bipolar transistor.

1 Introduction

Self-heating effects are a major concern in modern semiconductor devices, where the on-going miniaturization of feature size leads to increased power loss densities. The optimal design of semiconductor devices relies on numerical simulations, based on thermodynamically consistent models for the coupled electro-thermal transport processes. The standard model for the simulation of self-consistent charge and heat transport processes is the non-isothermal drift-diffusion system [1–3], which couples the semiconductor device equations to a heat transport equation. The magnitude of the thermoelectric cross effects (Seebeck effect, Thomson–Peltier effect) is governed by the Seebeck coefficient (also *thermopower*), which quantifies the thermoelectric voltage induced by a temperature gradient. Recently [2], the non-isothermal drift-diffusion system has been studied using the so-called *Kelvin formula* for the thermopower [4], which has two important implications: First, the Seebeck term in the current density expressions can be entirely absorbed in a temperature-dependent diffusion constant via a generalized Einstein relation. Second, the heat generation rate involves solely the three classically known self-heating effects without any further (transient) contribution. The model equations and its key features are described in Sect. 2. In Sect. 3, we present a finite volume discretization based on a novel, non-isothermal generalization of the Scharfetter–Gummel scheme for the discrete fluxes. The scheme holds for Fermi–Dirac statistics and preserves numerous structural and thermodynamic properties of the continuous system.

2 Non-isothermal drift-diffusion system

We consider the non-isothermal drift-diffusion system on $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$,

$$-\nabla \cdot \varepsilon \nabla \Phi = q(C + p - n), \quad (1)$$

$$q \partial_t n - \nabla \cdot \mathbf{j}_n = -qR, \quad (2)$$

$$q \partial_t p + \nabla \cdot \mathbf{j}_p = -qR, \quad (3)$$

$$c_V \partial_t T - \nabla \cdot \kappa \nabla T = H. \quad (4)$$

Poisson's Eq. (1) describes the electrostatic potential Φ generated by the electron density n , the density of valence band holes p and the built-in doping profile C . Here, q is the elementary charge and ε is the (absolute) permittivity of the material. The transport and recombination dynamics of the electrons and holes are modeled by the continuity Eqs. (2)–(3), where $\mathbf{j}_{n/p}$ are the electrical current densities and R is the (net-)recombination rate, which comprises several radiative and non-radiative processes [5, 6]. Finally, c_V is the volumetric heat capacity, κ is the thermal conductivity and H is the heat generation rate.

The carrier densities are related with the quasi-Fermi potentials $\varphi_{n/p}$, the electrostatic potential Φ and the (absolute) temperature T via the state equations

$$n = N_c(T) \mathcal{F} \left(\frac{q(\Phi - \varphi_n) - E_c(T)}{k_B T} \right), \quad p = N_v(T) \mathcal{F} \left(\frac{E_v(T) - q(\Phi - \varphi_p)}{k_B T} \right), \quad (5)$$

where $N_{c/v}$ are the effective density of states, $E_{c/v}$ are the band edge energies of the conduction and the valence band, respectively, and k_B is Boltzmann's constant. The function \mathcal{F} describes the occupation probability of the electronic states. In the case of non-degenerate semiconductors (Maxwell–Boltzmann statistics), $\mathcal{F}(\eta) = \exp(\eta)$ is an exponential function. At high carrier densities, where degeneration effects due to the Pauli exclusion principle (Fermi–Dirac statistics) must be taken into account, \mathcal{F} is typically given by the Fermi–Dirac integral $F_{1/2}$ [6]. The approach outlined below, does not rely on the specific form of \mathcal{F} and is applicable to materials with arbitrary density of states and degenerate or non-degenerate statistics [2].

2.1 Kelvin formula for the thermopower

The electrical current densities are modeled as

$$\mathbf{j}_n = -\sigma_n (\nabla \varphi_n + P_n \nabla T), \quad \mathbf{j}_p = -\sigma_p (\nabla \varphi_p + P_p \nabla T), \quad (6)$$

where $\sigma_{n/p}$ are the electrical conductivities and $P_{n/p}$ are the thermopowers of the material. In this paper, we choose the thermopowers according to the Kelvin formula as variational derivatives of the entropy \mathcal{S} with respect to the carrier densities

$$qP_n = -D_n \mathcal{S}(n, p, T), \quad qP_p = +D_p \mathcal{S}(n, p, T), \quad (7)$$

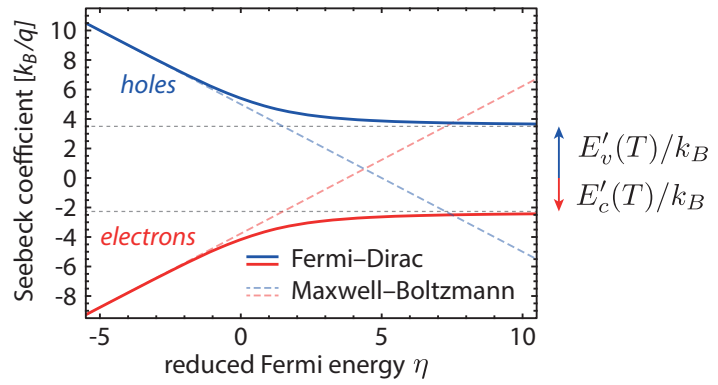
where D denotes the Gâteaux derivative. The Kelvin formula is the low frequency and long wavelength limit of the microscopically exact Kubo formula [4]. It was shown to provide a good approximation for several materials at sufficiently high temperature. The entropy is obtained from the free energy $\mathcal{F}(n, p, T)$ of the system.

We assume the free energy functional [1, 2]

$$\begin{aligned} \mathcal{F}(n, p, T) = & \int_{\Omega} dV \left(k_B T \mathcal{F}^{-1} \left(\frac{n}{N_c} \right) n - k_B T N_c \mathcal{G} \left(\mathcal{F}^{-1} \left(\frac{n}{N_c} \right) \right) + E_c(T) n \right. \\ & \left. + k_B T \mathcal{F}^{-1} \left(\frac{p}{N_v} \right) p - k_B T N_v \mathcal{G} \left(\mathcal{F}^{-1} \left(\frac{p}{N_v} \right) \right) - E_v(T) p \right) \\ & + \int_{\Omega} dV f_L(T) + \frac{1}{2} \int_{\Omega} dV \int_{\Omega} dV' G(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}) \rho(\mathbf{r}') + \int_{\Omega} dV \Phi_{\text{ext}} \rho, \end{aligned} \quad (8)$$

where the first two lines describe the free energy of the non-interacting electron-hole plasma (quasi-free Fermi gas), f_L is the free energy of the lattice phonons (ideal Bose gas), \mathcal{G} is the antiderivative of \mathcal{F}

Fig. 1. Thermopowers $P_{n/p}$ according to Eqs. (9) as functions of the reduced Fermi energy η (argument of \mathcal{F} in Eqs. (5)) in units of k_B/q . The thermopowers are plotted for $\mathcal{F}(\eta) = F_{1/2}(\eta)$ and $N_{c/v} \propto T^{3/2}$. The picture is taken from [2].



(i.e., $\mathcal{G}'(\eta) = \mathcal{F}'(\eta)$), $G(\mathbf{r}, \mathbf{r}')$ is the Green's function of Poisson's equation and $\rho = q(p - n)$ is the mobile charge density. The potential Φ_{ext} is generated by the built-in doping-profile and the applied bias.

The free energy (8) recovers the state equations (5) via the variational derivative with respect to the carrier densities $D_{n/p}\mathcal{F} := \mp q\varphi_{n/p}$, which is the defining relation for the quasi-Fermi potentials, see [2]. The entropy functional is defined as the derivative of the free energy (8) with respect to the temperature: $\mathcal{S}(n, p, T) = -\partial_T \mathcal{F}(n, p, T)$. Evaluation of Eq. (7) yields the thermopowers

$$P_n(n, T) = -\frac{k_B}{q} \left(\frac{TN'_c(T)}{N_c(T)} g\left(\frac{n}{N_c(T)}\right) - \mathcal{F}^{-1}\left(\frac{n}{N_c(T)}\right) - \frac{1}{k_B} E'_c(T) \right), \quad (9a)$$

$$P_p(p, T) = +\frac{k_B}{q} \left(\frac{TN'_v(T)}{N_v(T)} g\left(\frac{p}{N_v(T)}\right) - \mathcal{F}^{-1}\left(\frac{p}{N_v(T)}\right) + \frac{1}{k_B} E'_v(T) \right). \quad (9b)$$

The temperature-dependency of the band edge energies can be modeled using, e.g., the Varshni model [2, 5]. The function

$$g(x) = x \left(\mathcal{F}^{-1} \right)'(x) \quad (10)$$

quantifies the degeneration of the carriers ($g > 1$ for Fermi–Dirac statistics; $g \equiv 1$ for Maxwell–Boltzmann statistics). See Fig. 1 for a plot of the Seebeck coefficients (9).

2.2 Drift-diffusion currents and heat generation rate

The Kelvin formula has two important implications, which lead to a very simple and appealing form of the thermoelectric cross effects in the system (1)–(4).

First, we rewrite the electrical current densities by passing from the thermodynamic form (6) to the drift-diffusion form. By explicitly evaluating the gradient of the quasi-Fermi potentials using the state equations (5), one observes that the Seebeck terms $\mathbf{j}_{n/p}|_{\text{Seebeck}} = -\sigma_{n/p} P_{n/p} \nabla T$ cancel out *exactly* from the expressions [2]. Using the conductivities $\sigma_n = qM_n n$ and $\sigma_p = qM_p p$ (with mobilities $M_{n/p}$), one arrives at

$$\mathbf{j}_n = -qM_n n \nabla \Phi + qD_n(n, T) \nabla n, \quad \mathbf{j}_p = -qM_p p \nabla \Phi - qD_p(p, T) \nabla p. \quad (11)$$

We emphasize that in Eq. (11) – even though there is no explicit thermal driving force $\propto \nabla T$ – the Seebeck effect is fully taken into account via the (temperature-dependent) diffusion coefficients $D_{n/p}$. The latter obey the generalized Einstein relations [7]

$$qD_n = k_B T M_n g(n/N_c(T)), \quad qD_p = k_B T M_p g(p/N_v(T)). \quad (12)$$

Here, the degeneration factor (10) describes a nonlinear enhancement of the diffusion current due to the degeneration of the electron-hole plasma. The flux discretization described in Sect. 3.1 is based on the drift-diffusion form (11).

The second implication of the Kelvin formula concerns the heat generation rate H . The commonly accepted model for H , which was derived by Wachutka [3] from fundamental laws of linear irreversible thermodynamics, takes a particularly simple form, when assuming the Kelvin formula for the thermopower. One obtains (see Appendix A)

$$H = \sum_{\lambda \in \{n,p\}} \frac{1}{\sigma_\lambda} \|\mathbf{j}_\lambda\|^2 - \sum_{\lambda \in \{n,p\}} T \mathbf{j}_\lambda \cdot \nabla P_\lambda + q(\varphi_p + TP_p - \varphi_n - TP_n) R, \quad (13)$$

which involves solely the three classically known self-heating effects, namely Joule heating (first term), the Thomson–Peltier effect (second term) and recombination heating (last term). Any further (transient) contributions, which necessarily arise for thermopowers different from the Kelvin formula (7), do not occur in the model.

3 Finite volume discretization

We assume a boundary conforming Delaunay triangulation of the computational domain $\Omega \subset \mathbb{R}^d$, $d = \{1, 2, 3\}$, and obtain the finite volume discretization [6] of the (stationary) system (1)–(4) by integration over the (restricted) Voronoï cells as

$$- \sum_{L \in N(K)} s_{K,L} \varepsilon (\Phi_L - \Phi_K) = q |\Omega_K| (C_K + p_K - n_K), \quad (14a)$$

$$- \sum_{L \in N(K)} s_{K,L} J_{n,K,L} = -q |\Omega_K| R_K, \quad (14b)$$

$$+ \sum_{L \in N(K)} s_{K,L} J_{p,K,L} = -q |\Omega_K| R_K, \quad (14c)$$

$$- \sum_{L \in N(K)} s_{K,L} \kappa_{K,L} (T_L - T_K) = \frac{1}{2} \sum_{L \in N(K)} s_{K,L} (H_{J,K,L} + H_{T-P,K,L}) + |\Omega_K| H_{R,K}. \quad (14d)$$

Here, $|\Omega_K|$ is the volume of the K -th Voronoï cell, $s_{K,L} = |\partial\Omega_K \cap \partial\Omega_L| / \|\mathbf{r}_L - \mathbf{r}_K\|$ is a geometric factor and $N(K)$ is the set of adjacent nodes of K . The subscripts K, L indicate evaluation on the respective nodes or edges. The discrete heat sources are

$$H_{J,K,L} = - \sum_{\lambda \in \{n,p\}} J_{\lambda,K,L} (\varphi_{\lambda,L} - \varphi_{\lambda,K} + P_{\lambda,K,L} (T_L - T_K)), \quad (15a)$$

$$H_{T-P,K,L} = - \sum_{\lambda \in \{n,p\}} T_{K,L} J_{\lambda,K,L} (P_{\lambda,L} - P_{\lambda,K}), \quad (15b)$$

$$H_{R,K} = q (\varphi_{p,K} + T_K P_{p,K} - \varphi_{n,K} - T_K P_{n,K}) R_K, \quad (15c)$$

where we used a technique involving a weakly converging gradient developed in [8] for the discretization of the Joule and Thomson–Peltier terms (see [2] for details).

3.1 Generalized Scharfetter–Gummel scheme

A robust discretization of the flux projections $J_{n/p,K,L} = (\mathbf{r}_L - \mathbf{r}_K) \cdot \mathbf{j}_{n/p}$ is obtained by integrating Eq. (11) along the edge $\overline{KL} := \{\mathbf{r}(x) = x \mathbf{r}_L + (1-x) \mathbf{r}_K, x \in [0, 1]\}$, while assuming the electric field, the current density and the mobility to be constant along \overline{KL} . The temperature is assumed to be an affine function between adjacent nodes: $T(x) = x T_L + (1-x) T_K, x \in [0, 1]$. In the case of Fermi–Dirac statistics (with $g \neq 1$), the resulting two-point boundary value problem on $x \in [0, 1]$

$$k_B T(x) g \left(\frac{n(x)}{N_c(T(x))} \right) \frac{dn}{dx} = q (\Phi_L - \Phi_K) n(x) + \frac{J_{n,K,L}}{M_{n,K,L}}, \quad n(0) = n_K, \quad n(1) = n_L,$$

can be solved approximately, by freezing the degeneracy factor (10) to a suitable average $g_{n/p,K,L}$ [7, 9]. One obtains the non-isothermal Scharfetter–Gummel scheme

$$J_{n,K,L} = M_{n,K,L} k_B T_{K,L} g_{n,K,L} (n_L B(X_{n,K,L}) - n_K B(-X_{n,K,L})), \quad (16)$$

with $X_{n,K,L} = q (\Phi_L - \Phi_K) / (k_B T_{K,L} g_{n,K,L})$ and the Bernoulli function $B(x) = x / (\exp(x) - 1)$ (holes analogously). The averaged degeneracy factor (consistent with the thermodynamic equilibrium [7, 9]) and the logarithmic mean temperature read

$$g_{n,K,L} = \frac{\eta_{n,L} - \eta_{n,K}}{\log(\mathcal{F}(\eta_{n,L}) / \mathcal{F}(\eta_{n,K}))}, \quad T_{K,L} = \Lambda(T_L, T_K) = \frac{T_L - T_K}{\log(T_L / T_K)}. \quad (17)$$

The scheme (16) is a non-isothermal generalization of the scheme developed in [7, 9].

3.2 Structure-preserving properties

The discrete system (14)–(16) has several structure-preserving properties that hold without any smallness assumption. The conservation of charge is immediately guaranteed by the finite volume discretization [6]. Moreover, the scheme (16) is robust in both the drift- and diffusion dominated limits, as it interpolates between the upwind scheme for $X_{n,K,L} \rightarrow \pm\infty$ (strong electric field) and a central difference scheme for $X_{n,K,L} = 0$ (pure diffusion). The latter involves a discrete analogue of the nonlinear diffusion constant (12) using $g_{n,K,L}$ as in Eq. (17). For the analysis of further properties, which address the consistency with thermodynamics, it is convenient to recast the formula (16) into a discrete analogue of its thermodynamic form (6):

$$J_{n,K,L} = -\sigma_{n,K,L} (\varphi_{n,L} - \varphi_{n,K} + P_{n,K,L} (T_L - T_K)). \quad (18)$$

The edge-averaged discrete conductivity, which is implicitly taken by the Scharfetter–Gummel discretization, is a “tilted” logarithmic mean Λ of the carrier densities

$$\sigma_{n,K,L} = \frac{q M_{n,K,L}}{\text{sinhc}(\frac{1}{2} X_{n,K,L})} \Lambda \left(n_L \exp\left(-\frac{1}{2} X_{n,K,L}\right), n_K \exp\left(+\frac{1}{2} X_{n,K,L}\right) \right), \quad (19)$$

with $\text{sinhc}(x) = \sinh(x)/x$. The thermopower $P_{n,K,L}$, which is required in Eq. (15a), reads

$$P_{n,K,L} = -\frac{k_B}{q} \left[\log \left(\frac{N_c(T_L)}{N_c(T_K)} \right) \frac{g_{n,K,L}}{\log(T_L/T_K)} - \frac{1}{k_B} \frac{E_c(T_L) - E_c(T_K)}{T_L - T_K} - \frac{(T_L - T_{K,L}) \eta_{n,L} - (T_K - T_{K,L}) \eta_{n,K}}{T_L - T_K} \right]. \quad (20)$$

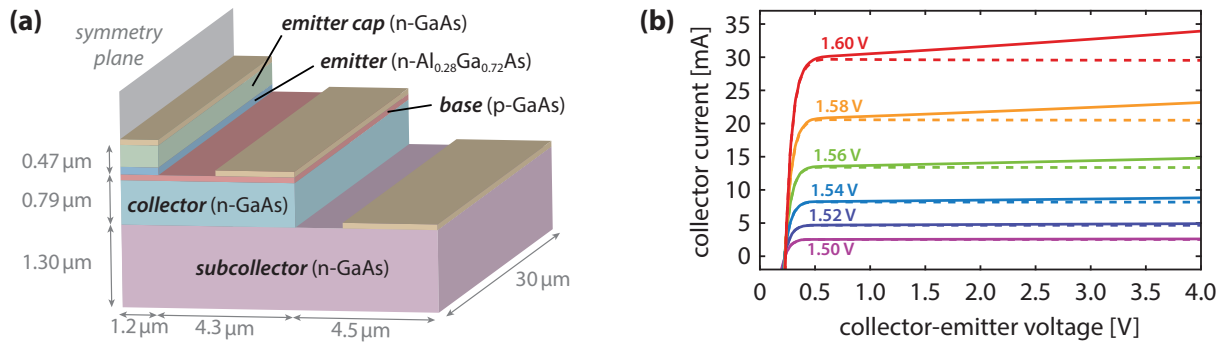


Fig. 2. (a) Cross section of a GaAs/AlGaAs-HBT. Due to symmetry, only half of the device is simulated. The doping densities are: $N_D^+ = 4 \times 10^{19} \text{ cm}^{-3}$ (emitter cap), $N_D^+ = 2 \times 10^{17} \text{ cm}^{-3}$ (emitter), $N_A^- = 3 \times 10^{19} \text{ cm}^{-3}$ (base), $N_D^+ = 2 \times 10^{16} \text{ cm}^{-3}$ (collector) and $N_D^+ = 5 \times 10^{18} \text{ cm}^{-3}$ (subcollector). (b) Calculated collector current I_C as a function of the collector-emitter voltage U_{CE} for different base-emitter voltages U_{BE} with (solid lines) and without (dashed) self-heating effects.

The scheme is manifestly consistent with the thermodynamic equilibrium (no current for $\varphi_{n,K} = \varphi_{n,L}$ and $T_K = T_L$) and the limiting cases of either vanishing chemical ($\varphi_{n,K} = \varphi_{n,L}$: pure Seebeck current) or thermal ($T_K = T_L$: isothermal drift-diffusion) driving forces. The discretization guarantees the non-negativity of the Joule heat term

$$H_{J,K,L} = \sum_{\lambda \in \{n,p\}} \sigma_{\lambda,K,L} |\varphi_{\lambda,L} - \varphi_{\lambda,K} + P_{\lambda,K,L} (T_L - T_K)|^2 \geq 0 \quad (21)$$

(using Eqs. (15a) and (18)) and subsequently also the consistency with the second law of thermodynamics on the discrete level [2]. Due to its structure-preserving properties, the scheme (16) was found to be significantly more accurate than the conventional non-isothermal Scharfetter–Gummel-type discretization approach. See [2] for a detailed analysis.

4 Numerical simulation of a heterojunction bipolar transistor

The approach is demonstrated by numerical simulations of the GaAs/AlGaAs-based heterojunction bipolar transistor (HBT) shown in Fig. 2 (a). We assume ideal ohmic contacts with perfect heat sinking ($T_{\text{cont}} = 300 \text{ K}$) and homogeneous Neumann boundary conditions else. The material parameters, including temperature-dependent models for the band edge energies, mobilities and the thermal conductivity, are taken from [5]. The validity of the Kelvin formula for GaAs was studied in [2]. The calculated current-voltage curves (with and without self-heating effects) are shown in Fig. 2 (b).

The temperature distribution and the heat generation rate are plotted in Fig. 3 for different collector-emitter voltages. The Thomson–Peltier effect is found to cool the AlGaAs/GaAs heterojunctions (emitter/emitter cap and emitter/base junction, blue color in Fig. 3 (b, d)) and heats up the collector/subcollector junction. With increasing current densities (i.e., increasing collector-emitter voltage), the relative importance of Joule heating increases, until it becomes the dominant effect. This leads to a strong temperature increase in the collector region close to the symmetry axis. Recombination processes additionally heat the base region below the base/emitter junction, but were found to be of minor importance in the present study.

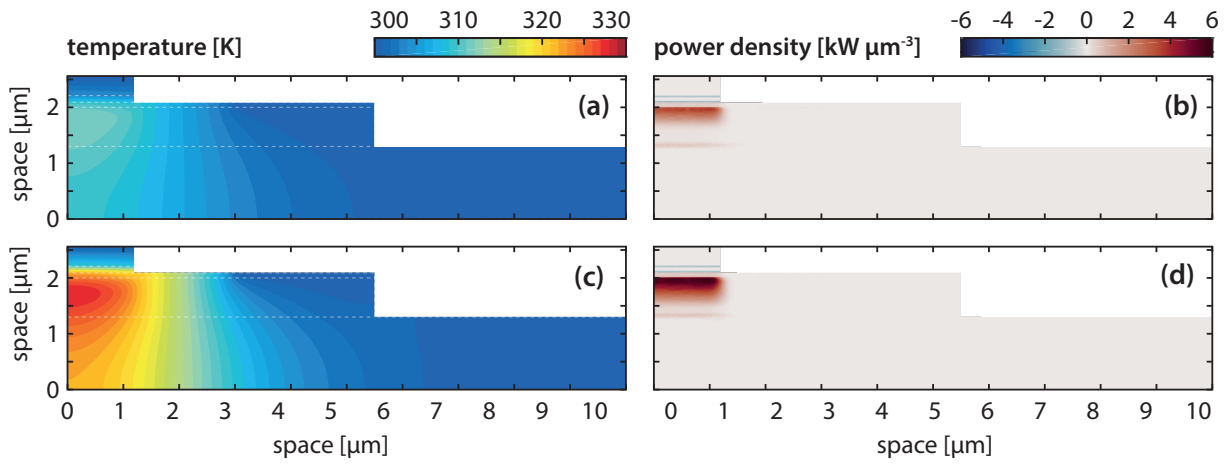


Fig. 3. Simulated temperature distribution and self-heating power density H at stationary operation with (a, b) $U_{CE} = 2$ V and (c, d) $U_{CE} = 4$ V. The basis-emitter voltage is $U_{BE} = 1.6$ V in both cases.

5 Conclusions

The Kelvin formula for the thermopower yields a remarkably simple form of the non-isothermal drift-diffusion system. The specific form of the current density expressions, which contain the thermal driving forces only implicitly, allow for a non-isothermal generalization of the Scharfetter–Gummel scheme for Fermi–Dirac statistics that was previously presented in [7, 9]. The discrete flux scheme is consistent with fundamental thermodynamic relations on the discrete level.

A Derivation of the heat equation

In the following, the heat equation (4) will be derived from an integral form of the total energy balance. The total energy is obtained from the free energy and the definition of the entropy (see Sect. (2.1)) as

$$\mathcal{E}(n, p, T) = \mathcal{F}(n, p, T) + TS(n, p, T) = \mathcal{F}(n, p, T) - T\partial_T \mathcal{F}(n, p, T).$$

Using the free energy functional (8), one obtains

$$\begin{aligned} \mathcal{E}(n, p, T) = & \int_{\Omega} dV \left(\frac{TN'_c(T)}{N_c(T)} k_B T N_c(T) \mathcal{G} \left(\mathcal{F}^{-1} \left(\frac{n}{N_c} \right) \right) + (E_c(T) - TE'_c(T)) n \right. \\ & \left. + \frac{TN'_v(T)}{N_v(T)} k_B T N_v(T) \mathcal{G} \left(\mathcal{F}^{-1} \left(\frac{p}{N_v} \right) \right) - (E_v(T) - TE'_v(T)) p \right) \\ & + \frac{1}{2} \int_{\Omega} dV \int_{\Omega} dV' G(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}) \rho(\mathbf{r}') + \int_{\Omega} dV \Phi_{\text{ext}} \rho + \int_{\Omega} dV u_L(T), \end{aligned} \quad (22)$$

where $u_L = f_L(T) - T\partial_T f_L(T)$ is the energy density of the lattice phonons.

The (volumetric) heat capacity of the system is defined as the variational derivative of the total energy (22) with respect to the temperature

$$D_T \mathcal{E}(n, p, T) = c_V. \quad (23a)$$

Moreover, one obtains

$$\begin{aligned} D_n \mathcal{E}(n, p, T) &= -q\varphi_n + k_B T \left(\frac{TN'_c(T)}{N_c(T)} g \left(\frac{n}{N_c(T)} \right) - \mathcal{F}^{-1} \left(\frac{n}{N_c(T)} \right) - \frac{1}{k_B} E'_c(T) \right), \\ D_p \mathcal{E}(n, p, T) &= +q\varphi_p + k_B T \left(\frac{TN'_v(T)}{N_v(T)} g \left(\frac{p}{N_v(T)} \right) - \mathcal{F}^{-1} \left(\frac{p}{N_v(T)} \right) + \frac{1}{k_B} E'_v(T) \right), \end{aligned}$$

which, if we assume the thermopowers according to the Kelvin formula (9), can be written as

$$D_n \mathcal{E}(n, p, T) = -q(\varphi_n + TP_n), \quad (23b)$$

$$D_p \mathcal{E}(n, p, T) = +q(\varphi_p + TP_p). \quad (23c)$$

The total time derivative of the energy functional (22) reads

$$\begin{aligned} \frac{d}{dt} \mathcal{E}(n, p, T) &= \int_{\Omega} dV \left(D_T \mathcal{E}(n, p, T) \frac{\partial T}{\partial t} + D_n \mathcal{E}(n, p, T) \frac{\partial n}{\partial t} + D_p \mathcal{E}(n, p, T) \frac{\partial p}{\partial t} \right) \\ &= \int_{\Omega} dV \left(c_V \frac{\partial T}{\partial t} - q(\varphi_p + TP_p - \varphi_n - TP_n) R \right. \\ &\quad \left. + \mathbf{j}_n \cdot \nabla(\varphi_n + TP_n) + \mathbf{j}_p \cdot \nabla(\varphi_p + TP_p) \right) \\ &\quad - \oint_{\partial\Omega} d\mathbf{A} \cdot ((\varphi_n + TP_n)\mathbf{j}_n + (\varphi_p + TP_p)\mathbf{j}_p), \end{aligned}$$

where we used Eq. (23) and the continuity equations (2)–(3).

The energy dissipated from the system is given by the heat and electrical energy fluxes leaving the domain through the boundary

$$\frac{d}{dt} \mathcal{E}(n, p, T) = - \oint_{\partial\Omega} d\mathbf{A} \cdot \mathbf{j}_Q - \int_{\Gamma_D} d\mathbf{A} \cdot (\varphi_n \mathbf{j}_n + \varphi_p \mathbf{j}_p), \quad (24)$$

where the heat flux density is known as $\mathbf{j}_Q = -\kappa \nabla T + TP_n \mathbf{j}_n + TP_p \mathbf{j}_p$ [2]. Here, $\Gamma_D \subset \partial\Omega$ denotes the electrical contacts. On the remaining part of the boundary $\Gamma = \partial\Omega \setminus \Gamma_D$, we assume no-flux boundary conditions $\mathbf{n} \cdot \mathbf{j}_{n/p} = 0$, as the charge carriers can not leave the domain there. Finally, using the divergence theorem, we obtain the heat transport equation as a local form of the energy balance equation (24)

$$c_V \frac{\partial T}{\partial t} - \nabla \cdot \kappa \nabla T = -\mathbf{j}_n \cdot \nabla(\varphi_n + TP_n) - \mathbf{j}_p \cdot \nabla(\varphi_p + TP_p) - q(\varphi_p + TP_p - \varphi_n - TP_n)R,$$

where the right hand side coincides with the heat generation rate as given in Eq. (13).

Note that the appealing form (13) of the heat generation rate is a consequence from using the Kelvin formula for the thermopowers in Eqs. (23b)–(23c). For different models for the thermopowers, additional (transient) terms will occur in the heat generation rate [2].

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